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**High order discontinuous Galerkin methods for
simulating miscible displacement process in porous
media with a focus on minimal regularity**

by

Jizhou Li

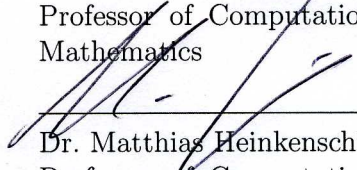
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Doctor of Philosophy

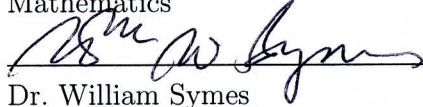
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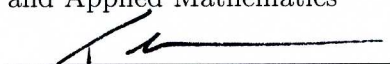
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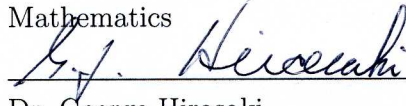
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MAY 2015

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ABSTRACT

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In my thesis, I formulate, analyze and implement high order discontinuous Galerkin methods for simulating miscible displacement in porous media. The analysis concerning the stability and convergence under the minimal regularity assumption is established to provide theoretical foundations for using discontinuous Galerkin discretization to solve miscible displacement problems. The numerical experiments demonstrate the robustness and accuracy of the proposed methods. The performance study for large scale simulations with highly heterogeneous porous media suggests strong scalability which indicates the efficiency of the numerical algorithm. The simulations performed using the algorithms for physically unstable flow show that higher order methods proposed in thesis are more suitable for simulating such phenomenon than the commonly used cell-center finite volume method.

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Q. What is your only comfort in life and in death?

A. That I am not my own, but belong body and soul, in life and in death to my faithful Savior, Jesus Christ... —The Heidelberg Catechism, 1563

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*Dedicated to my beloved wife Sunhild Li-Theiss. Without whom this thesis can
finish sooner...*

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Introduction

1.1 Miscible displacement process

With the increasing demand of fossil fuel, coming up with smarter ways to produce the crude oil becomes essential for the oil and gas industry. Enhanced oil recovery (EOR) is the key discipline for introducing a wide range of techniques to improve oil production after primary and secondary recovery. One of the most common techniques is called miscible displacement process or miscible flooding. The end goal of the miscible displacement process is to increase the production of the amount of remaining oil still trapped in the pores. The means by which we achieve this end is to inject the fluid that can be mixed with the residing oil and that forms a single-phase fluid mixture. Fluid such as CO_2 , propane and butane are commonly used. By using the miscible fluid, the interfacial tension between the residing oil and injected fluid can be eliminated completely; thereby, reducing the residual saturation to the lowest possible value. As a result, it maximizes the amount of oil that we can displace. The miscible flooding has long been investigated since the 1950's and has significantly improved production [1].

Miscible displacement occurs more than just in EOR. It can also be used to study pollutant tracking, ground water contamination, CO_2 sequestration and other fluid transport

phenomena.

The mathematical model consists of a coupled nonlinear system of partial differential equations with the pressure-velocity equations for the Darcy's law and a concentration equation derived from mass conservation given as follows,

$$\nabla \cdot \mathbf{u} = q^I - q^P, \quad \text{in } \Omega \times (0, T), \quad (1.1)$$

$$\mathbf{u} = -\mathbb{K}(c)(\nabla p - \rho(c)\mathbf{g}), \quad \text{in } \Omega \times (0, T), \quad (1.2)$$

$$\partial_t(\phi c) - \text{div}(\mathbb{D}(\mathbf{u})\nabla c - c\mathbf{u}) = q^I\hat{c} - q^Pc, \quad \text{in } \Omega \times (0, T), \quad (1.3)$$

where the physical unknowns are p the fluid pressure, $\mathbf{u}$ the velocity and c the concentration of the solvent.

The flow and transport processes can be driven by the functions q^I and q^P , which represent injection wells and production wells respectively. The other coefficients in the system are the fluid density $\rho(c)$, the gravity vector $\mathbf{g}$, the porosity of the media ϕ , the diffusion-dispersion matrix $\mathbb{D}(\mathbf{u})$, the injected concentration $\hat{c}$, and the tensor $\mathbb{K}(c)$, which is the ratio between the permeability tensor $\mathbf{k}$ and the fluid viscosity $\mu(c)$. The initial concentration is denoted by c_0 .

1.2 Reservoir simulations

In 1962, Peaceman and Rachford [2] developed a reservoir simulator using the finite difference method to simulate the miscible displacement process. With the advancement of computer technology, the computer based reservoir simulator became a very important tool to quantify the cost and benefit of oil recovery projects. Reservoir simulators stretched their capabilities onto multi-phase, multi-component and multi-physics simulations, and at the same time incorporating complex geological models and well information to address real world engineering problems.

Today, with the advancement of parallel computing capability, the development of the reservoir simulator has become an enormous project for research development in the oil and gas industry, and in the scientific community, attracting experts from various disciplines.

One of the most important aspects of the reservoir simulator is related to the discretization and gridding which are the main focus points of my thesis.

1.3 My contributions on simulation of miscible flooding

I propose high order discontinuous Galerkin (DG) discretization strategies for simulating the miscible displacement process. In this work, I establish the stability and convergence of the numerical methods proposed. From the simulation point of view, I demonstrate the capability of the numerical methods to address large scale simulations for the physical phenomenons. I also give detailed descriptions of the design of the simulation algorithm to obtain strong scalability. The numerical experiment demonstrates that, in fact, the high order methods are more adequate for simulating the miscible displacement while, at the same time guaranteeing efficiency and high fidelity solutions.

The content of the thesis is as follows. In this next chapter, I survey the existing literature concerning high order DG methods for reservoir simulation. Next, I discuss some commonly used discretizations for the fluid transport in porous media and also present the advanced discretization strategies I use for simulating miscible displacement. In chapter 4, the stability of the numerical methods proposed are established under the minimal regularity assumption. In chapter 5, I provide the proof for the convergence of the numerical solutions, also under the minimal regularity assumption—followed by the discussion of the design of the linear solver and its performance in chapter 6. Numerical experiments are presented in chapter 7, to demonstrate the advantage of the high order algorithm in contrast with the commonly used finite-volume method. In chapter 8, I specifically discuss the simulation of the viscous finger

effect and the importance of using the high order method for simulating such phenomenon . The last chapters, I present performance results for the large scale simulations and present final conclusions.

Literature Reviews

The study of advanced discretization using the Discontinuous Galerkin method (DG) for flow in porous media was initiated by Rivière, Wheeler and Banaś in the year 2000 [3, 4], though it was not the first time for DG to be used for solving the porous media flow [5]. Their work demonstrates how the high order mass-conservative method significantly reduces the effect of the computation grid on the quality of the numerical solutions for subsurface modeling and provides an alternative to the commonly used numerical discretization techniques, including the finite volume (FV) and finite difference (FD) methods. With the low sensitivity to the grid orientation effect, it becomes much easier to incorporate complex geology for reservoir simulation. On the other hand, the DG method introduces additional issues that researchers have worked to address for the past 15 years. The four main issues concerning DG for the reservoir simulation are:

- Construct mass-conservative continuous flux approximation;
- Handle overshoot and undershoot effect;
- Obtain efficient solver for the physical system;
- Establish convergence and stability of the numerical scheme.

Within the last 15 years, various DG discretization concepts have been proposed to address those four main concerns.

2.1 Numerical discretization

The first two issues concerning DG for reservoir flow rely on the discretization strategy. I have listed several approaches and their variations as a proposition to fix these numerical issues.

2.1.1 Sequential & semi-sequential DG-DG approach

This type of technique is designed for decoupled reservoir flow systems. Typically, we first solve the Darcy's flow equation for the pressure using DG; then, reconstruct the velocity based on the pressure computed and use it to solve for the fluid transport system. We call the decoupling methodology IMPES, or sequential, when we solve the pressure with implicit time-stepping and saturation, or concentration, with explicit time-stepping. Another decoupling approach is the semi-sequential approach, where we first solve for the pressure implicitly, and reconstruct the flux to solve the fluid transport also implicitly. The reason for such flux reconstruction is due to the requirement for maintaining a compatible global mass-conservation property [6]. If we simply use the flux computed using DG discretization for the Darcy's flow, then only Incomplete Interior Penalty Galerkin (IIPG) and Local DG (LDG) can satisfy such compatibility properties, which can be extremely restrictive in terms of implementation and theoretical analysis. Consequently, Eslinger, in his dissertation [7] and paper with Wheeler [8], presented a decoupled scheme based on the local DG (LDG) for compressible fluids and problems with different capillary curves for two-phase flow. Despite the compatibility property, in earlier literature by Rivière, Sun, and Wheeler [9, 10] for the semi-sequential decoupling, the velocity was constructed directly from the pressure gradient for moderately heterogeneous porous media with permeability varying from roughly 10^{-11}

to 10^{-12} m^2 . In this case, the slope-limiter was required.

The two flux reconstruction techniques are proposed by Ern, Nicaise, Vohralik, Bastian and Rivière [11, 12]. Unlike the flux computed directly using DG discretization, which is discontinuous in the normal direction on faces of the neighboring element, the reconstructed flux maintains mass-conservation and is continuous in the normal direction of the face. Therefore, it is more accurate. The techniques have been used in [13, 14, 15, 16] to solve both the single-phase and two-phase flow in porous media.

Both the sequential and semi-sequential decoupling approaches are used in the literature [13, 14, 15, 16]. No slope-limiter is required for the semi-sequential approach.

Another technique often used along with flux reconstruction is the weighted averages introduced in [17] by Ern et al. They apply it in the DG scheme for the average terms on the interior faces to handle discontinuous and anisotropic permeability.

Most recently, this type of approach is used to study the gravity-driven viscous fingering flow [18] with sequential decoupling. Explicit Runge-Kutta was used for solving the fluid transport. No slope-limiter nor flux reconstruction were used in the study. The heterogeneity of the permeability varied only in the magnitude of 10 which is similar to the results in the earlier literature [9, 10] as described before.

2.1.2 MFE-DG approach

Another well-known discretization strategy proposed by and Sun, Rivière and Wheeler [19] uses mixed finite element method for the Darcy's flow; thereby, computing the pressure and velocity simultaneously. The method takes advantage of the mixed finite element (MFE) method for solving the elliptic system and DG for solving the fluid transport. The discretization, hybridization, and time stepping strategy were further developed by Nayagum, Hoteit and Firoozabadi [20, 21, 22, 23, 24], by using a sequential approach with Runge-Kutta explicit time-stepping for the fluid transport. A slope-limiter is required to post-process the fluid saturation, which definitely reduces the accuracy in space.

To this day, the MFE-DG approach has been used by Hoteit, Firoozabadi and Sun to simulate multi-component fluid flow in unfractured and fractured media [22], two-phase compositional flow [21, 23, 25, 26, 27], two-phase flow [28] with different capillary pressure curves, two-phase flow [29, 30] with fracture media, and three-phase flow [31, 32, 33].

A fully-implicit scheme proposed by Bartel, Jensen and Müller [34] is also made possible with the combination of the MFE and DG discretization, since unlike the flux reconstruction approach we have to compute the pressure in order to reconstruct the flux. They also extend the approach to second order Crank-Nicolson semi-sequential time stepping for miscible displacement simulations. Li and Rivière [35, 36] proposed a higher order implicit Runge-Kutta time-stepping strategy based DG in time for the MFE-DG approach. Similar approaches such as the mixed DG-DG have also been proposed [37] to impose the continuity of the flux in the normal direction weakly.

However, for large scale simulations, the higher order mixed finite element methods using either Raviart-Thomas ($\mathcal{RT}$) basis of order two or three or Brezzi-Douglas-Marini ($\mathcal{BDM}$) basis of order two or higher, have rarely been used due to the complexity of generating the finite element space and the fact that hybridization is required for MFE to avoid solving large semi-definite saddle-point systems.

2.1.3 Fully-implicit DG-DG approach

Rivière and Epshteyn [38, 39] first used a fully-implicit approach to solve two-phase flow in porous media. The interior penalty discontinuous Galerkin (IPDG) method is used to discretize both pressure and saturation. Even without the slope-limiter and upwind stabilization, the convergence of numerical solutions is achieved. Another finding in their results is that the formulations of the problem can affect the quality of the solution. In particular, one formulation proposed in their work for the two-phase flow is very sensitive to the penalty parameter; whereas, the other formulation is robust on the unstructured grid and heterogeneous media.

Bastian [40] proposes another fully-implicit scheme with the capillary pressure-wetting-phase pressure p_c - p_w formulation. The DG discretization uses upwind stabilization and the flux on interior faces are evaluated by taking the average of the pressure gradient with an additional penalty term. The weighted average is taken from Ern's result [17] to accommodate the heterogeneous permeability. First, second, and third order implicit time-updatings are employed. No slope-limiter or any post-processing technique is required. Another formulation comes from the Diplomarbeit dissertation by Grüninger [41, 42] using a fully-implicit DG approach to discretize non-wetting-phase saturation-wetting-phase saturation s_o - p_w formulation of the two-phase flow. The result also uses the idea of the weighted average.

A fully-implicit approach with DG in time was used to study miscible displacement simulation by Chen, Steeb, Diebels [43]. The coupled system is more expensive to solve, however, it is compensated by allowing larger time step and mesh size for more complex physical phenomenon such as viscous fingering. A fully-implicit approach was also used for the miscible displacement simulation by Huang and Scovazzi [44, 45] to study the miscible viscous fingering effect. The discretization's capability to address heterogeneous porous media is not mentioned.

The approach was most recently used to solve black-oil model by Rivière and Rankin in [46].

The existing literature suggested that by using the fully-implicit DG-DG approach, we can eliminate the overshoot and undershoot for miscible displacement, as we refine the mesh because of diffusion term. For multi-phase flow, the overshoot and undershoot will remain bounded, but they still present under mesh refinement. Therefore, in order to guarantee positivity of the saturation we have to use positivity preserving slope-limiter.

2.2 Computational efficiency

In general, the discontinuous Galerkin method is more expensive in comparison with commonly used finite volume and finite difference methods. During the last 15 years, there has been tremendous effort put into developing an efficient algorithm to achieve good performance for large scaling simulations. One trade-off with the high order method, however, is that one can obtain the same level of accuracy on a coarser grid, which may result in short assembling time and a smaller linear system.

One of the most effective means to attain efficiency is through adaptive mesh refinement. From the very first publication using DG for porous media flow, the flexibility of mesh adaptability was demonstrated [4]. The adaptive mesh refinement was used for single-phase reactive transport in porous media in [47] and two-phase flow [48]. The results suggest that with the adaptive mesh refinement the degree of freedom of the system can be 10 times smaller than using uniform mesh refinement while still maintaining the same level of accuracy.

In terms of p -adaptation, work has been done to couple the finite volume (FV) with DG [49, 50, 51]. The coupled approach not only relaxed the gridding, it also reduced the computational cost.

With the high order DG method, the resulting linear system for the simulation of the reservoir flow becomes larger and more ill conditioned. Also, the highly heterogeneous permeability poses additional difficulty for the linear solver. The algebraic multigrid (AMG) solver introduced by Bastian, Blatt and Scheichl [52, 53] addressed the issue with linear solve. This AMG preconditioning technique has been used in [40] for a fully-implicit coupled flow system. The AMG preconditioner for the full system is able to solve the Jacobian system within a few iterations. The AMG solver has also been used to solve the system resulted from MFE discretization in [54] to attain efficiency for works on permeability upscaling. Most recently, a similar AMG preconditioning approach was presented by [55], with some differences on the subspace correction and the aggravation approach.

For the coupled nonlinear system resulting from the multi-phase and multi-component flow problems, Natvig and Lie [56, 57, 58] introduced the reordering technique for the Newton-Raphson nonlinear solver algorithmically reducing the runtime and the memory requirements to speed up the solver. The reordering technique has been applied to large scale simulations of multi-phase and multi-component flows in porous media in their result and was applied to solve flow problems in fractured media [59].

Overall, from the computational aspect, it is quite promising to achieve efficiency using the DG method to address the simulations in porous media flow.

2.3 Theoretical analysis

With the introduction of finite element spaces, which are discontinuous on the face between two neighboring elements for DG, new challenges have been posed in terms of establishing a solid theoretical foundation for the high order method. The ground work was laid by Arnold, Brezzi, Cockburn and Marini [60] introducing a unified approach to study the whole class of IPDG methods for second-order elliptic problems. The hp -error estimate was derived for the reactive-transport equations for the porous media flow by assuming that the Darcy's velocity was given [61, 62]. Following the error estimate, another hp -error estimate was obtained for the coupled miscible displacement system [10] using the DG-DG approach with pure Neumann boundary condition. It was extended to both Neumann and Dirichlet boundary conditions [63]. A priori error analysis was done in [64]. Error estimate was established for the fully-implicit MFE-DG approach in [19] using the “cut-off” operator for the unbounded diffusion-dispersion tensor and in [65, 66] without using the “cut-off” operator, but completely neglecting the dispersion and a result without using the “cut-off” operator while considering the dispersion by means of an induction hypothesis [67] and superconvergence results [68, 69] for both compressible and incompressible miscible displacement. An error estimate for the mixed-DG-DG fully-implicit approach was also established in [37].

The analyses that have been done so far do not apply to the case with solutions under minimal regularity. Without the additional regularity assumption for the solutions, there is simply no convergence result from the literature listed so far. To bridge this theoretical gap, Bartels, Jensen and Müller [34] proposed a fully-implicit Euler method in time, with MFE, and a symmetric DG in space. The convergence analysis is obtained by applying the standard Aubin-Lions lemma to the interpolated functional spaces that they constructed. In the scheme [34], the diffusion-dispersion matrix is projected onto the space of piecewise polynomial matrices. In addition, the penalty parameter depends on the shape regularity of the mesh and polynomial degree of the approximation space. The work was extended to a Crank-Nicolson time discretization by Jensen and Müller [70] with the system being decoupled and solved using a semi-sequential approach, while still maintaining the second-order approximation. Another result by Rivière and Walkington [71] titled “Convergence of a discontinuous Galerkin method for the miscible displacement equation under low regularity” studied the convergence of the numerical solutions for miscible displacement equations under minimal regularity. In this case, however, the analysis was done with DG in time, and with MFE for pressure and velocity, and the finite element method (FEM) for concentration. One noticeable result in their analysis was a generalized compactness theorem that enabled them to establish compactness with functions that are discontinuous in time. Li, Rivière and Walkington [72] have proposed a numerical scheme with MFE-DG and DG in time for solving miscible displacement equations. The convergence of the numerical solutions to the low regularity solutions has been proven. An even more general compactness theorem has been developed as a result to address function spaces that are discontinuous in both space and time. Under the minimal regularity assumption, the convergence of the numerical solutions using DG for the Darcy’s flow type of heterogeneous diffusion problem was obtained by Ern and Di Pietro [73, 74]. The convergence analysis for mass-conservative flux reconstruction for DG was done [75, 12], which laid the groundwork for using sequential and semi-sequential DG-DG approaches, which I discuss in my thesis.

Among all the existing literature concerning two-phase flow with DG discretization, very few theoretical analyses have ever been provided. Rivière and Epshteyn [76] have provided a theoretical proof of stability and convergence with a fully-implicit global pressure formulation. The convergence rate is obtained in their error analysis. For 4 years, this result was the only existing theoretical analysis using DG for solving two-phase flow problems in porous media. The result was established for 2D cases, which to some extent, indicates the technicality of establishing stability and convergence of the problem. Most recently, the MFE-DG approach has been analyzed for two-phase flow problems [77]. Also, the more commonly used DG-DG fully-implicit and IMPES approaches were analyzed by obtaining error estimate in [78, 79]. All these recent results on two-phase flow were presented by Sun and Kou.

No other theoretical analysis has been done for any other multi-phase or multi-component flow in porous media using DG. Here is where my literature search concerning discontinuous Galerkin methods for porous media flow comes to an end.

2.4 Summary

In summary, the various approaches mentioned above offer solutions for the four main issues for using DG to solve porous media flow problems. Here, I list the issues with related solutions provided by existing scientific literature:

- Construct the mass-conservative continuous flux approximation
 - MFE for computing the flux
 - $\mathcal{RT}$ flux reconstruction
 - $\mathcal{BDM}$ flux reconstruction
- Handle overshoot and undershoot effect
 - Slope-limiter

- Fully-implicit approach
- Obtain an efficient solver for the physical system
 - Reordering technique
 - AMG solver
- Establish convergence and stability of the numerical scheme
 - DG-DG and MFE-DG approaches for two-phase flow
 - Fully-implicit DG-DG approach for miscible displacement
 - Fully-implicit MFE-DG approach for miscible displacement under low regularity
 - Semi-sequential MFE-DG approach for miscible displacement under low regularity

In the next chapter, I will discuss the discretization strategies for the miscible displacement problem.

Discretizations

In this chapter, I give a detailed description of the spacial discretizations and time updating strategies used for solving the PDEs system resulted from the miscible displacement problem. Before discussing the discretization, I first present the formulations of the problems being solved and its related parameters.

3.1 Problem formulation

Let $[0, T]$ be a time interval and $\Omega \subset \mathbb{R}^d$ be the region occupied by the porous medium in which a polymer solvent is being displaced. Under the assumption of incompressibility, the fluid pressure p and velocity $\mathbf{u}$ satisfy the following equations

$$\nabla \cdot \mathbf{u} = q^I - q^P, \quad \text{in } \Omega \times (0, T), \quad (3.1)$$

$$\mathbf{u} = -\mathbb{K}(c)(\nabla p - \rho(c)\mathbf{g}), \quad \text{in } \Omega \times (0, T). \quad (3.2)$$

The concentration c of the solvent satisfies

$$\partial_t(\phi c) - \operatorname{div}(\mathbb{D}(\mathbf{u})\nabla c - c\mathbf{u}) = q^I \hat{c} - q^P c, \quad \text{in } \Omega \times (0, T). \quad (3.3)$$

The coefficients in the model are the injection q^I and production q^P functions, the fluid density $\rho(c)$, the gravity vector $\mathbf{g}$, the porosity of the medium ϕ , the diffusion-dispersion tensor $\mathbb{D}(\mathbf{u})$, the injected concentration $\hat{c}$, and the tensor $\mathbb{K}(c)$, which is the ratio between the permeability tensor $\mathbf{k}$ and the fluid viscosity $\mu(c)$.

The system is completed by the following boundary conditions.

$$\begin{aligned} p &= p_D \text{ on } \Gamma_D, & \mathbf{u} \cdot \mathbf{n} &= \mathbf{u}_N \cdot \mathbf{n} \text{ on } \Gamma_N, \\ \text{and } c &= c_{in} \text{ on } \Gamma_{in}, & \mathbb{D}(\mathbf{u})\nabla c \cdot \mathbf{n} &= q_{out} \text{ on } \Gamma_{out} \end{aligned}$$

If the boundary condition is set to be no flow boundary condition, i.e. $\Gamma_N = \partial\Omega$, then the system is completed by an additional constraint on the pressure for uniqueness and we also need a compatibility condition,

$$\int_{\partial\Omega} \mathbf{u}_N \cdot \mathbf{n} = \int_{\Omega} (q^I - q^P)$$

with the initial condition

$$c(x, 0) = c_0(x), \quad x \in \Omega.$$

Assumption 3.1.1. 1. $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain, $d = 2$ or 3 .

2. $\mathbb{K} : \Omega \times \mathbb{R} \rightarrow \mathbb{R}^{d \times d}$ is symmetric, Carathéodory (measurable in the first argument and continuous in the second almost everywhere), uniformly bounded and elliptic. That is, there exist constants $0 < k_0 < k_1$ such that

$$k_0 |\xi|^2 \leq \xi^T \mathbb{K}(x, c) \xi \leq k_1 |\xi|^2, \quad \xi \in \mathbb{R}^d, (x, c) \in \Omega \times \mathbb{R},$$

where $|\xi|$ denotes the Euclidean norm. The spatial dependence is omitted below; $\mathbb{K}(c) \equiv \mathbb{K}(x, c)$.

3. $\mathbb{D} : \Omega \times \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ is Carathéodory, symmetric valued, and Lipschitz continuous in

the second variable, and there exist constants $0 < d_0 < d_1$ such that

$$d_0(1 + |\mathbf{u}|) |\xi|^2 \leq \xi^T \mathbb{D}(x, \mathbf{u}) \xi \leq d_1(1 + |\mathbf{u}|) |\xi|^2, \quad (x, \mathbf{u}) \in \Omega \times \mathfrak{R}^d, \quad \xi \in \mathfrak{R}^d. \quad (3.4)$$

For simplicity, the spatial dependence is omitted in the rest of the thesis; $\mathbb{D}(\mathbf{u}) \equiv \mathbb{D}(x, \mathbf{u})$.

4. $\hat{c} \in L^\infty(\Omega)$, $\phi \in L^\infty(\Omega)$ and $\phi_0 < \phi < \phi_1$ for some positive constants ϕ_0, ϕ_1 .
5. $q^I, q^P \in L^\infty[0, T; L^2(\Omega)]$ with $q^I, q^P \geq 0$ and $\int_\Omega q^I(x, t) = \int_\Omega q^P(x, t)$ for $t \in [0, T]$.
6. There exist positive constants ρ_0, ρ_1 such that the function $\rho : \mathfrak{R} \rightarrow \mathfrak{R}$ is Lipschitz continuous and $\rho_0 \leq \rho \leq \rho_1$.

Next, I proceed to discuss the weak formulations based on the problem frameworks that were just presented.

3.2 Weak formulations

Two different weak formulations are presented for the miscible displacement problem. Following is the mixed formulation with pressure, velocity and concentration as unknowns.

Find the triple $(\mathbf{u}, p, c)$ in $L^\infty(0, T; H_{\Gamma_N}(\Omega; \text{div})) \times L^\infty(0, T; L^2(\Omega)) \times (L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)'))$ such that

$$\int_0^T ((\mathbb{K}^{-1}(c)\mathbf{u}, \mathbf{v}) - (p, \nabla \cdot \mathbf{v})) = \int_0^T (\rho(c)\mathbf{g}, \mathbf{v}) - \int_0^T (p_D, \mathbf{v} \cdot \mathbf{n})_{\Gamma_D} \quad (3.5)$$

$$\int_0^T (\nabla \cdot \mathbf{u}, q) = \int_0^T (q^I - q^P, q) \quad (3.6)$$

$$\int_0^T (-(\phi c, \partial_t w) + (\mathbb{D}(\mathbf{u})\nabla c, \nabla w) + (\mathbf{u} \cdot \nabla c, w) + (q^I c, w)) \quad (3.7)$$

$$= (\phi c_0, w(0)) + \int_0^T ((q^I \hat{c}, w) + (q_{out}, w)_{\Gamma_{out}})$$

For all $(\mathbf{v}, q) \in L^1(0, T; H_{\Gamma_N}(\Omega; \text{div})) \times L^1(0, T; L^2(\Omega))$ and for all

$$w \in \{H^1(0, T; H_{\Gamma_{out}}^2(\Omega)) \cap H^1(0, T; H_{\Gamma_{out}}^1(\Omega)') | w(T) = 0\}$$

Most of the convergence analyses for the numerical solutions under the low regularity assumption are done in [34, 35, 72, 71] within the mixed formulation framework, where the existence of the weak solution is still unknown. The mixed finite element and discontinuous Galerkin (MFE-DG) discretization can be used as spacial discretization. Whereas, if we treat only pressure and concentration as unknown and the velocity is obtained by taking the gradient of the pressure, then there is result in terms of the existence of the weak solutions [80]. In this case, the weak formulation is given as follow.

Find the triple $(\mathbf{u}, p, c)$ in $L^\infty(0, T; L^2(\Omega)) \times L^\infty(0, T; H^1(\Omega)) \times (L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)'))$ such that,

$$\int_0^T (\mathbb{K}(c) \nabla p, \nabla q) = \int_0^T ((q^I - q^P, q) - (\mathbf{u}_N \cdot \mathbf{n}, q)_{\Gamma_N} + (\mathbb{K}(c) \rho(c) \mathbf{g}, \nabla q)) \quad (3.8)$$

$$\mathbf{u} = -\mathbb{K}(c) \nabla p \quad (3.9)$$

$$\begin{aligned} \int_0^T (-\phi c, \partial_t w) + (\mathbb{D}(\mathbf{u}) \nabla c, \nabla w) + (\mathbf{u} \cdot \nabla c, w) + (q^I c, w) \\ = (\phi c_0, w(0)) + \int_0^T ((q^I \hat{c}, w) + (q_{out}, w)_{\Gamma_{out}}) \end{aligned} \quad (3.10)$$

For all $q \in L^1(0, T; H_{\Gamma_D}^1(\Omega))$ and for all

$$w \in \{H^1(0, T; H_{\Gamma_{out}}^2(\Omega)) \cap H^1(0, T; H_{\Gamma_{out}}^1(\Omega)') | w(T) = 0\}$$

This weak form is more appropriate in terms of establishing the convergence under low regularity condition for the numerical solutions which I examine in a later chapter using DG-DG discretization.

Remark 3.2.1. The weak forms for the concentration (3.7) and (3.10) do not require the

concentration solutions to be in $H^1(0, T; H^2(\Omega)')$. The result [80] for the existence of the solutions, however, has established the weak solution to be in $H^1(0, T; H^2(\Omega)')$.

3.3 Notation

Before I introduce the discretization, it is helpful to introduce some useful notation. First, Q_T is used to denote the space-time domain $\Omega \times (0, T)$. Let $\{t_j\}_{j=0}^N$ be a family of partitions of $[0, T]$ that are quasi-uniform; i.e., there exists $\nu \in (0, 1]$ such that

$$\nu k \leq \min_{1 \leq j \leq N} (t_j - t_{j-1}), \quad \text{where} \quad k = \max_{1 \leq j \leq N} (t_j - t_{j-1}).$$

For the time step on each interval is denote as,

$$k_j = t_j - t_{j-1}$$

If the numerical solutions are discontinuous in time, then the jump of a function v at time t^j is denoted by $[v^j]_t$:

$$v_+^j = \lim_{\epsilon \downarrow 0} v(\cdot, t_j + \epsilon), \quad v_-^j = \lim_{\epsilon \downarrow 0} v(\cdot, t_j - \epsilon), \quad [v^j]_t = v_+^j - v_-^j.$$

If the numerical solution of the concentration is discontinuous across mesh elements, to define the jump $[\cdot]$ and average $\{\cdot\}$ of a discontinuous function we let Γ_h denote the set of interior faces. Then, for each $e \in \Gamma_h$ fix a normal vector $\mathbf{n}_e$ and let E_+^e and E_-^e denote the neighboring elements such that $\mathbf{n}_e$ points from E_+^e to E_-^e . Thus, we have

$$\{v\} = \frac{v|_{E_+^e} + v|_{E_-^e}}{2}, \quad \text{and} \quad [v] = v|_{E_+^e} - v|_{E_-^e}.$$

The broken Sobolev spaces are denoted by $W^{s,p}(\mathcal{E}_h)$ and let $H^s(\mathcal{E}_h) = W^{s,2}(\mathcal{E}_h)$.

The norms on $H^1(\mathcal{E}_h)$ and $W^{1,4}(\mathcal{E}_h)$ are defined as

$$\begin{aligned} \|v\|_{H^1(\mathcal{E}_h)} &= \left(\|v\|_{L^2(\Omega)}^2 + \sum_{E \in \mathcal{E}_h} \|\nabla v\|_{L^2(E)}^2 + \sum_{e \in \Gamma_h} h^{-1} \|[v]\|_{L^2(e)}^2 \right)^{1/2}, \\ \|v\|_{W^{1,4}(\mathcal{E}_h)} &= \left(\|v\|_{L^4(\Omega)}^4 + \sum_{E \in \mathcal{E}_h} \|\nabla v\|_{L^4(E)}^4 + \sum_{e \in \Gamma_h} h^{-3} \|[v]\|_{L^4(e)}^4 \right)^{1/4}. \end{aligned}$$

The L^2 inner-product on $\mathcal{E}_h$ and Γ_h are:

$$(\cdot, \cdot)_{\mathcal{E}_h} = \sum_{E \in \mathcal{E}_h} (\cdot, \cdot)_E, \quad (\cdot, \cdot)_{\Gamma_h} = \sum_{e \in \Gamma_h} (\cdot, \cdot)_e.$$

The notation " $\lesssim$ " denotes less or equal with the constant independent of mesh size. Examples of the usage of the notation are given in section B.2.1. We also use the notation $\mathcal{P}_k$ to denote the polynomial of the degree k . With the notation defined, the discretizations can be discussed.

3.4 Discretization of the Darcy's flow

Recall the Darcy's flow is given by,

$$\begin{aligned} \mathbf{u} &= -\mathbb{K}(\nabla p - \rho \mathbf{g}) \text{ in } \Omega \subset \mathbb{R}^d \\ \nabla \cdot \mathbf{u} &= q^I - q^P \text{ in } \Omega \subset \mathbb{R}^d \end{aligned}$$

with boundary condition,

$$p = p_D \text{ on } \Gamma_D, \quad \mathbf{u} \cdot \mathbf{n} = \mathbf{u}_N \cdot \mathbf{n} \text{ on } \Gamma_N$$

I first consider using finite element discretization.

3.4.1 Finite element discretization

A typical finite element (FEM) discretization for the pressure requires following weak form,

$$\begin{aligned} - \int_{\Omega} \nabla \cdot \mathbb{K}(\nabla p - \rho \mathbf{g}) q &= \int_{\Omega} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q - \int_{\partial\Omega} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n} q \\ &= \int_{\Omega} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q + \int_{\Gamma_N} \mathbf{u}_N \cdot \mathbf{n} q \end{aligned}$$

for all test functions $q \in H_{\Gamma_D}^1(\Omega) = \{\varphi \in H^1(\Omega) : \varphi = 0 \text{ on } \Gamma_D\}$. The equality above is derived directly from integration by part. Hence, we have the system

$$\int_{\Omega} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q + \int_{\Gamma_N} \mathbf{u}_N \cdot \mathbf{n} q = \int_{\Omega} f q$$

Then the system can be discretized according to the weak formulation by approximating p using p_h and have,

$$\int_{\Omega} \mathbb{K}(\nabla p_h - \rho \mathbf{g}) \cdot \nabla q_h + \int_{\Gamma_N} \mathbf{u}_N \cdot \mathbf{n} q_h = \int_{\Omega} f q_h$$

where $p_h, q_h \in \{\varphi \in H_0^1(\Omega) : \varphi \in \mathcal{P}_k(\Omega)\}$. For the finite element basis, we refer the reader to Appendix A section A.2

However, the discretization using the FEM is not locally mass conservative. Written explicitly in mathematical notation, we have

$$- \int_{\partial E} \mathbb{K}(\nabla p_h - \rho \mathbf{g}) \cdot \mathbf{n} \neq \int_E (q^I - q^P).$$

The inability to maintain the local mass conservation triggers unphysical global oscillations of the numerical solutions when used to solve fluid flow problems [34]. One way to maintain local mass conservation without using the post-processing technique on FEM is to use the

mixed finite element method.

3.4.2 Mixed finite element method

The weak formulation puts into consideration pressure and velocity simultaneously:

$$\begin{aligned} \int_{\Omega} \nabla \cdot \mathbf{u} q &= \int_{\Omega} (q^I - q^P) q \\ \int_{\Omega} \mathbb{K}^{-1} \mathbf{u} \cdot \mathbf{v} - \int_{\Omega} p \nabla \cdot \mathbf{v} &= \int_{\Omega} \rho(c) \mathbf{g} \cdot \mathbf{v} - \int_{\Gamma_D} p_D \mathbf{v} \cdot \mathbf{n} \end{aligned}$$

with $\mathbf{u}, \mathbf{v} \in H_{\Gamma_N}(\Omega; \text{div}) = \{\varphi \in H(\Omega, \text{div}) : \varphi \cdot \mathbf{n} = 0 \text{ on } \Gamma_N\}$ and $p, q \in L^2(\Omega)$. The discretization can be constructed based on the weak formulation:

$$\begin{aligned} \int_{\Omega} \nabla \cdot \mathbf{u}_h q_h &= \int_{\Omega} (q^I - q^P) q_h \\ \int_{\Omega} \mathbb{K}^{-1} \mathbf{u}_h \cdot \mathbf{v}_h - \int_{\Omega} p_h \nabla \cdot \mathbf{v}_h &= \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{v}_h - \int_{\Gamma_D} p_D \mathbf{v}_h \cdot \mathbf{n} \end{aligned}$$

where $\mathbf{u}_h, \mathbf{v}_h \in \mathcal{RT}_k(\Omega) = \{\varphi \in H_0(\Omega, \text{div}) : \varphi \in \mathcal{P}_k(E)^d + \mathbf{x}\mathcal{P}_k(E) \ \forall E \in \mathcal{E}_h\}$ and $p_h, q_h \in \{\phi \in L^2(\Omega) : \phi \in \mathcal{P}_k(E) \ \forall E \in \mathcal{E}_h\}$. The bilinear form can for the discretization can be written as,

$$\begin{aligned} a(\mathbf{u}_h, \mathbf{v}_h) - b(p_h, \mathbf{v}_h) &= (\rho \mathbf{g}, \mathbf{v}_h) - (p_D, \mathbf{v}_h \cdot \mathbf{n})_{\Gamma_D} \\ b(q_h, \mathbf{u}_h) &= (q^I - q^P, q_h) \end{aligned} \tag{3.11}$$

Other mixed finite element spaces can be used for the velocity approximation such as $\mathcal{BDM}_k(\Omega)$. For the construction of the mixed finite element basis such as Raviart-Thomas basis, we refer the reader to Appendix A section A.3. Notice, the local mass conservation can be maintained. One can verify the mass conservation by choosing

$$q_h = 1_E,$$

then we have

$$\int_{\partial E} \mathbf{u}_h \cdot \mathbf{n} = \int_E \nabla \cdot \mathbf{u}_h = \int_E (q^I - q^P).$$

Therefore, it is a suitable discretization for porous media flow problems. In addition to the property of maintaining local mass conservation, the velocity obtained by using a mixed finite element is also continuous in the normal direction at the face between two neighboring elements.

Also, notice that the linear system resulted from MFE discretization is a larger symmetric positive semidefinite saddle-point system rather than the symmetric positive definite system by FEM.

i.e. the system becomes

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{0} \end{pmatrix},$$

which poses certain difficulties in solving the system. In general, hybridization or preconditioning techniques that exploit the block structure are used to reduce the size of the system. To avoid solving the saddle-point problem, while also maintaining the local mass conservation, discontinuous Galerkin (DG) is a suitable candidate.

3.4.3 DG discretization

Instead of deriving the weak formulation for FEM using integration by part over the entire domain, we derive DG from the integration by part on each element. First, we define $\mathcal{E}_h$ to be the set of all elements of the domain Ω and Γ_h to be the set of all interior faces. Hence, for each $E \in \mathcal{E}_h$ we have:

$$-\int_E \nabla \cdot \mathbb{K}(\nabla p - \rho \mathbf{g}) q = \int_E \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q - \int_{\partial E} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n} q$$

So, we can now sum up all the element in $\mathcal{E}_h$:

$$-\sum_{E \in \mathcal{E}_h} \int_E \nabla \cdot \mathbb{K}(\nabla p - \rho \mathbf{g}) q = \sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q - \sum_{E \in \mathcal{E}_h} \int_{\partial E} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_E q \quad (3.12)$$

Let $\mathbf{n}_e$ be a normal vector on each face $e \in \Gamma_h$ where the direction of the $\mathbf{n}_e$ is fixed to one specific direction. We define $E^\pm$ to be the element such that $e \in \partial E^\pm$ and $\mathbf{n}_e$ is the outward normal of E^+ . We now examine the term $-\sum_{E \in \mathcal{E}_h} \int_{\partial E} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_E q$:

$$\begin{aligned} -\sum_{E \in \mathcal{E}_h} \int_{\partial E} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_E q &= -\sum_{e \in \Gamma_h \cup \Gamma_D \cup \Gamma_N} \int_e [\mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_e q] \\ &= -\sum_{e \in \Gamma_h \cup \Gamma_D} \int_e [\mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_e q] + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q \end{aligned} \quad (3.13)$$

where

$$[\varphi] = \begin{cases} \varphi^+ - \varphi^- & \text{on } e \in \Gamma_h \text{ where } \varphi^\pm \text{ is basis value accessed from } E^\pm \\ \varphi & \text{on } e \in \partial\Omega \end{cases}$$

Define the average

$$\{\varphi\} = \begin{cases} \frac{1}{2}(\varphi^+ + \varphi^-) & \text{on } e \in \Gamma_h \\ \varphi & \text{on } e \in \partial\Omega \end{cases}$$

Since we are still in the continuum level, according to the regularity argument, the solution p satisfies:

$$[p] = 0 \text{ and } \mathbb{K} \nabla p \cdot \mathbf{n}_e = \{\mathbb{K} \nabla p \cdot \mathbf{n}_e\} \text{ a.e. on } \Gamma_h \text{ for all } p \in H^1(\Omega) \quad (3.14)$$

and from (3.13) we have,

$$-\sum_{E \in \mathcal{E}_h} \int_{\partial E} \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n} q = -\sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_e\} [q] + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q$$

So, the weak formulation (3.12) becomes:

$$\sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q - \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_e\} [q] + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q$$

Again by the regularity argument (3.14), we have following properties,

$$\begin{aligned} \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K} \nabla q \cdot \mathbf{n}_e\} [p] - \sum_{e \in \Gamma_D} \int_e \mathbb{K} \nabla q \cdot \mathbf{n}_e p_D &= 0 \\ \sum_{e \in \Gamma_h \cup \Gamma_D} \gamma_e \int_e [p][q] - \sum_{e \in \Gamma_D} \gamma_e \int_e p_D q &= 0 \end{aligned}$$

where γ_e is the penalty parameter, typically set to be

$$\gamma_e = \frac{\sigma}{|e|^{d-1}} \text{ or } \sigma h_e^{-1}, \text{ where } \sigma \text{ is a constant}$$

So, the weak formulation for the pressure is obtained as follow,

$$\begin{aligned} B_d(p, q) &= \sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \nabla q - \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(\nabla p - \rho \mathbf{g}) \cdot \mathbf{n}_e\} [q] + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q \\ &\quad + \theta \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K} \nabla q \cdot \mathbf{n}_e\} [p] - \theta \sum_{e \in \Gamma_D} \int_e \mathbb{K} \nabla q \cdot \mathbf{n}_e p_D \\ &\quad + \sum_{e \in \Gamma_h \cup \Gamma_D} \gamma_e \int_e [p][q] - \sum_{e \in \Gamma_D} \gamma_e \int_e p_D q \end{aligned}$$

Therefore, the weak form becomes

$$B_d(p, q) = (q^I - q^P, q)$$

When $\theta = -1$ we have a symmetric weak form. We call this Symmetric Interior Penalty Galerkin (SIPG). When $\theta = 1$ the weak form is non-symmetric. This is called Non-symmetric Interior Penalty Galerkin (NIPG). When $\theta = 0$ the entire term drops. This is called Incomplete Interior Penalty Galerkin (IIPG). Among those three weak forms, NIPG gives the most stable scheme regardless of the penalty term γ_e . When the penalty parameter $\gamma_e = 0$, the scheme is also known as Oden-Babuška-Baumann (OBB) DG [81]. Whereas, SIPG and IIPG require the adjustment of the penalty parameter to guarantee the stability.

We discretize the pressure using piecewise polynomial bases,

$$p_h, q_h \in \{\varphi \in H^1(\mathcal{E}_h) : \varphi \in \mathcal{P}_k(E)\}$$

For additional details concerning the basis functions for DG, we refer the reader to Appendix A section A.2. We have the discretization,

$$B_d(p_h, q_h) = (q^I - q^P, q_h) \quad (3.15)$$

For the assembling of the linear system and numerical integration, we refer reader to Appendix A section A.1. We can verify the local mass conservation by setting $q_h = 1_E$, then we have

$$-\int_{\partial E} \{\mathbb{K}(\nabla p_h - \rho \mathbf{g})\} \cdot \mathbf{n} + \int_{\partial E} \gamma_e[p_h] = \int_E q^I - q^P$$

where flux can be defined as

$$\begin{aligned} \mathbf{u}_h^{DG} &= -\mathbb{K}(\nabla p_h - \rho \mathbf{g}) \text{ on } E \\ \mathbf{u}_h^{DG} \cdot \mathbf{n} &= -\{\mathbb{K}(\nabla p_h - \rho \mathbf{g})\} \cdot \mathbf{n} + \gamma_e[p_h] \text{ on } \partial E \end{aligned}$$

Hence, according to the way the flux is constructed and the regularity of the solutions, local mass conservation is preserved; However, the flux can be inaccurate on the face of the element [12]. In particular, for miscible displacement problem we have to evaluate $\mathbb{D}(\mathbf{u}_h)\nabla c_h \cdot \mathbf{n}$, which is undefined by the way we construct the flux. Some more appropriate ways to reconstruct the flux are discussed in a later section.

Next, I present some additional modifications to the DG discretization to address several numerical issues for the problem related to porous media flow.

3.4.3.1 Weighted average

To enhance the quality of the simulation with varying permeability, I present here a common practice developed by Ern and et al [17, 74]. When integrating over the face element, instead of taking the arithmetic average, we take the weight average according to the permeability tensor on each adjacent element. Therefore,

$$B_d(p_h, q_h) = (q^I - q^P, q_h) \quad (3.16)$$

where,

$$\begin{aligned} B_d(p_h, q_h) = & \sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(\nabla p_h - \rho \mathbf{g}) \cdot \nabla q_h - \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(\nabla p_h - \rho \mathbf{g}) \cdot \mathbf{n}_e\}_\omega [q_h] \\ & + \theta \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K} \nabla q_h \cdot \mathbf{n}_e\}_\omega [p_h] - \theta \sum_{e \in \Gamma_D} \int_e \mathbb{K} \nabla q_h \cdot \mathbf{n}_e p_D \\ & + \sum_{e \in \Gamma_h \cup \Gamma_D} \gamma_{e,\omega} \int_e [p_h][q_h] - \sum_{e \in \Gamma_D} \gamma_{e,\omega} \int_e p_D q_h + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q_h \end{aligned}$$

where $\{\varphi\}_\omega$ is given by,

$$\{\varphi\}_\omega = \omega^+ \varphi^+ + \omega^- \varphi^-$$

for some weights $\omega^+ + \omega^- = 1$, $w^\pm \geq 0$. And the weights are given as

$$w^\pm = \frac{\delta_K^\mp}{\delta_K^+ + \delta_K^-}$$

with

$$\delta^\pm = \mathbf{n}_e^T \mathbb{K}^\pm \mathbf{n}_e$$

And the corresponding penalty parameter $\gamma_{e,\omega}$ is

$$\gamma_{e,\omega} = m \frac{2\delta_K^+ \delta_K^-}{\delta_K^+ + \delta_K^-} \frac{k(k+d-1) |e|}{\min(|E^+|, |E^-|)}$$

where k is the order of approximation in space and m is a positive constant to adjust in order to have the best convergence rate and condition number for the linear system. The choice of the weight and penalty parameter is supposed to yield a robust error estimate with respect to the diffusivity. The weighted average weakly imposes the continuity of the flux in [17]; thereby, improving the stability and convergence of the solution.

3.4.3.2 Flux Reconstruction

One disadvantage for using DG is that the normal component of velocity field is not continuous on the interior faces; Hence, when using sequential or semi-sequential time updating where the fluid transport equation requires accurate evaluations of the velocity, it is better to construct continuous flux while maintaining mass conservation properties.

One technique proposed by Bastian and Rivière [12], referred to as $\mathcal{BDM}$ flux reconstruction, for the purpose of this thesis, has been used in single-phase and two-phase flow. Here, we give some detailed descriptions of the flux reconstruction.

We denote the velocity directly obtained from DG as

$$\mathbf{u}_h^{DG} = -\mathbb{K}(\nabla p_h - \rho \mathbf{g}), \text{ with } p_h \in \mathcal{P}_k(\mathcal{E}_h)$$

The reconstructed velocity $\mathbf{u}_h^* \in \mathcal{P}_{k-1}^d(\mathcal{E}_h)$ have to satisfy following

$$\int_e \mathbf{u}_h^* \cdot \mathbf{n}_e z_h = \int_e \{\mathbf{u}_h^{DG}\} \cdot \mathbf{n}_e z_h, \quad \forall z \in \mathcal{P}_{k-1}(e), \quad \forall e \in \partial E \quad (3.17)$$

$$\int_E \mathbf{u}_h^* \cdot \nabla w_h = \int_E \mathbf{u}_h^{DG} \cdot \nabla w_h, \quad \forall w_h \in \mathcal{P}_{k-2}(E) \quad (3.18)$$

$$\int_E \mathbf{u}_h^* \cdot \nabla \times \phi_h = \int_E \mathbf{u}_h^{DG} \cdot \nabla \times \phi_h, \quad \forall \phi_h \in M_k(E) \quad (3.19)$$

where

$$M_k(E) = \{\phi \in \mathcal{P}_k(E) : \phi_h|_{\partial E} = 0\}$$

The conditions above uniquely define a mass conservative $\mathbf{u}_h^*$ that is continuous in the normal components. By this construction, $\mathbf{u}_h^* \in \mathcal{BDM}_{k-1}(\Omega)$, the flux reconstruction is designed for OBB DG discretization which is basically NIPG without the penalty term, but it can be generalized for other types of DG.

Ern and et al. [75] proposed a more accurate flux reconstruction because the reconstruction offers the optimal error estimate for the divergence of the flux. We refer the technique as $\mathcal{RT}$ flux reconstruction. The construction is as follows:

Let $\mathbf{u}_h^* \in \mathcal{RT}_k(\Omega)$ such that

$$\int_e \mathbf{u}_h^* \cdot \mathbf{n}_e q_h = \int_e (\{\mathbf{u}_h^{DG}\}_\omega \cdot \mathbf{n}_e + \gamma_e[p_h]) q_h, \quad \forall q_h \in \mathcal{P}_k(e), \quad \forall e \in \partial E \quad (3.20)$$

$$\int_E \mathbf{u}_h^* \cdot \mathbf{v} = \int_E \mathbf{u}_h^{DG} \cdot \mathbf{v}_h + \theta \sum_{e \in \partial E} \omega_{E,e} \int_e \mathbb{K} \mathbf{v}_h \cdot \mathbf{n}_e [p_h], \quad \forall \mathbf{v}_h \in \mathcal{P}_{k-1}^d(E) \quad (3.21)$$

These conditions, again, uniquely determine a mass conservative and continuous flux.

In both cases, the flux reconstructions are very efficient post-processing techniques since they can be done locally on each element and face. For the construction of the Raviart-

Thomas finite element on the quadrilateral element, we refer to the Appendix A section A.3.

3.4.3.3 Slope-limiter

Another numerical issue for using high order discretization for porous media flow is the effect of overshoot and undershoot at the location where large gradient of the solution occurs. In some cases, the overshoot and undershoot affect the quality of the numerical solutions so drastically, that, they requires to completely eliminate the overshoot and undershoot. The slope-limiter is designed to address this issue. In this part, I discuss the construction of the slope-limiter. Let us consider the construction of the slope-limiter on a 2D Cartesian grid. We denote DG solution by c_h^{DG} . On the element $E = (x_n, x_{n+1}) \times (y_m, y_{m+1})$, we can expand the solution

$$\begin{aligned} c_h^{DG}(x, y) = & a_0^{n,m} + a_1^{n,m} \psi_n(x) + a_2^{n,m} \xi_m(y) + a_3^{n,m} \psi_n(x) \xi_m(y) \\ & + a_4^{n,m} \left(\psi_n(x)^2 - \frac{1}{3} \right) + a_5^{n,m} \left(\xi_m(y)^2 - \frac{1}{3} \right) + \dots \end{aligned}$$

where the basis are given as

$$\psi_n(x) = \frac{x - \frac{x_n + x_{n+1}}{2}}{\frac{x_{n+1} - x_n}{2}}, \quad \xi_m(y) = \frac{y - \frac{y_m + y_{m+1}}{2}}{\frac{y_{m+1} - y_m}{2}}$$

Since we use the orthogonal polynomial as the bases of the DG solution, we have the local mass matrix is given explicitly by

$$M = |E| \operatorname{diag} \left(1, \frac{1}{3}, \frac{1}{3}, \frac{1}{9}, \frac{4}{45}, \frac{4}{45}, \dots \right)$$

It is straightforward for us to obtain the coefficients. Since the coefficients we need are $a_0^{n,m}$, $a_1^{n,m}$, $a_2^{n,m}$, we can be computed as follows

$$a_0^{n,m} = \frac{1}{|E|} \int_E c^{DG}, \quad a_1^{n,m} = \frac{3}{|E|} \int_E c^{DG} \psi_n, \quad a_2^{n,m} = \frac{3}{|E|} \int_E c^{DG} \xi_m \quad (3.22)$$

Then, we can detect overshoots or undershoots by comparing $a_1^{n,m}, a_2^{n,m}$ with some constant parameter M_{lim} . If the overshoot or undershoot is detected, we can compute the neighboring averages $a_0^{n-1,m}, a_0^{n+1,m}, a_0^{n,m-1}, a_0^{n,m+1}$ and construct new slope $\bar{a}_1^{n,m}, \bar{a}_2^{n,m}$. The solution after the post-processing is given to be

$$c_h^*(x, y) = a_0^{n,m} + \bar{a}_1^{n,m} \psi_n(x) + \bar{a}_2^{n,m} \xi_m(y)$$

The specific way to construct the new slope can be found in [82, 83]. The algorithm is given as follow:

```

for All the elements  $E = (x_n, x_{n+1}) \times (y_m, y_{m+1}) \in \mathcal{E}_h$  do
    Compute  $a_0^{n,m}, a_1^{n,m}, a_2^{n,m}$  using (3.22);
    if  $|a_1^{n,m}| > M_{lim}$  then
        Compute  $a_0^{n-1,m}, a_0^{n+1,m}$  using (3.22);
        Reconstruct  $\bar{a}_1^{n,m}$  using minmod algorithm;
    end
    if  $a_1^{n,m} \neq \bar{a}_1^{n,m}$  then
         $c_h^* = a_0^{n,m} + \bar{a}_1^{n,m} \psi_n(x) + a_2^{n,m} \xi_m(y);$ 
         $a_1^{n,m} = \bar{a}_1^{n,m}$ 
    end
    if  $|a_2^{n,m}| > M_{lim}$  then
        Compute  $a_0^{n,m-1}, a_0^{n,m+1}$  using (3.22);
        Reconstruct  $\bar{a}_2^{n,m}$  using minmod algorithm;
    end
    if  $a_2^{n,m} \neq \bar{a}_2^{n,m}$  then
         $c_h^* = a_0^{n,m} + a_1^{n,m} \psi_n(x) + \bar{a}_2^{n,m} \xi_m(y)$ 
    end
end

```

Algorithm 1: Slope-limiter

In addition to limiting the slope, the slope-limiter can detect the non-physical solution such as negative saturation or concentration, thereby, making certain adjustment to preserve

positivity.

3.4.4 Finite volume discretization

Finite volume discretization is a commonly used discretization for the porous media flow problem. There are in fact various types of finite volume methods. Here, I only present the cell-center finite volume (CCFV) method which can be seen as a DG method with piecewise constant approximations. We simply restrict the approximation to be

$$p_h, q_h \in \mathcal{P}_0(\mathcal{E}_h).$$

Then, from 3.16, we have

$$B_d(p_h, q_h) = \sum_{e \in \Gamma_h \cup \Gamma_D} \gamma_e \int_e [p_h][q_h] - \sum_{e \in \Gamma_D} \gamma_e \int_e p_D q_h + \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N \cdot \mathbf{n}_e q_h = (q^I - q^P, q_h)$$

By setting $\frac{\gamma_e}{|e|}$ to be transmissibility $\mathbb{T}$, we have CCFV method, i.e.

$$\sum_{e \in \partial E} \mathbb{T}(p_h^+ - p_h^-) = \int_E q^I - q^P \text{ for each interior element } E$$

The advantage of using CCFV method is that it maintains mass conservation and monotonicity of the numerical solutions. However, this low order discretization suffers significantly from the grid orientation effect and permeability anisotropy as I demonstrate in the chapter on numerical experiments.

Apart from the discretizations I have discussed above, there are other advanced discretization strategies that can be used for porous media flow simulations such as the multi-point flux approximation (MPFA) method. MPFA is an extension of the CCFV with 2nd-order approximation. It is more suitable for handling the case with grid distortion and permeability anisotropy.

	CCFV	MPFA	FEM	MFE	DG
Local mass conservation	✓	✓	×	✓	✓
Grid distortion	×	✓	✓	✓	✓
Anisotropy	×	✓	✓	✓	✓
High order	×	✓	✓	✓	✓
Convergence for minimal regularity	×	×	✓	✓	✓

Table 3.1: Discretization strategies comparison

Table 3.1 gives an overview of the numerical methods I described and the numerical issues that they address. For the rest of the thesis, I specifically focus on the two types of discretization namely the MFE method in (3.11), and the DG method in (3.16) with $\mathcal{RT}$ flux reconstruction. Extensive treatment for convergence of the solution and the quality of numerical simulation is discussed in the chapters that follow.

In the following section, I address the DG discretization for solving the fluid transport equation.

3.5 Discretization of the fluid transport

In the previous section I have discussed several numerical discretization approaches for Darcy's flow and their related numerical issues. In this section, I solely use DG discretization for the fluid transport. Recall, the fluid transport is given by

$$\phi \partial_t c - \nabla \cdot (\mathbb{D}(\mathbf{u}) \nabla c - \mathbf{u}c) = q^I \hat{c} - q^P c \text{ in } \Omega$$

with boundary condition:

$$c = c_{in} \text{ on } \Gamma_{in} \text{ and } \mathbb{D}(\mathbf{u}) \cdot \mathbf{n} = q_{out} \text{ on } \Gamma_{out}$$

and initial condition:

$$c(\cdot, 0) = c_0$$

For the DG discretization, we first consider using the upwind approximation for the convection.

3.5.1 Upwind stabilization DG

The discretization arises out of the most natural weak formulation. For the diffusion term, we have:

$$\begin{aligned} B_{di}(c, w; \mathbf{u}) = & \sum_{E \in \mathcal{E}_h} \int_E \mathbb{D}(\mathbf{u}) \nabla c \cdot \nabla w - \sum_{e \in \Gamma_h \cup \Gamma_{in}} \int_e \{ \mathbb{D}(\mathbf{u}) \nabla c \cdot \mathbf{n}_e \} [w] - \sum_{e \in \Gamma_{out}} \int_e q_{out} w \\ & + \theta \sum_{e \in \Gamma_h \cup \Gamma_{in}} \int_e \{ \mathbb{D}(\mathbf{u}) \nabla w \cdot \mathbf{n}_e \} [c] - \theta \sum_{e \in \Gamma_{in}} \int_e \mathbb{D}(\mathbf{u}) \nabla w \cdot \mathbf{n}_e c_{in} \\ & + \sum_{e \in \Gamma_h \cup \Gamma_{in}} \frac{\sigma}{h_e} \int_e [c][w] - \sum_{e \in \Gamma_{in}} \frac{\sigma}{h_e} \int_e c_{in} w \end{aligned}$$

For the convection term we have:

$$B_c(c, w; \mathbf{u}) = - \sum_{E \in \mathcal{E}_h} \int_E \mathbf{u} c \cdot \nabla w + \sum_{e \in \Gamma_h \cup \Gamma_{out}} \int_e \mathbf{u} \cdot \mathbf{n}_e c^{up}[w] + \sum_{e \in \Gamma_{in}} \int_e c_{in} \mathbf{u} \cdot \mathbf{n}_e w$$

where the upwind term is given as:

$$\varphi^{up} = \begin{cases} \varphi^+ & \text{if } \mathbf{u} \cdot \mathbf{n}_e \geq 0 \\ \varphi^- & \text{otherwise} \end{cases}$$

Therefore, we have the spacial discretization

$$(\phi \partial_t c_h, w_h) + B_{tr}(c_h, w_h; \mathbf{u}_h) = \ell_{tr}(w_h) \quad (3.23)$$

with $B_{tr}(c_h, w_h; \mathbf{u}_h) = B_{di}(c_h, w_h; \mathbf{u}_h) + B_c(c_h, w_h; \mathbf{u}_h)$ and $\ell_{tr}(w_h) = (q^I \hat{c} - q^P c_h, w_h)$.

3.5.2 Lax-Friedrichs stabilization DG

The scheme I present next is based on the Lax-Friedrichs flux splitting. The scheme is more helpful for theoretical analysis.

First, the transport equation can be rewritten as follows:

$$\partial_t(\phi c) - \nabla \cdot (\mathbb{D}(\mathbf{u}) \nabla c - (1/2) c \mathbf{u}) + (1/2) \mathbf{u} \cdot \nabla c + (1/2)(q^I + q^P) c = q^I \hat{c}.$$

The diffusion term is given as:

$$\begin{aligned} B_{di}(c_h, w_h; \mathbf{u}_h) &= (\mathbb{D}(\mathbf{u}_h) \nabla c_h, \nabla w_h)_{\mathcal{E}_h} - ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \\ &\quad + \epsilon([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} + (\sigma h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h], [w_h])_{\Gamma_h}. \end{aligned} \quad (3.24)$$

The convection-source term is given to be:

$$\begin{aligned} B_{cq}(c_h, w_h; \mathbf{u}_h) &= \frac{1}{2} \left((\mathbf{u}_h \cdot \nabla c_h, w_h)_{\mathcal{E}_h} - (\mathbf{u}_h c_h, \nabla w_h)_{\mathcal{E}_h} + ((q^I + q^P) c_h, w_h) \right. \\ &\quad \left. + (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_{\Gamma_h} - (w_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} \right). \end{aligned} \quad (3.25)$$

The downwind term follows the same concept as the upwind term:

$$\varphi^{\text{down}} = \begin{cases} \varphi^+ & \text{if } \mathbf{u} \cdot \mathbf{n}_e \leq 0 \\ \varphi^- & \text{otherwise} \end{cases}$$

Therefore, the spacial discretization is shown to be:

$$(\phi \partial_t c_h, w_h) + B_{tr}(c_h, w_h; \mathbf{u}_h) = \ell_{tr}(w_h) \quad (3.26)$$

with $B_{tr}(c_h, w_h; \mathbf{u}_h) = B_{di}(c_h, w_h; \mathbf{u}_h) + B_{cq}(c_h, w_h; \mathbf{u}_h)$ and $\ell_{tr}(w_h) = (q^I \hat{c}, w_h)$.

In the remaining section, I present the fully discrete scheme for the miscible displacement problem.

3.6 Fully discrete scheme for the miscible displacement model

In the previous section, I have introduced the spacial discretizations for each component of the miscible displacement problem. Now, I introduce the time-stepping techniques to incorporate the time stepping scheme into the miscible displacement model. The resulting algorithms can be implemented to simulate the miscible flooding.

3.6.1 MFE-DG discretization with DG in time

The numerical scheme with DG in time can be written as follows.

Finding $\mathbf{u}_h \in \mathcal{P}_\ell(t_{j-1}, t_j; \mathbf{U}_h)$, $p_h \in \mathcal{P}_\ell(t_{j-1}, t_j; P_h)$, $c_h \in P_\ell(t_{j-1}, t_j; C_h)$, satisfying

$$\int_{t_{j-1}}^{t_j} ((\mathbb{K}^{-1}(c_h) \mathbf{u}_h, \mathbf{v}_h) - (p_h, \nabla \cdot \mathbf{v}_h)) = \int_{t_{j-1}}^{t_j} (\rho(c_h) \mathbf{g}, \mathbf{v}_h), \quad (3.27)$$

$$\int_{t_{j-1}}^{t_j} (q_h, \nabla \cdot \mathbf{u}_h) = \int_{t_{j-1}}^{t_j} (q^I - q^P, q_h), \quad (3.28)$$

$$\int_{t_{j-1}}^{t_j} ((\phi \partial_t c_h, w_h) + B_{tr}(c_h, w_h; \mathbf{u}_h)) + ([c_h^{j-1}]_t, \phi w_{h+}^{j-1}) = \int_{t_{j-1}}^{t_j} (\hat{c} q^I, w_h), \quad (3.29)$$

The scheme is fully implicit; therefore, it is necessary to solve a nonlinear coupled system at each time step. In terms of the implementation, we can recast (3.29) as follows:

$$\int_{t_{j-1}}^{t_j} (\partial_t c_h, w_h) + \left([c_h^{j-1}]_t, w_{h+}^{j-1} \right) = \int_{t_{j-1}}^{t_j} (F_h(c_h), w_h)$$

Using integration by parts, we have:

$$(c_{h-}^j, w_{h-}^j) = (c_{h-}^{j-1}, w_{h+}^{j-1}) + \int_{t_{j-1}}^{t_j} (c_h, \partial_t w_h) + \int_{t_{j-1}}^{t_j} (F_h(c_h), w_h) \quad (3.30)$$

Thus, simply by selecting the polynomial basis functions for the approximation in time and numerical quadrature for the integration over time, we can construct time stepping schemes that can be easily implemented.

For example, if we select basis functions over the reference interval in time $[0, 1]$ to be

$$\left\{ 1, t, \frac{1}{2}(3t^2 - 1) \right\}$$

and we use the Radau II quadrature with quadrature points and weights

$$Q = \left\{ \frac{1}{3}, 1 \right\} \text{ and } W = \left\{ \frac{3}{4}, \frac{1}{4} \right\}$$

Then, we have the time updating based on Butcher's table as

1/3	1/3	0
1	1	0
	3/4	1/4

which is a third-order method.

If we select the basis function to be,

$$\left\{1, t, \frac{1}{2}(3t^2 - 1)\right\}$$

and if we use the Lobatto III quadrature with quadrature points and weights

$$Q = \left\{0, \frac{1}{2}, 1\right\} \text{ and } W = \left\{\frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right\}.$$

Then, we have a time updating based on Butcher's table as

0	0	0	0
1/2	1/4	1/4	0
1	0	1	0
	1/6	2/3	1/6

which is a fourth-order method.

The algorithm for time updating for the entire problem is given as

```

for  $j = 1 : N$  and  $\mathbf{v}_h \in \mathbf{U}_h$ ,  $q_h \in P_h$ , and  $w_h \in C_h$  do
    Set  $c_h^{(0)} = c_h(\cdot, t_{j-1})$ ;
    for  $i = 1 : s - 1$  where  $s - 1$  is the number of the intermediate points do
        Find  $(\mathbf{u}_h^{(i)}, p_h^{(i)}) \in (\mathbf{U}_h, P_h)$  such that
        
$$(\mathbb{K}^{-1}(c_h^{(0)})\mathbf{u}_h^{(i)}, \mathbf{v}_h) - (p_h^{(i)}, \text{div}(\mathbf{v}_h)) = (\rho(c_h^{(0)})\mathbf{g}, \mathbf{v}_h)$$


$$(q_h, \text{div}(\mathbf{u}_h^{(i)})) = ((q^I - q^P)(t_j^{(i)}), q_h)$$

        Find  $c_h^{(i)} \in C_h$  such that

$$(\phi \frac{c_h^{(i)} - c_h^{j-1}}{d_i k_j}, w_h) + \sum_{k=1}^i a_{i,k} B_{tr}(c_h^{(k)}, w_h; \mathbf{u}_h^{(k)}) = \sum_{k=1}^i a_{i,k} ((\hat{c}q^I)(t_j^{(k)}), w_h)$$

    end
    Find  $(\mathbf{u}_h^{(s)}, p_h^{(s)}) \in (\mathbf{U}_h, P_h)$  such that
    
$$(\mathbb{K}^{-1}(c_h^{(0)})\mathbf{u}_h^{(s)}, \mathbf{v}_h) - (p_h^{(s)}, \text{div}(\mathbf{v}_h)) = (\rho(c_h^{(0)})\mathbf{g}, \mathbf{v}_h)$$


$$(q_h, \text{div}(\mathbf{u}_h^{(s)})) = ((q^I - q^P)(t_j^{(s)}), q_h)$$

    Update  $c_h(\cdot, t_j) = c_h^j$  by solving

$$(\phi \frac{c_h^j - c_h^{j-1}}{k_j}, w_h) + \sum_{i=1}^{s-1} b_i B_{tr}(c_h^{(i)}, w_h; \mathbf{u}_h^{(i)}) = \sum_{i=1}^{s-1} b_i ((\hat{c}q^I)(t_j^{(i)}), w_h)$$

end

```

The intermediate time steps are defined as $t_j^{(i)} = t_{j-1} + d_i k_j$. The coefficients $a_{i,k}$'s, b_i 's and d_i 's are taken from the Butcher's table for the Runge-Kutta method:

$$\begin{array}{c|c} d & \mathbf{A} \\ \hline & b^T \end{array}$$

Algorithm 2: Discontinuous Galerkin in time updating

The algorithm we just presented for the Discontinuous Galerkin in time updating is essentially an implicit Runge-Kutta time updating scheme. Next, we take a look at some more conventional time stepping methods such as the implicit Euler method and the Crank-Nicolson method.

3.6.2 DG-DG with implicit Euler decoupling

For the DG-DG spatial discretization with implicit Euler in time, we have

Data: Initial condition, boundary condition, well information, etc.

initialize $t_0 = 0; k_1; c_h^0;$

while $j = 1 : N$ **do**

Solve Darcy system $B_d(p_h^j, q_h; c_h^{j-1}) = \ell_d^j(q_h; c_h^{j-1});$

Reconstruct velocity $\mathbf{u}_h^j$ using $\mathcal{RT}$ flux reconstruction by solving:

$$(\mathbf{u}_h^j, \mathbf{v}_h)_E = -(\mathbb{K}(\bar{c}_h^{j-1})(\nabla p_h^j - \rho(\bar{c}_h^{j-1})\mathbf{g}), \mathbf{v}_h)_E + \theta(\omega_{E,e}\mathbb{K}(\bar{c}_h^{j-1})\mathbf{v}_h \cdot \mathbf{n}_e, [p_h^j])_{\partial E};$$

$$(\mathbf{u}_h^j \cdot \mathbf{n}_e, q_h)_e = -(\{\mathbb{K}(\bar{c}_h^{j-1})(\nabla p_h^j - \rho(\bar{c}_h^{j-1})\mathbf{g})\}_\omega \cdot \mathbf{n}_e, q_h)_e + \gamma_e([p_h^j], q_h)_e;$$

Solve transport system for c_h^j with given $\mathbf{u}_h^j$ with implicit Euler;

$$\left(\phi \frac{c_h^j - c_h^{j-1}}{k_j}, w_h\right) + B_{tr}(c_h^j, w_h; \mathbf{u}_h^j) = \ell_{tr}^j(w_h);$$

$$t_{j+1} = t_j + k_j;$$

end

Algorithm 3: Implicit Euler decoupling for DG-DG

where we have,

$$\begin{aligned} B_d(p_h, q_h) &= \sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(c_h^{j-1}) \nabla p_h \cdot \nabla q_h - \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(c_h^{j-1}) \nabla p_h \cdot \mathbf{n}_e\}_\omega [q_h] \\ &\quad + \theta \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(c_h^{j-1}) \nabla q_h \cdot \mathbf{n}_e\}_\omega [p_h] + \sum_{e \in \Gamma_h \cup \Gamma_D} \gamma_{e,\omega} \int_e [p_h][q_h] \end{aligned}$$

and

$$\begin{aligned} \ell_d^j(q_h; c_h^{j-1}) &= \sum_{E \in \mathcal{E}_h} \int_E \mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) \mathbf{g} \cdot \nabla q_h - \sum_{e \in \Gamma_h \cup \Gamma_D} \int_e \{\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) \mathbf{g} \cdot \mathbf{n}_e\}_\omega [q_h] \\ &\quad + \theta \sum_{e \in \Gamma_D} \int_e \mathbb{K}(c_h^{j-1}) \nabla q_h \cdot \mathbf{n}_e p_D^j + \sum_{e \in \Gamma_D} \gamma_{e,\omega} \int_e p_D^j q_h - \sum_{e \in \Gamma_N} \int_e \mathbf{u}_N^j \cdot \mathbf{n}_e q_h \\ &\quad + ((q_h^I - q_h^P)^j, q_h) \end{aligned}$$

The source term is given to be as follow,

$$q_h^I = \frac{1}{k_j} \int_{t_{j-1}}^{t_j} q^I, \quad q_h^P = \frac{1}{k_j} \int_{t_{j-1}}^{t_j} q^P \quad \text{and} \quad \hat{c}_h = \frac{1}{k_j} \int_{t_{j-1}}^{t_j} \hat{c} \quad (3.31)$$

which is simply the L^2 -projection in time for the input data. If there is additional regularity for the input data, then we can simply use the point-wise evaluation at t_j over the interval $[t_{j-1}, t_j]$. Since the problem itself does not provide any additional regularity in time for the source functions, using L^2 -projection as the input data in the numerical scheme is required for us to establish convergence and stability of the numerical solutions.

For the flux reconstruction, $\bar{c}_h$ is the spacial piecewise averaging approximation of the solution c_h . We can also obtain high order approximation in time using the Crank-Nicolson decoupling approach.

3.6.3 DG-DG with Crank-Nicolson decoupling

For DG-DG discretization, we have

Data: Initial condition, boundary condition, well information, etc.

initialize $t_0 = 0; k_0; c_h^0$;

Set $c_h^{(0)} = c_h^0$;

Compute c_h^1 using implicit Euler algorithm over $[0, k_0]$;

for $j = 1 : N$ **do**

Solve Darcy system $B_d(p_h^j, q_h; c_h^j) = \ell_d^j(q_h; c_h^j)$;

Reconstruct velocity $\mathbf{u}_h^j$ using $\mathcal{RT}$ flux reconstruction by solving:

$$(\mathbf{u}_h^j, \mathbf{v}_h)_E = -(\mathbb{K}(\bar{c}_h^j)(\nabla p_h^j - \rho(\bar{c}_h^{j-1})\mathbf{g}), \mathbf{v}_h)_E + \theta(\omega_{E,e}\mathbb{K}(\bar{c}_h^j)\mathbf{v}_h \cdot \mathbf{n}_e, [p_h^j])_{\partial E};$$

$$(\mathbf{u}_h^j \cdot \mathbf{n}_e, q_h)_e = -(\{(\mathbb{K}(\bar{c}_h^j)\nabla p_h^j - \rho(\bar{c}_h^{j-1})\mathbf{g})\}_\omega \cdot \mathbf{n}_e, q_h)_e + \gamma_e([p_h^j], q_h)_e;$$

Compute $\check{\mathbf{u}}_h^{j+1} = \frac{3}{2}\mathbf{u}_h^j - \frac{1}{2}\mathbf{u}_h^{j-1}$;

Solve transport system for c_h^{j+1} with given $\check{\mathbf{u}}_h^{j+1}$ using Crank-Nicolson;

$$\left(\phi \frac{c_h^j - c_h^{j-1}}{k_j}, w_h\right) + B_{tr}\left(\frac{c_h^j + c_h^{j-1}}{2}, w_h; \check{\mathbf{u}}_h^j\right) = \ell_{tr}^j(w_h);$$

$t_{j+1} = t_j + k_j$;

end

Algorithm 4: Crank-Nicolson decoupling for MFE-DG

The Darcy system and source terms are the same as (3.31).

3.6.4 MFE-DG with implicit Euler decoupling

For the implicit Euler time updating with the MFE-DG spacial discretization, the algorithm is given as follow. We have

Data: Initial condition, boundary condition, well information, etc.

initialize $t_0 = 0; k_1; c_h^0;$

while $j = 1 : N$ **do**

 Solve Darcy system;

$$(\mathbb{K}^{-1}(c_h^{j-1})\mathbf{u}_h^j, \mathbf{v}_h) - (p_h^j, \text{div}(\mathbf{v}_h)) = (\rho(c_h^{j-1})\mathbf{g}, \mathbf{v}_h);$$

$$(q_h, \text{div}(\mathbf{u}_h^j)) = ((q_h^I - q_h^P)^j, q_h);$$

 Solve transport system for c_h^j with given $\mathbf{u}_h^j$ with implicit Euler;

$$\left(\phi \frac{c_h^j - c_h^{j-1}}{k_j}, w_h\right) + B_{tr}(c_h^j, w_h; \mathbf{u}_h^j) = \ell_{tr}^j(w_h);$$

$$t_{j+1} = t_j + k_j;$$

end

Algorithm 5: Implicit Euler decoupling for MFE-DG

The algorithm just presented is different from [34]. In our case, the coupled nonlinear systems have been decoupled into two linear systems and are solved sequentially. The source terms are the same as (3.31).

3.6.5 MFE-DG with Crank-Nicolson decoupling

For the Crank-Nicolson time updating, the algorithm is given as follows:

Data: Initial condition, boundary condition, well information, etc.

initialize $t_0 = 0; k_0; c_h^0$;

Set $c_h^{(0)} = c_h^0$;

Compute c_h^1 using implicit Euler algorithm over $[0, k_0]$;

for $j = 1 : N$ **do**

 Solve Darcy system;

$$(\mathbb{K}^{-1}(c_h^j) \mathbf{u}_h^j, \mathbf{v}_h) - (p_h^j, \operatorname{div}(\mathbf{v}_h)) = (\rho(c_h^j) \mathbf{g}, \mathbf{v}_h);$$

$$(q_h, \operatorname{div}(\mathbf{u}_h^j)) = ((q_h^I - q_h^P)^j, q_h);$$

$$\text{Compute } \check{\mathbf{u}}_h^{j+1} = \frac{3}{2} \mathbf{u}_h^j - \frac{1}{2} \mathbf{u}_h^{j-1};$$

 Solve transport system for c_h^{j+1} with given $\check{\mathbf{u}}_h^{j+1}$ using Crank-Nicolson;

$$\left(\phi \frac{c_h^j - c_h^{j-1}}{k_j}, w_h \right) + B_{tr} \left(\frac{c_h^j + c_h^{j-1}}{2}, w_h; \check{\mathbf{u}}_h^j \right) = \ell_{tr}^j(w_h);$$

$$t_{j+1} = t_j + k_j;$$

end

Algorithm 6: Crank-Nicolson decoupling for MFE-DG

The algorithm given is based on [70]. The extrapolated velocity $\check{\mathbf{u}}_h^{j+1}$ is needed to maintain the second-order convergence rate in time [84]. The source terms are the same as (3.31).

The next chapter examine the stability of the numerical solutions provided by each of the numerical schemes just presented.

Stability Analysis

In this chapter, I establish stability of the numerical solutions provided by MFE-DG and DG-DG discretizations proposed in Section 3.6. For simplicity, assume the following no flow boundary conditions:

$$\mathbf{u} \cdot \mathbf{n} = 0 \text{ and } \mathbb{D}(\mathbf{u}) \nabla c \cdot \mathbf{n} = 0 \text{ on } \partial\Omega$$

To be well-posed, the following compatibility conditions are introduced,

$$\int_{\Omega} q^I = \int_{\Omega} q^P \text{ and } \int_{\Omega} p = 0.$$

First, I restate the weak formulations in light of the boundary conditions imposed for simplicity.

4.1 Weak formulations

I present two weak formulations for the purpose of establishing convergence of numerical solutions for using both MFE-DG and DG-DG discretizations.

We first give the mixed weak formulation of the problem, for the solutions triplets

$$(\mathbf{u}, p, c) \in L^\infty(0, T; H(\Omega; \text{div})) \times L^\infty(0, T; L_0^2(\Omega)) \times (L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)'))$$

$$\int_0^T ((\mathbb{K}^{-1}(c)\mathbf{u}, \mathbf{v}) - (p, \nabla \cdot \mathbf{v})) = \int_0^T (\rho(c)\mathbf{g}, \mathbf{v}) \quad (4.1)$$

$$\int_0^T (\nabla \cdot \mathbf{u}, q) = \int_0^T (q^I - q^P, q) \quad (4.2)$$

$$\int_0^T (-\phi c, \partial_t w) + (\mathbb{D}(\mathbf{u})\nabla c, \nabla w) + (\mathbf{u} \cdot \nabla c, w) + (q^I c, w) = (\phi c_0, w(0)) + \int_0^T (q^I \hat{c}, w) \quad (4.3)$$

for all $(\mathbf{v}, q) \in L^1(0, T; H(\Omega; \text{div})) \times L^1(0, T; L^2(\Omega))$ and for all $w \in \{H^1(0, T; H^2(\Omega)) \cap H^1(0, T; H^1(\Omega)') | w(T) = 0\}$.

Another weak formulation is presented as, (for the triplet):

$$(\mathbf{u}, p, c) \in L^\infty(0, T; L^2(\Omega)^d) \times L^\infty(0, T; H_0^1(\Omega)) \times (L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)'))$$

$$\int_0^T (\mathbb{K}(c)\nabla p, \nabla q) = \int_0^T ((q^I - q^P, q) + (\mathbb{K}(c)\rho(c)\mathbf{g}, \nabla q)) \quad (4.4)$$

$$\mathbf{u} = -\mathbb{K}(c)\nabla p \quad (4.5)$$

$$\int_0^T (-\phi c, \partial_t w) + (\mathbb{D}(\mathbf{u})\nabla c, \nabla w) + (\mathbf{u} \cdot \nabla c, w) + (q^I c, w) = (\phi c_0, w(0)) + \int_0^T (q^I \hat{c}, w) \quad (4.6)$$

for all $q \in L^1(0, T; H^1(\Omega))$ and $w \in \{H^1(0, T; H^1(\Omega)) \cap H^1(0, T; H^1(\Omega)') | w(T) = 0\}$ with the Sobolev spaces defined as,

$$L_0^2(\Omega) = \left\{ \varphi \in L^2(\Omega) : \int_\Omega \varphi = 0 \right\}$$

and

$$H_0^1(\Omega) = \left\{ \varphi \in H^1(\Omega) : \int_{\Omega} \varphi = 0 \right\}$$

The rest of the analysis concerning the stability and convergence of the solutions are based on the formulations given above.

4.2 Stability analysis for MFE-DG with DG in time

I consider in this section, the stability analysis for the discretization strategy presented in (3.27)-(3.29) where we have a fully-implicit scheme with MFE for the pressure and velocity, DG for the concentration and DG in time.

4.2.1 Stability for pressure and velocity

The stability of the fluid pressure and velocity follows the same argument as in the result of Walkington and Rivière's work [71]. The derivation is directly taken from my master thesis work [35]. For completeness, recall the existing results.

Lemma 4.2.1. *There exists a constant $m > 0$ depending only upon Ω such that*

$$\sup_{\mathbf{u}_h \in \mathbf{U}_h} \frac{\int_{\Omega} p_h \operatorname{div}(\mathbf{u}_h)}{\|\mathbf{u}_h\|_{H(\Omega; \operatorname{div})}} \geq m \|p_h\|_{L^2(\Omega)}, \quad p_h \in P_h$$

In particular, if $Z_h = \{\mathbf{u}_h \in \mathbf{U}_h \mid \operatorname{div}(\mathbf{u}_h) = 0\}$ and $\mathbf{U}_h = Z_h \oplus Z_h^\perp$ is the orthogonal decomposition, then there exists a linear operator $L_h : P_h \rightarrow Z_h^\perp$ with $\|L_h\|_{\mathcal{L}(P_h, \mathbf{U}_h)} \leq 1$ such that

$$m \|p_h\|_{L^2(\Omega)}^2 \leq \int_{\Omega} p_h \operatorname{div}(L_h(p_h)), \quad p_h \in P_h$$

and if $\mathbf{u}_h \in Z_h^\perp$ then $m \|\mathbf{u}_h\|_{H(\Omega; \operatorname{div})} \leq \|\operatorname{div}(\mathbf{u}_h)\|_{L^2(\Omega)}$.

Lemma 4.2.2. *Let V be a linear space and $(\cdot, \cdot)_V$ be a (semi) inner product on V ; $w \geq 0$ be a non-zero element of $L^1(0, 1)$; and $0 < a < b$. Then there exists a constant $M_\ell > 0$, depending only upon ℓ and w , such that for all $u \in \mathcal{P}_\ell(a, b; V)$*

$$\|u\|_{L^p(a, b; V)} \leq (b - a)^{1/p-1/2} \left(M_\ell \int_a^b w((t - a)/(b - a)) \|u(t)\|_V^2 dt \right)^{1/2}, \quad 1 \leq p \leq \infty$$

In particular, if $1/p + 1/p' = 1$ then

$$\|u\|_{L^p(a, b; V)} \|u\|_{L^{p'}(a, b; V)} \leq M_\ell \int_a^b w((t - a)/(b - a)) \|w(t)\|_V^2$$

Now, I state and prove the stability for the pressure and velocity.

Theorem 4.2.3. *There exists a constant $M > 0$ independent of h and k such that solutions of the numerical scheme satisfy the following bounds.*

- *If $1 \leq p, q \leq \infty$ and $q^I, q^P \in L^p(0, T; L^q(\Omega))$, then*

$$\|\operatorname{div}(\mathbf{u}_h)\|_{L^p(0, T; L^q(\Omega))} \leq M (\|q^I\|_{L^p(0, T; L^q(\Omega))} + \|q^P\|_{L^p(0, T; L^q(\Omega))})$$

- *If $1 \leq p \leq \infty$, $q^I, q^P \in L^p(0, T; L^2(\Omega))$, then*

$$\begin{aligned} \|\mathbf{u}_h\|_{L^p(0, T; H(\Omega, \operatorname{div}))} + \|p_h\|_{L^p(0, T; L^2(\Omega))} &\leq M (\|q^I\|_{L^p(0, T; L^2(\Omega))} + \|q^P\|_{L^p(0, T; L^2(\Omega))} \\ &\quad + \|\rho_1 \mathbf{g}\|_{L^p(0, T; L^2(\Omega))}) \end{aligned}$$

Proof. For each $E \in \mathcal{E}_h$, let $\Pi_h : L^2(t_{j-1}, t_j; L^2(E)) \rightarrow \mathcal{P}_\ell(t_{j-1}, t_j; \mathcal{P}_k(E))$ denote the L^2 projection. A parent element calculation shows that there exists a constant $M > 0$ depending only on the parent element such that

$$\|\Pi_h(q^I - q^P)\|_{L^p(t_{j-1}, t_j, L^q(E))} \leq M \|q^I - q^P\|_{L^p(t_{j-1}, t_j, L^q(E))}, \quad 1 \leq p, q \leq \infty$$

Since $\operatorname{div}(\mathbf{u}_h) \in P_h$ it follows from (3.28) that

$$\operatorname{div}(\mathbf{u}_h) = \Pi_h(q^I - q^P)$$

Next, we introduce the orthogonal decomposition $\mathbf{U}_h = Z_h \oplus Z_h^\perp$, therefore, letting $\mathbf{u}_h = \mathbf{z}_h + \mathbf{u}_h^\perp$ be the decomposition of $\mathbf{u}_h$. From Lemma 4.2.1, we find

$$M \|\mathbf{u}_h^\perp\|_{H(\Omega; \operatorname{div})} \leq \|\operatorname{div}(\mathbf{u}_h^\perp)\|_{L^2(\Omega)} = \|\operatorname{div}(\mathbf{u}_h)\|_{L^2(\Omega)}$$

and, since $\operatorname{div}(\mathbf{u}_h) = \Pi_h(q^I - q^P)$, it follows that

$$\begin{aligned} \|\mathbf{u}_h^\perp\|_{L^p(t_{j-1}, t_j; H(\Omega; \operatorname{div}))} &\leq M \|\operatorname{div}(\mathbf{u}_h)\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} \\ &\leq M (\|q^I\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|q^P\|_{L^p(t_{j-1}, t_j; L^2(\Omega))}) \end{aligned}$$

To estimate $\mathbf{z}_h$, select it to be the test function in (4.1), and we have:

$$\int_{t_{j-1}}^{t_j} (\mathbb{K}^{-1}(c_h)(\mathbf{z}_h + \mathbf{u}_h^\perp), \mathbf{v}_h) = \int_{t_{j-1}}^{t_j} (\mathbb{K}^{-1}(c_h)\mathbf{u}_h, \mathbf{v}_h) = \int_{t_{j-1}}^{t_j} (\rho(c_h)g, \mathbf{v}_h)$$

Upon rescaling that $\|\mathbf{z}_h\|_{H(\Omega; \operatorname{div})} = \|\mathbf{z}_h\|_{L^2(\Omega)}$, and the assumption on $\mathbb{K}$, it follows that

$$\begin{aligned} \|\mathbf{z}_h\|_{L^2(t_{j-1}, t_j; \operatorname{div}(\Omega, \operatorname{div}))}^2 &\leq M \int_{t_{j-1}}^{t_j} (\mathbb{K}^{-1}(c_h)\mathbf{z}_h, \mathbf{z}_h) \\ &\leq M \left(\left| \int_{t_{j-1}}^{t_j} (\rho(c_h)g, \mathbf{v}_h) \right| + \left| \int_{t_{j-1}}^{t_j} (\mathbb{K}^{-1}(c_h)\mathbf{u}_h^\perp, \mathbf{v}_h) \right| \right) \\ &\leq M \|\mathbf{z}_h\|_{L^{p'}(t_{j-1}, t_j; H(\Omega; \operatorname{div}))} (\|\rho_1 \mathbf{g}\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|\mathbf{u}_h^\perp\|_{L^p(t_{j-1}, t_j; L^2(\Omega))}) \end{aligned}$$

Since $1/p + 1/p' = 1$ we can use Hölder's inequality:

$$\|\mathbf{z}_h\|_{L^p(t_{j-1}, t_j; \operatorname{div}(\Omega, \operatorname{div}))} \leq M (\|\rho_1 \mathbf{g}\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|\mathbf{u}_h^\perp\|_{L^p(t_{j-1}, t_j; L^2(\Omega))})$$

We can construct the bound

$$\|\mathbf{z}_h\|_{L^p(t_{j-1}, t_j; \text{div}(\Omega, \text{div}))} \leq M \left(\|\rho_1 \mathbf{g}\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|q^I\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|q^P\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} \right)$$

from which we can find the bound for $\|\mathbf{z}_h\|_{L^p(t_{j-1}, t_j; \text{div}(\Omega, \text{div}))}$. Since the operator $L_h : P_h \rightarrow Z_h^\perp$ in Lemma 4.2.1 is independent of time, it follows that $L_h(p_h) \in \mathcal{P}_\ell(t_{j-1}, t_j, \mathbf{U}_h)$. We may then set $\mathbf{v}_h = L_h(p_h)$ in (3.27) to find:

$$M \int_{t_{j-1}}^{t_j} \|p_h\|_{L^2(\Omega)}^2 \leq \int_{t_{j-1}}^{t_j} (p_h, \text{div}(L_h(p_h))) = \int_{t_{j-1}}^{t_j} ((\mathbb{K}^{-1}(c_h) \mathbf{u}_h, L_h(p_h)) - (\rho(c_h)g, L_h(p_h)))$$

By Lemma 4.2.2, we have:

$$\begin{aligned} \|p_h\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} &\leq M \left(\|\mathbf{u}_h\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|\rho_1 \mathbf{g}\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} \right) \\ &\leq M \left(\|\rho_1 \mathbf{g}\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|q^I\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} + \|q^P\|_{L^p(t_{j-1}, t_j; L^2(\Omega))} \right) \end{aligned}$$

□

4.2.2 Stability of concentration

In this section, I show that the scheme is stable for the concentration. We recall the discretization for the Lax-Friedrich DG scheme proposed in (3.26). I first consider using DG in time.

Define the energy semi-norm $\|\cdot\|_{C_h}$ in the following way:

$$\|v\|_{C_h} = \left(\sum_{E \in \mathcal{E}_h} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla v\|_{L^2(E)}^2 + \sum_{e \in \Gamma_h} h^{-1} \|(1 + \{|\mathbf{u}_h|\})^{1/2} [v]\|_{L^2(e)}^2 \right)^{1/2} \quad (4.7)$$

I first show the coercivity of the diffusion term in the following lemma.

Lemma 4.2.4. *There always exists a penalty parameter $\sigma > 0$ such that*

$$B_{di}(w_h, w_h; \mathbf{u}_h) \geq \frac{1}{2} \|w_h\|_{C_h}^2, \quad \forall w_h \in C_h$$

Proof. From our numerical scheme, we have

$$\begin{aligned} B_{di}(w_h, w_h; \mathbf{u}_h) &= (\mathbb{D}(\mathbf{u}_h) \nabla w_h, \nabla w_h) + (\epsilon - 1)([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} \\ &\quad + (\sigma h^{-1}(1 + \{|\mathbf{u}_h|\})[w_h], [w_h])_{\Gamma_h} \end{aligned}$$

According to the results from Appendix B in (B.18)

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} \leq M \left(\sum_{e \in \Gamma_h} h^{-1} \|(1 + \{|\mathbf{u}_h|\})^{1/2} [w_h]\|_{L^2(e)}^2 \right)^{1/2} \|D^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(\mathcal{E}_h)}$$

for a constant M independent upon h .

We use Young's inequality to obtain,

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} \leq \frac{\delta \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(\mathcal{E}_h)}^2}{2} + \frac{M^2}{2\delta} \sum_{e \in \Gamma_h} h^{-1} \|(1 + \{|\mathbf{u}_h|\})^{1/2} [w_h]\|_{L^2(e)}^2$$

for all $\delta > 0$.

Thus,

$$\begin{aligned} B_{di}(w_h, w_h; \mathbf{u}_h) &\geq (1 + \frac{\delta}{2}(\epsilon - 1)) \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(\mathcal{E}_h)}^2 \\ &\quad + \sum_{e \in \Gamma_h} \left(\sigma + \frac{\epsilon - 1}{2\delta} M^2 \right) h^{-1} \|(1 + \{|\mathbf{u}_h|\})^{1/2} [w_h]\|_{L^2(e)}^2 \end{aligned}$$

If $\epsilon = 1$, immediately one obtains $B_{di}(w_h, w_h; \mathbf{u}_h) = \|w_h\|_{C_h}^2$; (since $\epsilon = 1$ in this case)

If $\epsilon = 0$, choose $\delta = 1$ and $\sigma \geq \frac{1}{2}(1 + M^2)$;

If $\epsilon = -1$, choose $\delta = \frac{1}{2}$ and $\sigma \geq \frac{1}{2} + 2M^2$.

These criteria will guarantee $B_{di}(w_h, w_h; \mathbf{u}_h) \geq \frac{1}{2} \|w_h\|_{C_h}^2$. □

We just showed the coercivity of the diffusion term. Now, with the help of this property, we will proceed by proving the stability of the concentration solution.

Theorem 4.2.5. *The numerical scheme is stable with respect to the fluid concentration, so that $\|c_h\|_{\ell^\infty(L^2(\Omega))}$, $\|c_h\|_{L^2(0,T;C_h)}$ and $\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))}$ are bounded independent of h and k . In particular, we have:*

$$\begin{aligned} \max_{1 \leq n \leq N} \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \sum_{j=1}^N \|[\phi^{1/2} c_h^{j-1}]\|_{L^2(\Omega)}^2 + \int_0^T \left(\|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \right. \\ \left. + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h} \right) \leq \|\phi^{1/2} c_{h-}^0\|_{L^2(\Omega)}^2 + \int_0^T \|\sqrt{q^I} \hat{c}\|_{L^2(\Omega)}^2 \end{aligned}$$

Proof. According to the result in Lemma 4.2.4, we have

$$B_{di}(c_h, c_h; \mathbf{u}_h) \geq \frac{1}{2} \|c_h\|_{C_h}^2$$

Also according to our numerical scheme,

$$\begin{aligned} B_{cq}(c_h, w_h; \mathbf{u}_h) = \frac{1}{2} \left((\mathbf{u}_h \nabla c_h, w_h) - (\mathbf{u}_h c_h, \nabla w_h) + ((q^I + q^P) c_h, w_h) \right. \\ \left. + (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_{\Gamma_h} - (w_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} \right) \end{aligned}$$

then, we have

$$\begin{aligned} B_{cq}(c_h, c_h; \mathbf{u}_h) = \frac{1}{2} \left((\mathbf{u} \nabla c_h, c_h)_{\mathcal{E}_h} - (\mathbf{u}_h c_h, \nabla c_h)_{\mathcal{E}_h} + ((q^I + q^P) c_h, c_h) \right. \\ \left. + (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} - (c_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} \right) \\ = \frac{1}{2} \left((q^I + q^P) c_h, c_h \right) + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h} \end{aligned}$$

We can conclude:

$$B_{cq}(c_h, c_h; \mathbf{u}_h) = \frac{1}{2} \left((q^I + q^P) c_h, c_h \right) + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h} \quad (4.8)$$

Now, we expand the numerical scheme:

$$\begin{aligned} \int_{t_{j-1}}^{t_j} ((\phi \partial_t c_h, c_h) + B_{di}(c_h, c_h; \mathbf{u}_h) + B_{cq}(c_h, c_h; \mathbf{u}_h)) + (c_{h+}^{j-1}, \phi c_{h+}^{j-1}) \\ = (c_{h-}^{j-1}, \phi c_{h+}^{j-1}) + \int_{t_{j-1}}^{t_j} (\hat{c}q^I, c_h) \end{aligned}$$

Notice,

$$\int_{t_{j-1}}^{t_j} (\phi \partial_t c_h, c_h) = \int_{t_{j-1}}^{t_j} \frac{1}{2} \partial_t (\phi c_h, c_h) = \frac{1}{2} (\phi c_{h-}^j, c_{h-}^j) - \frac{1}{2} (\phi c_{h+}^{j-1}, c_{h+}^{j-1})$$

Thus, we have

$$\begin{aligned} \int_{t_{j-1}}^{t_j} (\phi \partial_t c_h, c_h) + (c_{h+}^{j-1}, \phi c_{h+}^{j-1}) &= \frac{1}{2} (\phi c_{h-}^j, c_{h-}^j) + \frac{1}{2} (\phi c_{h+}^{j-1}, c_{h+}^{j-1}) \\ &= \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|^2 + \frac{1}{2} (\phi [c_h^{j-1}]_t, [c_h^{j-1}]_t) + (\phi c_{h+}^{j-1}, c_{h-}^{j-1}) - \frac{1}{2} (\phi c_{h-}^{j-1}, c_{h-}^{j-1}) \\ &= \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|^2 + \frac{1}{2} \|\phi^{1/2} [c_h^{j-1}]_t\|^2 + (\phi c_{h+}^{j-1}, c_{h-}^{j-1}) - \frac{1}{2} \|\phi^{1/2} c_{h-}^{j-1}\|^2 \end{aligned}$$

Therefore,

$$\begin{aligned} \int_{t_{j-1}}^{t_j} (B_{di}(c_h, c_h; \mathbf{u}_h) + B_{cq}(c_h, c_h; \mathbf{u}_h)) + \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|^2 + \frac{1}{2} \|\phi^{1/2} [c_h^{j-1}]_t\|^2 \\ + (\phi c_{h+}^{j-1}, c_{h-}^{j-1}) - \frac{1}{2} \|\phi^{1/2} c_{h-}^{j-1}\|^2 = (c_{h-}^{j-1}, \phi c_{h+}^{j-1}) + \int_{t_{j-1}}^{t_j} (\hat{c}q^I, c_h) \end{aligned}$$

Hence, we obtain

$$\begin{aligned} \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \frac{1}{2} \|\phi^{1/2} [c_h^{j-1}]_t\|_{L^2(\Omega)}^2 + \int_{t_{j-1}}^{t_j} (B_{di}(c_h, c_h; \mathbf{u}_h) + B_{cq}(c_h, c_h; \mathbf{u}_h)) \\ = \frac{1}{2} \|\phi^{1/2} c_{h-}^{j-1}\|_{L^2(\Omega)}^2 + \int_{t_{j-1}}^{t_j} (\hat{c}q^I, c_h) \end{aligned}$$

The equation above can be simplified by Lemma 4.2.4 and 4.8.

$$\begin{aligned} & \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \frac{1}{2} \|[\phi^{1/2} c_h^{j-1}]_t\|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{t_{j-1}}^{t_j} (\|c_h\|_{C_h}^2 + ((q^I + q^P)c_h, c_h) \\ & + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h}) \leq \frac{1}{2} \|\phi^{1/2} c_{h-}^{j-1}\|_{L^2(\Omega)}^2 + \int_{t_{j-1}}^{t_j} (\hat{c} q^I, c_h) \end{aligned} \quad (4.9)$$

Now, again Cauchy-Schwarz's inequality and Young's inequality can be used to obtain

$$(\hat{c} q^I, c_h) \leq \|\hat{c} \sqrt{q^I}\|_{L^2(\Omega)} \|\sqrt{q^I} c_h\|_{L^2(\Omega)} \leq \frac{\|\sqrt{q^I} c_h\|_{L^2(\Omega)}^2}{2} + \frac{\|\hat{c} \sqrt{q^I}\|_{L^2(\Omega)}^2}{2}$$

Now, substituting this term into (4.9):

$$\begin{aligned} & \frac{1}{2} \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \frac{1}{2} \|[\phi^{1/2} c_h^{j-1}]_t\|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{t_{j-1}}^{t_j} (\|c_h\|_{C_h}^2 + ((q^I + q^P)c_h, c_h) \\ & + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h}) \leq \frac{1}{2} \|\phi^{1/2} c_{h-}^{j-1}\|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{t_{j-1}}^{t_j} \|\sqrt{q^I} c_h\|_{L^2(\Omega)}^2 + \frac{1}{2} \int_{t_{j-1}}^{t_j} \|\hat{c} \sqrt{q^I}\|_{L^2(\Omega)}^2 \end{aligned}$$

Therefore,

$$\begin{aligned} & \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \|[\phi^{1/2} c_h^{j-1}]_t\|_{L^2(\Omega)}^2 + \int_{t_{j-1}}^{t_j} \left(\|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h} \right) \\ & \leq \|\phi^{1/2} c_{h-}^{j-1}\|_{L^2(\Omega)}^2 + \int_{t_{j-1}}^{t_j} \|\sqrt{q^I} \hat{c}\|_{L^2(\Omega)}^2. \end{aligned}$$

We sum up, overall, the time interval and obtain:

$$\begin{aligned} & \max_{1 \leq n \leq N} \|\phi^{1/2} c_{h-}^j\|_{L^2(\Omega)}^2 + \sum_{j=1}^N \|[\phi^{1/2} c_h^{j-1}]_t\|_{L^2(\Omega)}^2 + \int_0^T \left(\|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \right. \\ & \left. + (|\mathbf{u}_h \cdot \mathbf{n}_e| [c_h], [c_h])_{\Gamma_h} \right) \leq \|\phi^{1/2} c_{h-}^0\|_{L^2(\Omega)}^2 + \int_0^T \|\sqrt{q^I} \hat{c}\|_{L^2(\Omega)}^2 \end{aligned}$$

Therefore, the scheme is stable for the concentration. Now, we show that

$\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))}$ is bounded, with the broken Sobolev space defined as

$$H^1(\mathcal{E}_h) = \{\varphi \in L^2(\Omega) : \varphi_E \in H^1(E), E \in \mathcal{E}_h\}$$

Define the semi-norm for $H^1(\mathcal{E}_h)$ to be

$$|v|_{H^1(\mathcal{E}_h)} = \left(\sum_{E \in \mathcal{E}_h} \|\nabla v\|_{L^2(E)}^2 + \sum_{e \in \Gamma_h} h^{-1} \|[v]\|_{L^2(e)}^2 \right)^{1/2}$$

and recall that the $H^1(\mathcal{E}_h)$ norm is defined to be

$$\|v\|_{H^1(\mathcal{E}_h)} = \left(\|v\|_{L^2(\Omega)}^2 + |v|_{H^1(\mathcal{E}_h)}^2 \right)^{1/2}$$

We first consider the case when $\int_{\Omega} q^P = 0$ over a certain time interval. Since this implies $q^P = 0$ and $q^I = 0$, it means we have to impose additional constraints for the concentration such as

$$\int_{\Omega} c_h = 0$$

for the well-posedness of the solution according to (3.27)-(3.29). Therefore, according to Poincaré's inequality,

$$\int_A \|c_h\|_{L^2(\Omega)}^2 \leq C_p^2 \int_A |c_h|_{H^1(\mathcal{E}_h)}^2$$

where A is the interval such that

$$\int_{\Omega} q^P = 0.$$

Consider $\int_{\Omega} q^P > 0$, then apply the Poincaré's inequality for the broken Sobolev space from [85, 86].

$$\|c_h\|_{L^2(\Omega)} \leq C_p \left(|c_h|_{H^1(\mathcal{E}_h)}^2 + \left(\int_{\Omega} \sqrt{q^P} c_h \right)^2 \right)^{1/2}$$

where C_p is the Poincaré constant independent of h on a regular mesh. We use Cauchy-Schwarz's inequality and obtain

$$\|c_h\|_{L^2(\Omega)} \leq C \left(|c_h|_{H^1(\mathcal{E}_h)}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \right)^{1/2}$$

Therefore,

$$\|c_h\|_{H^1(\mathcal{E}_h)} \lesssim \left(|c_h|_{H^1(\mathcal{E}_h)}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \right)^{1/2} \lesssim \left(\|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \right)^{1/2}$$

Hence, we have

$$\int_{A^c} \|c_h\|_{H^1(\mathcal{E}_h)}^2 \lesssim \int_0^T \|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2$$

Therefore, $\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))}$ is bounded as well. $\square$

4.3 Stability analysis for DG-DG with implicit Euler decoupling

4.3.1 Stability of pressure and velocity

Again for simplicity, I consider the case without the use of weighted average. Recall the DG discretization for pressure in Algorithm 3, where we have

$$B_d(p_h^j, q_h; c_h^{j-1}) = \ell_d^j(q_h; c_h^{j-1}).$$

We define $H_0^1(\mathcal{E}_h)$ to be,

$$H_0^1(\mathcal{E}_h) = \left\{ \varphi \in H^1(\mathcal{E}_h) : \int_{\Omega} \varphi = 0 \right\}$$

The norm for $H_0^1(\mathcal{E}_h)$ is defined to be,

$$\|\varphi\|_{H_0^1(\mathcal{E}_h)} = \left(\sum_{E \in \mathcal{E}_h} \|\nabla \varphi\|_{L^2(E)}^2 + \sum_{e \in \Gamma_h} h^{-1} \|[\varphi]\|_{L^2(e)}^2 \right)^{1/2}.$$

By the Poincaré's inequality from [85, 86], one can verify it is indeed a norm for $H_0^1(\mathcal{E}_h)$.

Now, I establish a bound of the pressure and velocity solutions.

Theorem 4.3.1. *There exists a constant $M > 0$ independent of h and k such that solutions of the numerical scheme presented in Algorithm 3 satisfy the following bounds.*

- For all $q^I, q^P \in L^2(0, T; L^2(\Omega))$, then

$$\|div(\mathbf{u}_h)\|_{L^2(0, T; L^2(\Omega))} \leq M (\|q^I\|_{L^2(0, T; L^2(\Omega))} + \|q^P\|_{L^2(0, T; L^2(\Omega))})$$

- For all $q^I, q^P \in L^2(0, T; L^2(\Omega))$, then

$$\begin{aligned} \|\mathbf{u}_h\|_{L^2(0, T; H(\Omega, div))} + \|p_h\|_{L^2(0, T; H_0^1(\mathcal{E}_h))} &\leq M (\|q^I\|_{L^2(0, T; L^2(\Omega))} + \|q^P\|_{L^2(0, T; L^2(\Omega))}) \\ &\quad + \|\rho_1 \mathbf{g}\|_{L^2(0, T; L^2(\Omega))} \end{aligned}$$

Proof. From DG discretization, we have

$$\begin{aligned} B_d(p_h, p_h; c_h) = & \sum_{E \in \mathcal{E}_h} \|\mathbb{K}(c_h) \nabla p_h\|_{L^2(E)}^2 + (\theta - 1) \sum_{e \in \Gamma_h} (\{\mathbb{K}(c_h)^{1/2} \nabla p_h \cdot \mathbf{n}_e\}, [p_h])_e + \sum_{e \in \Gamma_h} \sigma h^{-1} \|[p_h]\|_{L^2(e)}^2 \end{aligned}$$

Thus, we can obtain a lower bound for the bilinear form,

$$\begin{aligned} B_d(p_h, p_h; c_h) \geq & \left(1 - \frac{\delta}{2} |1 - \theta|\right) k_0 \sum_{E \in \mathcal{E}_h} \|\nabla p_h\|_{L^2(E)}^2 + \sum_{e \in \Gamma_h} \left(\sigma - \frac{C_t^2 k_1^2 n_0}{2\delta k_0} |1 - \theta|\right) h^{-1} \|[p_h]\|_{L^2(e)}^2 \end{aligned}$$

for all $\delta > 0$. Next, we have

$$B_d(p_h^j, p_h^j; c_h^{j-1}) \geq \frac{1}{2} \|p_h^j\|_{H_0^1(\mathcal{E}_h)}^2$$

where p_h^j is the piecewise constant approximation in time over the interval $[t_{j-1}, t_j]$.

Then, we can derive an upper bound for $\ell_d^j(p_h^j; c_h^{j-1})$, where we have,

$$\begin{aligned} \ell_d^j(p_h^j; c_h^{j-1}) &\leq \frac{\delta k_0}{2C_t^2 k_1^2 n_0} \|(q_h^I - q_h^P)^j\|_{L^2(\Omega)}^2 + \frac{C_t^2 k_1^2 n_0}{2\delta k_0} \|p_h^j\|_{L^2(\Omega)}^2 + \frac{k_1 \delta}{2} \|\rho \mathbf{g}\|_{L^2(\Omega)}^2 \\ &\quad + \frac{C_t^2 k_1^2 n_0}{2\delta k_0} \sum_{e \in \Gamma_h} h^{-1} \| [p_h^j] \|_{L^2(e)}^2 \end{aligned}$$

for all $\delta > 0$ according to the trace inequality and Young's inequality.

For the source term:

$$\begin{aligned} \int_0^T \|q_h^I - q_h^P\|_{L^2(\Omega)}^2 &= \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|(q_h^I - q_h^P)^j\|_{L^2(\Omega)}^2 = \sum_{j=1}^N \int_{t_{j-1}}^{t_j} ((q_h^I - q_h^P)^j, q^I - q^P) \\ &\leq \left(\int_0^T \|q_h^I - q_h^P\|_{L^2(\Omega)}^2 \right)^{1/2} \left(\int_0^T \|q^I - q^P\|_{L^2(\Omega)}^2 \right)^{1/2} \end{aligned}$$

Hence, we have

$$\|q_h^I - q_h^P\|_{L^2(0,T;L^2(\Omega))} \leq \|q^I - q^P\|_{L^2(0,T;L^2(\Omega))} \quad (4.10)$$

Similarly, we also have:

$$\|q_h^I\|_{L^2(0,T;L^2(\Omega))} \leq \|q^I\|_{L^2(0,T;L^2(\Omega))} \quad (4.11)$$

$$\|q_h^P\|_{L^2(0,T;L^2(\Omega))} \leq \|q^P\|_{L^2(0,T;L^2(\Omega))} \quad (4.12)$$

So, for the right-hand-side we have:

$$\begin{aligned} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \ell^j(p_h^j; c_h^{j-1}) &\leq \frac{\delta k_0}{2C_t^2 k_1^2 n_0} \|q^I - q^P\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{C_t^2 k_1^2 n_0}{2\delta k_0} \|p_h\|_{L^2(0,T;L^2(\Omega))}^2 \\ &\quad + \frac{k_1 \delta}{2} \|\rho \mathbf{g}\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{C_t^2 k_1^2 n_0}{2\delta k_0} \int_0^T \sum_{e \in \Gamma_h} h^{-1} \|[p_h^j]\|_{L^2(e)}^2 \end{aligned} \quad (4.13)$$

From Poincaré's inequality, we have:

$$\|\varphi\|_{L^2(\Omega)} \leq C_p \|\varphi\|_{H_0^1(\mathcal{E}_h)} \text{ for all } \varphi \in H_0^1(\mathcal{E}_h)$$

for all $\delta > 0$.

Therefore, from (4.10), (4.13) and (4.14) we have

$$\begin{aligned} \frac{1}{2} \|p_h\|_{L^2(0,T;H_0^1(\mathcal{E}_h))}^2 &\leq \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_d(p_h^j, p_h^j; c_h^{j-1}) = \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \ell_d^j(p_h^j; c_h^{j-1}) \\ &\leq \frac{\delta k_0 C_p^2}{2C_t^2 k_1^2 n_0} \|q^I - q^P\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{C_t^2 k_1 n_0}{2\delta k_0} \|p_h\|_{L^2(0,T;H_0^1(\mathcal{E}_h))}^2 + \frac{k_1 \delta}{2} \|\rho_1 \mathbf{g}\|_{L^2(0,T;L^2(\Omega))}^2 \end{aligned}$$

We have therefore derived an upper bound for the pressure:

$$\|p_h^j\|_{H_0^1(\mathcal{E}_h)} \leq M (\|q^I\|_{L^2(\Omega)} + \|q^P\|_{L^2(\Omega)} + \|\rho_1 \mathbf{g}\|_{L^2(\Omega)})$$

For the velocity term $\mathbf{u}_h$, according to the flux reconstruction in Algorithm 3, we have:

$$\begin{aligned} \|\mathbf{u}_h\|_{L^2(\Omega)}^2 &\leq |(\mathbb{K} \nabla p_h, \mathbf{u}_h)_{\mathcal{E}_h}| + |\theta| |(\{\mathbb{K}\} \mathbf{u}_h \cdot \mathbf{n}_e, [p_h])_{\Gamma_h}| + |(\mathbb{K} \rho \mathbf{g}, \mathbf{u}_h)_{\mathcal{E}_h}| \\ &\leq \frac{k_1 \delta}{2} \|\nabla p_h\|_{L^2(\mathcal{E}_h)}^2 + \frac{k_1}{2\delta} (2 + C_t^2) \|\mathbf{u}_h\|_{L^2(\Omega)}^2 + \frac{k_1 \delta}{2} \sum_{e \in \Gamma_h} h^{-1} \|[p_h]\|_{L^2(e)}^2 + \frac{k_1 \delta}{2} \|\rho_1 \mathbf{g}\|_{L^2(\Omega)}^2 \\ &\leq \frac{k_1 \delta}{2} \|p_h\|_{H_0^1(\mathcal{E}_h)}^2 + \frac{k_1}{2\delta} (2 + C_t^2) \|\mathbf{u}_h\|_{L^2(\Omega)}^2 + \frac{k_1 \delta}{2} \|\rho_1 \mathbf{g}\|_{L^2(\Omega)}^2 \end{aligned}$$

for all $\delta > 0$ by Young's inequality. Therefore, we also have an upper bound for the velocity

term,

$$\|\mathbf{u}_h^j\|_{L^2(\Omega)} \leq M \left(\|p_h^j\|_{H_0^1(\mathcal{E}_h)} + \|\rho_1 \mathbf{g}\|_{L^2(\Omega)} \right) \leq M \left(\|(q_h^I)^j\|_{L^2(\Omega)} + \|(q_h^P)^j\|_{L^2(\Omega)} + \|\rho_1 \mathbf{g}\|_{L^2(\Omega)} \right)$$

According to [75], the reconstructed flux satisfies the following property:

$$\nabla \cdot \mathbf{u}_h^j = \pi_h(q_h^I - q_h^P)^j$$

where π_h is the L^2 -projection in space.

Then, we can obtain an upper bound for $\nabla \cdot \mathbf{u}_h$,

$$\|\nabla \cdot \mathbf{u}_h^j\|_{L^2(\Omega)} \leq M \left(\|(q_h^I)^j\|_{L^2(\Omega)} + \|(q_h^P)^j\|_{L^2(\Omega)} \right)$$

We can simply integrate over the time interval $[0, T]$ and use the result (4.11), (4.12) to obtain,

$$\|\operatorname{div}(\mathbf{u}_h)\|_{L^2(0,T;L^2(\Omega))} \leq M \left(\|q^I\|_{L^2(0,T;L^2(\Omega))} + \|q^P\|_{L^2(0,T;L^2(\Omega))} \right)$$

$$\begin{aligned} \|\mathbf{u}_h\|_{L^2(0,T;H(\Omega,\operatorname{div}))} + \|p_h\|_{L^2(0,T;H_0^1(\mathcal{E}_h))} &\leq M \left(\|q^I\|_{L^2(0,T;L^2(\Omega))} + \|q^P\|_{L^2(0,T;L^2(\Omega))} \right. \\ &\quad \left. + \|\rho_1 \mathbf{g}\|_{L^2(0,T;L^2(\Omega))} \right) \end{aligned}$$

for all q^I, q^P in $L^2(0, T; L^2(\Omega))$. And since we know the input source term q^I, q^P are in $L^\infty(0, T; L^2(\Omega))$; we can obtain the stability for the pressure and velocity. $\square$

Remark 4.3.2. In comparison with DG in time, the upper bound for pressure and velocity using the implicit Euler decoupling is L^2 in time instead of L^∞ . The reason for this is because we take the L^2 projection in time for the source information in our numerical scheme.

4.3.2 Stability of concentration

The stability result for the implicit Euler scheme for the concentration has been established in [34]. We simply state the stability result here.

Theorem 4.3.3. *For all $j = 1, 2, \dots, N$, we have the following bound for the concentration solution computed using Algorithm 3:*

$$\begin{aligned} \|\phi^{1/2} c_h^j\|_{L^2(\Omega)}^2 + \int_0^{t_j} k \|\phi^{1/2} \partial_t c_h\|_{L^2(\Omega)}^2 + \|c_h\|_{C_h}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 dt \\ \leq \|\phi^{1/2} c_h^0\|_{L^2(\Omega)}^2 + \int_0^{t_j} \|\sqrt{q^I} \hat{c}\|^2 dt \end{aligned}$$

where $k = \max_{i=1, \dots, j} \{k_i\}$.

Corollary 4.3.4. *There is a positive constant $M > 0$ such that for the concentration computed using Algorithm 3, we have:*

$$\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))} \leq M$$

Proof. According to Theorem 4.3.3 we have,

$$\int_0^T \|c_h\|_{H^1(\mathcal{E}_h)}^2 + \|\sqrt{q^P} c_h\|_{L^2(\Omega)}^2 \leq \|\phi^{1/2} c_h^0\|_{L^2(\Omega)}^2 + \int_0^T \|\sqrt{q^I} \hat{c}\|^2.$$

With the same argument as in Theorem 4.2.5 using Poincaré's inequality and bounding the term where there is no injection and production. We have an upper bound for $\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))}$.

□

4.4 Stability analysis for DG-DG with Crank-Nicolson decoupling scheme

4.4.1 Stability of pressure and velocity

The stability of the pressure and the velocity for the Crank-Nicolson decoupling scheme, according to the Algorithm 4, we have almost exactly the same result as the case with the implicit Euler time stepping, because the bilinear form in each interval is

$$B_d(p_h^j, q_h; c_h^j) = \ell_d^j(q_h; c_h^j).$$

With the same argument as in Theorem 4.3.1, we have following result.

Theorem 4.4.1. *There exists a constant $M > 0$ independent of h and k such that the pressure and velocity solutions of the numerical scheme presented in Algorithm 4 satisfy the following bounds.*

- For all $q^I, q^P \in L^2(0, T; L^2(\Omega))$, then

$$\|div(\mathbf{u}_h)\|_{L^2(0, T; L^2(\Omega))} \leq M (\|q^I\|_{L^2(0, T; L^2(\Omega))} + \|q^P\|_{L^2(0, T; L^2(\Omega))})$$

- For all $q^I, q^P \in L^2(0, T; L^2(\Omega))$, then

$$\begin{aligned} \|\mathbf{u}_h\|_{L^2(0, T; H(\Omega, div))} + \|p_h\|_{L^2(0, T; H_0^1(\mathcal{E}_h))} &\leq M (\|q^I\|_{L^2(0, T; L^2(\Omega))} + \|q^P\|_{L^2(0, T; L^2(\Omega))} \\ &\quad + \|\rho_1 \mathbf{g}\|_{L^2(0, T; L^2(\Omega))}) \end{aligned}$$

4.4.2 Stability of concentration

The stability result for the Crank-Nicolson scheme for the concentration has been established in [70]. The stability result is simply stated here. For the Crank-Nicolson scheme, we have

Theorem 4.4.2. *For all $j = 2, \dots, N$, we have:*

$$\|\phi^{1/2} c_h^j\|_{L^2(\Omega)}^2 + \int_{t_1}^{t_j} \|\bar{c}_h\|_{C_h}^2 + \|\sqrt{\bar{q}^P} \bar{c}_h\|_{L^2(\Omega)}^2 dt \leq \|\phi^{1/2} c_h^1\|_{L^2(\Omega)}^2 + \int_{t_1}^{t_j} \|\sqrt{\bar{q}^I} \bar{c}\|^2 dt \quad (4.14)$$

where $k = \max_{i=1, \dots, j} \{k_i\}$.

As a consequence, we also have the upper bound for the concentration solution in $L^2(0, T; H^1(\mathcal{E}_h))$. For the proof, we refer to Corollary 4.3.4.

Corollary 4.4.3. *There is a positive constant $M > 0$ such that for the concentration computed using Algorithm 4 we have:*

$$\|\bar{c}_h\|_{L^2(0, T; H^1(\mathcal{E}_h))} \leq M$$

4.5 Stability analysis for MFE-DG with implicit Euler and Crank-Nicolson decoupling schemes

For the stability analysis of the MFE-DG with implicit Euler and Crank-Nicolson decoupling schemes, I refer the reader to the results in [34] and [70].

Convergence Analysis

In this chapter, I establish the convergence of the numerical solutions under low regularity condition. Under the low regularity, one has to rely upon the compactness result to establish subsequential convergence. The Aubin-Lions compactness theorem is extremely useful in establishing the compact embedding of the Sobolev spaces. However, the Aubin-Lions compactness theorem is restricted to function spaces that are continuous in time. Hence, the Aubin-Lions compactness theorem works for Implicit Euler and Crank-Nicolson time updating. For DG in time, I have generalized the compactness theorem so that it works on Sobolev spaces with discontinuous functions in time.

With the help of the compactness result, I demonstrate the convergence of pressure and velocity using Mixed-Finite Element (MFE) discretization and also using discontinuous Galerkin (DG) discretization with flux reconstruction. Then, I proceed to prove the convergence of the concentration to the weak solution using DG discretization.

5.1 Compactness theorems

The Aubin-Lions compactness theorem [87] states:

Theorem 5.1.1 (Aubin-Lions compactness theorem). *Consider Banach spaces B_0 , B_1 , B_2 such that $B_0 \hookrightarrow B_1$ is compact and $B_1 \hookrightarrow B_2$ is continuous. Assume that B_0 is reflexive*

and separable. Then $W = \{u \in L^2(0, T; B_0) : \partial_t u \in L^2(0, T; B_2)\}$ is compactly embedded into $L^2(0, T; B_1)$.

The generalized compactness theorem is presented as follows [72]:

Theorem 5.1.2. *Let H be a Hilbert space with inner-product $(\cdot, \cdot)_H$ and V and W be Banach spaces equipped with norms $\|\cdot\|_V$ and $\|\cdot\|_W$. Assume that $W \subset H$ is dense and*

$$W \hookrightarrow V \hookrightarrow H \hookrightarrow W'$$

are dense embeddings with V compactly embedded in H . The space W' denotes the dual space of W . Let $h \in (0, \infty)$ be a (mesh) parameter and for each $h > 0$ let $W(\mathcal{E}_h)$ be a Banach space with $W \hookrightarrow W(\mathcal{E}_h) \hookrightarrow V$ where the embedding constants are independent of h .

For each h , let $W_h \subset W(\mathcal{E}_h)$ be a closed subspace and let $\{t_j\}_{j=0}^N$ be a quasi-uniform family of partitions of $[0, T]$. Let $\pi_h : H \rightarrow W_h$ denote the orthogonal projection, and assume that its restriction to $W(\mathcal{E}_h)$ is stable in the sense that there exists a constant $M > 0$ independent of h such that $\|\pi_h w\|_{W(\mathcal{E}_h)} \leq M \|w\|_{W(\mathcal{E}_h)}$ for $w \in W(\mathcal{E}_h)$.

Fix $\ell \geq 0$ an integer and $1 < p < \infty$, $1 \leq q < \infty$, with $1/p + 1/q \geq 1$, and assume that

- 1. For each $h > 0$, $w_h \in \{w_h \in L^p(0, T; W_h) \mid w_h|_{(t_{j-1}, t_j)_h} \in \mathcal{P}_\ell(t_{j-1}, t_j; W_h)\}$ and on each interval satisfies*

$$\forall z_h \in \mathcal{P}_\ell(t_{j-1}, t_j; W_h), \quad \int_{t_{j-1}}^{t_j} (\partial_t w_h, z_h)_H + (w_{h+}^{j-1} - w_{h-}^{j-1}, z_{h+}^{j-1})_H = \int_{t_{j-1}}^{t_j} F_h(z_h).$$

- 2. The sequence $\{w_h\}_{h>0}$ is bounded in $L^p(0, T; V)$.*

- 3. For each $h > 0$, $F_h \in L^q(0, T; W'_h)$ and $\{\|F_h\|_{L^q(0, T; W'_h)}\}_{h>0} \subset \mathfrak{R}$ is bounded.*

Then the set $\{w_h\}_{h>0}$ is precompact in $L^p(0, T; H) \cap L^r(0, T; W')$ for each $1 \leq r < \infty$.

Proof. First, fix $\delta > 0$ and consider the space $L^p(\delta, T; W(\mathcal{E}_h))$. Its dual space is $L^{p'}(\delta, T; W(\mathcal{E}_h)')$ with $1/p + 1/p' = 1$. Since the function $t \rightarrow w_h(t) - w_h(t - \delta)$ belongs to W_h , use the definition

of the projection π_h onto W_h and its stability on $W(\mathcal{E}_h)$ to have:

$$\begin{aligned}
\left(\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'_h}^{p'} dt \right)^{1/p'} &= \sup_{v \in L^p(\delta, T; W(\mathcal{E}_h))} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), v)_H dt}{\|v\|_{L^p(\delta, T; W(\mathcal{E}_h))}} \\
&= \sup_{v \in L^p(\delta, T; W(\mathcal{E}_h))} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), \pi_h v)_H dt}{\|v\|_{L^p(\delta, T; W(\mathcal{E}_h))}} \\
&= \sup_{v \in L^p(\delta, T; W(\mathcal{E}_h))} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), \pi_h v)_H dt}{\|\pi_h v\|_{L^p(\delta, T; W(\mathcal{E}_h))}} \frac{\|\pi_h v\|_{L^p(\delta, T; W(\mathcal{E}_h))}}{\|v\|_{L^p(\delta, T; W(\mathcal{E}_h))}} \\
&\leq M \sup_{v \in L^p(\delta, T; W(\mathcal{E}_h))} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), \pi_h v)_H dt}{\|\pi_h v\|_{L^p(\delta, T; W(\mathcal{E}_h))}}.
\end{aligned}$$

This implies

$$\left(\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'_h}^{p'} dt \right)^{1/p'} \leq M \sup_{v \in L^p(\delta, T; W_h)} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), v)_H dt}{\|v\|_{L^p(\delta, T; W(\mathcal{E}_h))}}. \quad (5.1)$$

Lemma 3.9 of [71] then gives that

$$\sup_{v_h \in L^p(\delta, T; W_h)} \frac{\int_{\delta}^T (w_h(t) - w_h(t - \delta), v_h)_H dt}{\|v_h\|_{L^p(\delta, T; W(\mathcal{E}_h))}} \leq M(\ell, \nu) \|F_h\|_{L^q(0, T; W'_h)} \max(k, \delta)^{1/q'} \delta^{1/p'}.$$

Thus equation (5.1) becomes (with a different constant M that depends on $\|\pi_h\|_{\mathcal{L}(W(\mathcal{E}_h), W_h)}$)

$$\left(\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'_h}^{p'} dt \right)^{1/p'} \leq M(\ell, \nu) \|F_h\|_{L^q(0, T; W'_h)} \max(k, \delta)^{1/q'} \delta^{1/p'}.$$

Next, since $W \hookrightarrow W(\mathcal{E}_h)$, there is a constant $M > 0$ such that

$$\|w_h(t) - w_h(t - \delta)\|_{W'} \leq M \|w_h(t) - w_h(t - \delta)\|_{W'_h}.$$

Therefore, we have

$$\left(\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'}^{p'} dt \right)^{1/p'} \leq M(\ell, \nu) \|F_h\|_{L^q(0, T; W'_h)} \max(k, \delta)^{1/q'} \delta^{1/p'}. \quad (5.2)$$

By assumption, $\|F_h\|_{L^q(0,T;W'_h)}$ is uniformly bounded. We now show that $\{w_h\}_{h>0}$ is equicontinuous in $L^{p'}(0,T;W')$.

Fix $\epsilon > 0$. We want to show there is $\delta_0 > 0$ such that

$$\left(\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'}^{p'} dt \right)^{1/p'} \leq \epsilon, \quad \forall h > 0, \forall \delta < \delta_0. \quad (5.3)$$

Since $p > 1$, we have $p' < \infty$. If $q = 1$, we choose δ_0 such that $M\delta_0^{1/p'} < \epsilon$. If $q > 1$, it suffices to find δ_0 such that

$$M \max(k, \delta_0)^{1/q'} \delta_0^{1/p'} < \epsilon.$$

We can assume that $\delta_0 < k$ and take

$$\delta_0 = \min \left(\frac{1}{2} \left(\frac{\epsilon}{Mk^{1/q'}} \right)^{p'}, k \right).$$

Consider now the case $q > 1$, then $q' < \infty$. It suffices to find δ_0 such that

$$M \max(k, \delta_0)^{1/q'} \delta_0^{1/p'} < \epsilon.$$

We can assume that $\delta_0 < k$ and choose

$$\delta_0 = \min \left(\frac{1}{2} \left(\frac{\epsilon}{Mk^{1/q'}} \right)^{p'}, k \right).$$

By assumption $\{w_h\}_{h>0}$ is bounded in $L^p(0,T;V)$ with $p > 1$. This implies that $\{w_h\}_{h>0}$ is bounded in $L^1(0,T;V)$. In addition, we showed that $\{w_h\}_{h>0}$ is equicontinuous in $L^{p'}(0,T;W')$ for $1 < p' < \infty$. Then, from Theorem 3.2 of [88], we conclude that for all $0 < \theta < T/2$, the set $\{w_h|_{(\theta,T-\theta)}\}_{h>0}$ is precompact in $L^{p'}(\theta,T-\theta;W')$.

Equation (5.2), with the assumption $0 < \delta < T$, gives:

$$\int_{\delta}^T \|w_h(t) - w_h(t - \delta)\|_{W'}^{p'} dt \leq M\delta.$$

Using Lemma 3.4 in [88], we conclude that $\{w_h\}_{h>0}$ is uniformly bounded in $L^r(0, T; W')$ for any $1 \leq r < \infty$. Therefore uniform integrability holds and this implies that $\{w_h\}_{h>0}$ is precompact in $L^{p'}(0, T; W')$. Now, the fact that $\{w_h\}_{h>0}$ is bounded in $L^r(0, T; W')$ for any $1 \leq r < \infty$, and that $\{w_h\}_{h>0}$ is precompact in $L^{p'}(0, T; W')$, implies that $\{w_h\}_{h>0}$ is precompact in $L^r(0, T; W')$ for any $1 \leq r < \infty$.

Finally it remains to show that $\{w_h\}_{h>0}$ is precompact in $L^p(0, T; H)$. From [87] the fact that $V \hookrightarrow H \hookrightarrow W'$ implies that for all $\epsilon > 0$ there exists $M(\epsilon) > 0$ such that

$$\|w_h(t)\|_H \leq \epsilon \|w_h(t)\|_V + M(\epsilon) \|w_h(t)\|_{W'}.$$

So,

$$\|w_h\|_{L^p(0, T; H)} \leq \epsilon \|w_h\|_{L^p(0, T; V)} + M(\epsilon) \|w_h\|_{L^p(0, T; W')}.$$

Since $\{w_h\}_{h>0}$ is bounded in $L^p(0, T; V)$ and precompact in $L^p(0, T; W')$, it easily follows that it is also precompact in $L^p(0, T; H)$. $\square$

5.1.1 Compactness of the solutions with DG in time

One important and challenging step in proving convergence of the numerical approximation of the concentration is to show compactness of $\{c_h\}_{h>0}$. This is stated in the following theorem, which is a non-trivial application of Theorem 5.1.2.

Theorem 5.1.3. *Suppose the maximal time step k tends to zero with the mesh parameter h . Then the concentration $\{c_h\}_{h>0}$ computed using the numerical scheme (3.29) are precompact in $L^2(0, T; L^2(\Omega)) \cap L^r(0, T; W^{1,4}(\Omega)')$ for all $1 \leq r < \infty$.*

Proof. Apply Theorem 5.1.2 with the following choice of spaces:

$$W = W^{1,4}(\Omega), \quad V = BV(\Omega) \cap L^4(\Omega), \quad H = L^2(\Omega), \quad W(\mathcal{E}_h) = W^{1,4}(\mathcal{E}_h), \quad W_h = C_h.$$

The spaces W , V and H are clearly Banach spaces and it is easy to check that $W(\mathcal{E}_h)$

equipped with the following norm is a Banach space.

$$\|w\|_{W(\mathcal{E}_h)} = \|w\|_{W^{1,4}(\mathcal{E}_h)}. \quad (5.4)$$

From [34] and [71], we also have that $W \subset H$ is dense, and that $W \hookrightarrow V \hookrightarrow H \hookrightarrow W'$ are dense embeddings with V compactly embedded in H . Next we easily see that $W^{1,4}(\Omega)$ is embedded in $W^{1,4}(\mathcal{E}_h)$, which is itself embedded in V , with embedding constants independent of h . It remains to check the assumptions of Theorem 5.1.2. The fact that the L^2 projection, $\pi_h : L^2(\Omega) \rightarrow C_h$ is stable in $W^{1,4}(\mathcal{E}_h)$ is proved in Lemma 5.1.4. Assumption 1 in Theorem 5.1.2 is immediately satisfied if the inner-product on H is the weighted L^2 inner-product with weight ϕ , and if we define the function F_h as:

$$F_h(w_h) = (\hat{c}q^I, w_h) - B_{di}(c_h, w_h; \mathbf{u}_h) - B_{cq}(c_h, w_h; \mathbf{u}_h). \quad (5.5)$$

Assumption 2 is satisfied for $p = 2$, since the boundedness of $\{c_h\}_{h>0}$ in $L^2(0, T; V)$ is a consequence of the embedding of $H^1(\mathcal{E}_h)$ into V and the boundedness of $\{\|c_h\|_{L^2(0, T; H^1(\mathcal{E}_h))}\}_{h>0}$. Finally, it remains to check Assumption 3 of Theorem 5.1.2. This requires upper bounds for the forms B_d, B_{cq} , that are proved in Lemma B.2.17. Since $\hat{c} \in L^\infty(\Omega)$, one can easily obtain

$$(\hat{c}q^I, w_h) \lesssim \|q^I\|_{L^2(\Omega)} \|w_h\|_{L^4(\Omega)}.$$

Therefore, by Lemma B.2.17 we have,

$$\begin{aligned} |F_h(w_h)| &\leq M \|w_h\|_{W^{1,4}(\mathcal{E}_h)} \left((1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2}) \|c_h\|_{C_h} + \|q^I\|_{L^2(\Omega)} \right. \\ &\quad \left. + (\|q^I + q^P\|_{L^2(\Omega)} + \|\mathbf{u}_h\|_{L^2(\Omega)}) \|c_h\|_{L^4(\Omega)} \right), \end{aligned} \quad (5.6)$$

with the constant M independent of the mesh size.

From [34], [89], [90], [73] and (3.4),

$$\|c_h\|_{L^4(\Omega)} \lesssim \|c_h\|_{H^1(\mathcal{E}_h)}, \quad (5.7)$$

hence, using Cauchy-Schwarz's inequality, one can obtain

$$\begin{aligned} \int_0^T |F_h(w_h)| &\leq M \int_0^T \|w_h\|_{W^{1,4}(\mathcal{E}_h)} \left((1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2}) \|c_h\|_{C_h} + \|q^I\|_{L^2(\Omega)} \right. \\ &\quad \left. + (\|q^I + q^P\|_{L^2(\Omega)} + \|\mathbf{u}_h\|_{L^2(\Omega)}) \|c_h\|_{L^4(\Omega)} \right) \\ &\leq M \left((1 + \|\mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))}^{1/2}) \|c_h\|_{L^2(0,T;C_h)} \right. \\ &\quad \left. + \|q^I\|_{L^\infty(0,T;L^2(\Omega))} + (\|q^I + q^P\|_{L^\infty(0,T;L^2(\Omega))} \right. \\ &\quad \left. + \|\mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))}) \|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))} \right) \|w_h\|_{L^4(0,T;W^{1,4}(\mathcal{E}_h))}. \end{aligned}$$

Therefore, F_h belongs to $L^1(0, T; W'_h)$ and we have

$$\begin{aligned} \|F_h\|_{L^1(0,T;W'_h)} &\leq M \left((1 + \|\mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))}^{1/2}) \|c_h\|_{L^2(0,T;C_h)} + \|q^I\|_{L^\infty(0,T;L^2(\Omega))} \right. \\ &\quad \left. + (\|q^I + q^P\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))}) \|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))} \right). \end{aligned}$$

Furthermore, according to the stability analysis in Theorem 4.2.3 and Theorem 4.2.5, we know that $\|\mathbf{u}_h\|_{L^\infty(0,T;L^2(\Omega))}$, $\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))}$ and $\|c_h\|_{L^2(0,T;C_h)}$ are bounded by a constant independent of h and k . Therefore, $\{\|F_h\|_{L^1(0,T;W'_h)}\}_{h>0}$ is bounded.

□

Lemma 5.1.4. *The L^2 projection*

$$\pi_h : L^2(\Omega) \rightarrow C_h$$

is stable in $W(\mathcal{E}_h) = W^{1,4}(\mathcal{E}_h)$, i.e. there is a constant $M > 0$ independent of h such that

$$\|\pi_h w\|_{W(\mathcal{E}_h)} \leq M \|w\|_{W(\mathcal{E}_h)}, \quad \forall w \in W(\mathcal{E}_h).$$

Proof. Fix $w \in W^{1,4}(\mathcal{E}_h)$. For the term $\|\pi_h w\|_{L^4(\Omega)}$, use an inverse inequality, the stability of π_h in L^2 and Cauchy-Schwarz's inequality to obtain

$$\|\pi_h w\|_{L^4(\Omega)}^4 = \sum_{E \in \mathcal{E}_h} \|\pi_h w\|_{L^4(E)}^4 \lesssim \sum_{E \in \mathcal{E}_h} h^{-d} \|\pi_h w\|_{L^2(E)}^4 \lesssim \sum_{E \in \mathcal{E}_h} h^{-d} \|w\|_{L^2(E)}^4 \lesssim \|w\|_{L^4(\Omega)}^4. \quad (5.8)$$

Next, let $\bar{w}$ denote the average of w on each element, i.e.

$$\bar{w}|_E = \frac{1}{|E|} \int_E w, \quad \forall E \in \mathcal{E}_h.$$

Thus, we have

$$\begin{aligned} & \left(\sum_{E \in \mathcal{E}_h} \|\nabla \pi_h w\|_{L^4(E)}^4 + \sum_{e \in \Gamma_h} h^{-3} \|[\pi_h w]\|_{L^4(e)}^4 \right)^{1/4} \leq \left(\sum_{e \in \Gamma_h} h^{-3} \|[\pi_h \bar{w}]\|_{L^4(e)}^4 \right)^{1/4} \\ & \quad + \left(\sum_{E \in \mathcal{E}_h} \|\nabla \pi_h (w - \bar{w})\|_{L^4(E)}^4 + \sum_{e \in \Gamma_h} h^{-3} \|[\pi_h (w - \bar{w})]\|_{L^4(e)}^4 \right)^{1/4}. \end{aligned}$$

For the first term in the upper bound, we have

$$\|[\pi_h \bar{w}]\|_{L^4(e)} = \|[\bar{w}]\|_{L^4(e)} \leq \|w - \bar{w}\|_{L^4(e)} + \|w\|_{L^4(e)}.$$

From [91], we have

$$\sum_{e \in \Gamma_h} h^{-3} \|w - \bar{w}\|_{L^4(e)}^4 \lesssim \sum_{E \in \mathcal{E}_h} \|\nabla w\|_{L^4(E)}^4.$$

Hence, we have

$$\sum_{e \in \Gamma_h} h^{-3} \|[\pi_h \bar{w}]\|_{L^4(e)}^4 \lesssim \sum_{E \in \mathcal{E}_h} \|\nabla w\|_{L^4(E)}^4 + \sum_{e \in \Gamma_h} h^{-3} \|[w]\|_{L^4(e)}^4.$$

Using the same derivation as in (5.8), we have:

$$\sum_{E \in \mathcal{E}_h} \|\nabla \pi_h(w - \bar{w})\|_{L^4(E)}^4 = \sum_{E \in \mathcal{E}_h} \|\nabla \pi_h w\|_{L^4(E)}^4 \lesssim \sum_{E \in \mathcal{E}_h} \|\nabla w\|_{L^4(E)}^4.$$

Furthermore, by trace and inverse inequalities we obtain

$$\begin{aligned} \|\pi_h(w - \bar{w})\|_{L^4(e)} &\leq M h_E^{-1/4} \|\pi_h(w - \bar{w})\|_{L^4(E)} \leq M h_E^{-1/4} h_E^{-d/4} \|\pi_h(w - \bar{w})\|_{L^2(E)} \\ &\leq M h_E^{-1/4} h_E^{-d/4} \|w - \bar{w}\|_{L^2(E)} \leq M h_E^{1/4} h_E^{-d/4} h_E^{-1/2} \|w - \bar{w}\|_{L^2(E)} \\ &\leq M h_E^{1/4} h_E^{-d/4} h_E^{1/2} \|\nabla w\|_{L^2(E)} \leq M h_E^{1/4} h_E^{-d/4} h_E^{1/2} h_E^{d/4} \|\nabla w\|_{L^4(E)} \\ &\leq M h^{3/4} \|\nabla w\|_{L^4(E)}. \end{aligned}$$

Hence, we have

$$\sum_{e \in \Gamma_h} h^{-3} \|[\pi_h(w - \bar{w})]\|_{L^4(e)}^4 \leq M \sum_{E \in \mathcal{E}_h} \|\nabla w\|_{L^4(E)}^4.$$

So, we can conclude by combining all the bounds above. $\square$

In the next theorem, I give more information about the accumulation points of the concentration solutions.

Theorem 5.1.5. *Suppose that the maximal time step k and mesh size h tend to zero with mesh parameter. Then upon passage to a subsequence, the concentrations $\{c_h\}_h$ computed using the scheme (3.27)-(3.29) over a regular family of meshes converge strongly in $L^2(0, T; L^2(\Omega))$ to $c \in L^2(0, T; H^1(\Omega))$ and $\{\nabla c_h\}_h$ converges weakly in $L^2(0, T; H^{-1}(\Omega))$ to ∇c .*

Proof. From Theorem 5.1.3 we know $\{c_h\}_{h>0}$ is precompact in

$L^2(0, T; L^2(\Omega)) \cap L^r(0, T; W^{1,4}(\Omega)')$ for all $1 \leq r < \infty$. There exists a subsequence $\{c_h\}_h$ that converges to $c \in L^2(0, T; L^2(\Omega))$ strongly in $L^2(0, T; L^2(\Omega))$. From the stability result in Theorem 4.2.5, we also know there exists $M > 0$ such that $\|c_h\|_{L^2(0, T; H^1(\mathcal{E}_h))} < M$. Therefore, from Theorem 6.1 in [34] we have there exists a subsequence $\{\nabla c_h\}_h$ that converges weakly in $L^2(0, T; H^{-1}(\Omega))$ to ∇c . $\square$

Simply having the weak convergence of the gradient is not enough to suggest the convergence of the numerical solutions to the weak solution. Therefore, it is necessary for us to introduce the discrete gradient to further our study on the convergence of the numerical solutions.

First, we shall introduce the lifting operator. Following [73], for any face e in Γ_h and any function $\varphi \in L^2(e)$, we define the lifting $\mathbf{r}_e(\varphi) \in \mathcal{P}_\ell(\mathcal{E}_h)^d$ by

$$\int_{\Omega} \mathbf{r}_e(\varphi) \cdot \mathbf{v}_h = \int_e \{\mathbf{v}_h \cdot \mathbf{n}_e\} \varphi \quad \forall \mathbf{v}_h \in \mathcal{P}_\ell(\mathcal{E}_h)^d. \quad (5.9)$$

We observe that the support of $\mathbf{r}_e$ is the union of the elements sharing the edge e . In other words, for any E in $\mathcal{E}_h$,

$$\mathbf{r}_e(\varphi)|_E = \mathbf{0} \quad \text{if } e \notin \partial E.$$

Then, for any w_h in $H^1(\mathcal{E}_h)$, we set

$$\mathbf{R}_h([w_h]) = \sum_{e \in \Gamma_h} \mathbf{r}_e([w_h]),$$

and define the discrete gradient $\mathbf{G}_h$ in each element E by

$$\mathbf{G}_h(w_h) = \nabla w_h - \mathbf{R}_h([w_h]) \quad (5.10)$$

such that

$$(\mathbf{G}(w_h), \mathbf{v}_h) = (\nabla w_h, \mathbf{v}_h)_{\mathcal{E}_h} - ([w_h], \{\mathbf{v}_h \cdot \mathbf{n}_e\})_{\Gamma_h}, \quad \text{for all } \mathbf{v}_h \in \mathcal{P}_\ell(\mathcal{E}_h)^d \quad (5.11)$$

and the discrete gradient can be extended to

$$(\mathbf{G}(w_h), \mathbf{v}) = (\nabla w_h, \mathbf{v})_{\mathcal{E}_h} - ([w_h], \{\pi_h \mathbf{v} \cdot \mathbf{n}_e\})_{\Gamma_h}, \quad \text{for all } \mathbf{v} \in L^2(\Omega)^d \quad (5.12)$$

for functions in $L^2(\Omega)$.

With the help of the discrete gradient we have additional convergence result in terms of the gradient.

Theorem 5.1.6. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using the numerical scheme (3.27)-(3.29). Then, there exist $c \in L^2(0, T; H^1(\Omega))$ such that with maximal mesh size and time step h, k tend to zero by passing a subsequence, we have*

$$c_h \text{ converges to } c \text{ strongly in } L^2(0, T; L^2(\Omega)),$$

$$\mathbf{G}_h(c_h) \text{ converges to } \nabla c \text{ weakly in } L^2(0, T; L^2(\Omega)).$$

Proof. The uniform boundedness of $\{\|c_h\|_{L^2(0, T; H^1(\mathcal{E}_h))}\}_{h>0}$ implies that the sequence $\{\mathbf{G}(c_h)\}_{h>0}$ is bounded; therefore, there exists subsequence $\{\mathbf{G}(c_h)\}_{h>0}$ such that it converges weakly to $\mathbf{v}$ in $L^2(0, T; L^2(\Omega))$. According to the definition of the discrete gradient in (5.11) we know that, in fact, $\{\mathbf{G}(c_h)\}_{h>0}$ converges weakly to ∇c according [74]. The proof can also be found in Theorem 6.3 in [34]. $\square$

Remark 5.1.7. In [34], we are given an example of a sequence of functions as in Figure 5.1 to show the necessity of using the discrete gradient.

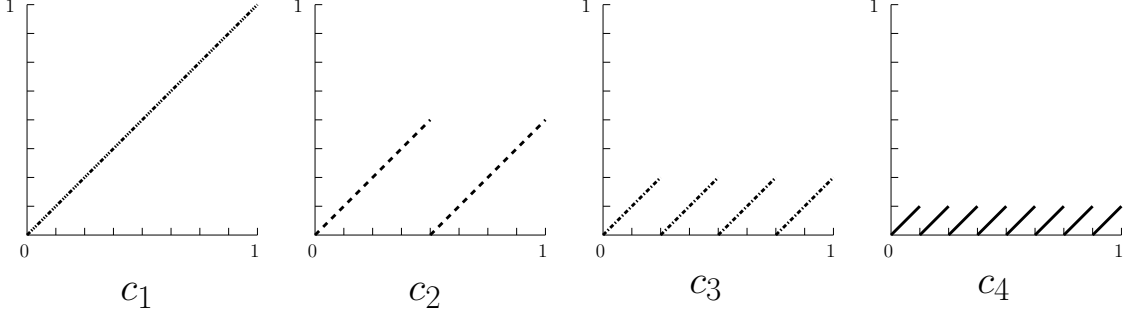


Figure 5.1: Function c_n with $n = 1, 2, 3, 4$

where we have $c_n \rightarrow c = 0$ strongly in $L^2(\Omega)$ and $c \in H^1(\Omega)$, but clearly we do not have $\nabla c_n \rightharpoonup \nabla c$ weakly in $L^2(\Omega)$. If we consider the discrete gradient, then we have

$$(\mathbf{G}_h(c_n), I_n \mathbf{v}) = (\nabla c_n, I_n \mathbf{v})_{\mathcal{E}_h} - ([c_n], I_n \mathbf{v} \cdot \mathbf{n}_e)_{\Gamma_h} = \int_0^1 I_n \mathbf{v} - \frac{1}{2^{n-1}} \sum_{i=1}^{2^{n-1}} I_n \mathbf{v} \left(\frac{i}{2^{n-1}} \right)$$

where $I_h \mathbf{v}$ is the Lagrange interpolate of smooth function $\mathbf{v}$; thus, we have

$$\lim_{n \rightarrow \infty} (\mathbf{G}_h(c_n), I_n \mathbf{v}) = \lim_{n \rightarrow \infty} \int_0^1 I_n \mathbf{v} - \lim_{n \rightarrow \infty} \frac{1}{2^{n-1}} \sum_{i=1}^{2^{n-1}} \mathbf{v} \left(\frac{i}{2^{n-1}} \right) = \lim_{n \rightarrow \infty} \int_0^1 (I_n \mathbf{v} - \mathbf{v}) = 0$$

Therefore, we have:

$$\lim_{n \rightarrow \infty} (\mathbf{G}_h(c_n), \mathbf{v}) = \lim_{n \rightarrow \infty} (\mathbf{G}_h(c_n), I_n \mathbf{v}) = (\nabla c, \mathbf{v})$$

So, indeed we have the convergence of the discrete gradient, but not the gradient of the piecewise function. Examples in 2D and 3D can also be easily generated.

5.1.2 Compactness of the solutions with implicit Euler

For the Implicit Euler decoupling in Algorithm 3 and Algorithm 5, since we now have the solution function that is continuous in time by defining the concentration c_h as,

$$c_h(t) = c_h^j \frac{t - t_{j-1}}{k_j} - c_h^{j-1} \frac{t - t_j}{k_j} \text{ over interval } (t_{j-1}, t_j). \quad (5.13)$$

We can use the Aubin-Lions compactness theorem.

We consider the numerical schemes proposed in Algorithm 3 and Algorithm 5, since both algorithms share the same discretization for the concentration.

Lemma 5.1.8. *Let c_h be the concentration solutions obtained from either Algorithm 3 or Algorithm 5, then*

$$c_h \in L^2(0, T; H^2(\Omega)')$$

Proof. Notice that the discretization for the concentration can be written as

$$\int_0^T (\phi \partial_t c_h, w_h) = \int_0^T F_h(w_h) \quad (5.14)$$

where $F_h(w_h)$ over each interval (t_{j-1}, t_j) is given by:

$$F_h(w_h) = (\tilde{c}_h^j(q_h^I)^j, w_h) - B_{di}(c_h^j, w_h; \mathbf{u}_h^j) - B_{cq}(c_h^j, w_h; \mathbf{u}_h^j). \quad (5.15)$$

Therefore, the same upper bound as in (5.6) applies, and we have

$$F_h(w_h) \leq M \|w_h\|_{W^{1,4}(\mathcal{E}_h)} \quad (5.16)$$

with $M > 0$ independent of the mesh size.

Lemma B.2.18 implies that

$$F_h(w_h) \leq M \left(\sum_{E \in \mathcal{E}_h} \|w_h\|_{H^2(E)}^2 \right)^{1/2} \quad (5.17)$$

Now, let $w \in C_0^\infty(0, T; C^\infty(\Omega))$ and $w_h = \pi_h w$ where π_h is the L^2 -projection in space,

$$\text{i.e. } w_h(\cdot, t) = \pi_h w(\cdot, t),$$

Then, according to Lemma B.1.2, we have

$$F_h(w_h) \lesssim \left(\sum_{E \in \mathcal{E}_h} \|w_h - w\|_{H^2(E)}^2 \right)^{1/2} + \left(\sum_{E \in \mathcal{E}_h} \|w\|_{H^2(E)}^2 \right)^{1/2} \lesssim \left(\sum_{E \in \mathcal{E}_h} \|w\|_{H^2(E)}^2 \right)^{1/2} = \|w\|_{H^2(\Omega)}$$

Finally, by the definition of the L^2 projection,

$$\int_0^T (\phi \partial_t c_h, w) = \int_0^T (\phi \partial_t c_h, w_h) = \int_0^T F_h(w_h) \lesssim \int_0^T \|w\|_{H^2(\Omega)} \lesssim \|w\|_{L^2(0, T; H^2(\Omega))}$$

Therefore, $c_h \in L^2(0, T; H^2(\Omega)')$. □

Remark 5.1.9. In fact, for the implicit Euler decoupling, we can even show $c_h \in L^2(0, T; H^2(\Omega)')$ with mesh adaptation in each time step because of the stability result in Theorem 4.3.3 also provides an upper bound for the $\partial_t c_h$. Since mesh adaptation is beyond the scope of the thesis, I will not pursue the subject any further.

I now establish the compactness of the numerical solution for the concentration in the next result using Aubin-Lions compactness theorem.

Theorem 5.1.10. *Let $\{c_h\}_{h>0}$ be a sequence of the numerical solutions for the concentration obtained using Algorithm 3 or Algorithm 5; then, $\{c_h\}_{h>0}$ is precompact in $L^2(0, T; L^2(\Omega))$.*

Proof. According to Theorem 4.3.3, we know that there exist a constant $M > 0$ independent

of mesh size or time step such that

$$\|c_h\|_{L^2(0,T;H^1(\mathcal{E}_h))} < M$$

Therefore, $c_h \in L^2(0, T; BV(\Omega))$ since we have

$$\|\varphi\|_{BV(\Omega)} \leq \|\varphi\|_{L^1(\Omega)} + \|\nabla \varphi\|_{L^1(\Omega)} + \|[\varphi]\|_{L^2(\Gamma_h)} \lesssim \|\varphi\|_{H^1(\mathcal{E}_h)}$$

Thus,

$$c_h \in L^2(0, T; [BV(\Omega) \cap L^4(\Omega), L^4(\Omega)]_{1/2}).$$

Also, from Lemma 5.1.8 we know that

$$c_h \in L^2(0, T; H^2(\Omega)').$$

According to [34], we have

$$[BV(\Omega) \cap L^4(\Omega), L^4(\Omega)]_{1/2} \hookrightarrow L^2(\Omega) \hookrightarrow H^2(\Omega)'$$

with $[BV(\Omega) \cap L^4(\Omega), L^4(\Omega)]_{1/2}$ being both separable and reflexive; therefore, according Aubin-Lions compactness theorem in Theorem 5.1.1, the solutions set $\{c_h\}_{h>0}$ is precompact in $L^2(0, T; L^2(\Omega))$. $\square$

Theorem 5.1.11. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 3 or Algorithm 5; then, there exist $c \in L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)')$ such that with maximal time step k and mesh size h tend to zero. By passing a subsequence, we*

have

$$\begin{aligned}
c_h &\rightarrow c \text{ strongly in } L^2(0, T; L^2(\Omega)), \\
\partial_t c_h &\text{ converges to } \partial_t c \text{ weakly in } L^2(0, T; H^2(\Omega)'), \\
\nabla c_h &\text{ converges to } \nabla c \text{ weakly in } L^2(0, T; H^{-1}(\Omega)), \\
\mathbf{G}_h(c_h) &\text{ converges to } \nabla c \text{ weakly in } L^2(0, T; L^2(\Omega)).
\end{aligned}$$

If $c_h^0 \rightarrow c_0$ in $H^2(\Omega)'$; then, the c satisfies the initial condition.

Proof. Since $\{c_h\}_{h>0}$ is precompact in $L^2(0, T; L^2(\Omega))$, the proof is taken exactly from [34]. $\square$

5.1.3 Compactness of the solutions with Crank-Nicolson

The compactness of the concentration solutions obtained through Algorithm 4 and Algorithm 6 with Crank-Nicolson decoupling can be established using the same technique introduced for the implicit Euler time stepping.

Lemma 5.1.12. *Let c_h be the concentration solutions obtained from either Algorithm 4 or Algorithm 6; then:*

$$c_h \in L^2(0, T; H^2(\Omega)')$$

Proof. Notice, that the discretization for the concentration can written as

$$\int_0^T (\phi \partial_t c_h, w_h) = \int_0^T F_h(w_h) \quad (5.18)$$

where $F_h(w_h)$ over each interval (t_{j-1}, t_j) is given by,

$$F_h(w_h) = \left(\frac{1}{4} ((q_h^I)^j + (q_h^I)^{j-1}) (\tilde{c}_h^j + \tilde{c}_h^{j-1}), w_h \right) - B_{di}(c_h^j, w_h; \check{\mathbf{u}}_h^j) - B_{cq}(c_h^j, w_h; \check{\mathbf{u}}_h^j). \quad (5.19)$$

Therefore, we can follow exactly the same proof as Lemma 5.1.8 to show $c_h \in L^2(0, T; H^2(\Omega)')$.

□

Next, we have the compactness of the numerical solutions.

Theorem 5.1.13. *Let $\{c_h\}_{h>0}$ be a sequence of the numerical solutions for the concentration obtained using Algorithm 4 or Algorithm 6; then, $\{c_h\}_{h>0}$ is precompact in $L^2(0, T; L^2(\Omega))$.*

Proof. The proof is the same as in Theorem 5.1.10.

□

Finally, we have the convergence of the numerical solutions.

Theorem 5.1.14. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 4 or Algorithm 6; then, there exist $c \in L^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^2(\Omega)')$ such that with maximal time step k and mesh size h , tend to zero. By passing a subsequence we have:*

$$\begin{aligned} c_h &\text{ converges to } c \text{ strongly in } L^2(0, T; L^2(\Omega)), \\ \partial_t c_h &\text{ converges to } \partial_t c \text{ weakly in } L^2(0, T; H^2(\Omega)'), \\ \nabla c_h &\text{ converges to } \nabla c \text{ weakly in } L^2(0, T; H^{-1}(\Omega)), \\ \mathbf{G}_h(c_h) &\text{ converges to } \nabla c \text{ weakly in } L^2(0, T; L^2(\Omega)). \end{aligned}$$

If $c_h^0 \rightarrow c_0$ in $H^2(\Omega)'$, then, the c satisfies the initial condition.

5.2 Convergence of MFE-DG with DG in time

By establishing the compactness of the concentration solution, we can now show the convergence of the numerical solutions to the solutions of the weak problem (4.1)-(4.3). We begin by establishing the convergence of the pressure and velocity.

5.2.1 Convergence of pressure and velocity

We show the convergence of velocity and pressure using the exact argument from [88]. The proof is taken exactly from my master's thesis [35] for the sake of completion.

Theorem 5.2.1. *Given the data, parameters and numerical scheme. Assume the maximal time step k tends to zero with the mesh parameter. Suppose that the sequence $\{c_h\}_{h>0} \subset L^2(0, T; L^2(\Omega))$ converges to c in $L^2(0, T; L^2(\Omega))$; then, the velocity and pressure computed using the scheme (3.27)-(3.29) over the regular family of meshes converges strongly to the solutions of the weak forms (4.1) and (4.2).*

Proof. For completeness, we repeat the proof given in [71]. Let $\mathbb{U} = L^2(0, T; H(\Omega; \text{div}))$ and $\mathbb{P} = L^2(0, T; L^2(\Omega))$. Denote the finite element subspaces to be

$$\begin{aligned}\mathbb{U}_h &= \{\mathbf{u}_h \in \mathbb{U} \mid \mathbf{u}_h|_{(t_{j-1}, t_j)} \in \mathcal{P}_\ell(t_{j-1}, t_j; \mathbf{U}_h)\}, \text{ and} \\ \mathbb{P}_h &= \{p_h \in \mathbb{P} \mid p_h|_{(t_{j-1}, t_j)} \in \mathcal{P}_\ell(t_{j-1}, t_j; P_h)\}\end{aligned}$$

By Lemma 4.2.3, we know the numerical approximation $\{(\mathbf{u}_h, p_h)\}_{h>0}$ are bounded in $\mathbb{U} \times \mathbb{P}$; so, we may pass to a subsequence for which $(\mathbf{u}_h, p_h)$ converges weakly to a pair $(\mathbf{u}, p)$ in $\mathbb{U} \times \mathbb{P}$. Also, we can use dominate convergence theorem to show $\mu(c_h) \rightarrow \mu(c)$ in $L^r(0, T; L^r(\Omega))$ for each $1 \leq r < \infty$.

To show $(\mathbf{u}, p)$ is the weak solution of the mixed problem, we fix $(\mathbf{v}, q) \in C^\infty([0, T] \times \bar{\Omega}) \cap (\mathbb{U} \times \mathbb{P})$. Approximation theory tells us that there exists a sequence $((\mathbf{v}_h, q_h))_h \subset \mathbb{U}_h \times \mathbb{P}_h$ such that $(\mathbf{v}_h, q_h) \rightarrow (\mathbf{v}, q)$ in $W^{1,\infty}((0, T) \times \Omega)$; Hence, we can pass the limit term-by-term in equation (4.1) and (4.2) to show that

$$\begin{aligned}\int_0^T (\mathbb{K}^{-1}(c)\mathbf{u}, v) - (p, \text{div}(v)) &= \int_0^T (\rho(c)g, v) \\ \int_0^T (q, \text{div}(\mathbf{u})) &= \int_0^T (q^I - q^P, q)\end{aligned}$$

Since $C^\infty([0, T] \times \bar{\Omega}) \cap (\mathbb{U} \times \mathbb{P})$ is dense in $\mathbb{U} \times \mathbb{P}$, it follows that $(\mathbf{u}, p)$ is a weak solution of the mixed problem.

In order to show strong convergence we introduce the notation $b(\cdot, \cdot; c)$ such that for a fixed $c \in L^2(0, T; L^2(\Omega))$ we have $b(\cdot, \cdot; c) : (\mathbb{U} \times \mathbb{P})^2 \rightarrow \mathbb{R}$ where

$$b((\mathbf{u}, p), (\mathbf{v}, q); c) = \int_0^T ((\mathbb{K}^{-1}(c)\mathbf{u}, \mathbf{v}) - (p, \operatorname{div}(\mathbf{v})) + (q, \operatorname{div}(\mathbf{u})))$$

Lemma 4.2.1 shows that $b(\cdot, \cdot; c)$ is coercive on $\mathbb{U}_h \times \mathbb{P}_h$. Clearly, $b(\cdot, \cdot; c)$ is continuous. Hence, we can use the Strang's Lemma

$$\begin{aligned} \|(\mathbf{u} - \mathbf{u}_h, p - p_h)\|_{\mathbb{U} \times \mathbb{P}} &\leq \inf_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \|(\mathbf{u} - \mathbf{v}_h, p - q_h)\|_{\mathbb{U} \times \mathbb{P}} \\ &\quad + \sup_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \frac{|b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c) - b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c_h)|}{\|(\mathbf{v}_h, q_h)\|_{\mathbb{U} \times \mathbb{P}}} \end{aligned}$$

Since we have

$$b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c) - b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c_h) = \int_0^T (\mathbb{K}^{-1}(c) - \mathbb{K}^{-1}(c_h))\mathbf{u}, \mathbf{v}_h)$$

so

$$\begin{aligned} \|(\mathbf{u} - \mathbf{u}_h, p - p_h)\|_{\mathbb{U} \times \mathbb{P}} &\leq \inf_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \|(\mathbf{u} - \mathbf{v}_h, p - q_h)\|_{\mathbb{U} \times \mathbb{P}} + \|(\mathbb{K}^{-1}(c) - \mathbb{K}^{-1}(c_h))\mathbf{u}\|_{L^2(0, T; L^2(\Omega))} \end{aligned}$$

The assumptions on $\mathbb{K}$ guarantee that $|\mathbb{K}^{-1}(c_h)\mathbf{u}|^2$ converges pointwise to $|\mathbb{K}^{-1}(c)\mathbf{u}|^2$, and since $\mathbb{K}^{-1}$ takes values in a compact set it follows that $|\mathbb{K}^{-1}(c_h)\mathbf{u}|^2 \leq M|\mathbf{u}|^2$. Apply the dominated convergence theorem shows $\mathbb{K}^{-1}(c_h)\mathbf{u} \rightarrow \mathbb{K}^{-1}(c)\mathbf{u}$ in $L^2(0, T; L^2(\Omega))$, and strong convergence of the velocity and pressure follows. $\square$

5.2.2 Convergence of concentration

With the convergence of the pressure and velocity established, we can now show the convergence of the concentration.

Theorem 5.2.2. *Suppose that the maximal time step k and h tend to zero with the mesh parameter. Then, upon passage to a subsequence, the concentrations $\{c_h\}_h$ computed using the scheme (3.29) with SIPG namely $\epsilon = 1$ over a regular family of meshes converge strongly in $L^2(0, T; L^2(\Omega))$ to $c \in L^2(0, T; H^1(\Omega))$; which satisfies the weak formulation (4.3).*

Proof. The uniform boundedness of $\{\|c_h\|_{L^2(0, T; H^1(\mathcal{E}_h))}\}_{h>0}$, obtained from Theorem 4.2.5, implies that every accumulation point of $\{c_h\}_{h>0}$ in $L^2(0, T; L^2(\Omega))$ belongs to $L^2(0, T; H^1(\Omega))$, and that there exists a subsequence, still denoted by $\{c_h\}_{h>0}$, such that $\{\nabla c_h\}_{h>0}$ converges weakly in $L^2(0, T; H^{-1}(\Omega))$ to ∇c (see Theorem 7.1 [34]). Let $w \in C^\infty(0, T; C^\infty(\Omega))$ and $w(T) = 0$. Approximation theory guarantees existence of $w_h \in C(0, T; L^2(\Omega))$ such that $w_h|_{(t_{j-1}, t_j)}$ belongs to $\mathcal{P}_\ell(t_{j-1}, t_j; C_h)$, with $w_h(T) = 0$ and such that the sequence $\{w_h\}_{h>0}$ converges strongly to w in the following sense

$$\lim_{h \rightarrow 0} \|w_h - w\|_{L^\infty(0, T; L^\infty(\Omega))} = 0,$$

$$\lim_{h \rightarrow 0} \|\nabla w_h - \nabla w\|_{L^\infty(0, T; L^\infty(\Omega))} = 0. \quad (5.20)$$

Integrating the temporal term in (3.29), summing over n , and using the fact that $w_h(T) = 0$, yields

$$\int_0^T (-(\phi c_h, \partial_t w_h) + B_{di}(c_h, w_h; \mathbf{u}_h) + B_{cq}(c_h, w_h; \mathbf{u}_h)) = (\phi c_{h-}^0, w_h(0)) + \int_0^T (\hat{c} q^I, w_h). \quad (5.21)$$

We now pass to the limit term by term in (5.21). We clearly have

$$\begin{aligned}\lim_{h \rightarrow 0} \int_0^T (\phi c_h, \partial_t w_h) &= \int_0^T (\phi c, \partial_t w), \\ \lim_{h \rightarrow 0} (\phi c_{h-}^0, w_h(0)) &= (\phi c_0, w(0)), \\ \lim_{h \rightarrow 0} \int_0^T (\hat{c} q^I, w_h) &= \int_0^T (\hat{c} q^I, w).\end{aligned}$$

Next we show that

$$\int_0^T (\nabla c, \mathbb{D}(\mathbf{u}) \nabla w) = \lim_{h \rightarrow 0} \int_0^T B_{di}(c_h, w_h; \mathbf{u}_h). \quad (5.22)$$

The proof of this result is technical and requires the introduction of the operator $\mathbb{D}_h$ and the discrete gradient introduced in (5.10). The matrix $\mathbb{D}_h(\mathbf{v})$ is a piecewise constant matrix defined by

$$\mathbb{D}_h(\mathbf{v})|_E = \mathbb{D}(\tilde{\mathbf{v}}|_E), \quad \tilde{\mathbf{v}}|_E = \frac{1}{|E|} \int_E \mathbf{v}, \quad \forall E \in \mathcal{E}_h.$$

By the Lipschitz continuity of the diffusion-dispersion tensor $\mathbb{D}$, we have

$$\begin{aligned}\|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u})\|_{L^2(\Omega)} &= \|\mathbb{D}(\tilde{\mathbf{u}}_h) - \mathbb{D}(\mathbf{u})\|_{L^2(\Omega)} \lesssim \|\tilde{\mathbf{u}}_h - \mathbf{u}\|_{L^2(\Omega)} \\ &\lesssim \|\tilde{\mathbf{u}}_h - \tilde{\mathbf{u}}\|_{L^2(\Omega)} + \|\tilde{\mathbf{u}} - \mathbf{u}\|_{L^2(\Omega)}.\end{aligned}$$

Since $\tilde{\mathbf{u}}$ is the piecewise constant approximation of $\mathbf{u}$, then

$$\lim_{h \rightarrow 0} \int_0^T \|\tilde{\mathbf{u}} - \mathbf{u}\|_{L^2(\Omega)}^2 = 0. \quad (5.23)$$

Furthermore,

$$\|\tilde{\mathbf{u}}_h - \tilde{\mathbf{u}}\|_{L^2(\Omega)} \leq \|\mathbf{u}_h - \mathbf{u}\|_{L^2(\Omega)}.$$

Since the sequence $\{\mathbf{u}_h\}_h$ converges strongly to $\mathbf{u}$ in $L^2(0, T; L^2(\Omega))$, according to the The-

orem 5.2.1, we have

$$\lim_{h \rightarrow 0} \int_0^T \|\tilde{\mathbf{u}}_h - \tilde{\mathbf{u}}\|_{L^2(\Omega)}^2 = 0.$$

Therefore, we can conclude

$$\lim_{h \rightarrow 0} \int_0^T \|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u})\|_{L^2(\Omega)}^2 = 0. \quad (5.24)$$

Since we also have the property,

$$\lim_{h \rightarrow 0} \int_0^T \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}(\mathbf{u})\|_{L^2(\Omega)}^2 = 0. \quad (5.25)$$

Consequently we have

$$\lim_{h \rightarrow 0} \int_0^T \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)\|_{L^2(\Omega)}^2 = 0. \quad (5.26)$$

From the property (5.26), we have

$$\begin{aligned} \lim_{h \rightarrow 0} \int_0^T (\nabla c_h, \mathbb{D}(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} &= \lim_{h \rightarrow 0} \int_0^T (\nabla c_h, (\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla w_h)_{\mathcal{E}_h} \\ &\quad + \lim_{h \rightarrow 0} \int_0^T (\nabla c_h, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} \\ &= \lim_{h \rightarrow 0} \int_0^T (\nabla c_h, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h}. \end{aligned} \quad (5.27)$$

Additionally, from the property (5.24) and (5.20), we have

$$\int_0^T (\nabla c, \mathbb{D}(\mathbf{u}) \nabla w) = \lim_{h \rightarrow 0} \int_0^T (\nabla c, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h}. \quad (5.28)$$

We also observe:

$$\begin{aligned}
\int_0^T |(\mathbf{G}(c_h), \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} - (\nabla c, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h}| &\leq \int_0^T |(\mathbf{G}(c_h) - \nabla c, \mathbb{D}(\mathbf{u}) \nabla w)_{\mathcal{E}_h}| \\
&+ \int_0^T |(\mathbf{G}(c_h), (\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u})) \nabla w_h)_{\mathcal{E}_h}| + |(\mathbf{G}(c_h), \mathbb{D}(\mathbf{u})(\nabla w_h - \nabla w))_{\mathcal{E}_h}| \\
&+ \int_0^T |(\nabla c, (\mathbb{D}(\mathbf{u}) - \mathbb{D}_h(\mathbf{u}_h)) \nabla w)_{\mathcal{E}_h}| + |(\nabla c, \mathbb{D}_h(\mathbf{u}_h)(\nabla w - \nabla w_h))_{\mathcal{E}_h}|.
\end{aligned}$$

Therefore, we have from (5.20), (5.24) and the weak convergence of $\{\mathbf{G}(c_h)\}_h$ to ∇c according to Theorem 5.1.6.

$$\lim_{h \rightarrow 0} \int_0^T (\nabla c, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} = \lim_{h \rightarrow 0} \int_0^T (\mathbf{G}(c_h), \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h}. \quad (5.29)$$

Thus, we conclude with (5.28), (5.29) and (5.11)

$$\begin{aligned}
\int_0^T (\nabla c, \mathbb{D}(\mathbf{u}) \nabla w) &= \lim_{h \rightarrow 0} \int_0^T (\nabla c, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} = \lim_{h \rightarrow 0} \int_0^T (\mathbf{G}(c_h), \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} \\
&= \lim_{h \rightarrow 0} \int_0^T \left((\nabla c_h, \mathbb{D}_h(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} - ([c_h], \{\mathbb{D}_h(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\}_{\Gamma_h}) \right). \quad (5.30)
\end{aligned}$$

Using a trace inequality, we write

$$\begin{aligned}
&\int_0^T ([c_h], \{(\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla w_h \cdot \mathbf{n}_e\}_{\Gamma_h}) \\
&\lesssim \int_0^T \|c_h\|_{C_h} \left(\sum_{e \in \Gamma_h} h \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)\|_{L^2(e)}^2 \right)^{1/2} \|\nabla w_h\|_{L^\infty(\Omega)} \\
&\lesssim \int_0^T \|c_h\|_{C_h} \|\mathbf{u}_h - \tilde{\mathbf{u}}_h\|_{L^2(\Omega)} (\|\nabla w\|_{L^\infty(\Omega)} + \|\nabla w - \nabla w_h\|_{L^\infty(\Omega)}).
\end{aligned}$$

From the stability of c_h in $L^2(0, T; C_h)$ and (5.20), we obtain

$$\lim_{h \rightarrow 0} \int_0^T ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\}_{\Gamma_h}) = \lim_{h \rightarrow 0} \int_0^T ([c_h], \{\mathbb{D}_h(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\}_{\Gamma_h}). \quad (5.31)$$

Thus (5.27), (5.30) and (5.31) imply

$$\int_0^T (\nabla c, \mathbb{D}(\mathbf{u}) \nabla w) = \lim_{h \rightarrow 0} \int_0^T (\nabla c_h, \mathbb{D}(\mathbf{u}_h) \nabla w_h)_{\mathcal{E}_h} - ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h}. \quad (5.32)$$

Next, let us examine the term $([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h}$. Using (B.18) and Theorem 4.2.5, we have

$$\int_0^T ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim \left(\int_0^T \sum_{e \in \Gamma_h} \int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2}.$$

Then, with (B.26) and (B.27), we have

$$\int_0^T ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim \left(\int_0^T (1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^2) \right)^{1/4} \left(\int_0^T \sum_{e \in \Gamma_h} h^{-3} \| [w_h] \|_{L^4(e)}^4 \right)^{1/4}.$$

From Lemma 4.2.3 and an inverse inequality we have

$$\int_0^T ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim \left(\int_0^T h^{-(2+d)} \sum_{e \in \Gamma_h} \| [w_h] \|_{L^2(e)}^4 \right)^{1/4}.$$

We now apply Jensen's inequality and an approximation result

$$\begin{aligned} \int_0^T ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} &\lesssim \left(\int_0^T h^{-(2+d)} \left(\sum_{e \in \Gamma_h} \| [w_h] \|_{L^2(e)}^2 \right)^2 \right)^{1/4} \\ &\lesssim \left(\int_0^T h^{-(2+d)} \left(\sum_{e \in \Gamma_h} \| [w_h - w] \|_{L^2(e)}^2 \right)^2 \right)^{1/4} \\ &\lesssim \left(\int_0^T h^{4-d} \| w \|_{H^2(\Omega)}^4 \right)^{1/4} \lesssim h^{1/4} \left(\int_0^T \| w \|_{H^2(\Omega)}^4 \right)^{1/4}. \end{aligned}$$

Therefore, we have

$$\lim_{h \rightarrow 0} \int_0^T ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} = 0. \quad (5.33)$$

For the penalty term, we use a similar argument

$$\begin{aligned} & \int_0^T (\sigma h^{-1}(1 + \{|\mathbf{u}_h|\})[c_h], [w_h])_{\Gamma_h} \\ & \lesssim \left(\int_0^T (h^{-1}(1 + \{|\mathbf{u}_h|\})[w_h], [w_h])_{\Gamma_h} \right)^{1/2} \left(\int_0^T \|c_h\|_{C_h}^2 \right)^{1/2} \lesssim h^{1/4} \left(\int_0^T \|w\|_{H^2(\Omega)}^4 \right)^{1/4}. \end{aligned}$$

Therefore, we have

$$\lim_{h \rightarrow 0} \int_0^T (\sigma h^{-1}(1 + \{|\mathbf{u}_h|\})[c_h], [w_h])_{\Gamma_h} = 0. \quad (5.34)$$

Combining the results above, namely (5.32), (5.33), (5.34), yields (5.22). Next we show that

$$\frac{1}{2} \int_0^T ((\mathbf{u} \cdot \nabla c, w) - (c\mathbf{u}, \nabla w) + ((q^I + q^P)c, w)) = \lim_{h \rightarrow 0} \int_0^T B_{cq}(c_h, w_h; \mathbf{u}_h). \quad (5.35)$$

Since $\{\mathbf{u}_h\}_h$ converges strongly to $\mathbf{u}$ in $L^2(0, T; L^2(\Omega))$, it is easy to show that

$$\frac{1}{2} \int_0^T (-(c\mathbf{u}, \nabla w) + ((q^I + q^P)c, w)) = \lim_{h \rightarrow 0} \frac{1}{2} \int_0^T (-(c_h\mathbf{u}_h, \nabla w_h) + ((q^I + q^P)c_h, w_h)). \quad (5.36)$$

Using trace inequality and inverse inequality, we also have,

$$\begin{aligned} (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_{\Gamma_h} & \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)} \|c_h\|_{L^4(\Omega)} \left(\sum_{e \in \Gamma_h} h^{-\frac{d+1}{2}} \int_e [w_h - w]^2 \right)^{1/2} \\ & \lesssim h^{1/2} \|w\|_{H^2(\Omega)} \|\mathbf{u}_h\|_{L^2(\Omega)} \|c_h\|_{L^4(\Omega)}. \end{aligned}$$

With the stability bounds on $\mathbf{u}_h$ and c_h , we then have

$$\lim_{h \rightarrow 0} \int_0^T (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_{\Gamma_h} = 0. \quad (5.37)$$

Integrating by parts on each element and summing over all elements yields:

$$(c_h, \text{div}(\mathbf{u}_h w)) = -(\mathbf{u}_h \cdot \nabla c_h, w)_{\mathcal{E}_h} + (w \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h}. \quad (5.38)$$

We write

$$(c_h, \operatorname{div}(\mathbf{u}_h w)) - (c, \operatorname{div}(\mathbf{u} w)) = (c_h, (\operatorname{div}(\mathbf{u}_h) - \operatorname{div}(\mathbf{u}))w) + (c_h, (\mathbf{u}_h - \mathbf{u}) \cdot \nabla w).$$

We denote by $\pi_h(q^I - q^P)$ the L^2 -projections of $q^I - q^P$ respectively, in the space P_h . We remark that (3.28) yields

$$\operatorname{div}(\mathbf{u}_h) = \pi_h(q^I - q^P). \quad (5.39)$$

Therefore we have

$$\operatorname{div}(\mathbf{u}_h) - \operatorname{div}(\mathbf{u}) = \pi_h(q^I - q^P) - (q^I - q^P).$$

We can now obtain

$$\lim_{h \rightarrow 0} \int_0^T (c_h, \operatorname{div}(\mathbf{u}_h w)) = \int_0^T (c, \operatorname{div}(\mathbf{u} w)). \quad (5.40)$$

From (5.20), we have

$$\lim_{h \rightarrow 0} \int_0^T (\mathbf{u}_h \cdot \nabla c_h, w_h)_{\mathcal{E}_h} = \lim_{h \rightarrow 0} \int_0^T (\mathbf{u}_h \cdot \nabla c_h, w)_{\mathcal{E}_h}, \quad (5.41)$$

$$\lim_{h \rightarrow 0} \int_0^T (w_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} = \lim_{h \rightarrow 0} \int_0^T (w \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h}. \quad (5.42)$$

Thus, from the result obtained in (5.38), (5.40), (5.41) and (5.42) we have

$$\begin{aligned} \int_0^T (\mathbf{u} \cdot \nabla c, w) &= \int_0^T -(c, \operatorname{div}(\mathbf{u} w)) \\ &= \lim_{h \rightarrow 0} \int_0^T (\mathbf{u}_h \cdot \nabla c_h, w_h)_{\mathcal{E}_h} - (w_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h}. \end{aligned} \quad (5.43)$$

We have then proved (5.35) and we conclude that the limit c satisfies the weak problem. □

Next result, we are presenting much stronger convergence for the gradient of the concentration solution. We also extend our proof of the convergence to NIPG and IIPG provided

that we have additional regularity for the velocity such that $\mathbf{u}$ is bounded in $L^\infty(\Omega)$.

Theorem 5.2.3. *Suppose that the maximal time step k and h tend to zero with mesh parameter. Then upon passage to a subsequence, the concentrations $\{c_h\}_h$ computed using the scheme (3.27)-(3.29) with SIPG, NIPG and IIPG over a regular family of meshes converge strongly in $L^2(0, T; H^1(\mathcal{E}_h))$ to $c \in L^2(0, T; H^1(\Omega))$, i.e. we have*

$$\begin{aligned} c_h &\text{ converges to } c \text{ strongly in } L^2(0, T; L^2(\Omega)), \\ \nabla c_h &\text{ converges to } \nabla c \text{ strongly in } L^2(0, T; L^2(\Omega)), \\ \lim_{h, k \rightarrow 0} \int_0^T (h_e^{-1}[c_h], [c_h])_{\Gamma_h} &= 0, \end{aligned}$$

where c is the same accumulation point as in Theorem 5.1.6.

Proof. To simplify, let $A(c_h, w_h; \mathbf{u}_h)$ denote the bilinear form in the left-hand side by summing over all j from 1 to N ,

$$\begin{aligned} A(c_h, w_h; \mathbf{u}_h) &= \int_0^T \left((\phi \partial_t c_h, w_h) + B_{di}(c_h, w_h; \mathbf{u}_h) + B_{cq}(c_h, w_h; \mathbf{u}_h) \right) dt \\ &\quad + \sum_{j=1}^N ([c_h^{j-1}]_t, \phi w_{h+}^{j-1}) = \int_0^T (\hat{c} q^I, w_h). \end{aligned} \quad (5.44)$$

The stability Theorem 4.2.5 gives us a lower bound for $A(w_h, w_h; \mathbf{u}_h)$:

$$\begin{aligned} 2A(w_h, w_h; \mathbf{u}_h) &\geq \|\phi^{1/2} w_{h-}^N\|_{L^2(\Omega)}^2 + \sum_{j=1}^N \|\phi^{1/2} w_h^{j-1}\|_{L^2(\Omega)}^2 - \|\phi^{1/2} w_{h-}^0\|_{L^2(\Omega)}^2 \\ &\quad + 2 \int_0^T \|w_h\|_{C_h}^2 + \int_0^T \|(q^I + q^P)^{1/2} w_h\|_{L^2(\Omega)}^2 + \int_0^T \|\mathbf{u}_h \cdot \mathbf{n}_e\|^{1/2} [w_h]\|_{\Gamma_h}^2. \end{aligned} \quad (5.45)$$

A glance at (5.45) suggests to apply it to the difference between c_h and an interpolant of c , and use the discrete concentration equation (5.44) to derive a useful upper bound for the left-hand side. However, this upper bound requires higher regularity that can be expected

from c . Therefore, we shall proceed by density argument and start with a smooth function φ that is arbitrary for the moment but will approximate c further on. For each time t , we discretize φ in space by its Lagrange interpolant, $I_h\varphi$ in the space

$$V_h = \{q \in \mathcal{C}^0(\overline{\Omega}); \forall E \in \mathcal{E}_h, q|_E \in \mathbb{P}_1\}.$$

This is possible since the mesh is conforming and φ is smooth. We also set $(I_h\varphi)_-^0 = (I_h\varphi)_+^0$. On one hand, (5.45) gives a lower bound for $A(c_h - I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h)$. On the other hand, using (5.44), we can write

$$\begin{aligned} A(c_h - I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) &= A(c_h, c_h - I_h\varphi; \mathbf{u}_h) - A(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) \\ &= \int_0^T (\hat{c}q^I, c_h - I_h\varphi)dt - A(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h). \end{aligned}$$

By combining with (5.45), this gives:

$$\begin{aligned} &\|\phi^{1/2}(c_{h-}^N - (I_h\varphi)_-^N)\|_{L^2(\Omega)}^2 + \sum_{j=1}^N \|\phi^{1/2}(c_h - I_h\varphi)^{j-1}\|_{L^2(\Omega)}^2 + 2 \int_0^T \|c_h - I_h\varphi\|_{C_h}^2 \\ &+ \int_0^T \|(q^I + q^P)^{1/2}(c_h - I_h\varphi)\|_{L^2(\Omega)}^2 + \int_0^T \| |\mathbf{u}_h \cdot \mathbf{n}_e|^{1/2} [c_h - I_h\varphi] \|_{\Gamma_h}^2 \\ &\leq 2 \int_0^T (\hat{c}q^I, c_h - I_h\varphi)dt - 2A(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) + \|\phi^{1/2}(c_{h-}^0 - (I_h\varphi)_-^0)\|_{L^2(\Omega)}^2, \end{aligned}$$

and in particular,

$$\int_0^T \|c_h - I_h\varphi\|_{C_h}^2 \leq \int_0^T (\hat{c}q^I, c_h - I_h\varphi) - A(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) + \frac{1}{2} \|\phi^{1/2}(c_{h-}^0 - (I_h\varphi)_-^0)\|_{L^2(\Omega)}^2. \quad (5.46)$$

As we know that c_h tends to a function c weakly in $L^2(\Omega \times (0, T))$ and $I_h\varphi$ tends to φ strongly in $L^2(\Omega \times (0, T))$, we can pass to the limit in the first and last term of this right-hand side, and it remains to examine the middle term. Since $I_h\varphi$ has no discontinuity

in space or time, $A(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h)$ simplifies to

$$A(I_h\varphi, c_h - I_h\varphi) = \int_0^T \left((\phi \partial_t(I_h\varphi), c_h - I_h\varphi) + B_{di}(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) + B_{cq}(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) \right).$$

For the first term in the right-hand side, we note that

$$\frac{\partial}{\partial t} I_h\varphi = I_h\left(\frac{\partial}{\partial t}\varphi\right),$$

and since φ is smooth in space and time,

$$\int_0^T \|I_h(\partial_t\varphi) - \partial_t\varphi\|_{L^2(\Omega)}^2 \leq C^2 h^2 \|\partial_t\varphi\|_{L^2(0,T;H^1(\Omega))}^2.$$

Thus $\phi^{1/2}\partial_t(I_h\varphi)$ converges strongly in $L^2((0,T) \times \Omega)$ to $\phi^{1/2}\partial_t\varphi$, since ϕ is independent of time and bounded in space. Hence

$$\lim_{h \rightarrow 0} \int_0^T (\phi \partial_t I_h\varphi, c_h - I_h\varphi) = \int_0^T (\phi \partial_t\varphi, c - \varphi). \quad (5.47)$$

The continuity of $I_h\varphi$ simplifies the third term:

$$\begin{aligned} B_{cq}(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) &= \frac{1}{2} \left((\mathbf{u}_h \cdot \nabla I_h\varphi, c_h - I_h\varphi)_{\varepsilon_h} - (\mathbf{u}_h I_h\varphi, \nabla(c_h - I_h\varphi))_{\varepsilon_h} \right. \\ &\quad \left. + ((q^I + q^P)I_h\varphi, c_h - I_h\varphi) + ((I_h\varphi)\mathbf{u}_h \cdot \mathbf{n}_e, [c_h - I_h\varphi])_{\Gamma_h} \right). \end{aligned}$$

After an integration by parts, it reduces to

$$B_{cq}(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) = (\mathbf{u}_h \cdot \nabla I_h\varphi, c_h - I_h\varphi)_{\varepsilon_h} + \frac{1}{2}((q^I + q^P + \pi_h(q^I - q^P))I_h\varphi, c_h - I_h\varphi),$$

where $\pi_h(q^I - q^P)$ are the L^2 -projections of $q^I - q^P$ respectively, in the space P_h . Therefore, considering that $I_h\varphi$ converges to φ strongly in $L^\infty(0,T;W^{1,\infty}(\Omega))$ and $\mathbf{u}_h$ converges to $\mathbf{u}$

strongly in $L^2(0, T; L^2(\Omega)^d)$, we have

$$\lim_{h \rightarrow 0} \int_0^T B_{cq}(I_h \varphi, c_h - I_h \varphi; \mathbf{u}_h) = \int_0^T \left((\mathbf{u} \cdot \nabla \varphi, c - \varphi) + (q^I \varphi, c - \varphi) \right). \quad (5.48)$$

Hence it remains to study the second term. Again, it simplifies owing to the continuity of $I_h \varphi$:

$$B_{di}(I_h \varphi, c_h - I_h \varphi; \mathbf{u}_h) = (\mathbb{D}(\mathbf{u}_h) \nabla I_h \varphi, \nabla(c_h - I_h \varphi))_{\mathcal{E}_h} - ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla I_h \varphi \cdot \mathbf{n}_e\})_{\Gamma_h}.$$

We propose to express B_d in terms of the discrete gradients $\mathbf{G}_h$. But, as mentioned previously, this is achieved by replacing $\mathbb{D}(\mathbf{u}_h)$ by piecewise constants. Thus, we introduce $\mathbb{D}_h(\mathbf{u}_h)$ and write:

$$\begin{aligned} B_{di}(I_h \varphi, c_h - I_h \varphi; \mathbf{u}_h) &= (\mathbb{D}_h(\mathbf{u}_h) \nabla I_h \varphi, \nabla(c_h - I_h \varphi))_{\mathcal{E}_h} - ([c_h], \{\mathbb{D}_h(\mathbf{u}_h) \nabla I_h \varphi \cdot \mathbf{n}_e\})_{\Gamma_h} \\ &\quad + ((\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi, \nabla(c_h - I_h \varphi))_{\mathcal{E}_h} - ([c_h], \{(\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi \cdot \mathbf{n}_e\})_{\Gamma_h}. \end{aligned} \quad (5.49)$$

Let us bound first the terms in the second line. Since $\mathbb{D}(\mathbf{u}_h)$ is symmetric positive definite, in view of (B.6), we can write in any E ,

$$\begin{aligned} &((\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi, \nabla(c_h - I_h \varphi))_E \\ &\leq \|(\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi\|_{L^2(E)} \|\nabla(c_h - I_h \varphi)\|_{L^2(E)} \\ &\leq \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)\|_{L^2(E)} \|\nabla I_h \varphi\|_{L^\infty(E)} \|\nabla(c_h - I_h \varphi)\|_{L^2(E)} \end{aligned}$$

Now, (5.26) states that

$$\lim_{h, k \rightarrow 0} \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)\|_{L^2(0, T; L^2(\Omega)^d)} = 0.$$

Since the second and third factors are bounded, it follows that

$$\lim_{h,k \rightarrow 0} \int_0^T ((\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi, \nabla (c_h - I_h \varphi))_{\mathcal{E}_h} = 0. \quad (5.50)$$

The treatment of the second term is similar, but more involved, by using (B.6) and (B.7), we have

$$\begin{aligned} & \left| \int_e [c_h - I_h \varphi] \{ (\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi \cdot \mathbf{n}_e \} \right| \\ & \leq h_e^{-1/2} \| [c_h - I_h \varphi] \|_{L^2(e)} h_e^{1/2} \| \{ |(\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)) \nabla I_h \varphi \cdot \mathbf{n}_e|_2 \} \|_{L^2(e)} \\ & \leq h_e^{-1/2} \| [c_h - I_h \varphi] \|_{L^2(e)} h_e^{1/2} \| \{ |\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)|_2 \} \|_{L^2(e)} \| \{ \nabla I_h \varphi \} \|_{L^\infty(e)} \end{aligned}$$

Therefore

$$\begin{aligned} & \left| ([c_h - I_h \varphi], \{ (\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi \cdot \mathbf{n}_e \})_{\Gamma_h} \right| \\ & \leq \left(\sum_{e \in \Gamma_h} \frac{1}{h_e} \| (1 + \{ |\mathbf{u}_h|_2 \})^{1/2} [c_h - I_h \varphi] \|_{L^2(e)}^2 \right)^{1/2} \left(\sum_{e \in \Gamma_h} h_e \| \{ |\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)|_2 \} \|_{L^2(e)}^2 \right)^{1/2} \\ & \quad \times \| \nabla I_h \varphi \|_{L^\infty(\Omega)}. \end{aligned}$$

When integrating this inequality over time, as the first and last factors are bounded, Corollary B.2.8 implies that

$$\lim_{h,k \rightarrow 0} \int_0^T ([c_h - I_h \varphi], \{ (\mathbb{D}(\mathbf{u}_h) - \mathbb{D}_h(\mathbf{u}_h)) \nabla I_h \varphi \cdot \mathbf{n}_e \})_{\Gamma_h} = 0. \quad (5.51)$$

Hence the treatment of $B_{di}(I_h \varphi, c_h - I_h \varphi; \mathbf{u}_h)$ reduces to the two terms of the first line of (5.49). With the notation (5.10) for the discrete gradient, we have

$$\begin{aligned} & (\mathbb{D}_h(\mathbf{u}_h) \nabla I_h \varphi, \nabla (c_h - I_h \varphi))_{\mathcal{E}_h} - ([c_h], \{ \mathbb{D}_h(\mathbf{u}_h) \nabla I_h \varphi \cdot \mathbf{n}_e \})_{\Gamma_h} \\ & = (\nabla I_h \varphi, \mathbb{D}_h(\mathbf{u}_h) \mathbf{G}_h(c_h - I_h \varphi))_{\mathcal{E}_h}. \end{aligned} \quad (5.52)$$

The result follows immediately from the definitions discrete gradient (5.10) and the fact that $I_h\varphi$ has no jumps. Now consider

$$\int_0^T (\nabla I_h\varphi, \mathbb{D}_h(\mathbf{u}_h) \mathbf{G}_h(c_h - I_h\varphi))_{\mathcal{E}_h} dt.$$

On one hand, as $\mathbf{G}_h$ is the symmetric discrete gradient, we know that [73]

$$\lim_{h \rightarrow 0} \mathbf{G}_h(c_h - I_h\varphi) = \nabla(c - \varphi) \quad \text{weakly in } L^2(\Omega \times (0, T)).$$

On the other hand, from (5.24) we have,

$$\lim_{h \rightarrow 0} \|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u})\|_{L^2(\Omega \times (0, T))} = 0.$$

Finally, from approximation theorem using Lagrange interpolation we have,

$$\lim_{h \rightarrow 0} \|\nabla I_h\varphi - \nabla \varphi\|_{L^\infty(0, T; L^\infty(\Omega))} = 0.$$

Hence

$$\begin{aligned} \lim_{h \rightarrow 0} \int_0^T & \left[(\mathbb{D}_h(\mathbf{u}_h) \nabla I_h\varphi, \nabla(c_h - I_h\varphi))_{\mathcal{E}_h} - ([c_h], \{\mathbb{D}_h(\mathbf{u}_h) \nabla I_h\varphi \cdot \mathbf{n}_e\}_{\Gamma_h}) \right] \\ &= \int_0^T (\nabla \varphi, \mathbb{D}(\mathbf{u}) \nabla(c - \varphi)). \end{aligned} \quad (5.53)$$

Thus, by collecting (5.50), (5.51), and (5.53), we obtain

$$\lim_{h \rightarrow 0} \int_0^T B_{di}(I_h\varphi, c_h - I_h\varphi; \mathbf{u}_h) = \int_0^T (\nabla \varphi, \mathbb{D}(\mathbf{u}) \nabla(c - \varphi)). \quad (5.54)$$

Then, by combining (5.54), (5.47) and (5.48), we deduce

$$\begin{aligned} \lim_{h,k \rightarrow 0} A(I_h \varphi, c_h - I_h \varphi; \mathbf{u}_h) &= \int_0^T \left((\mathbf{u} \cdot \nabla \varphi, c - \varphi) + (q^I \varphi, c - \varphi) + (\nabla \varphi, \mathbb{D}(\mathbf{u}) \nabla (c - \varphi)) \right. \\ &\quad \left. + (\phi \partial_t \varphi, c - \varphi) \right). \end{aligned}$$

Hence, in view of (5.46), we derive for all sufficiently smooth φ :

$$\begin{aligned} \lim_{h,k \rightarrow 0} \int_0^T \|c_h - I_h \varphi\|_{C_h}^2 &\leq \int_0^T (\hat{c} q^I, c - \varphi) + \frac{1}{2} \|\phi^{1/2}(c_0 - \varphi(0))\|_{L^2(\Omega)}^2 \\ &\quad - \int_0^T \left((\mathbf{u} \cdot \nabla \varphi, c - \varphi) + (q^I \varphi, c - \varphi) + (\nabla \varphi, \mathbb{D}(\mathbf{u}) \nabla (c - \varphi)) \right. \\ &\quad \left. + (\phi \partial_t \varphi, c - \varphi) \right). \end{aligned} \tag{5.55}$$

This is true in particular for any sequence $(\varphi_s)_{s \geq 0}$ of smooth functions approximating c in $L^2(0, T; H^1(\Omega))$. Therefore

$$\lim_{h,k \rightarrow 0} \int_0^T \|c_h - I_h \varphi_s\|_{C_h}^2 = 0. \tag{5.56}$$

From here we deduce the strong convergence of c_h to c in the following sense. Then (5.55) implies on one hand

$$\nabla c_h \text{ converges to } \nabla c \text{ strongly in } L^2(\Omega \times (0, T))^d, \tag{5.57}$$

and on the other hand

$$\lim_{h \rightarrow 0} \left(\int_0^T \sum_{e \in \Gamma_h} \frac{1}{h_e} \|(1 + \{|\mathbf{u}_h|_2\})^{1/2} [c_h]\|_{L^2(e)}^2 \right)^{1/2} = 0. \tag{5.58}$$

□

Now we are in a position to pass to the limit in (3.29) to show the convergence numerical

solution for the concentration produced using SIPG, NIPG and IIPG.

Theorem 5.2.4. *Suppose that the maximal time step k and h tend to zero with mesh parameter. Then upon passage to a subsequence, the concentrations $\{c_h\}_h$ computed using the scheme (3.29) with SIPG, NIPG and IIPG over a regular family of meshes converge strongly in $L^2(0, T; H^1(\mathcal{E}_h))$ to $c \in L^2(0, T; H^1(\Omega))$, that satisfies the weak formulation (4.3). i.e. we have*

$$\begin{aligned} c_h &\text{ converges to } c \text{ strongly in } L^2(0, T; L^2(\Omega)), \\ \nabla c_h &\text{ converges to } \nabla c \text{ strongly in } L^2(0, T; L^2(\Omega)). \end{aligned}$$

Proof. Again, let φ be a smooth function in space and time satisfying $\varphi(T) = 0$. Let us test (3.29) with $w_h = I_h\varphi$ and integrate the first term by parts in time. This gives

$$\begin{aligned} \int_0^T \left(-(\phi c_h, \partial_t(I_h\varphi)) + B_{di}(c_h, I_h\varphi; \mathbf{u}_h) + B_{cq}(c_h, I_h\varphi; \mathbf{u}_h) \right) \\ = (\phi c_{h-}^0, I_h\varphi(0)) + \int_0^T (\hat{c}q^I, I_h\varphi). \end{aligned} \quad (5.59)$$

As far as the right-hand side is concerned, the regularity of φ and the convergence of the initial data imply

$$\lim_{h \rightarrow 0} \left((\phi c_{h-}^0, I_h\varphi(0)) + \int_0^T (\hat{c}q^I, I_h\varphi) \right) = (\phi c_0, \varphi(0)) + \int_0^T (\hat{c}q^I, \varphi).$$

Now, we examine the left-hand side. For the first term, we find immediately

$$\lim_{h \rightarrow 0} \int_0^T (\phi c_h, \partial_t(I_h\varphi)) = \int_0^T (\phi c, \partial_t\varphi).$$

With the notation $\nabla_h c_h$, the form B_d reduces to

$$B_{di}(c_h, I_h\varphi; \mathbf{u}_h) = (\mathbb{D}(\mathbf{u}_h) \nabla_h c_h, \nabla(I_h\varphi))_{\mathcal{E}_h} + \epsilon([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla I_h\varphi \cdot \mathbf{n}_e\})_{\Gamma_h}.$$

The strong convergences of $\nabla_h c_h$ in $L^2(0, T; L^2(\Omega)^d)$, of $\mathbb{D}(\mathbf{u}_h)$ in $L^2(0, T; L^2(\Omega)^{d \times d})$ and $I_h \varphi$ in $W^{1, \infty}(\Omega \times (0, T))$ readily imply that

$$\lim_{h, k \rightarrow 0} \int_0^T (\mathbb{D}(\mathbf{u}_h) \nabla_h c_h, \nabla(I_h \varphi))_{\varepsilon_h} = \int_0^T (\mathbb{D}(\mathbf{u}) \nabla c, \nabla \varphi).$$

By invoking the same reasons, applying (5.58), and the regularity of the mesh, we readily derive that the second term in B_d tends to zero.

Regarding B_{cq} , the regularity of $I_h(\varphi)$ yields

$$\begin{aligned} B_{cq}(c_h, I_h \varphi; \mathbf{u}_h) = & \frac{1}{2} \left((\mathbf{u}_h \cdot \nabla_h c_h, I_h \varphi)_{\varepsilon_h} - (\mathbf{u}_h c_h, \nabla I_h \varphi)_{\varepsilon_h} + ((q^I + q^P) c_h, I_h \varphi) \right. \\ & \left. - ((I_h \varphi) \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} \right). \end{aligned} \quad (5.60)$$

Then a similar argument gives

$$\lim_{h \rightarrow 0} \int_0^T B_{cq}(c_h, I_h \varphi; \mathbf{u}_h) = \frac{1}{2} \int_0^T \left((\mathbf{u} \cdot \nabla c, \varphi) - (\mathbf{u} c, \nabla \varphi) + ((q^I + q^P) c, \varphi) \right).$$

Hence, by collecting these limits, we find that the limit function c satisfies indeed (4.3):

$$\begin{aligned} \int_0^T \left(-(\phi c, \partial_t \varphi) + (\mathbb{D}(\mathbf{u}) \nabla c, \nabla \varphi) + \frac{1}{2} \left((\mathbf{u} \cdot \nabla c, \varphi) - (\mathbf{u} c, \nabla \varphi) + ((q^I + q^P) c, \varphi) \right) \right) \\ = (\phi c_0, \varphi(0)) + \int_0^T (\hat{c} q^I, \varphi), \end{aligned}$$

for all sufficiently smooth φ that vanishes at time T . □

5.3 Convergence of DG-DG with implicit Euler in time

5.3.1 Convergence of pressure and velocity

With implicit Euler in Algorithm 3, additional error is introduced in the decoupling. I begin by showing that the error occurs due to the decoupling is sufficiently small for us to maintain the convergence of the numerical solutions for the pressure and velocity. To put it more precisely, I show that the numerical solution c_h^{j-1} provides a good approximation not only for the function c in the time interval (t_{j-2}, t_{j-1}) , but also for the time interval (t_{j-1}, t_j) .

Lemma 5.3.1. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 3 with maximal time step k and mesh size h tend to zero, and c be an accumulating point for $\{c_h\}$, then we have*

$$\lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c\|_{L^2(\Omega)}^2 = 0$$

Proof. From theorem 5.1.11, we have

$$c_h \text{ converges to } c \text{ in } L^2(0, T; L^2(\Omega))$$

which means

$$\lim_{h,k \rightarrow 0} \int_0^T \|c_h - c\|_{L^2(\Omega)}^2 = 0 \quad (5.61)$$

where the

$$c_h = c_h^j \frac{t - t_{j-1}}{k_j} - c_h^{j-1} \frac{t - t_j}{k_j} \text{ over interval } (t_{j-1}, t_j) \quad (5.62)$$

Thus,

$$\sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c\|_{L^2(\Omega)}^2 \leq \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c_h\|_{L^2(\Omega)}^2 + \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h - c\|_{L^2(\Omega)}^2$$

For the second term converges to zero because of the convergence of the concentration solution. We can also derive an upper bound for the term as follows,

$$\sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c_h\|_{L^2(\Omega)}^2 = \sum_{j=1}^N \int_{t_{j-1}}^{t_j} k_j^2 \|\partial_t c_h^j\|_{L^2(\Omega)}^2 \leq k \int_0^{t_N} k \|\partial_t c_h\|_{L^2(\Omega)}^2.$$

The term $\int_0^{t_N} k \|\partial_t c_h\|_{L^2(\Omega)}^2$ is bounded according to Theorem 4.3.3. Now, as the time step $k \rightarrow 0$ and mesh size $h \rightarrow 0$, we have

$$\lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c_h\|_{L^2(\Omega)}^2 = 0, \quad (5.63)$$

which implies

$$\lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c\|_{L^2(\Omega)}^2 = 0.$$

We conclude c_h^{j-1} is a sufficiently good approximation for c in time interval (t_{j-1}, t_j) . The same argument can be used to show that c_h^j is also a sufficiently good approximation for c in time interval (t_{j-1}, t_j) $\square$

Lemma 5.3.1 shows that instead of using continuous piecewise linear approximation in time for the concentration, we can accurately approximate the concentration using piecewise constant in time.

In order for us to show the convergence of the numerical solution for the pressure, we first establish a weak convergence for the pressure solution.

Theorem 5.3.2. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using*

Algorithm 3 with maximal time step k and mesh size h tend to zero, then there exist $p \in L^2(0, T; H^1(\Omega))$ such that after passing a subsequence,

$$\begin{aligned} p_h &\text{ converges to } p \text{ weakly in } L^2(0, T; L^2(\Omega)), \\ \mathbf{G}_h(p_h) &\text{ converges to } \nabla p \text{ weakly in } L^2(0, T; L^2(\Omega)). \end{aligned}$$

Proof. First, we show the weak convergence of the pressure. By the stability argument in Theorem 4.3.1, we have p_h is bounded and $L^2(0, T; L^2(\Omega)) = L^2(Q_T)$ is a Hilbert space. Thus, there exist $p \in L^2(0, T; L^2(\Omega))$ such that

$$p_h \text{ converges to } p \text{ weakly in } L^2(0, T; L^2(\Omega))$$

Also, we have an upper boundary for the discrete gradient,

$$\int_0^T \|\mathbf{G}_h(p_h)\|_{L^2(\Omega)}^2 \lesssim \int_0^T \|p_h\|_{H^1(\mathcal{E}_h)}^2 < M$$

Hence, we also have a weakly convergence subsequence,

$$\mathbf{G}_h(p_h) \text{ converges to } v \text{ weakly in } L^2(0, T; L^2(\Omega))$$

Now, we want to show that, in fact, $v = \nabla p$. So, for all $\varphi \in C_0^\infty(0, T; C_0^\infty(\Omega))$, then we have

$$\begin{aligned} \int_{Q_T} \mathbf{G}_h(p_h) \varphi &= \int_0^T (\mathbf{G}_h(p_h), \varphi) = \int_0^T (\nabla p_h, \varphi) - \int_0^T (\{\pi_h \varphi\} \cdot \mathbf{n}_e, [p_h])_{\Gamma_h} \\ &= - \int_0^T (p_h, \nabla \cdot \varphi) - \int_0^T (\{\pi_h \varphi - \varphi\} \cdot \mathbf{n}_e, [p_h])_{\Gamma_h} \end{aligned}$$

By taking the limit and that $p_h \rightharpoonup p$ weakly, we have

$$\lim_{h,k \rightarrow 0} \int_{Q_T} \mathbf{G}_h(p_h) \varphi = - \lim_{h,k \rightarrow 0} \int_0^T (p_h, \nabla \cdot \varphi) = - \lim_{h,k \rightarrow 0} \int_0^T (p, \nabla \cdot \varphi) = \lim_{h,k \rightarrow 0} \int_0^T (\nabla p, \varphi)$$

□

Next result, we show the strong convergence of numerical solution with NIPG, IIPG and SIPG.

Theorem 5.3.3. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 3 with NIPG, IIPG and SIPG as the maximal mesh size h and time step size k tend to zero, then we have*

$$p_h \text{ converges to } p \text{ strongly in } L^p(0, T; H^1(\mathcal{E}_h))$$

where p is the solution of the weak problem.

Proof. Let φ be a smooth function in space and time and let $I_h\varphi$ be its Lagrange interpolation, then we have

$$\|\varphi - I_h\varphi\|_{L^\infty(0, T; L^\infty(\Omega))} = 0 \text{ and } \|\nabla\varphi - \nabla I_h\varphi\|_{L^\infty(0, T; L^\infty(\Omega))} = 0$$

then we have

$$\begin{aligned} \int_0^T B_{di}(p_h - I_h\varphi, p_h - I_h\varphi; c_h) &= \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_{di}(p_h^j - I_h\varphi, p_h^j - I_h\varphi; c_h^{j-1}) \\ &= \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \ell_d^j(p_h^j - I_h\varphi; c_h^{j-1}) - B_{di}(I_h\varphi, p_h^j - I_h\varphi; c_h^{j-1}) \end{aligned}$$

We examine the first term on the right-hand-side, first recall the definition of source terms (3.31), we have

$$\lim_{h, k \rightarrow 0} \|(q_h^I - q_h^P) - (q^I - q^P)\|_{L^2(0, T; L^2(\Omega))} = 0$$

Hence,

$$\begin{aligned}
\lim_{h,k \rightarrow 0} \int_0^T \ell_d(p_h^j - I_h \varphi; c_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \ell_d(p_h^j - I_h \varphi; c_h^{j-1}) \\
&= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) \mathbf{g}, \nabla(p_h^j - I_h \varphi)) + (q^I - q^P, p_h^j - I_h \varphi) \\
&\quad - \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\{\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) \mathbf{g}\} \cdot \mathbf{n}_e, [p_h^j - I_h \varphi])_{\Gamma_h} \\
&= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} ((\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) - \mathbb{K}_h(c_h^{j-1}) \rho_h(c_h^{j-1})) \mathbf{g}, \nabla(p_h^j - I_h \varphi)) \\
&\quad - \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\{(\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) - \mathbb{K}_h(c_h^{j-1}) \rho_h(c_h^{j-1})) \mathbf{g}\} \cdot \mathbf{n}_e, [p_h^j - I_h \varphi])_{\Gamma_h} \\
&\quad + \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\mathbb{K}_h(c_h^{j-1}) \rho_h(c_h^{j-1}) \mathbf{g}, \mathbf{G}_h(p_h^j - I_h \varphi)) \\
&\quad + \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} ((q_h^I - q_h^P)^j, p_h^j - I_h \varphi) \\
&= \int_0^T (\mathbb{K}(c) \rho(c) \mathbf{g}, \nabla p - \nabla \varphi) + \int_0^T (q^I - q^P, p - \varphi)
\end{aligned}$$

For the second term, we have

$$\begin{aligned}
\lim_{h,k \rightarrow 0} \int_0^T B_{di}(I_h \varphi, p_h - I_h \varphi; c_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_{di}(I_h \varphi, p_h^j - I_h \varphi; c_h^{j-1}) \\
&= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\nabla I_h \varphi, (\mathbb{K}(c_h^{j-1}) - \mathbb{K}_h(c_h^{j-1})) \nabla(p_h^j - I_h \varphi)) \\
&\quad - \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\{(\mathbb{K}(c_h^{j-1}) - \mathbb{K}_h(c_h^{j-1})) \nabla I_h \varphi\} \cdot \mathbf{n}_e, [p_h^j])_{\Gamma_h} \\
&\quad + \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\mathbf{G}_h(p_h^j - I_h \varphi), \mathbb{K}_h(c_h^{j-1}) \nabla I_h \varphi) \\
&= \int_0^T (\nabla p - \nabla \varphi, \mathbb{K}(c) \nabla \varphi)
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
\lim_{h,k \rightarrow 0} \frac{1}{2} \|p_h - I_h \varphi\|_{L^2(0,T;H^1(\mathcal{E}_h))}^2 &\leq \lim_{h,k \rightarrow 0} \int_0^T B_{di}(p_h - I_h \varphi, p_h - I_h \varphi; c_h) \\
&= \int_0^T (q^I - q^P, p - \varphi) \\
&\quad - \int_0^T (\nabla p - \nabla \varphi, \mathbb{K}(c) \nabla \varphi) + \int_0^T (\mathbb{K}(c) \rho(c) \mathbf{g}, \nabla p - \nabla \varphi)
\end{aligned}$$

By the density argument, we can pass through the sequence $(\varphi_s)_{s \geq 0}$ of smooth function approximating p in $L^2(0, T; H^1(\Omega))$. Therefore,

$$\lim_{h,k,s \rightarrow 0} \|p_h - I_h \varphi_s\|_{L^2(0,T;H^1(\mathcal{E}_h))}^2 = 0$$

Hence, we have

$$p_h \text{ converges to } p \text{ strongly in } L^2(0, T; L^2(\Omega)) \quad (5.64)$$

$$\nabla p_h \text{ converges to } \nabla p \text{ strongly in } L^2(0, T; L^2(\Omega)) \quad (5.65)$$

also we have for the jump term,

$$\lim_{h,k \rightarrow 0} \int_0^T (h_e^{-1} [p_h], [p_h])_{\Gamma_h} = 0 \quad (5.66)$$

□

Now, we can show in fact the pressure approximation converges to the weak solution.

Theorem 5.3.4. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 3 with maximal time step k and mesh size h tend to zero, the pressure approximation converges to weak solution in (4.4).*

Proof. Let $\varphi \in C_0^\infty(0, T; C^\infty(\Omega))$ and let $I_h \varphi_h$ be the Lagrange approximation of the φ over

each time interval. And according to (5.64), (5.65) and (5.66) we have

$$\begin{aligned}
\lim_{h,k \rightarrow 0} \int_0^T B_{di}(p_h, I_h \varphi; c_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_{di}(p_h^j, I_h \varphi; c_h^{j-1}) \\
&= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\nabla p_h^j, \mathbb{K}(c_h^{j-1}) \nabla I_h \varphi) + \theta(\{\mathbb{K}(c_h^{j-1}) \nabla I_h \varphi\} \cdot \mathbf{n}_e, [p_h^j]_{\Gamma_h}) \\
&= \int_0^T (\nabla p, \mathbb{K}(c) \nabla \varphi)
\end{aligned}$$

For the right-hand-side, we have

$$\begin{aligned}
\lim_{h,k \rightarrow 0} \int_0^T \ell_d(I_h \varphi; c_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \ell_d(I_h \varphi; c_h^{j-1}) \\
&= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\mathbb{K}(c_h^{j-1}) \rho(c_h^{j-1}) \mathbf{g}, \nabla I_h \varphi) + ((q_h^I - q_h^P)^j, I_h \varphi) \\
&= \int_0^T (\mathbb{K}(c) \rho(c) \mathbf{g}, \nabla \varphi) + \int_0^T (q^I - q^P, \varphi)
\end{aligned}$$

Therefore, the numerical solution for the pressure indeed converges to the weak solution of the miscible displacement problem. $\square$

After we establish the convergence of the pressure, we can also establish the convergence of the velocity as follow. Notice, the numerical solution p_h for the pressure is essentially piecewise constant in time which does not indicate any additional regularity in time.

Theorem 5.3.5. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions using algorithm with maximal time step k and mesh size h tend to zero, then we have*

$$\mathbf{u}_h \text{ converges to } \mathbf{u} \text{ strongly in } L^2(0, T; L^2(\Omega))$$

where $\mathbf{u} = -\mathbb{K}(c) \nabla p$ as in the weak formulation (4.5) and p is the solution of the weak problem (4.4).

Proof. By result in [75] and the construction of the flux, we have

$$\sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|\mathbf{u}_h^j - \mathbf{u}\|_{L^2(\Omega)}^2 \lesssim \int_0^T \|p_h - p\|_{L^2(\Omega)}^2$$

□

Corollary 5.3.6. *If $\mathbf{u} = -\mathbb{K}(c)\nabla p$ is in $H(\Omega; \text{div})$, then we have*

$$\mathbf{u}_h \text{ converges to } \mathbf{u} \text{ in } L^2(0, T; H(\Omega; \text{div}))$$

Proof. From [75], we know

$$\nabla \cdot \mathbf{u}_h^j = \pi_h(q_h^I - q_h^P)^j$$

Therefore,

$$\nabla \cdot \mathbf{u}_h^j = \pi_h(q_h^I - q_h^P)^j \text{ converges to } q^I - q^P = \nabla \cdot \mathbf{u} \text{ strongly in } L^2(0, T; L^2(\Omega))$$

□

Remark 5.3.7. Using DG discretization for the Darcy's flow relaxes the regularity of the velocity to be only in $L^2(0, T; L^2(\Omega))$ such that its existence is known [80]. Whereas using the MFE for the discretization requires the velocity to be in $H(\Omega; \text{div})$, but there is no theoretical result in terms of the existence of the solution in this case.

5.3.2 Convergence of concentration

The proof of the convergence of the concentration is very similar to the case with DG in time.

Theorem 5.3.8. *Suppose that the maximal time step k and h tend to zero with mesh parameter. Then upon passage to a subsequence, the concentrations $\{c_h\}_{h>0}$ computed using*

Algorithm 3 with SIPG over a regular family of meshes converge strongly in $L^2(0, T; L^2(\Omega))$ to $c \in L^2(0, T; H^1(\Omega))$, that satisfies the weak formulation (4.6).

Proof. Let w_h be the Lagrange interpolation function approximating $w \in C^\infty(0, T; C^\infty(\Omega))$.

Using the same argument as in Theorem 5.2.2 we have

$$\begin{aligned} \lim_{h,k \rightarrow 0} \int_0^T B_{di}(c_h, w_h; \mathbf{u}_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_{di}(c_h^j, w_h; \mathbf{u}_h^j) = \int_0^T (\mathbb{D}(\mathbf{u}) \nabla c, \nabla w) \\ \lim_{h,k \rightarrow 0} \int_0^T B_{cq}(c_h, w_h; \mathbf{u}_h) &= \lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} B_{cq}(c_h^j, w_h; \mathbf{u}_h^j) = \\ &= \frac{1}{2} \int_0^T \left((\mathbf{u} \cdot \nabla c, w) - (c \mathbf{u}, \nabla w) + ((q^I + q^P)c, w) \right) = \int_0^T \left((\mathbf{u} \cdot \nabla c, w) + (q^I c, w) \right) \end{aligned}$$

Also, we have

$$\begin{aligned} \lim_{h \rightarrow 0} \int_0^T (\phi \partial_t c_h, w_h) &= \lim_{h \rightarrow 0} \int_0^T (\phi \partial_t c_h, w) = - \lim_{h \rightarrow 0} \int_0^T (\phi c_h, \partial_t w) + (\phi c_h(0), w) \\ &= - \int_0^T (\phi c, \partial_t w) + (\phi c(0), w) \end{aligned}$$

So, we have

$$\lim_{h,k \rightarrow 0} \int_0^T B_{di}(c_h, w_h; \mathbf{u}_h) + B_{cq}(c_h, w_h; \mathbf{u}_h) = \int_0^T \left((\mathbb{D}(\mathbf{u}) \nabla c, \nabla w) + (\mathbf{u} \cdot \nabla c, w) + (q^I c, w) \right)$$

And we have the right-hand-side,

$$\lim_{h,k \rightarrow 0} \int_0^T (q_h^I \hat{c}_h, w_h) = \int_0^T (q^I \hat{c}, w)$$

Therefore, the numerical solution for the concentration converges to the solution to the weak problem. $\square$

5.4 Convergence of MFE-DG with implicit Euler in time

With the analysis we have presented for MFE-DG with DG in time and DG-DG with implicit Euler decoupling, the convergence analysis for the MFE-DG with implicit Euler in time has become very straightforward. In this section, we present the proof of the convergence.

5.4.1 Convergence of pressure and velocity

The convergence of the pressure and velocity for the MFE-DG with implicit Euler follows the same idea as DG-DG with implicit Euler. First, we have to show the decoupling provides sufficiently good approximation for the concentration.

Theorem 5.4.1. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 5 with maximal time step k and mesh size h tend to zero, and c be an accumulating point for $\{c_h\}$, then we have*

$$\lim_{h,k \rightarrow 0} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \|c_h^{j-1} - c\|_{L^2(\Omega)}^2$$

Proof. The proof is exactly the same as Theorem 5.3.1 since the discretization of the concentration has not changed. □

Next result is based on mixed finite element analysis.

Theorem 5.4.2. *Let $(\mathbf{u}_h, p_h, c_h)$ be a sequence of the numerical solutions computed using Algorithm 5, with h, k go to zero, then we have*

$$p_h \text{ converges to } p \text{ strong in } L^p(0, T; L^2(\Omega))$$

$$\mathbf{u}_h \text{ converges to } \mathbf{u} \text{ strong in } L^p(0, T; H(\Omega; \text{div}))$$

where $p, \mathbf{u}$ are the solutions of the weak formulation (4.1), (4.2), (4.3).

Proof. We use the same notation as in Theorem 5.2.1, where we have

$$\begin{aligned}\mathbb{U}_h &= \{\mathbf{u}_h \in \mathbb{U} \mid \mathbf{u}_h|_{(t_{j-1}, t_j)} \in \mathcal{P}_0(t_{j-1}, t_j; \mathbf{U}_h)\}, \text{ and} \\ \mathbb{P}_h &= \{p_h \in \mathbb{P} \mid p_h|_{(t_{j-1}, t_j)} \in \mathcal{P}_0(t_{j-1}, t_j; P_h)\}\end{aligned}$$

From Strang's Lemma we have,

$$\begin{aligned}\|(\mathbf{u} - \mathbf{u}_h, p - p_h)\|_{\mathbb{U} \times \mathbb{P}} &\leq \inf_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \|(\mathbf{u} - \mathbf{v}_h, p - q_h)\|_{\mathbb{U} \times \mathbb{P}} \\ &\quad + \sup_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \frac{|b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c) - b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c_h)|}{\|(\mathbf{v}_h, q_h)\|_{\mathbb{U} \times \mathbb{P}}}\end{aligned}$$

where,

$$b((\mathbf{u}, p), (\mathbf{v}, q); c) = \int_0^T ((\mathbb{K}^{-1}(c)\mathbf{u}, \mathbf{v}) - (p, \operatorname{div}(\mathbf{v})) + (q, \operatorname{div}(\mathbf{u})))$$

Since we have

$$b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c) - b((\mathbf{u}, p), (\mathbf{v}_h, q_h); c_h) = \sum_{j=1}^N \int_{t_{j-1}}^{t_j} (\mathbb{K}^{-1}(c) - \mathbb{K}^{-1}(c_h^{j-1}))\mathbf{u}, \mathbf{v}_h)$$

so

$$\begin{aligned}\|(\mathbf{u} - \mathbf{u}_h, p - p_h)\|_{\mathbb{U} \times \mathbb{P}} &\leq \inf_{(\mathbf{v}_h, q_h) \in \mathbb{U}_h \times \mathbb{P}_h} \|(\mathbf{u} - \mathbf{v}_h, p - q_h)\|_{\mathbb{U} \times \mathbb{P}} + \|(\mathbb{K}^{-1}(c) - \mathbb{K}^{-1}(c_h))\mathbf{u}\|_{L^2(0, T; L^2(\Omega))}\end{aligned}$$

The assumptions on $\mathbb{K}$ guarantee that $|\mathbb{K}^{-1}(c_h^{j-1})\mathbf{u}|^2$ converges pointwise to $|\mathbb{K}^{-1}(c)\mathbf{u}|^2$, and since $\mathbb{K}^{-1}$ takes values in a compact set it follows that $|\mathbb{K}^{-1}(c_h^{j-1})\mathbf{u}|^2 \leq M|\mathbf{u}|^2$. Apply the dominated convergence theorem shows $\mathbb{K}^{-1}(c_h^{j-1})\mathbf{u} \rightarrow \mathbb{K}^{-1}(c)\mathbf{u}$ in $L^2(0, T; L^2(\Omega))$, and strong convergence of the velocity and pressure follows. $\square$

5.4.2 Convergence of concentration

Theorem 5.4.3. *Suppose that the maximal time step k and h tend to zero with mesh parameter. Then upon passage to a subsequence, the concentrations $\{c_h\}_h$ computed using Algorithm 5 with SIPG over a regular family of meshes converge strongly in $L^2(0, T; L^2(\Omega))$ to $c \in L^2(0, T; H^1(\Omega))$, that satisfies the weak formulation (4.3).*

Proof. The proof is the same as in Theorem 5.2.2. □

5.5 Convergence of MFE-DG and DG-DG with Crank-Nicolson in time

The stability result presented in Theorem 4.4.2 for the Crank-Nicolson scheme does not provide additional information for the derivative in time for the concentration. As a consequence, we cannot obtain the result to show that c_h^{j-1} is a sufficiently good piecewise constant approximation for concentration over the interval (t_{j-1}, t_j) . So, in order to establish the convergence for Crank-Nicolson decoupling approach we have to assume additional regularity in time for the pressure and velocity. However, the assumption of the additional regularity is beyond the scope of this thesis. Therefore, no further discussion is given.

For the proof of convergence for the Algorithm 6 for MFE-DG with Crank-Nicolson decoupling, we refer to [70].

Linear solver

6.1 Overlapping domain decomposition

The parallelism aspect of the simulation is done using domain decomposition (DD). The domain is partitioned into each process. Hence, the entire assembling process is done in parallel. For the linear solver, the non-overlapping DD commonly used for the nodal basis in FEM simply requires us to keep track of the nodes' values at the interface for matrix-vector multiplication illustrated in Figure 6.1.

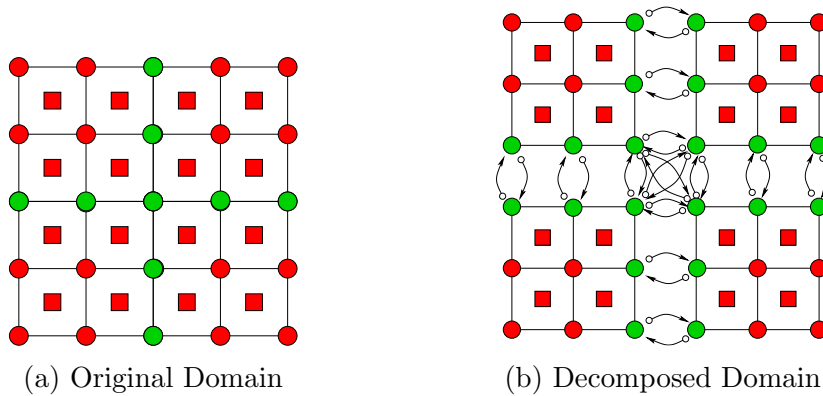


Figure 6.1: Non-overlapping domain decomposition

In our case, since we also want to consider the modal bases, we use overlapping DD by partitioning the domain into smaller subdomains with additional ghost cells. Then we use

the additive Schwarz alternating process, by setting the boundary of the ghost cells to be the previously computed values in corresponding cells from the neighboring subdomains and iterate until convergence is achieved as being illustrated Figure 6.2.

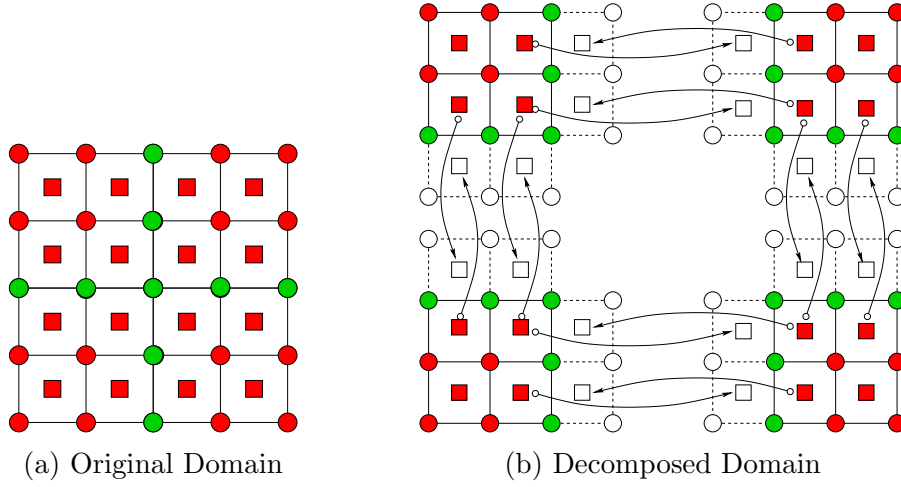


Figure 6.2: Overlapping domain decomposition

For the Darcy's flow using MFE, the saddle-point problem is still challenging to solve due to the semi-definite system. From the implementation perspective, I use MUMPS [92, 93] the parallel direct solver by linking DUNE [94, 95] with PETSc [96, 97, 98] environment. The overall performance of for the MFE-DG method for 2D homogeneous permeability model up to 32 processes is given in Figure 6.3.

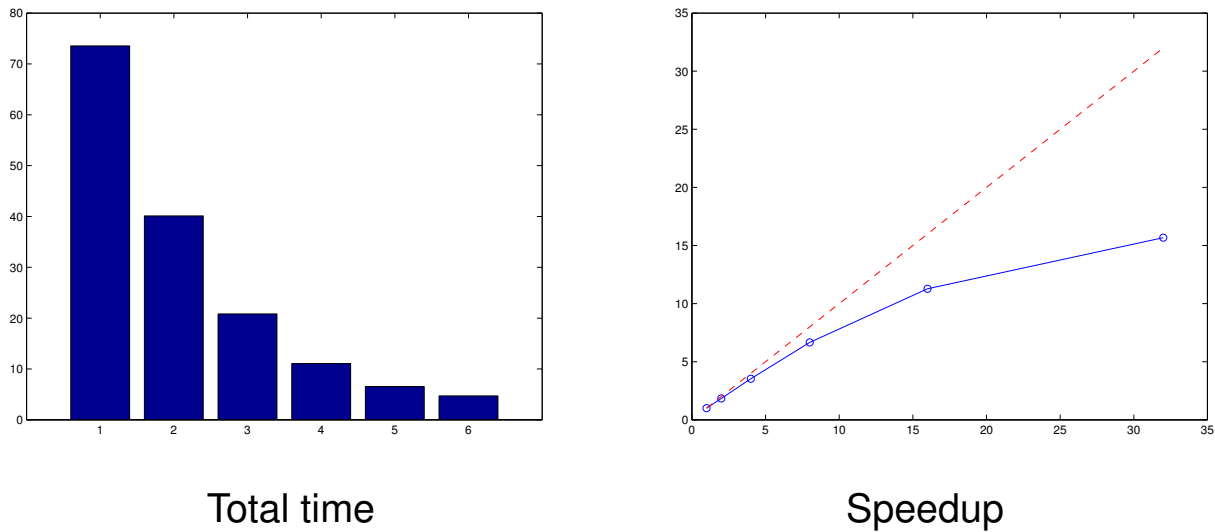


Figure 6.3: Overall performance of the MFE-DG

We do observe speedup, but the scaling terms to be poor. The poor scaling is due to the parallel direct solver for solving the saddle-point problem. However, solving the Darcy's system using DG can be efficiently implemented with AMG preconditioning as I discuss in the next section.

6.2 Algebraic multigrid preconditioner for DG

Before introducing the preconditioner for the miscible displacement problem, I first present a table of commonly used preconditioning techniques and their pros and cons.

	Type	Pros	Cons	Example
Direct Solver	LU decomposition	higher precision, reusable	not scalable	MUMPS, PARDISO, SuperLU, UMFPACK
ILU	approximated LU	cheap setup	not robust	Hyper, PaStiX
AMG	graph based coarsening	robust, scalable	expensive setup	BoomerAMG, AGMG

Table 6.1: Preconditioner comparison

The Darcy's system (3.16) resulting from the pressure equation is more difficult to solve than the transport system (3.26) because of the highly varying permeability field. We solve the transport system with domain decomposition preconditioned by ILU(0) with Restarted GMRES.

For the Darcy's system, ILU based preconditioning fails for the large scale simulation or the case with highly heterogeneous permeability. Whereas, using direct solver we encounter difficulty for obtaining scalability as being mentioned using MFE method. In this case, we construct our preconditioner using algebraic multigrid (AMG) algorithm based on the works [52, 53]. Without going into the details of the solver, we give an overview of our approach for the reader familiar with AMG. We use overlapping domain decomposition for the parallel implementation and subspace correction to reduce the first coarse level onto low order finite element space. The resulting coarser levels are constructed and solved by going through a V-cycle using non-smooth aggregation AMG. The coarsest level is solved using direct solver. We choose ILU(1) to be the smoother for the original system (3.16). On the coarse level SSOR is used as smoother. Our approach differs from [52] by the choice of nonconforming piecewise constant for the low order finite element space instead of continuous piecewise linears. This choice results in an M-matrix on the first coarsening level and a more robust

solver for highly heterogeneous porous media. For the reduction onto the piecewise constant space, the restrictive operator can be constructed as follows

$$\psi_{E_i} = \sum_{E_i \in \mathcal{E}_h} \sum_j \mathbf{R}_{E_i,j} \phi_{E_i,j}$$

with

$$\phi_{E_i,j} \in P_h \text{ and } \psi_{E_i} = \begin{cases} 1 & \text{on } E_i \\ 0 & \text{elsewhere} \end{cases}$$

Then the restrictive operator is

$$\mathbf{R}_0 = \begin{pmatrix} \mathbf{R}_{E_1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{E_2} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{R}_{E_n} \end{pmatrix}$$

The first coarse level can be constructed as

$$\mathbf{A}_0 = \mathbf{R}_0 \mathbf{A}_{DG} \mathbf{R}_0^T$$

where $\mathbf{A}_{DG}$ is the linear system from (3.16). BiCGStab or Restarted GMRES can be used to solve the preconditioned system.

6.3 Performance evaluation

To demonstrate the efficiency and the robustness of the solver, we consider a problem driven by flux boundary conditions at one side (velocity is $0.1m/s$), pressure on the other side ($p_D = 1000Pa$) and no-flow boundary condition on the rest of the boundary, as illustrated

in Figure 6.4. Viscosities are chosen as

$$\mu_s = 5.8 Pa \cdot s \text{ and } \mu_o = 2.9 Pa \cdot s \quad (6.1)$$

Following parameters are given for the diffusion-dispersion matrix and porosity,

$$d_m = 1.8 \times 10^{-7} m^2/s, \quad \alpha_l = 1.8 \times 10^{-5} m \text{ and } \alpha_t = 1.8 \times 10^{-6} m, \quad \phi = 0.2. \quad (6.2)$$

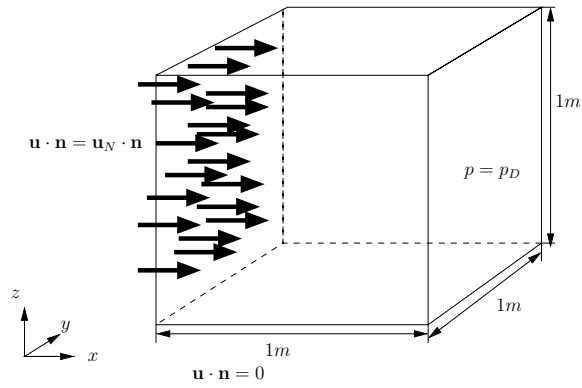


Figure 6.4: Flux driven problem

The permeability field, as illustrated in Figure 6.5, is discontinuous; the lens inside the domain has permeability equal to $10^{-4} m^2$ while the rest of the domain has permeability equal to $1 m^2$. The gravitational effect is neglected in this case.

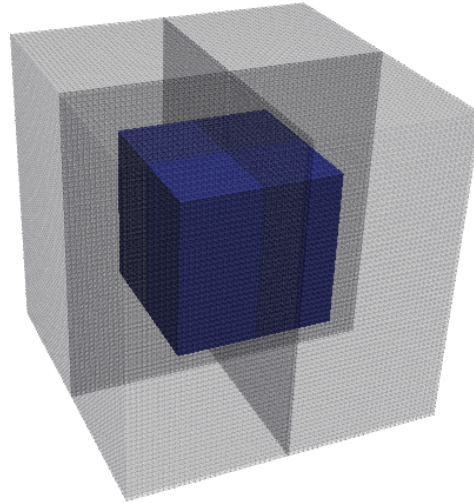


Figure 6.5: Discontinuous permeability field

We have implemented the discretization in parallel architecture IBM iDataPlex with Intel(R) Xeon(R) CPU X5660 2.80GHz processors. In Figure 6.6 we present the performance of the entire simulation for one time step up to 512 processors with piecewise quadratic approximation. The mesh contains 262,114 cells which yields 7,077,888 degrees of freedom for the Darcy's system and 2,621,140 degrees of freedom for the transport system.

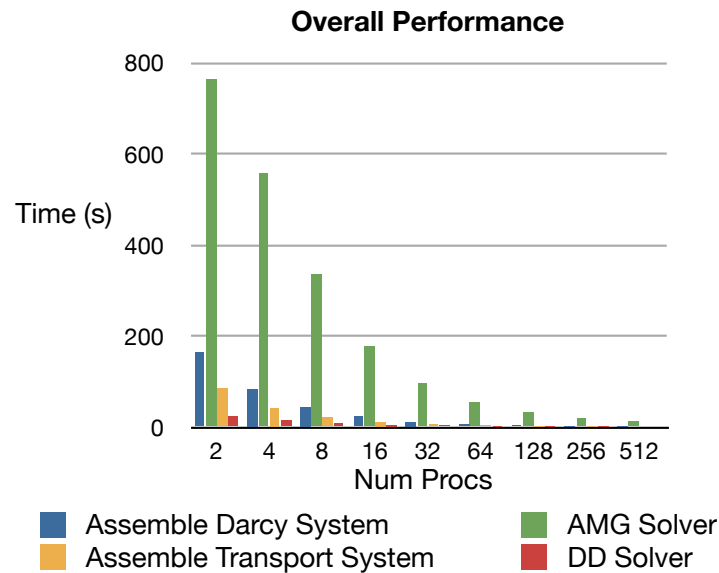


Figure 6.6: Overall performance

Figure 6.6 shows the computational time for each component of the solver. The most

time-consuming process is the AMG solver for the Darcy's system. This cost increases with the heterogeneities and discontinuities of the permeability field. Our proposed AMG solver performs well on the parallel cluster. Figure 6.7 suggests a linear trend of the speedup as we increase the number of the processors, which indicates strong scalability of the AMG solver.

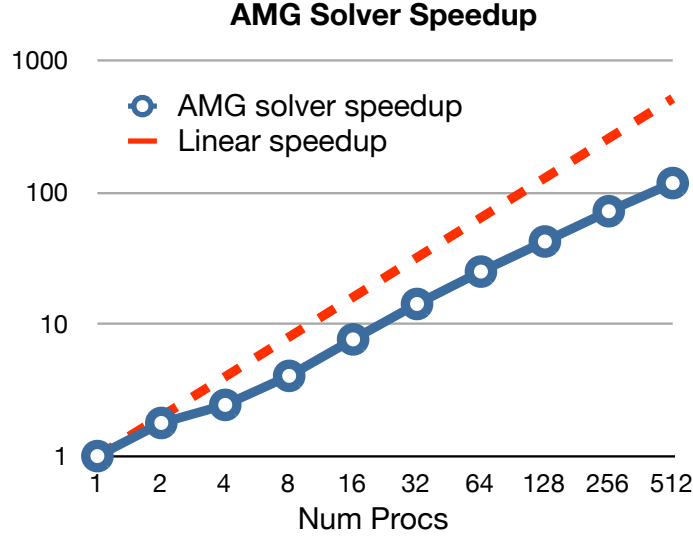


Figure 6.7: AMG solver speedup

The implementation was done within Distributed and Unified Numerics Environment (DUNE) [94, 95] and DUNE-PDELab [99]. The flexible C++ template based development environment allows for an efficient implementation of our method. For more detail information on the software including compilation and simulation capability, we refer reader to Appendix C.

Numerical Experiments

7.1 Simulation using MFE-DG

In this section, I present the simulation results using MFE-DG method.

7.1.1 Analytical problem and convergence study

Consider the miscible displacement problem in $\Omega = (0, 1)^2$ with the following analytical solutions:

$$\begin{aligned} p(x, y, t) &= \left(2 - e^{-x} (1 + x + x^2) - e^{-y} (1 + y + y^2)\right) e^{\frac{\pi t}{2}}, \\ c(x, y, t) &= \frac{1}{2} (\sin(2\pi x)^2 + \cos(2\pi y)^2) \sin\left(\frac{\pi t}{2}\right). \end{aligned}$$

For the diffusion-dispersion tensor we use the semi-empirical relation:

$$\mathbb{D}(\mathbf{u}) = d_m \mathbf{I} + |\mathbf{u}| (\alpha_l E(\mathbf{u}) + \alpha_t (\mathbf{I} - E(\mathbf{u}))), \quad (7.1)$$

where $E(\mathbf{u}) = \frac{\mathbf{u}\mathbf{u}^T}{|\mathbf{u}|^2}$ and we set,

$$d_m = 1.8 \times 10^{-7}, \quad \alpha_l = 1, 8 \times 10^{-5} \text{ and } \alpha_t = 1.8 \times 10^{-6}. \quad (7.2)$$

The parameters d_m , α_l and α_t are the molecular diffusion, longitudinal dispersivity and transverse dispersivity respectively. The other parameters are

$$\phi = 0.2, \mathbb{K}(c) = \frac{9.44 \times 10^{-3}}{(c(2.9)^{-0.25} + (1-c)(5.8)^{-0.25})^{-4}}, \mathbf{g} = 0. \quad (7.3)$$

Pressure and velocity				
h	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	1.50e-1	—	2.54e-4	—
2^{-2}	5.26e-2	1.52	9.89e-5	1.36
2^{-3}	1.89e-2	1.47	3.65e-5	1.44
2^{-4}	7.44e-3	1.35	1.60e-5	1.19
2^{-5}	3.36e-3	1.15	7.70e-6	1.06
Concentration				
h	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	1.78e-1	—	3.05e+0	—
2^{-2}	2.13e-2	3.07	4.86e-1	2.65
2^{-3}	1.57e-2	0.44	9.78e-1	-1.01
2^{-4}	4.03e-3	1.96	5.00e-1	0.96
2^{-5}	1.02e-3	1.99	2.52e-1	0.99

Table 7.1: Errors and rates for the method with RT₀-NIPG₁ and Lobatto III methods.

We observe that for a given mesh size h , the errors decrease as the order of the method increases (see Table 7.1, 7.2 and 7.3). The notation RT _{k} -NIPG _{p} means using Raviart-Thomas finite element basis of order k for the Darcy's system and p th-order NIPG for the transport

Pressure and velocity				
h	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	4.26e-2	—	1.04e-4	—
2^{-2}	1.55e-2	1.45	1.38e-5	2.91
2^{-3}	4.74e-3	1.71	6.19e-6	1.16
2^{-4}	1.30e-3	1.86	1.55e-6	2.00
2^{-5}	3.44e-4	1.93	3.86e-7	2.00
Concentration				
h	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	4.85e-2	—	1.04e+0	—
2^{-2}	2.13e-2	1.19	1.11e+0	-0.09
2^{-3}	2.10e-3	3.34	2.17e-1	2.35
2^{-4}	2.68e-4	2.97	5.53e-2	1.97
2^{-5}	3.38e-5	2.99	1.39e-2	2.00

Table 7.2: Errors and rates for the method $\text{RT}_1\text{-NIPG}_2$ and Lobatto III methods.

system. We also observe the expected optimal rates in space:

$$\|p(T) - p_h^N\|_{L^2(\Omega)} = \mathcal{O}(h^{k+1})$$

$$\|\mathbf{u}(T) - \mathbf{u}_h^N\|_{L^2(\Omega)} = \mathcal{O}(h^{k+1})$$

$$\|c(T) - c_h^N\|_{L^2(\Omega)} = \mathcal{O}(h^{r+1})$$

$$\|\nabla(c(T) - c_h^N)\|_{L^2(\mathcal{E}_h)} = \mathcal{O}(h^r)$$

Pressure and velocity				
h	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	1.09e-2	—	2.45e-5	—
2^{-2}	1.87e-3	2.55	8.59e-6	1.51
2^{-3}	2.56e-4	2.87	8.47e-7	3.34
2^{-4}	3.44e-5	2.89	1.04e-7	3.03
2^{-5}	4.93e-6	2.80	1.30e-8	3.00
Concentration				
h	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	4.88e-2	—	1.82e+0	—
2^{-2}	6.93e-4	6.14	4.48e-2	5.34
2^{-3}	2.08e-4	1.73	3.15e-2	0.51
2^{-4}	1.33e-5	3.97	4.02e-3	2.97
2^{-5}	9.68e-7	3.78	5.07e-4	2.99

Table 7.3: Errors and rates for the method with RT₂-NIPG₃ and Lobatto III methods.

In the next two tables we show that the choice of the symmetrization parameter ϵ in (3.24) does not have a visible effect on the errors and rates. We repeat the experiments above with either the SIPG method ($\epsilon = -1$) or the IIPG method ($\epsilon = 0$). Errors and rates are computed for the last two finer meshes (see Table 7.4 and Table 7.5).

	h	$\ p - p_h\ _{L^2(\Omega)}$	rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	rate
RT ₀ -SIPG ₁	2 ⁻⁴	7.44e-3	—	1.60e-5	—
	2 ⁻⁵	3.36e-3	1.15	7.70e-6	1.06
RT ₀ -IIPG ₁	2 ⁻⁴	7.44e-3	—	1.60e-5	—
	2 ⁻⁵	3.36e-3	1.15	7.70e-6	1.06
RT ₁ -SIPG ₂	2 ⁻⁴	1.30e-3	—	1.55e-6	—
	2 ⁻⁵	3.44e-4	1.93	3.86e-7	2.00
RT ₁ -IIPG ₂	2 ⁻⁴	1.30e-3	—	1.55e-6	—
	2 ⁻⁵	3.44e-4	1.93	3.86e-7	2.00
RT ₂ -SIPG ₃	2 ⁻⁴	3.44e-5	—	1.04e-7	—
	2 ⁻⁵	4.93e-6	2.80	1.30e-8	3.00
RT ₂ -IIPG ₃	2 ⁻⁴	3.44e-5	—	1.04e-7	—
	2 ⁻⁵	4.93e-6	2.80	1.30e-8	3.00

Table 7.4: Pressure and velocity: errors and rates for RT_k-SIPG_r and RT_k-IIPG_r methods and Lobatto III methods.

	h	$\ c - c_h\ _{L^2(\Omega)}$	rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	rate
RT ₀ -SIPG ₁	2 ⁻⁴	4.03e-3	–	5.00e-1	–
	2 ⁻⁵	1.02e-3	1.99	2.52e-1	0.99
RT ₀ -IIPG ₁	2 ⁻⁴	4.03e-3	–	5.00e-1	–
	2 ⁻⁵	1.02e-3	1.99	2.52e-1	0.99
RT ₁ -SIPG ₂	2 ⁻⁴	2.68e-4	–	5.53e-2	–
	2 ⁻⁵	3.38e-5	2.99	1.39e-2	2.00
RT ₁ -IIPG ₂	2 ⁻⁴	2.68e-4	–	5.53e-2	–
	2 ⁻⁵	3.38e-5	2.99	1.39e-2	2.00
RT ₂ -SIPG ₃	2 ⁻⁴	1.33e-5	–	4.02e-3	–
	2 ⁻⁵	9.68e-7	3.78	5.07e-4	2.99
RT ₂ -IIPG ₃	2 ⁻⁴	1.33e-5	–	4.02e-3	–
	2 ⁻⁵	9.68e-7	3.78	5.07e-4	2.99

Table 7.5: Concentration: errors and rates for RT_k-SIPG_r and RT_k-IIPG_r methods and Lobatto III methods.

We also varies the order of approximation in time from 1st to 3rd-order time stepping as we illustrated in Table 7.6, 7.7 and 7.8 with RT₂-NIPG₃ and mesh size $h = 0.015625$.

Pressure and velocity				
Δt	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	3.66e-2	—	3.32e-5	—
2^{-2}	2.08e-2	0.90	1.90e-5	0.90
2^{-3}	1.11e-2	0.95	1.02e-5	0.95
2^{-4}	5.75e-3	0.97	5.30e-6	0.97
2^{-5}	2.93e-3	0.99	2.70e-6	0.99
Concentration				
Δt	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	9.32e-2	—	5.24e-1	—
2^{-2}	5.37e-2	0.89	3.02e-1	0.89
2^{-3}	2.90e-2	0.94	1.63e-1	0.94
2^{-4}	1.51e-2	0.97	8.48e-2	0.97
2^{-5}	7.70e-3	0.98	4.33e-2	0.98

Table 7.6: Errors and rates with implicit Euler time-stepping method and RT₂-NIPG₃.

Pressure and velocity				
Δt	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	6.44e-2	—	6.21e-5	—
2^{-2}	1.61e-2	2.05	1.50e-5	2.06
2^{-3}	3.87e-3	2.01	3.59e-6	2.01
2^{-4}	9.60e-4	2.01	8.91e-7	2.00
2^{-5}	2.38e-4	2.05	2.22e-7	1.99
Concentration				
Δt	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	1.83e-1	—	1.03e+0	—
2^{-2}	4.31e-2	2.07	2.42e-1	2.06
2^{-3}	1.03e-2	2.01	5.78e-2	2.01
2^{-4}	2.54e-3	2.00	1.43e-2	2.00
2^{-5}	6.35e-4	2.00	3.57e-3	2.00

Table 7.7: Errors and rates with Gauss I time-stepping method and $\text{RT}_2\text{-NIPG}_3$.

Pressure and velocity				
Δt	$\ p - p_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \mathbf{u} - \mathbf{u}_h\ _{L^2(\Omega)}$	Cvg. rate
2^{-1}	1.12e-1	—	9.73e-5	—
2^{-2}	1.33e-2	3.30	1.23e-5	3.30
2^{-3}	1.35e-3	3.15	1.25e-6	3.16
2^{-4}	1.52e-4	2.92	1.39e-7	3.00
2^{-5}	2.00e-5	2.13	1.75e-8	1.55
Concentration				
Δt	$\ c - c_h\ _{L^2(\Omega)}$	Cvg. rate	$\ \nabla c - \nabla c_h\ _{L^2(\mathcal{E}_h)}$	Cvg. rate
2^{-1}	2.65e-1	—	1.49e+0	—
2^{-2}	3.48e-2	3.29	1.95e-1	3.29
2^{-3}	3.56e-3	3.16	2.00e-2	3.15
2^{-4}	3.98e-4	3.07	2.24e-3	3.02
2^{-5}	4.72e-5	2.98	2.76e-4	2.45

Table 7.8: Errors and rates with Radau II time-stepping method and $\text{RT}_2\text{-NIPG}_3$.

We observe higher order for convergence rate in time as well using the implicit Runge-Kutta time updating formulated using DG in time.

7.1.2 Grid distortion

In this part, we study the MFE-DG method in terms of its capability to address the grid distortion under hp -refinement on unstructured grid. Consider the quarter 5-spot problem, we observe in Figure 7.1.

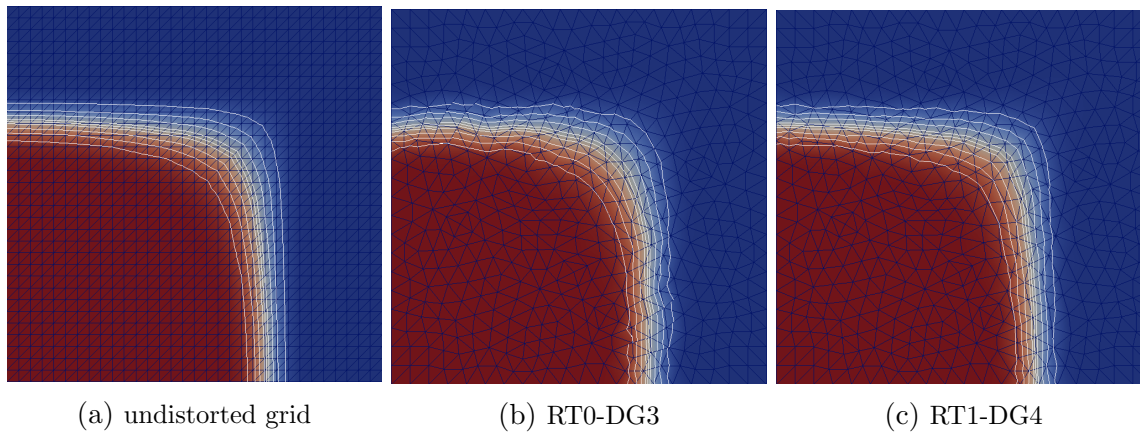


Figure 7.1: Grid distortion under p -refinement

Despite the fact that we use an unstructured grid, we still observe similar concentration front profile. Also, as we increase the order of the approximation, the solution becomes more consistent with the case with undistorted grid. Next result, we use h -refinement with RT_1-DG_2 approximation.

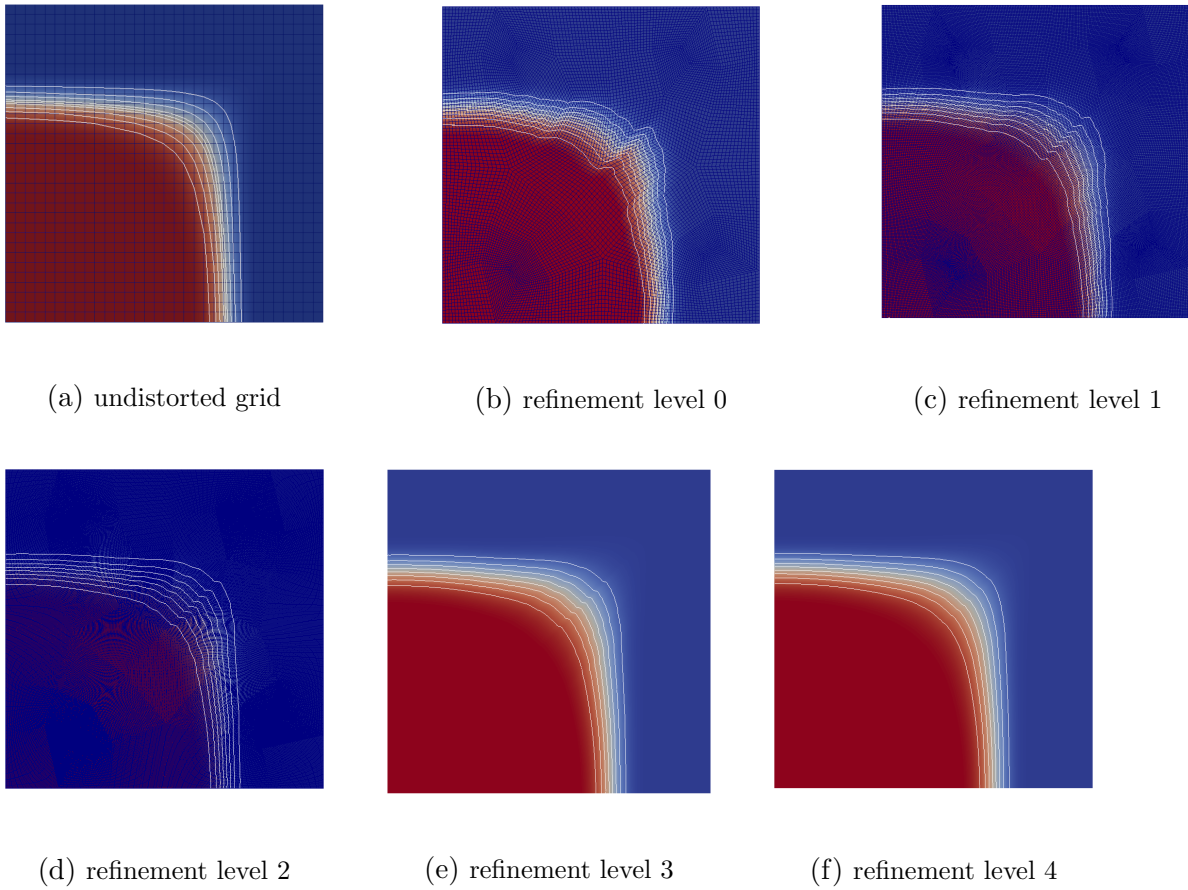


Figure 7.2: Convergence under h -refinement

As the Figure 7.2 demonstrated, the convergence of numerical solution under h -refinement on unstructured quadrilateral grid.

7.1.3 Permeability anisotropy

Another important aspect when incorporating realistic geological model for the simulation in porous media is the anisotropy of the permeability.

To test the numerical method's ability to produce correct solution for anisotropic permeability field, we consider the same model problem as in Figure 7.15 with the same input data except for permeability. Let $\mathbf{R}(\theta)$ denote the rotation matrix of angle θ . The permeability

is defined as

$$\mathbf{k} = \mathbf{R}(-\theta) \begin{pmatrix} 100 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{R}(\theta)$$

Figure 7.3 shows the spatial distribution of the permeability field; the angle θ is equal to 45° in the red regions and alternates between 90° and 0° in the green and blue regions. This experiment is based on a numerical experiment done in [100].

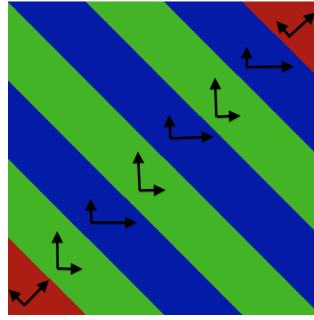


Figure 7.3: Anisotropic permeability setup

The simulation is illustrated in Figure 7.4,

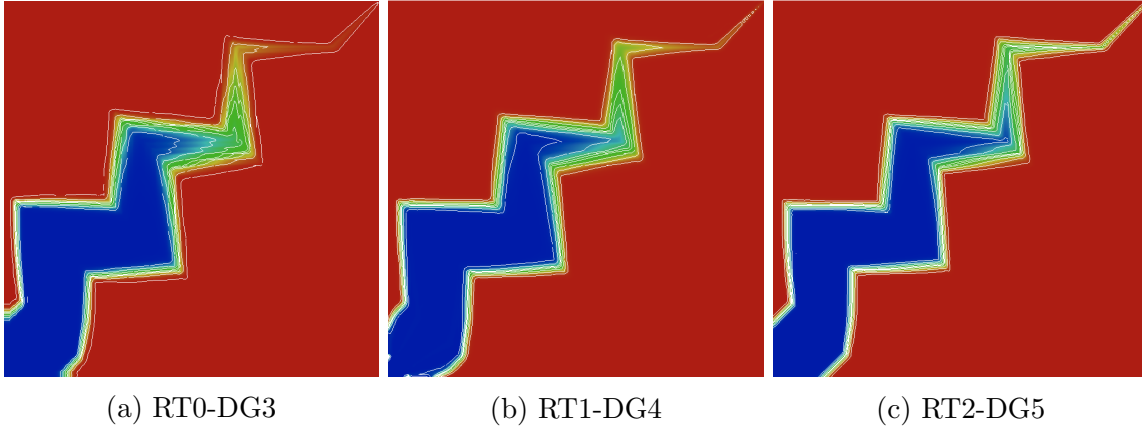


Figure 7.4: Anisotropic permeability simulation

where we are able to capture the zigzag flow pattern in based the anisotropic permeability field.

7.1.4 3D simulation

For the 3D simulation, we consider the permeability field sampled from the SPE10 model. In this case, we sample $32 \times 32 \times 32$ from SPE10 model with the permeability in z-direction the same as the permeability in xy-direction demonstrated in Figure 7.5.

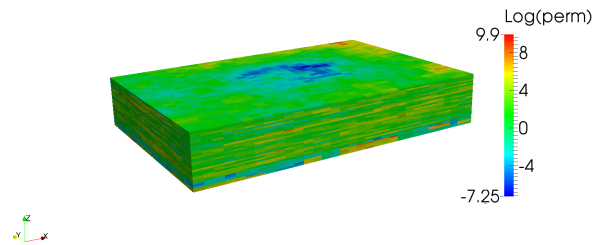


Figure 7.5: 3D permeability with unit mD

Notice, we sample most of the permeability from the Taber formation from the top layers of the SPE10 model. The simulation snapshots are illustrated as follows,

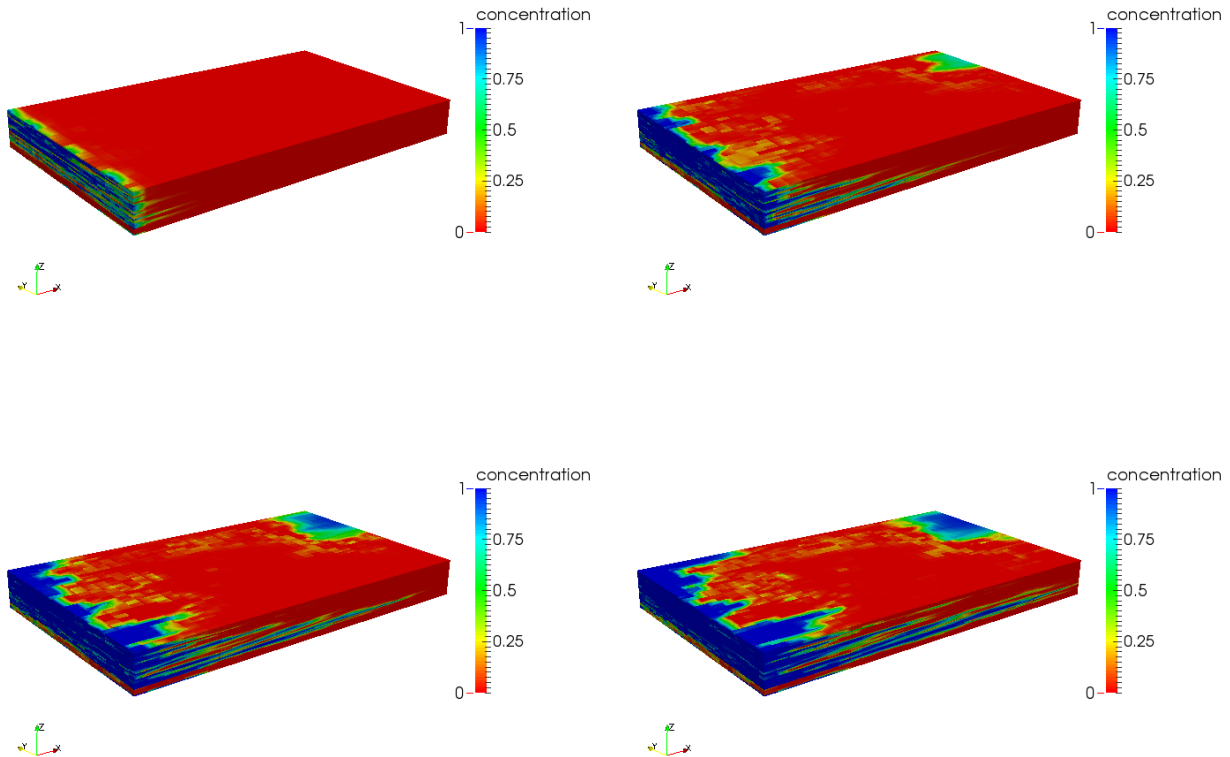


Figure 7.6: 3D model on $32 \times 32 \times 32$ grid

The simulation is done using RT_0 - DG_1 . Due to the improper scaling of the unit the actual time for the physical simulation is given. For the SPE10 problem, we will have further discussion in the chapter on large scale simulation.

7.2 Simulation using DG-DG

In this section, I present the simulation results using DG-DG method.

7.2.1 Convergence study

First, we conduct study on the convergence of the discretization by testing the method with the following analytic solutions over the unit square

$$p(x, y, t) = (2 + (-e^{-x}(1 + x + x^2) - e^{-y}(1 + y + y^2)))e^{\frac{\pi t}{2}}$$

$$c(x, y, t) = 0.5(\sin(2\pi x)^2 + \cos(2\pi y)^2) \sin(0.5\pi t).$$

The permeability is constant, $\mathbf{k} = 9.44 \times 10^{-3} m^2$, gravity is neglected and the viscosities are given by (7.1). We plot the L^2 norm of the errors in pressure, velocity and concentration, and the broken H_0^1 norm of the errors in concentration. We vary the order of the spatial discretization from one to four. Crank-Nicolson updating is used with $T = 0.5s$ and a uniform time step $\Delta t = 0.001s$.

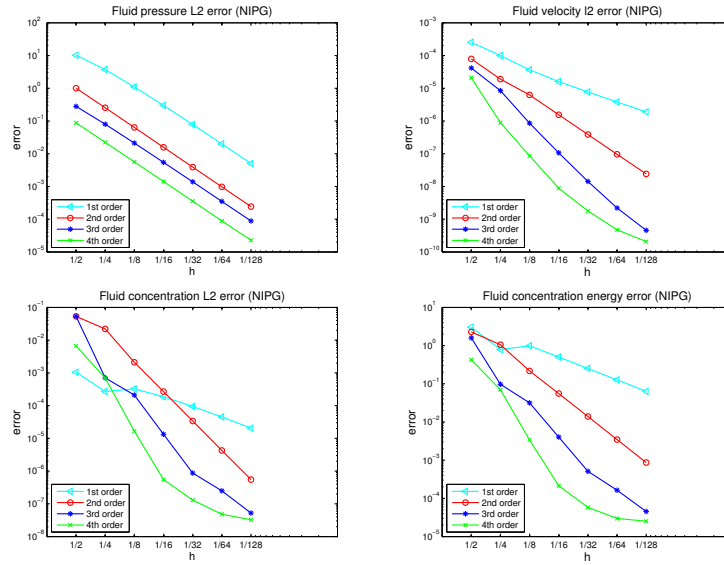


Figure 7.7: Error in spatial discretization for first, second, third and fourth order methods in space. A second order in time method is used.

We observe, as expected, a higher convergence rate and a greater level of accuracy as the order of the method increases. Next, we test the convergence in time by fixing spatial order (four) and grid (size $h = 1/128$). Figure 7.8 demonstrates optimal rates in time for both implicit Euler and Crank-Nicolson decoupled algorithms.

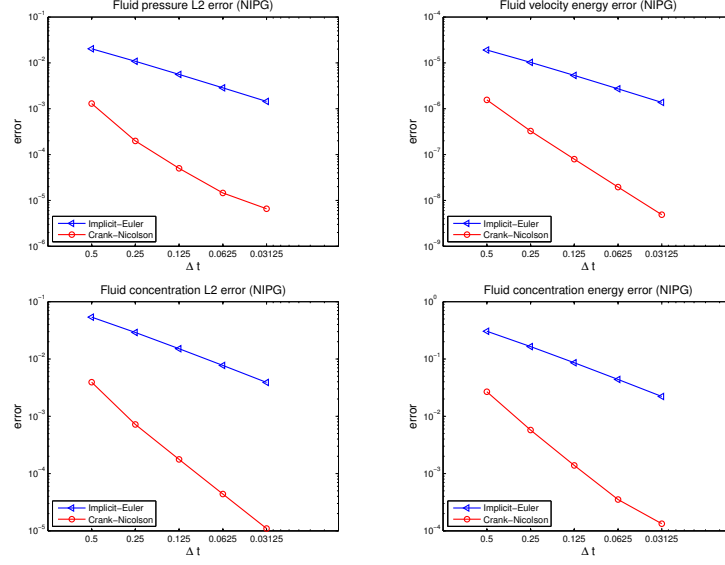


Figure 7.8: Error in time updating for first and second order methods in time. A fourth order method in space is used.

We remark that for smooth solutions the Crank-Nicolson scheme yields second order approximation in time. However, we have observed that for non-smooth realistic solutions, important overshoot and undershoot phenomena (about 10%) occur in the neighborhood of a sharp gradient. Slope limiters are needed to minimize the overshoot/undershoot amounts even if they remain bounded throughout the simulation. For the remainder of the thesis, we choose to use the implicit Euler scheme as overshoot/undershoot phenomena are negligible.

We also investigate the computational time required in order to achieve a given accuracy. We vary the order of the method as well as the mesh size. Results are shown in Figure 7.9.

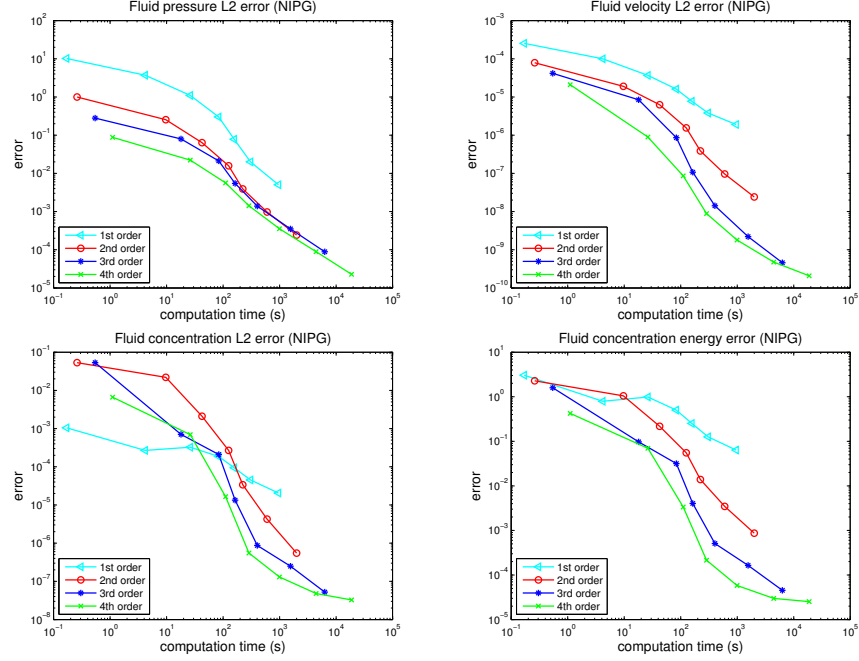


Figure 7.9: Computation time vs. accuracy

From the results, we see that choosing a higher order method on a coarse mesh can not only yield higher level of accuracy but can also be faster than a lower order method on a finer mesh. The comparison experiment is run in serial on Intel(R) Xeon(R) CPU X5660 2.80GHz.

7.2.2 Effect of flux reconstruction

In this part, we investigate the impact of flux reconstruction, more specifically how it improves the quality of the solution. First, we consider a simple 2D case with flux driven flow for a discontinuous permeability ($10^{-6}m^2$ in the lens and $1m^2$ throughout the rest of the domain, see Figure 7.10). The flux boundary condition is $\mathbf{u}_N \cdot \mathbf{n} = -0.1m/s$ on the left boundary of the domain and the pressure on the right boundary is $p_D = 1000Pa$. No flow boundary condition is imposed on the rest of the domain. The viscosity is the same as in (7.1). The time step is chosen as $\Delta t = 0.1s$. The second order method in space is employed.

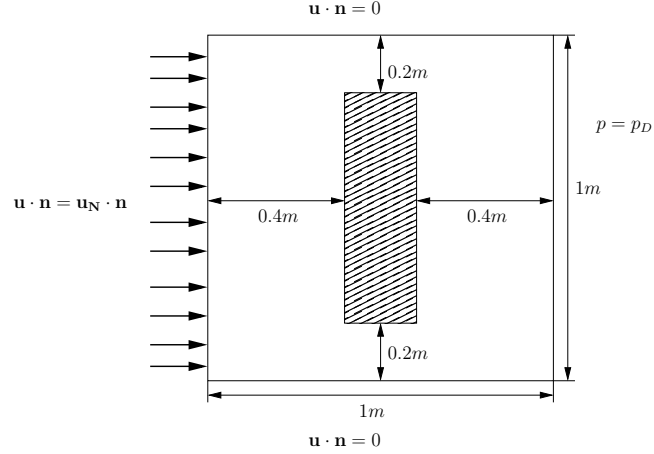
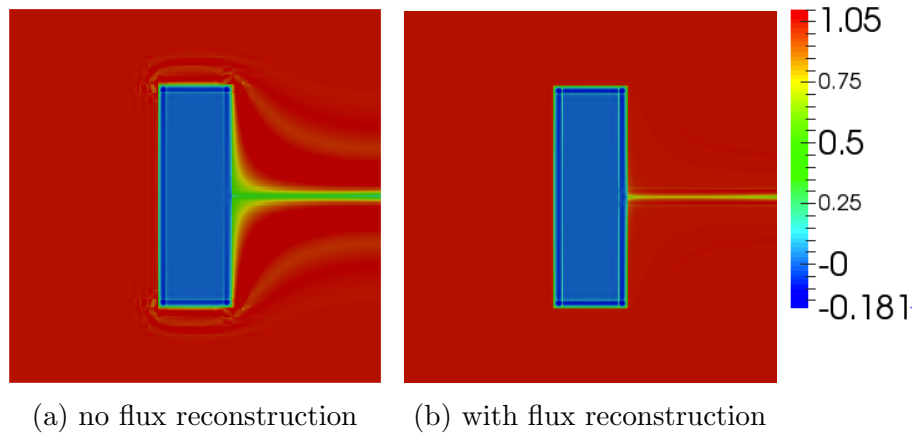


Figure 7.10: 2D flux driven problem with lens

For the case without the flux reconstruction, the velocity on the face is given by

$$\mathbf{u}_h^{DG} = \{\mathbf{u}_h\}_\omega$$

In Figure 7.11, we observe a significant contrast for the concentration profile at $T = 8s$ when flux reconstruction is activated or not.

Figure 7.11: Concentration profile with DG2 on 40×40 Cartesian grid

We can observe in Figure 7.11, that the flux reconstruction reduces the non-physical oscillations around the region where the permeability changes. The effect is more obvious in the case of highly varying permeability. In the next numerical experiment we use the perme-

ability field from layer 39 of the SPE10 model [101]. The highly discontinuous permeability is shown in Figure 7.12.

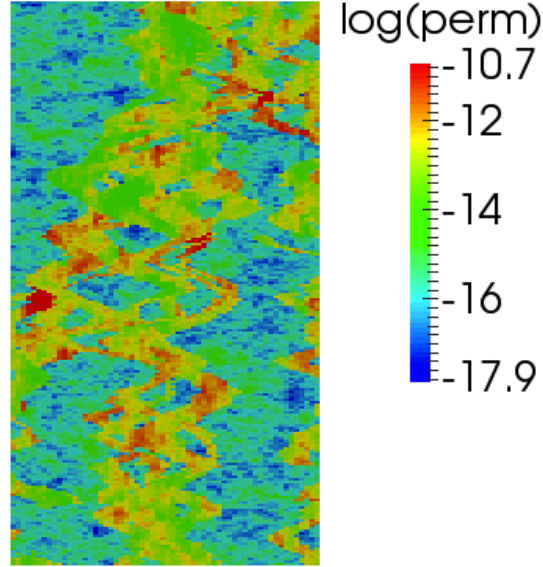


Figure 7.12: SPE10 permeability: layer 39 (log scale with unit m^2)

The flow is driven by injection and production wells: $\int_{\Omega} q^I = \int_{\Omega} q^P = 0.01 m^2/s$. We inject from the lower left corner and produce from the upper right corner of domain. No flow boundary condition is imposed. The rest of the parameters is the same as in the previous experiment. Figure 7.13 demonstrates a clear improvement of the numerical concentration if flux reconstruction is activated. The case without flux reconstruction produces poor results with severe overshoot and undershoot.

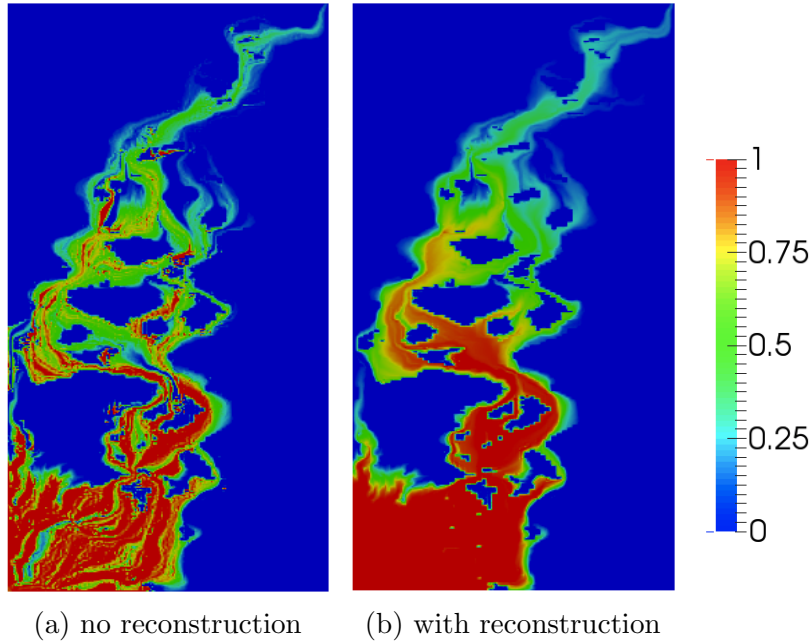


Figure 7.13: Concentration profile after 13 days, obtained with second order method

We conclude this section by noticing that, even for homogeneous porous media, solutions obtained with flux reconstruction are more accurate. We repeat the simple flux driven problem for a permeability equal to $1m^2$. Figure 7.14 compares the x-component velocity obtained with or without flux reconstruction at time $t = 0.8s$. In this homogeneous case, the exact velocity is $(0.1, 0)$. We observe a non-negligible error in the velocity without flux reconstruction. The error is larger at the location of the concentration front, and arises from the coupling between the Darcy's and transport systems.

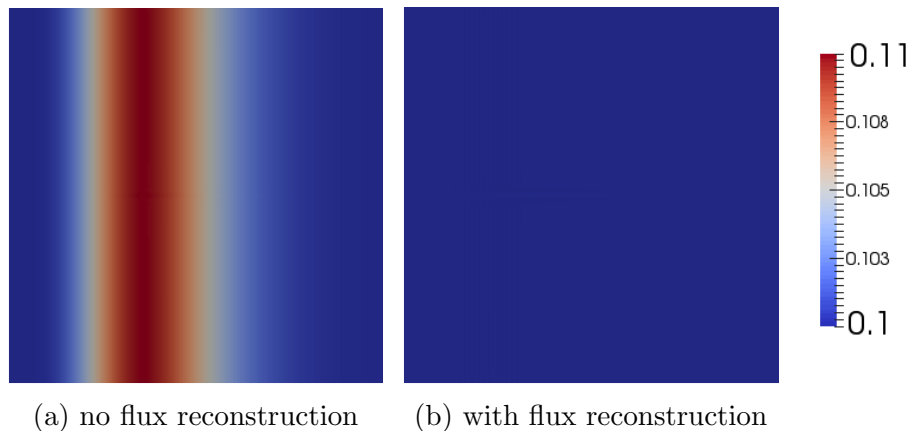


Figure 7.14: Velocity in x -direction with DG2 on 80×80 Cartesian grid

7.2.3 Grid orientation effect

In subsurface modeling, the complex geological formations can be too complicated to be appropriately approximated by structured grids. On the other hand, unstructured grids, although they can more vividly portrait the geological formations, are likely to yield grid distortions. In the following numerical experiments, we evaluate the quality of the DG discretization when using distorted unstructured grids.

The grid orientation effect for reservoir simulation was first observed by Garrett [102] and was subsequently investigated by Todd, O'dell and Hirasaki [103]. We consider the quarter five-spot problem illustrated in Figure 7.15.

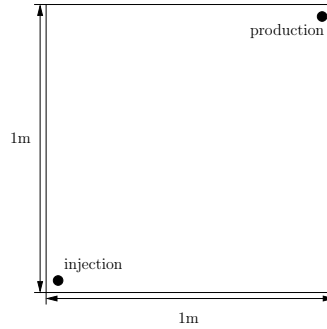


Figure 7.15: Quarter five-spot problem set-up

We consider injection and production rates given by $\int_{\Omega} q^I = \int_{\Omega} q^P = 0.18m^2/s$ and no flow boundary condition. The permeability is homogeneous ($1m^2$) and viscosity is set to be the same as (7.1). Our first test case is to consider grid distortion of 30° and -30° . The meshes that we use to test our method are shown in Figure 7.16. The experiment is based a numerical experiment conducted in [100].

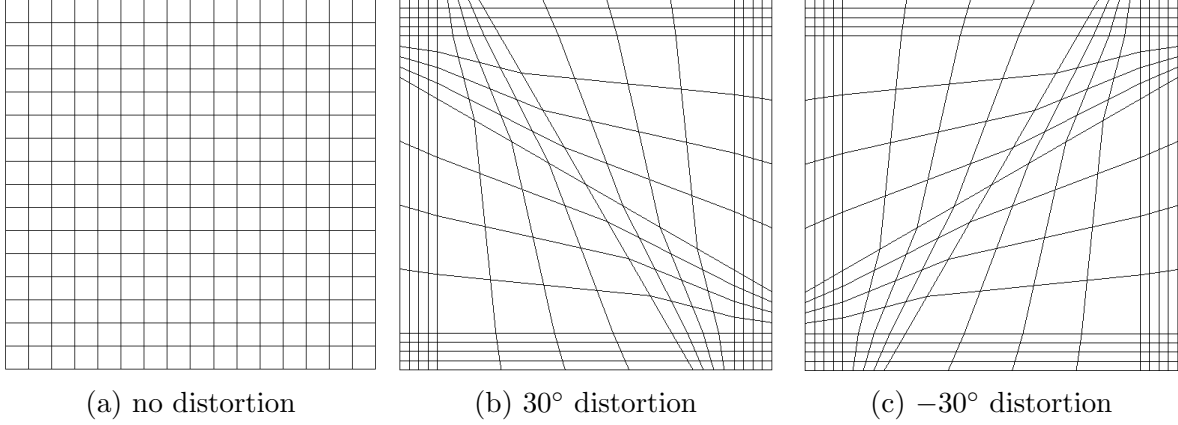
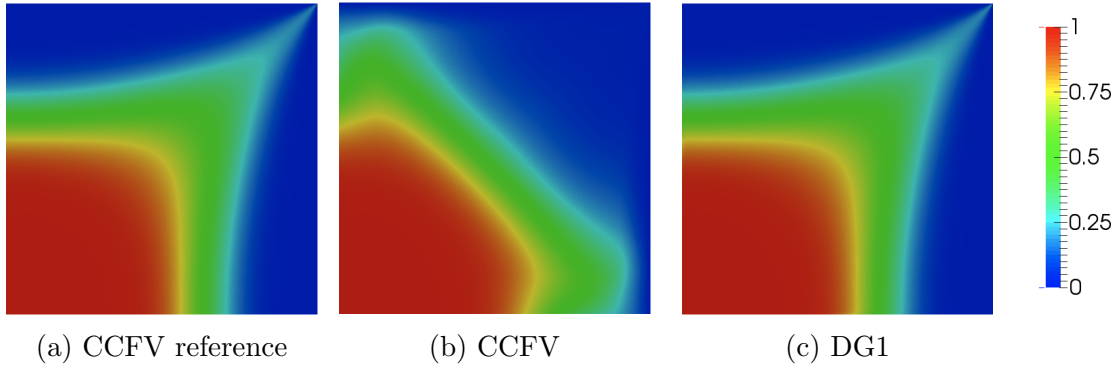


Figure 7.16: Meshes for grid distortions study

We compare the solutions obtained with our DG method of first order (DG1) to the solutions obtained with the cell-centered finite volume (CCFV) method. We also compute a reference CCFV solution on a 2048×2048 undistorted grid. We first compare the concentration profiles at time $t = 0.5s$ on the grid with 30° distortion.

Figure 7.17: Concentration profiles on grid with 30° distortion

We observe in Figure 7.17 that the profile produced by CCFV is significantly impacted by the distortion of the grid, whereas the DG solution is not sensitive to the grid distortion and can represent the reference solution well. Similar conclusions can be made from the comparisons on grid with -30° distortion, shown in Figure 7.18.

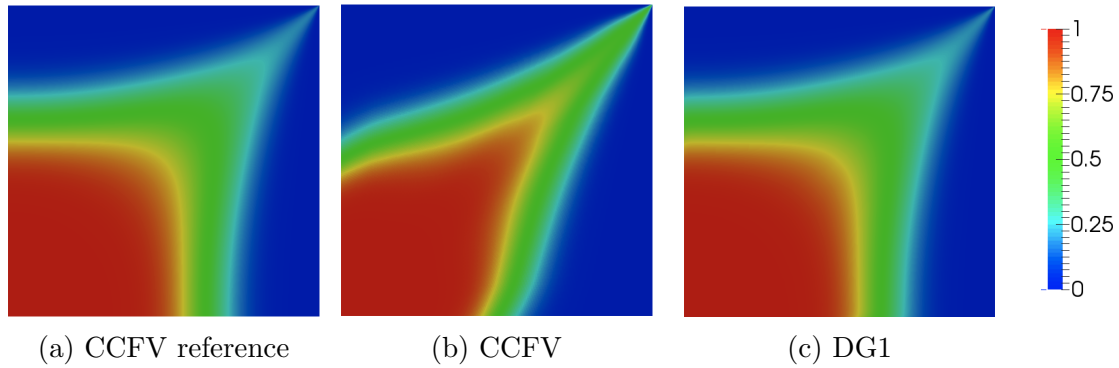


Figure 7.18: Concentration profiles on grid with -30° distortion

We now test the quality of the DG solutions obtained on quadrilateral and triangular meshes given in Figure 7.19.

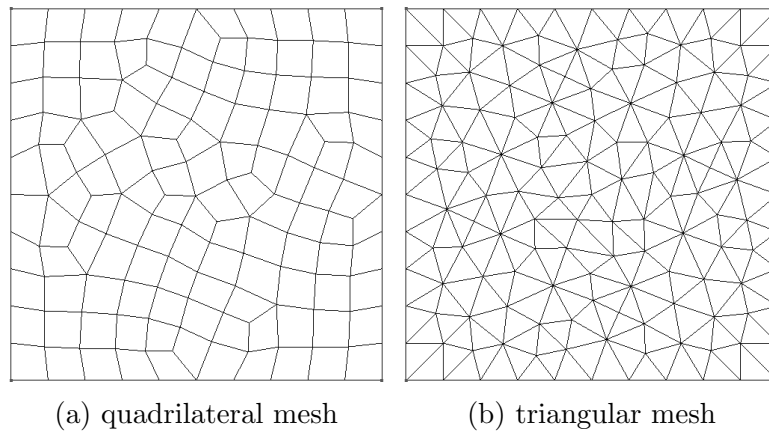


Figure 7.19: Unstructured meshes

The concentration profiles are shown on Figure 7.20 and 7.21 respectively. The CCFV solution is obtained on the coarse mesh that has been uniformly refined three times (h3) whereas the DG solution is obtained on the coarse mesh uniformly refined once (h1).

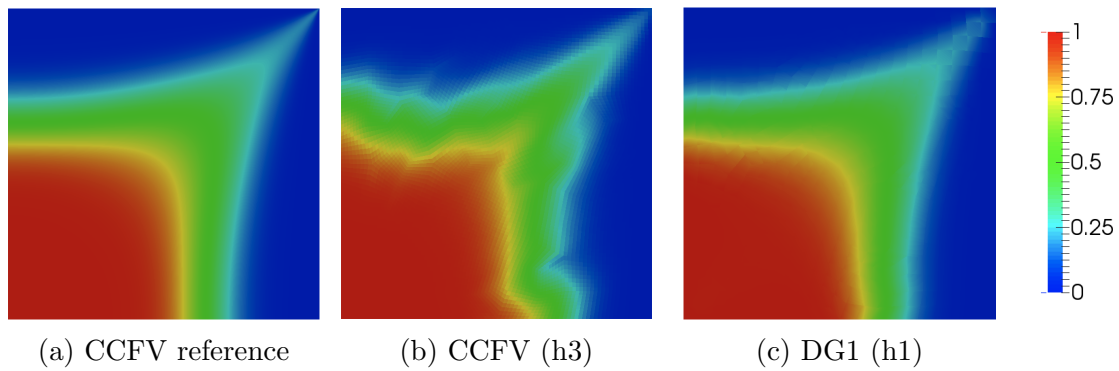


Figure 7.20: Concentration profiles on unstructured quadrilateral meshes

Both figures show that after three levels of refinement, the CCFV solution fails to converge to the reference solution whereas the DG solution converges on a mesh with one level of refinement.

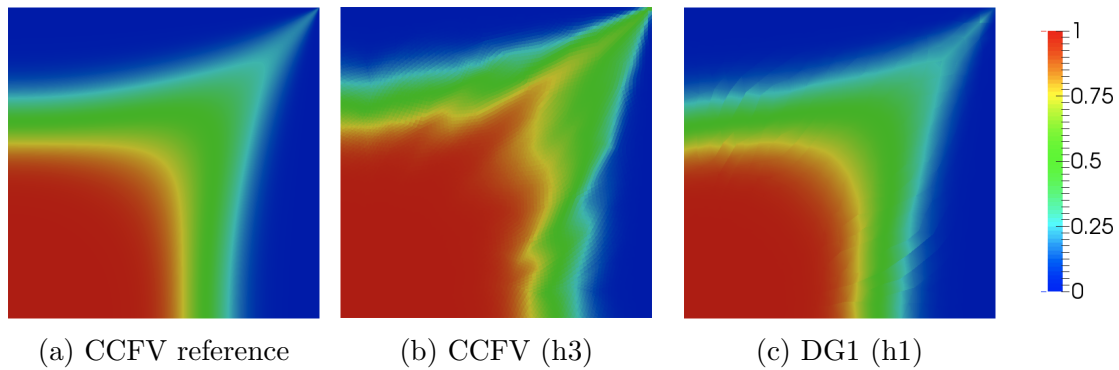


Figure 7.21: Concentration profiles on unstructured triangular meshes

Figure 7.22 and Figure 7.23 show convergence of the DG solutions using h-refinement.

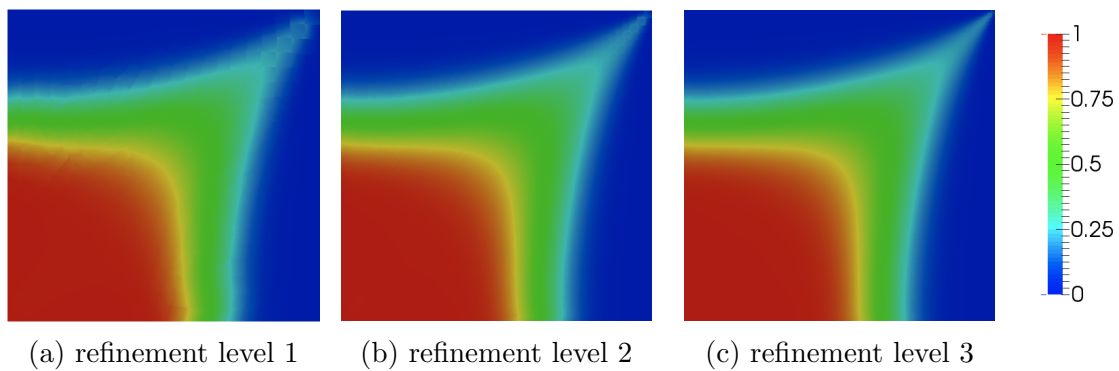


Figure 7.22: Convergence of DG1 solutions on successively refined quadrilateral meshes

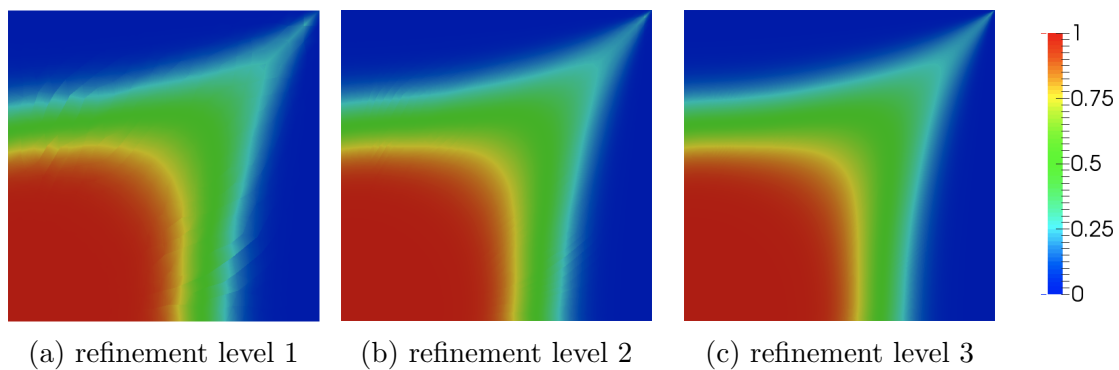


Figure 7.23: Convergence of DG1 solutions on successively refined triangular meshes

Figure 7.24 and Figure 7.25 show convergence of the DG solutions using p-refinement. Solutions are computed on coarse meshes shown in Figure 7.19.

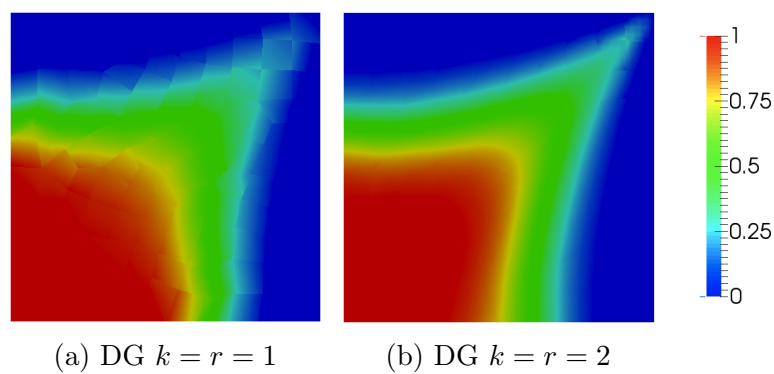


Figure 7.24: p-Convergence of DG solutions on coarse quadrilateral mesh

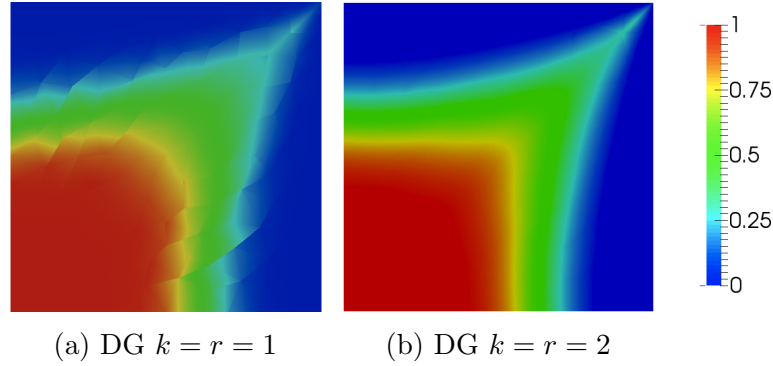


Figure 7.25: p-Convergence of DG solutions on coarse triangular mesh

Unstructured grid can better capture the complex geological formation as we will demonstrate in the next experiment that models a pinch-out geological formation. In Figure 7.26, the pinch-out is the white triangular region with high permeability of $1m^2$, and the shaded region has low permeability $10^{-10}m^2$.

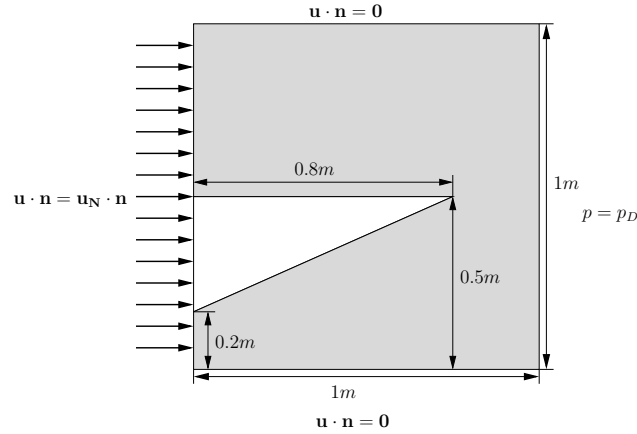


Figure 7.26: Pinch-out problem set-up and unstructured grid

Flow is driven by boundary conditions, identical to the ones in Figure 7.10. In order for CCFV to provide accurate solutions, we have to use k-orthogonal grid such as Cartesian grid. But, for this problem the k-orthogonal grid simply fails to capture the realistic geometry around the pinch-out location. The flexibility of DG methods is an advantage for this

particular set-up and enables us to both attain accurate geometry and solution accuracy. The unstructured grid that we use to realistically represent the geometry is illustrated in Figure 7.27.

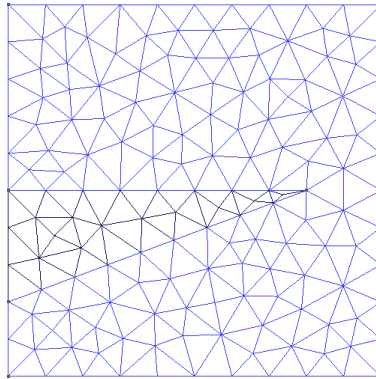


Figure 7.27: Unstructured mesh for pinch-out example

The concentration profiles obtained by either CCFV or DG at time $t = 0.3s$ are shown in Figure 7.28. The CCFV solutions are obtained on a mesh with five levels of bisection refinement of the coarse mesh. The second order DG solutions are obtained on a mesh with three levels of refinement. This yields for the Darcy's system 284,672 degrees of freedom for CCFV and 160,128 degrees of freedom for DG. The CCFV solution suffers from gridding effects and exhibits a large amount of diffusion in the pinch-out region.

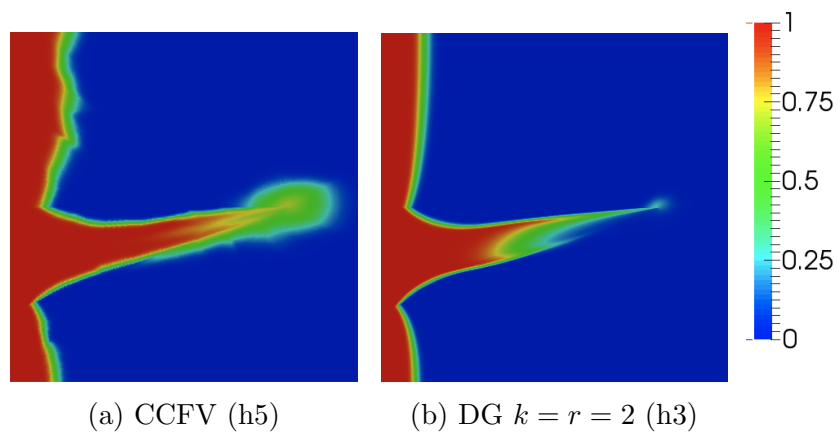


Figure 7.28: Concentration profiles

Throughout the test cases that we have conducted, we observe that the method we propose has low sensitivity with respect to grid distortion and can achieve convergence using h and p -refinement on unstructured grids.

7.2.4 Anisotropy permeability

Another important aspect when incorporating realistic geological model for the simulation in porous media is the anisotropy of the permeability.

To test the numerical method's ability to produce correct solution for anisotropic permeability field, we consider the same model problem as in Figure 7.15 with the same input data except for permeability. Let $\mathbf{R}(\theta)$ denote the rotation matrix of angle θ . The permeability is defined as

$$\mathbf{k} = \mathbf{R}(-\theta) \begin{pmatrix} 100 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{R}(\theta)$$

Figure 7.29 shows the spatial distribution of the permeability field; the angle θ is equal to 45° in the red regions and alternates between 90° and 0° in the green and blue regions. This experiment is based on a numerical experiment done in [100].

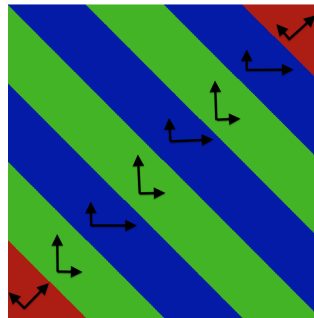


Figure 7.29: Anisotropic permeability set-up

Figure 7.30 shows the concentration profiles obtained on a Cartesian grid of size 256×256 at time $0.25s$. We compare the CCFV solution with the DG solutions of order one to five. We first observe that the CCFV solution fails to capture the successive changes in the principal

directions of the permeability matrix. We also note that as the polynomial degree increases the DG solution has less numerical diffusion. With the first order DG method, the channel flow is captured but with some amount of numerical diffusion. In contrast differences between the profiles obtained with DG of order two to five, are negligible or very small.

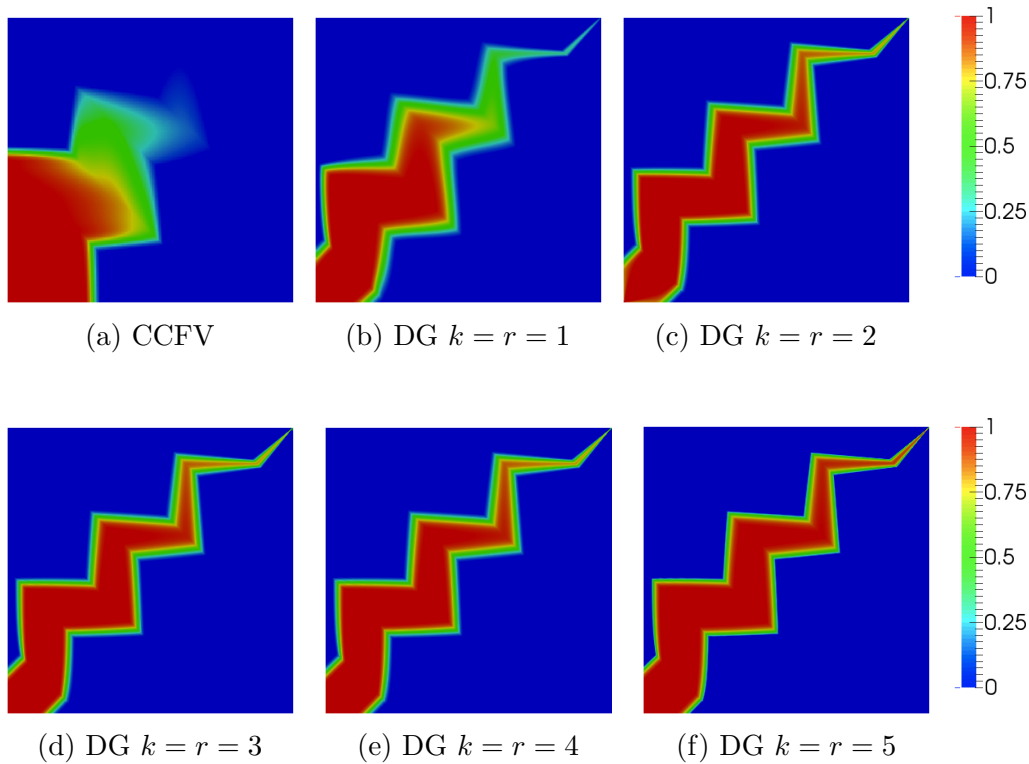


Figure 7.30: Comparison between CCFV and DG solutions for anisotropic medium

Since CCFV is a low order method, we show the solution profile obtained on a finer mesh (1024×1024) in Figure 7.31. Even on a finer mesh, the CCFV method performs poorly for such anisotropic medium. There is no tendency to converge to a realistic solution.

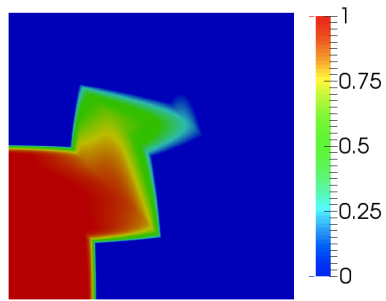


Figure 7.31: CCFV solution on finer mesh of size 1024×1024

Viscous Fingering Simulation

In this chapter, I want to focus the attention on a very interesting phenomenon called viscous fingering effect in miscible displacement process in porous media. In particular, after going through the physical concept of this phenomenon I present the simulation results using DG in comparison with commonly used CCFV method. I explore the *hp*-convergence of the viscous fingering in 2D and grid orientation effect in simulating viscous fingering in radial flow. Afterwards, I present some results for the study of the viscous fingering in 3D simulation. In the last section, I present the computational cost to justify the use of the high order DG.

8.1 Concept of the viscous fingering

In porous media flow, under the condition when the mobility ratio is greater than one i.e.

$$M = \frac{\mu_o}{\mu_s} > 1,$$

the flow becomes unstable. A what looks like irregular finger shapes started to emerge during the displacement process at the location where the injected solvent and residing fluid are in contact. We call this type of phenomenon viscous fingering. Such phenomenon, interestingly,

occurs even in homogeneous media. In our case, we are studying the viscous fingering in miscible flow.

The physics of viscous fingering can be understood in following simplified way. Consider the rectilinear miscible displacement, demonstrated in Figure 8.1.

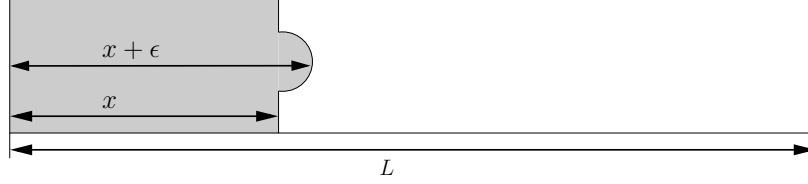


Figure 8.1: Viscous fingering concept

where we have the Darcy's law,

$$\frac{dx}{dt} = -\frac{k\Delta p}{\phi\mu_s(ML + (1 - M)x)}$$

when under certain perturbation ϵ ,

$$\frac{d(x + \epsilon)}{dt} = -\frac{k\Delta p}{\phi\mu_s(ML + (1 - M)(x + \epsilon))}$$

It follows that

$$\frac{d\epsilon}{dt} = \frac{k\Delta p(1 - M)\epsilon}{\phi\mu_s(ML + (1 - M)x)^2}$$

Therefore,

$$\epsilon(t) = \mathbf{e}^{St}$$

where

$$S = \frac{k\Delta p(1 - M)}{\phi\mu_s(ML + (1 - M)x)^2}$$

with Δp being the pressure difference and $\mu_s(ML + (1 - M)x)$ being the simplified viscous of the fluid mixture.

If we have $M < 1$, then the perturbation decays exponentially. Otherwise, when $M > 1$, i.e. when using less viscous fluid to displace more viscous residing fluid, the perturbation is amplified exponentially. In homogeneous porous media, even with microscopic variation of the permeability, it is enough perturbation to trigger the viscous fingering in the concentration profile under the case with mobility ratio greater than one.

The diffusion-dispersion also impacts the pattern of the viscous fingering profoundly. In particular, when the transverse dispersion is large, the fingering can be stabilized or reduced down to a few large fingers.

From the simulation point of view, additional challenges occurs when modeling the unstable flow. One challenge simply has to do with obtaining a reliable viscous finger pattern. Finite volume method is able simulation the unstable flow, but with different grid orientations namely the grid parallel to the flow or diagonal to the flow direction the viscous fingering pattern can be different with large mobility ratio. Another challenge is to ensure the trustworthiness of the simulation results, since with unstable flow a small numerical floating point error can be amplified and eventually pollute the entire solution. Also, with large mobility ratio the unstable system becomes harder to solve which can significantly limit the range of problem to only small mobility ratio whereas in reality the mobility ratio can go up 1000 or more. From efficiency point of view, we want to know if there is a gain using higher order method.

To be able to accurately simulate the finger growth could essentially improve the prediction of the breakthrough time and avoiding undesirable fingering pattern in the flow for both reservoir simulation and pollutant removal process.

8.2 2D viscous fingering simulation

The viscous fingering effect in 2D has been frequently studied both from engineering aspect and numerical aspect. Recently, a fully-implicit DG discretization has been investigated in

[44, 45]. The finding from their results is that CCFV is not adequate for the simulation of viscous finger effect as I demonstrate next. First, let us consider the rectlinear flow.

8.2.1 Rectlinear flow & hp -refinement

The model for the rectlinear flow can be regarded as the 2D cross-section of the 3D core flooding simulation in figure 8.2.

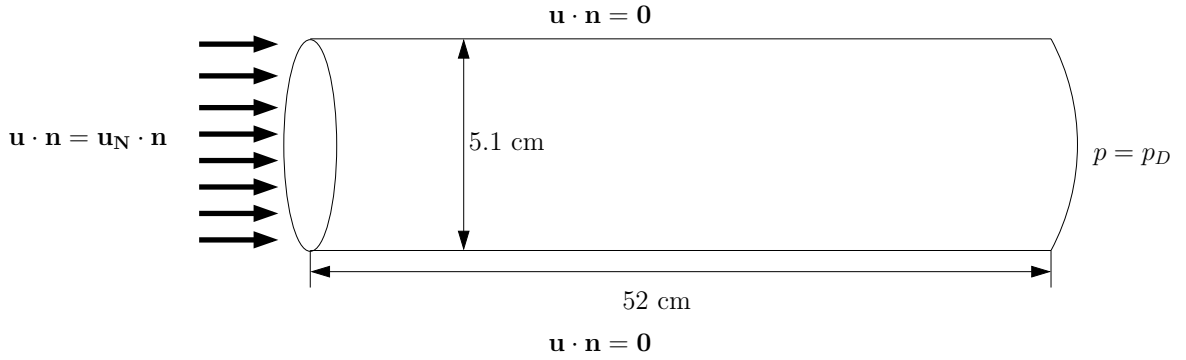


Figure 8.2: Core flooding problem setup

For the problem, we set the injection rate to be 1.53 mL/min and permeability to $3.720700841 \times 10^{-13} \text{ m}^2$. The mobility ratio is given to be 30.3 and the parameters for the diffusion dispersion tensor are

$$d_m = 1.8 \times 10^{-7} \text{ m}^2/\text{s}, \quad \alpha_l = 1,8 \times 10^{-5} \text{ m} \text{ and } \alpha_t = 1.8 \times 10^{-6} \text{ m}, \quad \phi = 0.2. \quad (8.1)$$

First, we examine the convergence of the fingering pattern under h -refinement.

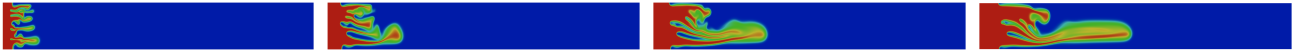


Figure 8.3: CCFV 20480×2048 dofs 41,943,040

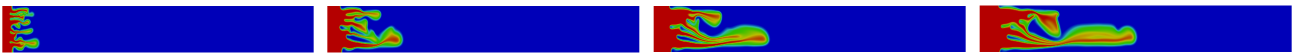
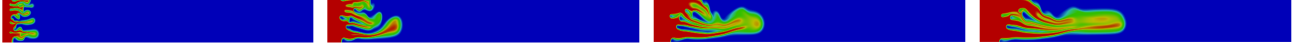
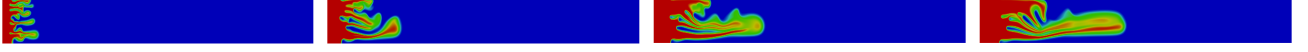
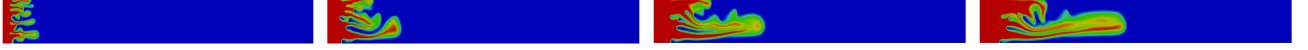
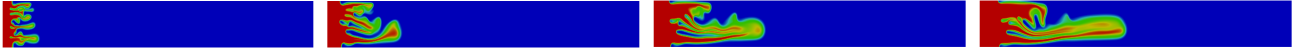
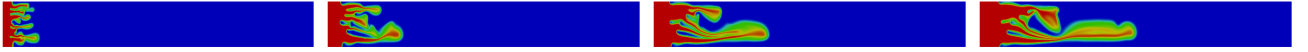
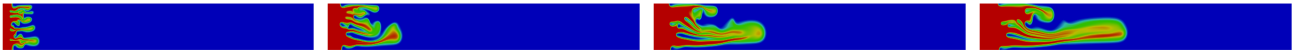
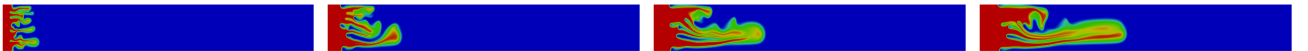


Figure 8.4: DG1 1280×128 dofs 655,360

Figure 8.5: DG1 2560×256 dofs 2,621,440Figure 8.6: DG1 5120×512 dofs 10,485,760Figure 8.7: DG1 10240×1024 dofs 41,943,040

The snapshot of the simulation is taken at time $0.5s$, $1.0s$, $1.5s$, $2.0s$. We observe the convergence of the fingering pattern as we refine the grid. Indeed, we have a consistent fingering pattern with grid sizes 5120×512 and 10240×1024 . Whereas, the solution provided by CCFV does not converge to the same pattern, despite the fact that the linear system has the same degree of freedom as the finest 1st-order DG approximation.

Now, let us examine the same viscous fingering simulation under p -refinement.

Figure 8.8: DG1 10240×1024 dofs 41,943,040Figure 8.9: DG1 1280×128 dofs 655,360Figure 8.10: DG2 1280×128 dofs 1,474,560Figure 8.11: DG3 1280×128 dofs 2,621,440Figure 8.12: DG4 1280×128 dofs 4,096,000

We observe the convergence under p -refinement on coarser grid with resulted linear system in 4th-order DG approximately 10 times smaller than 1st-order DG approximation which in fact takes less time solve as we demonstrate in the last section.

8.2.2 Radial flow & grid orientation effect

In this part, we consider the radial flow and the impact of grid orientation effect. For the simulation of the viscous fingering, due to instability of the flow. Even a small perturbation of the simulation can lead to very different fluid flow profile. We have full control of the perturbation that initially triggers the viscous fingerings, but the perturbation can also caused by numerical error. One of the most prevalent numerical errors come from the geometry of the grid. Many times simply by changing the direction of the grid can alter the shape of the fingers profoundly as we will see in our numerical experiments. The goal of using DG discretization is to reduce the grid orientation effect, thereby producing high fidelity simulation results.

We again consider the quarter of 5-spot problem, with permeability and porosity set to be

$$\mathbf{k} = 3.720700841 \times 10^{-13} m^2, \phi = 0.2$$

We still consider using the quarter-mixing rule with mobility ratio,

$$M = 303$$

The diffusion-dispersion parameter is given to be

$$d_m = 1.8 \times 10^{-5} m^2/s, \alpha_l = 1.8 \times 10^{-5} m, \alpha_t = 1.8 \times 10^{-5} m$$

The injection and production wells are set to be

$$q^I = \frac{7.2 \times 10^{-1}}{2\pi\sigma^2} \exp\left\{-\frac{(x - x_{well})^2 + (y - y_{well})^2}{2\sigma^2}\right\}, \sigma = 0.2$$

where $q^P = -q^I$ with the well location set to be the production well location. We perturb the initial permeability as follow,

$$\hat{\mathbf{k}} = \mathbf{k}(1 + 10^{-2}\cos(50\pi x)\cos(50\pi y)).$$

The Peclet number is estimated to be around $\mathbf{Pe} = 10^4$ and the time step size is set to be $\Delta t = 10^{-3}s$. We present the simulation results with parallel grid and diagonal grid. The parallel grid is Cartesian grid with cells oriented parallel to the flow direction, whereas the diagonal grid is Cartesian grid with cells oriented diagonal to the flow direction. First, let us evaluate the solution provided by CCFV method for the simulation of the viscous fingerings.

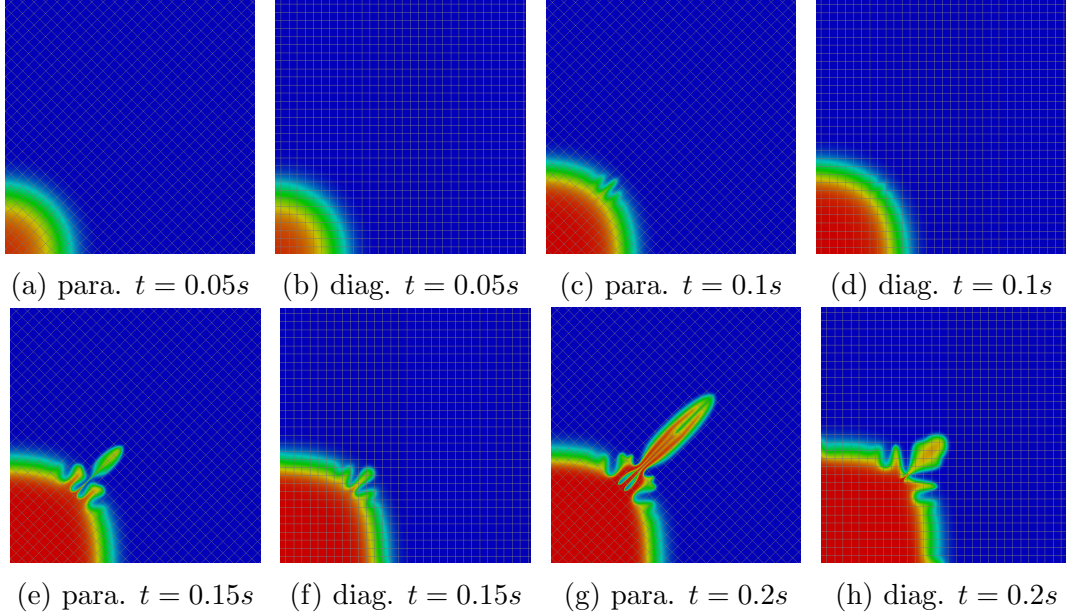


Figure 8.13: Viscous fingering with $M = 303$ CCFV $h = 9.77 \times 10^{-4}$

We observe that the solutions provided by CCFV method suffer severely from the grid orientation effect. In particular, the case with diagonal grid where the solution looks dras-

tically different from time $0.1s$, $0.15s$ and $0.2s$ as illustrated in Figure 8.13. Next, we use 1st-order DG approximation in Figure 8.14.

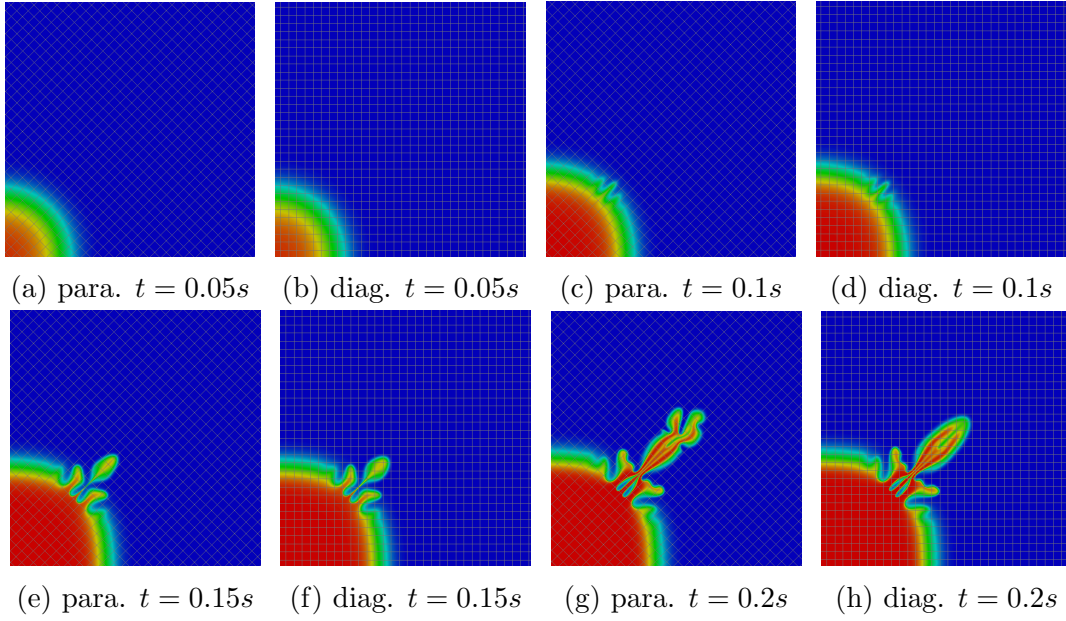


Figure 8.14: Viscous fingering with $M = 303$ DG1 $h = 9.77 \times 10^{-4}$

For the 1st-order DG approximation, we still see the grid orientation effect on the simulation of the viscous fingers. As time evolve, in particular at time $t = 0.2s$ where the simulations look very different between parallel and diagonal grid, but considerably better in the resemblance of the concentration profiles in earlier time comparing with CCFV method.

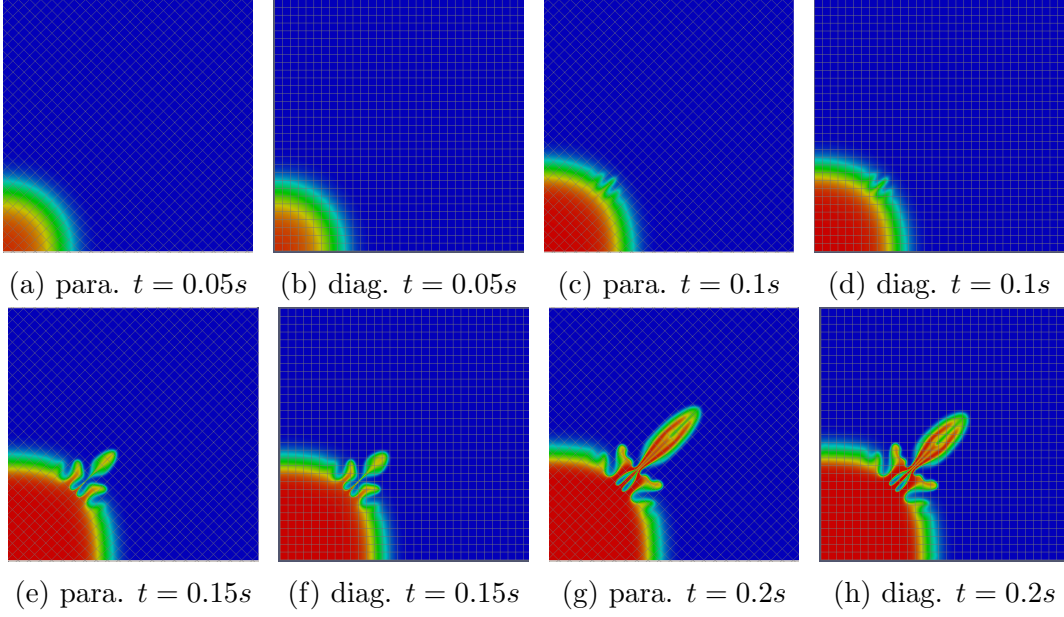


Figure 8.15: Viscous fingering with $M = 303$ DG2 $h = 2.76 \times 10^{-3}$

As we increase the order of approximation to 2nd-order DG and run the simulation on coarser grid in Figure 8.15, we now observe a similar pattern for the viscous fingering at all time for our simulations which suggest the necessity of using higher order method to simulate the viscous fingering to obtain reliable simulation result.

8.3 3D viscous fingering simulation

We also experiment on simulating 3D miscible viscous fingering. We consider the same core flooding model. We generate the unstructured grid using GMSH [104] for the cylindrical core illustrated in Figure 8.16.

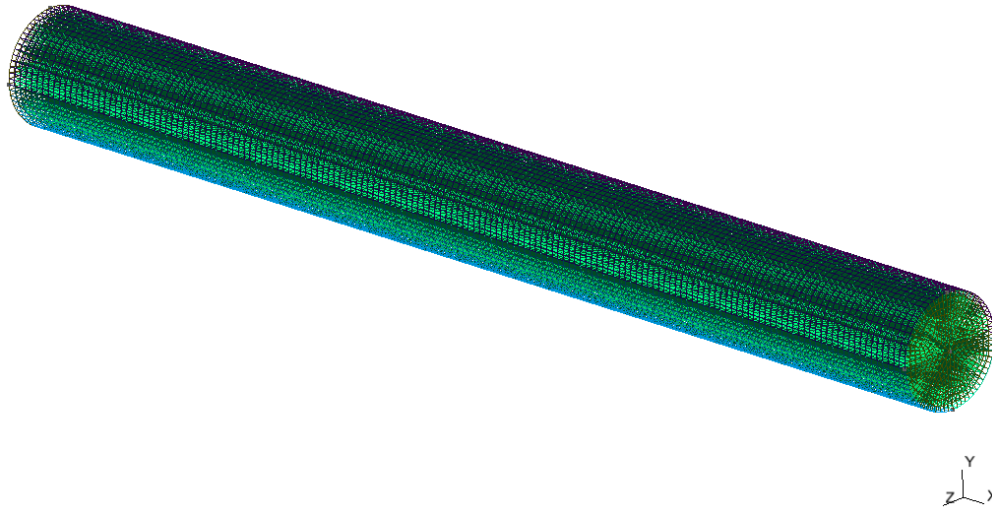


Figure 8.16: Mesh for 3D cylindrical core

We present the simulation result with 3,932,160 cells using DG1 with mobility

$$M = 30.3$$

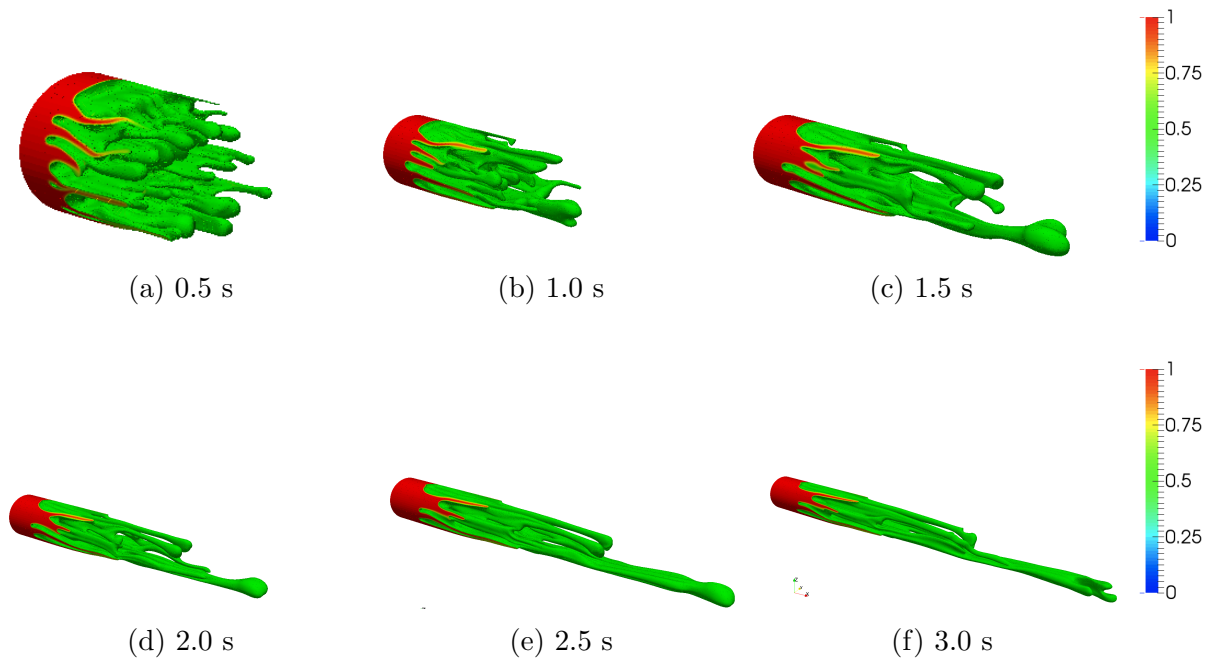


Figure 8.17: 3D viscous finger simulation over 3,932,160 cells DG1

Figure 8.17 demonstrates the capability of DG-DG numerical method for simulating 3D viscous fingering. In Figure 8.17, we observe the formation of the viscous fingers, and the spreading, the merging, the splitting and eventually the breakthrough of the fingers.

8.4 Computational cost

In this section, I demonstrate the advantage of the high order approximation for the viscous fingering simulation. I evaluate the performance the 2D viscous fingering simulation in section 8.2.1 running on parallel over 48 processes. The performance is demonstrated in Figure 8.18 with time evaluated in second.

Viscous fingering simulation per time step on 48 processes							
x	y	size	order	Assemble Darcy's system	AMG solver Darcy's system	Assemble transport system	DD solver transport system
1280	128	163840	1	0.091726	0.49026	0.096872	0.036834
2560	256	655360	1	0.3687	1.6312	0.381	0.45408
5120	512	2621440	1	1.50438	9.9872	1.54426	7.3868
10240	1024	10485760	1	6.381	116.77	6.3872	69.054
1280	128	163840	2	0.193884	1.0233	0.24528	0.119732
1280	128	163840	3	0.43196	2.613	0.65162	0.46058
1280	128	163840	4	0.88736	6.784	1.73176	2.6724

Figure 8.18: Performance of viscous fingering simulations

From Figure 8.18, we observe higher order method running on coarser grid is more efficient in terms of the computational cost per time step for assembling the linear systems and linear solvers.

Therefore, we conclude the chapter by claiming that the higher order DG is adequate for providing accurate and efficient numerical simulation for the viscous fingering simulation.

Large Scale Simulations

9.1 Three-dimensional heterogeneous medium

The experiments I have done so far have demonstrated the robustness and accuracy of the DG discretization while facing various numerical challenges. Next, I would like to test our discretization on some realistic physical data. I select the permeability field from the SPE10 model [101], which is well-known for its large heterogeneities varying from 10^{-10} to $10^{-18} m^2$. In addition, the bottom 50 layers of the permeability field represent the Upper Ness structure which include underground channels and pose additional challenges.

We consider the five-spot problem by placing injection and production wells as in Figure 9.1.

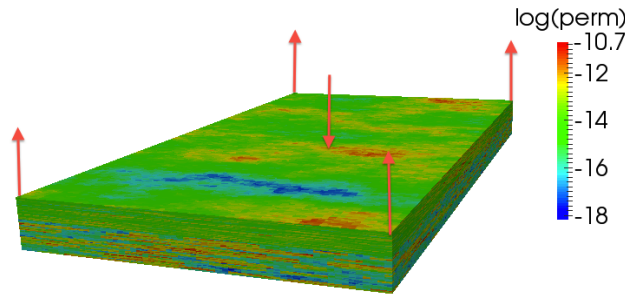


Figure 9.1: SPE10 permeability in m^2 and location of wells

We set the injection rate to be $\int_{\Omega} q^I = 1.7 m^3/s$ and production rate at each corner to

be $\int_{\Omega} q^P = 0.425 \text{ m}^3/s$. We keep the permeability in the z -direction the same as in the xy -direction. Gravitational force $\mathbf{g} = (0, 0, -9.8)^T \text{ m/s}^2$ is incorporated in the simulation. No flow boundary condition is imposed. Viscosities are

$$\mu_s = 10^{-3} \text{ Pa} \cdot \text{s} \text{ and } \mu_o = 9 \times 10^{-4} \text{ Pa} \cdot \text{s}$$

Densities are

$$\rho_s = \rho_o = 1000 \text{ kg/m}^3$$

We set a uniform time step to be 1 day and use piecewise quadratic approximation. The mesh consists of 1,220,000 elements. Snapshots of the concentration profiles over several days are shown in Figure 9.2. Concentrations are plotted above a threshold of 0.5.

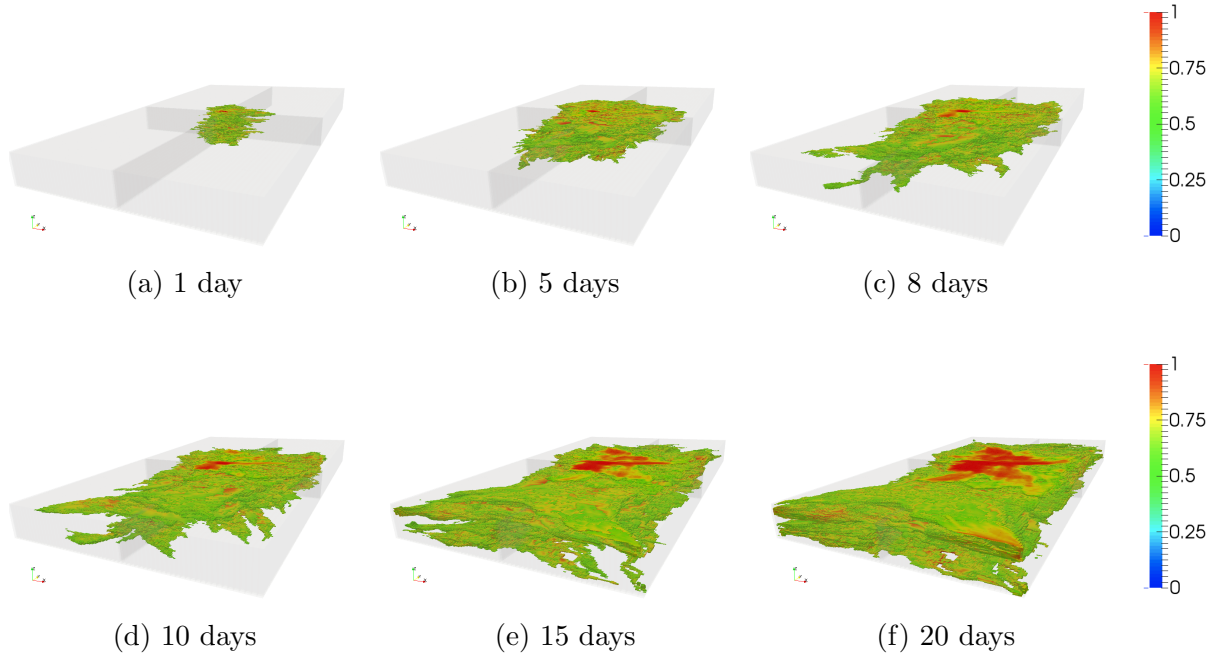


Figure 9.2: Concentration snapshots obtained with DG2

We observe in Figure 9.2 that the simulation results can realistically represent the channels in the bottom layer of the Upper Ness structure. To validate our simulation result, we

plot in Figure 9.3 the “water cut” profiles for the injected fluid at the production wells, with solutions obtained by 1st and 2nd order DG.

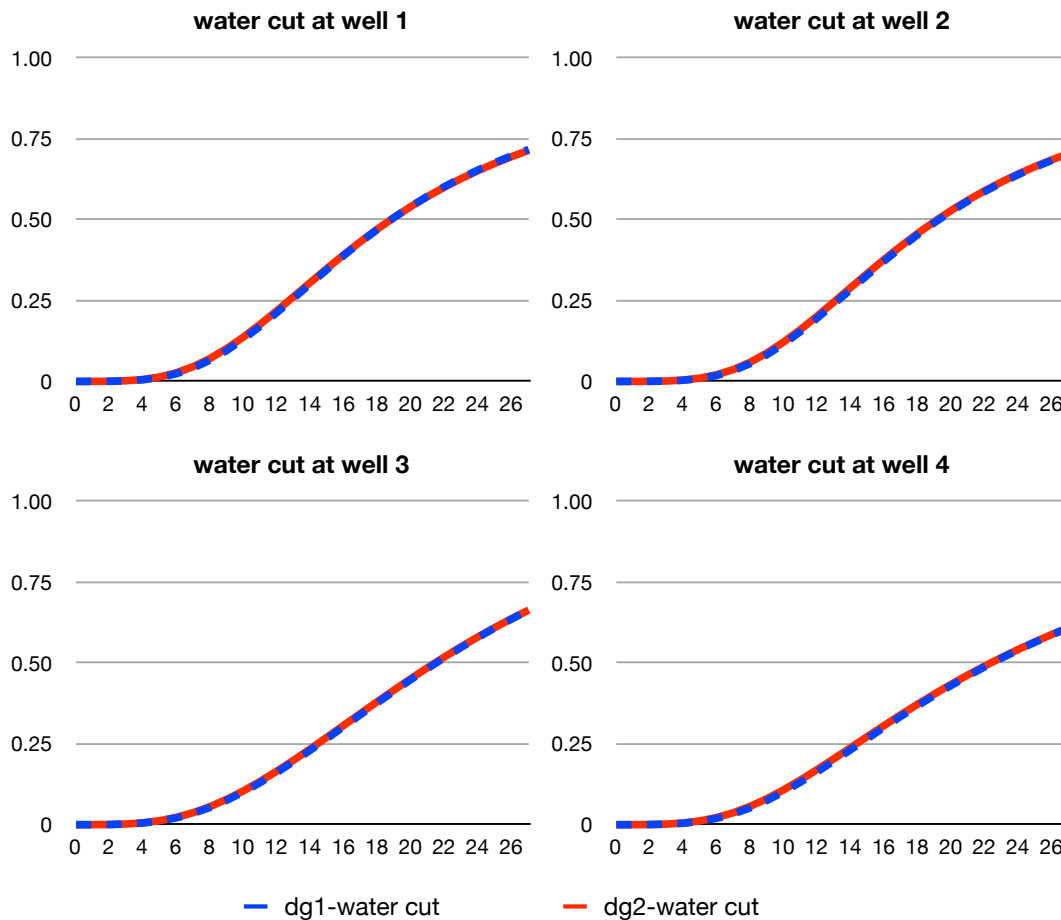


Figure 9.3: Water cut plot at the production wells

We observe in Figure 9.3 that the water cuts overlap. The plots give us confidence that the DG discretization can produce reliable results for large scale simulations. Also, the S-shape of the water cut curve is also realistic for the miscible displacement flooding which is different from multi-phase flow.

9.2 Performance evaluation

In this section, I evaluate the performance of solver when solving the SPE10 problem. The mesh consists of 1,220,000 elements. The Darcy's system has 30,294,000 degrees of freedom with 2nd-order Lagrange basis and the transport system 10,098,000 degrees of freedom with 2nd-order Orthogonal basis. The performance evaluation is done by taking 20 time steps with each time step to be 1 day for the same problem in previous section. In this case, we use Restarted GMRES for both Darcy's and transport system. The Darcy's system is preconditioned with aggregated AMG. The subspace correction is done by projecting the DG space to piecewise constant functions. ILU0 is used as the smoother for the finest system and Jacobi preconditioner is used as the smoother for the coarser system on each level. For the transport system, ILU0 is used as the preconditioner.

We observe in figure 9.4 the AMG solver is the most time consuming part in the overall performance. We then plot the AMG efficiency of the AMG solver. Interestingly, we observe a quite significant performance boost after running up to 32 processes which is quite unexpected consider the additional communications it requires. We then notice that in fact the number of the Krylov subspace iteration reduced significantly and eventually is reduced to 17 iterations per linear solve as we increase of the number of processes. This reduction is caused by the reduction of heterogeneity of the permeability in each subproblem. Therefore, for problem with highly varying heterogeneity like SPE10 problem, we observe domain decomposition technique not only can be used as a parallelism strategy, but also can be consider as a preconditioner to exploit the geological structure to achieve speedup.

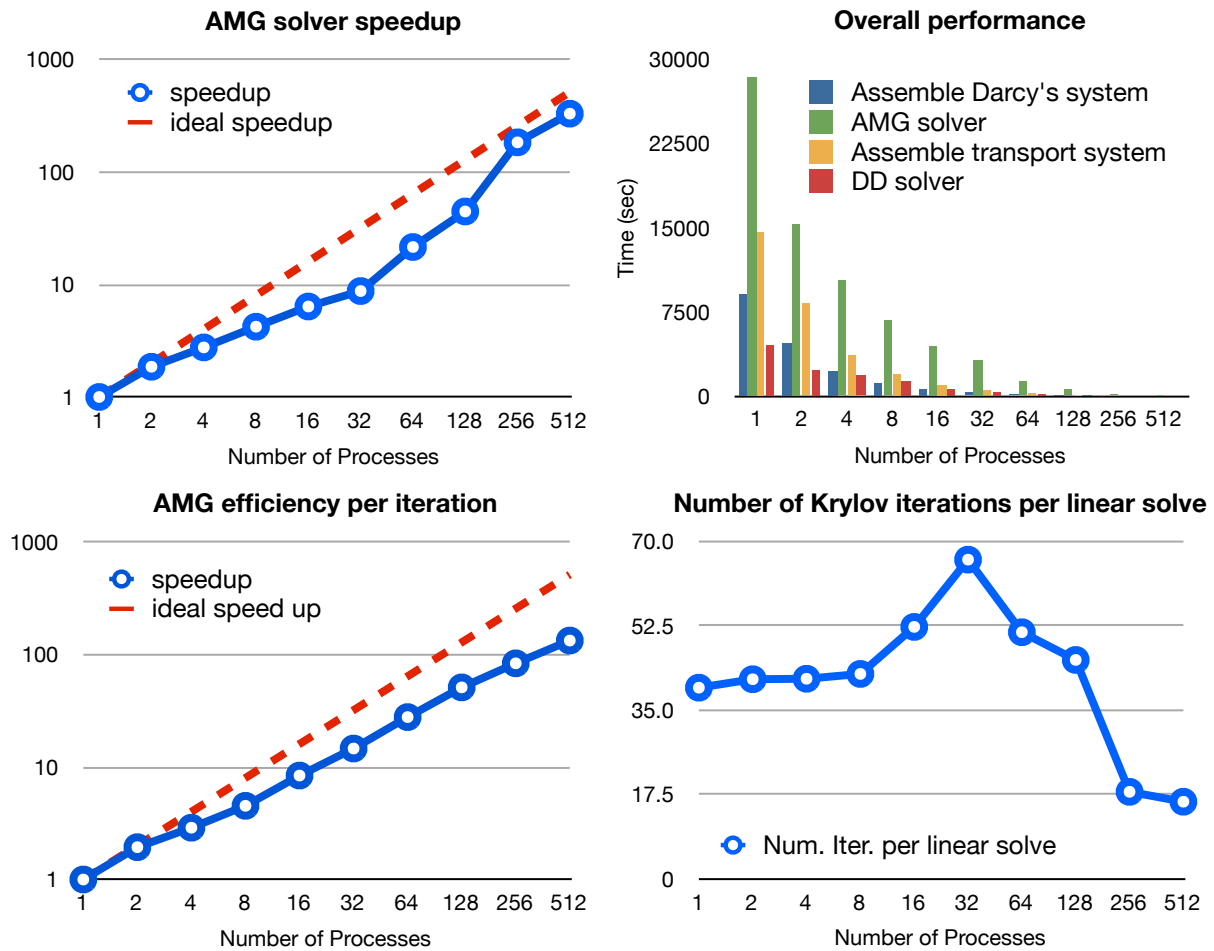


Figure 9.4: SPE10 model performance evaluation

In order for us to better evaluate the performance of AMG solver, we plot the speedup of AMG solver in each Krylov subspace iteration. And again we observe the linear trend in terms of the speedup. The efficiency is estimated to be 79% up to 512 processes.

Conclusions

In this thesis, I introduced high order methods using a MFE-DG approach with DG in time, and a semi-sequential DG-DG approach, with 1st and 2nd-order time-stepping, and flux reconstruction for solving miscible displacement equations. I have presented theoretical analyses for the numerical discretizations introduced. Both stability and convergence has been proven with minimal regularity assumption. The results grant a theoretical basis for the reliability of the associated numerical approaches for solving miscible displacement problems.

I have implemented numerical algorithms for solving miscible displacement problem based on the discretizations proposed. A series of numerical experiments demonstrate the robustness and accuracy of the numerical methods.

Both numerical algorithms were implemented in parallel. In particular, the semi-sequential DG-DG algorithm was solved using an overlapping domain decomposition with an AMG preconditioner and achieved strong scalability up to 512 processes.

I specifically examined the viscous fingering simulation using DG discretization. In contrast with the cell-center finite volume method, the high order DG method provided more reliable solutions and was considered to be more adequate for simulating the unstable flow phenomenon.

Apart from the specific challenges in miscible displacement problems, the study of single-

phase flow is the foundation for understanding multi-phase, and multi-component flow problems in porous media. The results and techniques I presented in the thesis can be extended to multi-phase and multi-component flows in porous media.

Numerical aspect of the finite element method

A.1 Numerical integration

For the integration of the basis function, it is possible in some case to obtain the analytical forms for the integral values. But, in general, it is not feasible. Hence, it is important to use numerical quadrature. The concept of the quadrature rule is as following. For example, if we want to compute the integral of function f over the domain $[0, 1]$. We can approximate the integral by the function values evaluate at some locations in the domain and time the some certain weight. In this example we have:

$$\int_0^1 f(x)dx \approx \sum_{k=1}^{N_Q} w_k f(s_k)$$

For higher dimensional quadrature rule follows the same concept,

$$\int_0^1 \int_0^1 f(x, y)dx dy \approx \sum_{k=1}^{N_Q} w_k f(s_{x,k}, s_{y,k})$$

Since the discretization itself is an approximation of the solution of the problem, as long as the order of approximation is no less than the order of the approximation of the polynomial basis for the discretization we can still achieve the same order of convergence rate.

Since we have to integrate element by element, for finite element method in general it would be extremely tedious if we construct quadrature rule on each element when computing the numerical integration. Therefore, we introduce the reference element and the transformation from reference element to physical element. Hence, the quadrature rule is constructed only once on the reference element. The element-wise integration is done on the reference element and transform to the physical element integration. Also, by defining the reference element we can construct basis functions on the reference element and transform them to be the local basis function on the physical element.

We now introduce the affine map from the reference element to the physical element as illustrated in the Figure A.1.

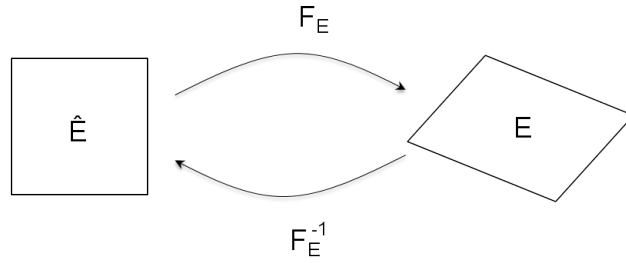


Figure A.1: Transformation between reference element and physical element

The transformation is the affine map,

$$F_E(\hat{x}) = B_E \hat{x} + b_E$$

where

$$B_E = \begin{pmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{y}} \\ \frac{\partial y}{\partial \hat{x}} & \frac{\partial y}{\partial \hat{y}} \end{pmatrix}$$

We have the transformation of the basis function,

$$\varphi(F_E(\hat{x})) = \hat{\varphi}(\hat{x}) \text{ and } \hat{\varphi}(F_E^{-1}(x)) = \varphi(x)$$

Then we can show that

$$\nabla \varphi(x) = \frac{dF_E^{-1}}{dx} \nabla \varphi(\hat{x}) = B_E^{-1} \nabla \varphi(\hat{x})$$

Now, the integration of any function f on any element E can be computed from the integration over the reference element $\hat{E}$, such that

$$\int_E f(x) dx = \int_{\hat{E}} f(F_E(\hat{x})) |\det B_E| d\hat{x} = \int_{\hat{E}} \hat{f}(\hat{x}) |\det B_E| d\hat{x}$$

In the same way we have,

$$\begin{aligned} \int_E \varphi_j(x) \cdot \varphi_i(x) dx &= \int_{\hat{E}} \hat{\varphi}_j(\hat{x}) \cdot \hat{\varphi}_i(\hat{x}) |\det B_E| d\hat{x} \\ \int_E \mathbb{K} \nabla \varphi_j(x) \cdot \nabla \varphi_i(x) dx &= \int_{\hat{E}} \mathbb{K} B_E^{-1} \nabla \hat{\varphi}_j(\hat{x}) \cdot B_E^{-1} \nabla \hat{\varphi}_i(\hat{x}) |\det B_E| d\hat{x} \end{aligned}$$

For the integration on the faces, we also have the following affine transformation illustrated in Figure A.2,

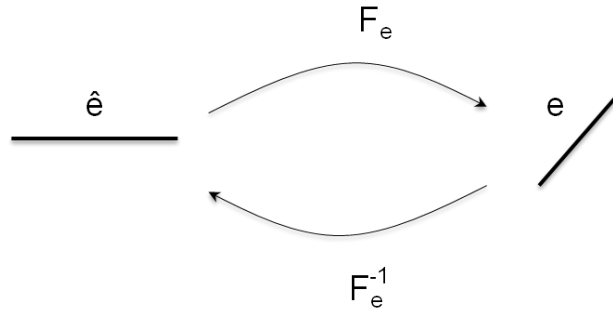


Figure A.2: Transformation between reference face and physical face

The transformation is given as,

$$F_e(\hat{x}) = B_e \hat{x} + b_e$$

where

$$B_e = \begin{pmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{y}} \\ \frac{\partial y}{\partial \hat{x}} & \frac{\partial y}{\partial \hat{y}} \end{pmatrix}$$

Define,

$$\tilde{\varphi}(\hat{x}) = \varphi(F_e^{-1}(\hat{x}))$$

We have the integration on the face as follows,

$$\begin{aligned} \int_e \varphi_j(x) \varphi_i(x) dx &= \int_{\hat{e}} \tilde{\varphi}_j(\hat{x}) \tilde{\varphi}_i(\hat{x}) |\det B_e| d\hat{x} \\ \int_e \mathbb{K} \nabla \varphi_j(x) \cdot \mathbf{n}_e \varphi_i(x) dx &= \int_{\hat{e}} \mathbb{K} B_e^{-1} \nabla \tilde{\varphi}_j(\hat{x}) \cdot \mathbf{n}_e \tilde{\varphi}_i(\hat{x}) |\det B_e| d\hat{x} \end{aligned}$$

Now, we can use the numerical quadrature to evaluate the integral. For the integral over the element we have,

$$\begin{aligned} \int_E \varphi_j(x) \varphi_i(x) dx &= \int_{\hat{E}} \hat{\varphi}_j(\hat{x}) \hat{\varphi}_i(\hat{x}) |\det B_E| d\hat{x} \approx |\det B_E| \sum_{k=1}^{N_Q} \hat{\varphi}_j(s_k) \hat{\varphi}_i(s_k) w_k \\ \int_E \mathbb{K} \nabla \varphi_j(x) \cdot \nabla \varphi_i(x) dx &= \int_{\hat{E}} \mathbb{K} B_E^{-1} \nabla \hat{\varphi}_j(\hat{x}) \cdot B_E^{-1} \nabla \hat{\varphi}_i(\hat{x}) |\det B_E| d\hat{x} \\ &\approx |\det B_E| \sum_{k=1}^{N_Q} \mathbb{K} B_E^{-1} \nabla \hat{\varphi}_j(s_k) \cdot B_E^{-1} \nabla \hat{\varphi}_i(s_k) w_k \end{aligned}$$

For the faces, we have

$$\begin{aligned}
 \int_e \varphi_j(x) \varphi_i(x) dx &= \int_{\hat{e}} \tilde{\varphi}_j(\hat{x}) \tilde{\varphi}_i(\hat{x}) |\det B_e| d\hat{x} \approx |\det B_e| \sum_{k=1}^{N_Q} \tilde{\varphi}_j(s_k) \tilde{\varphi}_i(s_k) w_k \\
 \int_e \mathbb{K} \nabla \varphi_j(x) \cdot \mathbf{n}_e \varphi_i(x) dx &= \int_{\hat{e}} \mathbb{K} B_e^{-1} \nabla \tilde{\varphi}_j(\hat{x}) \cdot \mathbf{n}_e \tilde{\varphi}_i(\hat{x}) |\det B_e| d\hat{x} \\
 &\approx |\det B_e| \sum_{k=1}^{N_Q} \mathbb{K} B_e^{-1} \nabla \tilde{\varphi}_j(s_k) \cdot \mathbf{n}_e \tilde{\varphi}_i(s_k) w_k
 \end{aligned}$$

For the quadrature rules, we refer readers to Appendix A in [83].

A.2 Finite element spaces

In this section, we would like to introduce various kinds DG finite element space without going into too much technical details. We begin by understanding the continuous finite element space. The continuous finite element space can be represented by nodal functions as following figure.

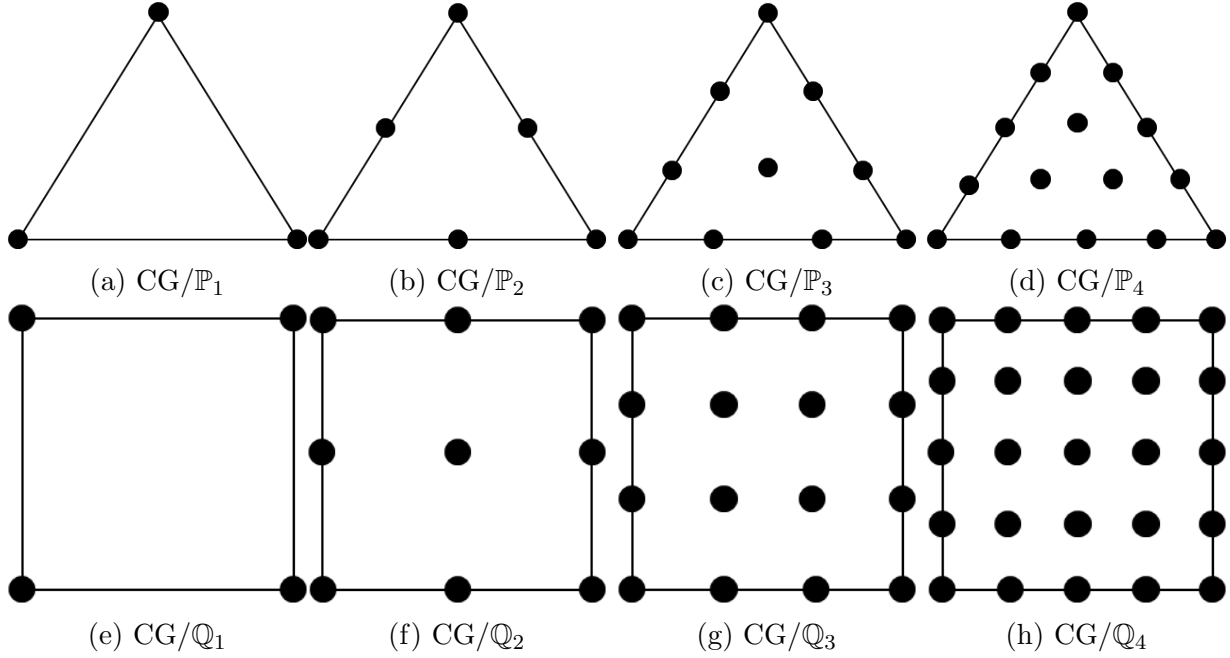


Figure A.3: Conforming finite element spaces

The continuity is required on each nodes in figure A.3. Hence, we have the adjacent elements illustrated in figure below.

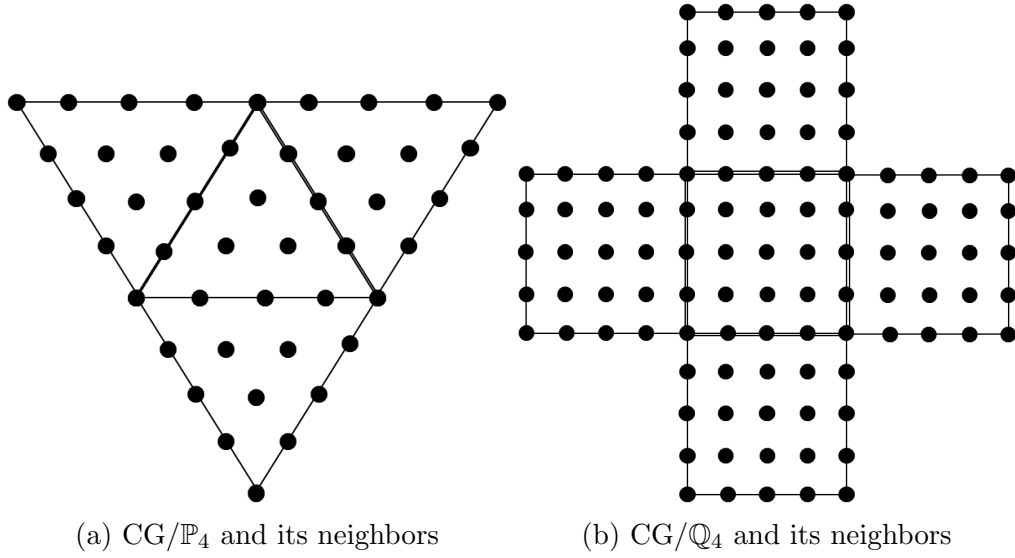


Figure A.4: Conforming finite element spaces and their neighbors

The solution has its value on each nodes. Because of the requirement of continuity, the basis functions are not localized apart from the interior nodes on each element. But, the finite element space guarantee the continuity of the solution on the face of all the elements. Each basis function are simply Lagrange polynomial taking value on one node and vanishing on other nodes.

Now, DG finite element space seeks to localize the basis functions in following way that in the weak formulation it introduces additional terms on the faces which results in more basis functions, but much more localized system. We can still use the nodal function to represent the finite element spaces as following.

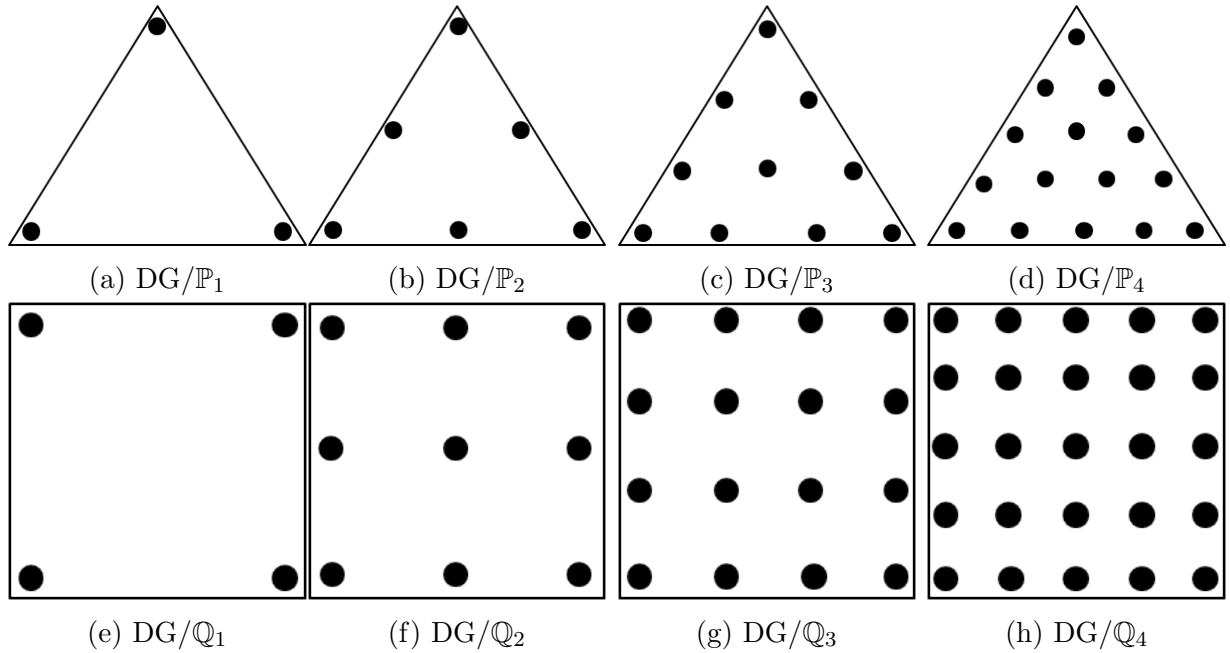


Figure A.5: Nonconforming finite element spaces (Lagrange basis)

And the adjacent elements are as follows.

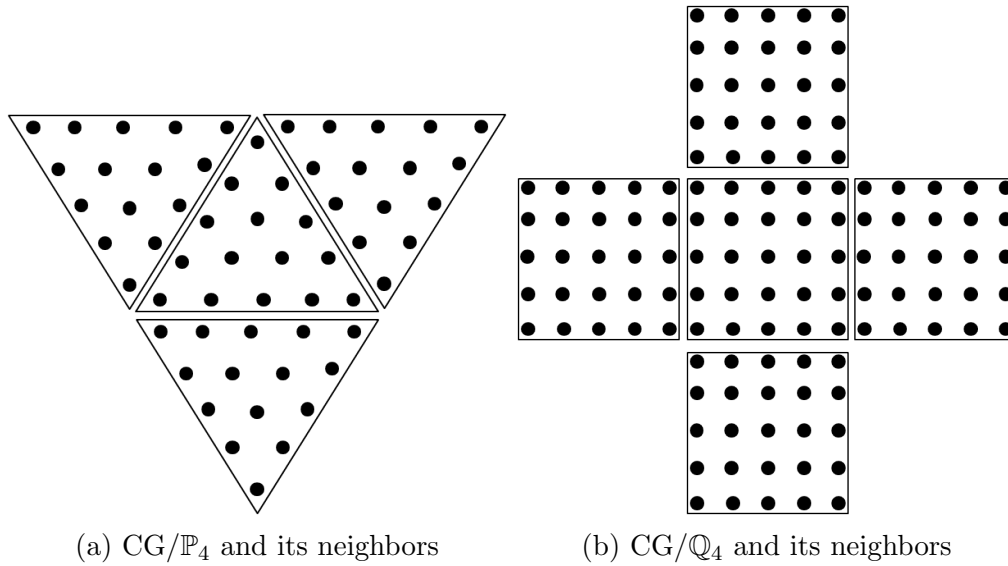


Figure A.6: Nonconforming finite element spaces and their neighbors (Lagrange basis)

In this case, the Lagrange basis is defined on each element and vanishing outside the element. Hence, the basis is localized on each element.

Not only do we have the advantage of the defining localized basis functions, we also have

more freedom of choosing the basis function on each element since the continuity on the face is no longer required. For example, we can define none nodal basis such as monomial space on both triangle and quadrilateral.

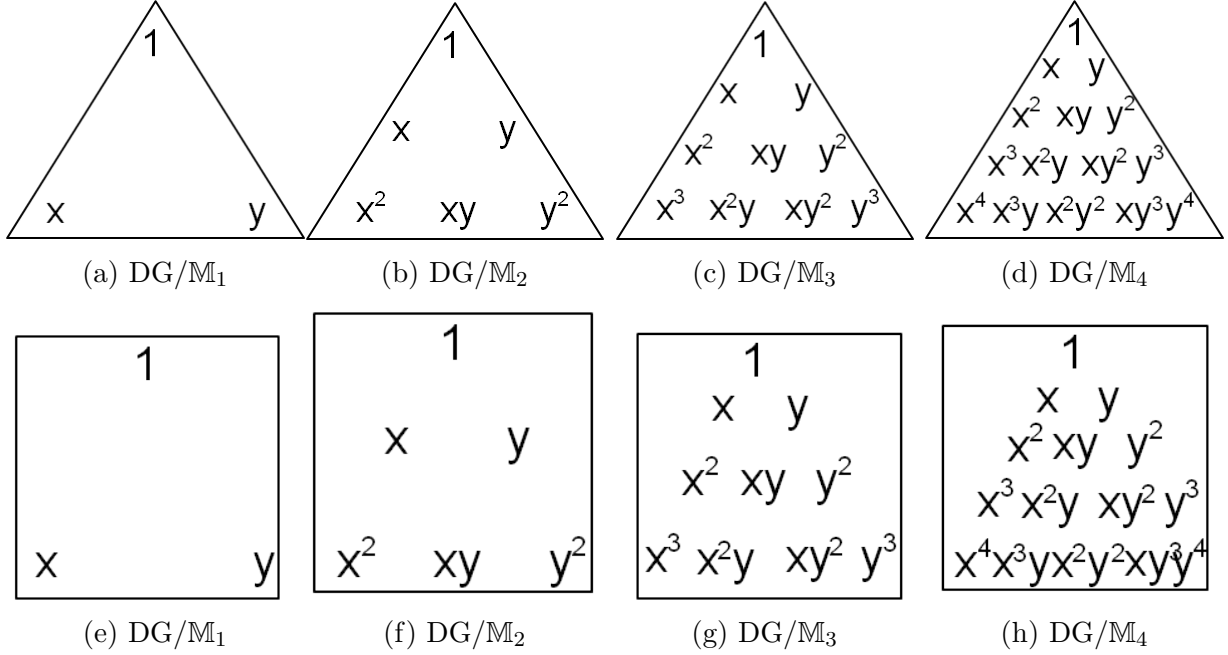


Figure A.7: Nonconforming finite element spaces (monomial basis)

In the same way, we can also construct basis function using orthogonal polynomial basis. In this case, with orthogonal basis function we have diagonal matrix as mass matrix.

A.3 Raviart-Thomas element construction on 2D quadrilateral element

The 2D $\mathcal{RT}$ space on rectangular element is give to be

$$\mathcal{RT}_{[k]}(E) = Q_{k+1,k}(E) \times Q_{k,k+1}(E)$$

where

$$Q_{r,s}(E) = \{\ell_i(x)\ell_j(y) : i = 0, \dots, r \text{ and } j = 0, \dots, s\}$$

with $\ell_i(x)$ to be the i th 1D basis.

And the Degree of freedom is given to be

$$\begin{aligned} (\mathbf{v} \cdot \mathbf{n}_e, q)_e \quad \forall q \in \mathcal{P}_k(e) \\ (\mathbf{v}, \mathbf{w})_E \quad \forall \mathbf{w} \in Q_{k-1,k} \times Q_{k,k-1}(E) \end{aligned}$$

In this case, we let the $\mathcal{P}_k(e)$ be span by the basis function

$$\mathcal{P}_k(e) = \{\ell_0, \ell_1, \dots, \ell_k\}$$

where ℓ_i is the Legendre polynomial of the order i with $\ell_i(0) = (-1)^i$ and $\ell_i(1) = 1$.

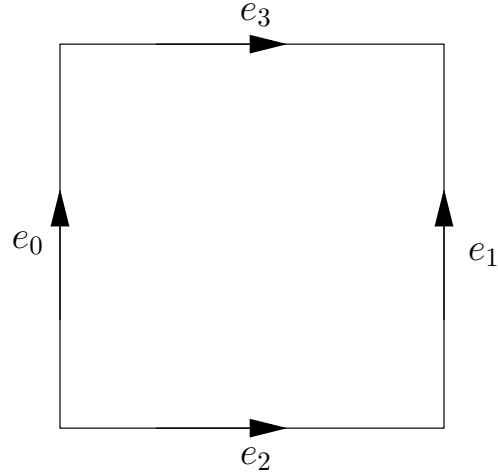


Figure A.8: Reference rectangular element

Given the reference rectangular element and direction of the integration as in figure A.8,

we have for example

$$\mathcal{P}_k(e_0) = \text{span}\{\ell_0(y), \ell_1(y), \dots, \ell_k(y)\}$$

$$\mathcal{P}_k(e_1) = \text{span}\{(-1)^0 \ell_0(y), (-1)^1 \ell_1(y), \dots, (-1)^k \ell_k(y)\}$$

$$\mathcal{P}_k(e_2) = \text{span}\{(-1)^0 \ell_0(x), (-1)^1 \ell_1(x), \dots, (-1)^k \ell_k(x)\}$$

$$\mathcal{P}_k(e_3) = \text{span}\{\ell_0(x), \ell_1(x), \dots, \ell_k(x)\}$$

We also set basis $Q_{k-1,k}(E) \times Q_{k,k-1}(E)$ to be

$$Q_{k-1,k}(E) \times Q_{k,k-1}(E) = \text{span}\{\mathbf{v} = \mathbf{e}_0 \sum_{i=0}^{k-1} \sum_{j=0}^k \alpha_{J_0(i,j)} \ell_i(x) \ell_j(y) + \mathbf{e}_1 \sum_{i=0}^k \sum_{j=0}^{k-1} \alpha_{J_1(i,j)} \ell_i(x) \ell_j(y)\}$$

And the we set the basis for $\mathcal{RT}_{[k]}(E) = Q_{k+1,k}(E) \times Q_{k,k+1}(E)$ to be

$$\begin{aligned} \mathcal{RT}_{[k]}(E) = \text{span}\{ & \mathbf{e}_0 \ell_i(x) \ell_j(y) \text{ with } i = 0, \dots, k+1, j = 0, \dots, k \text{ and} \\ & \mathbf{e}_1 \ell_i(x) \ell_j(y) \text{ with } i = 0, \dots, k, j = 0, \dots, k+1\} \end{aligned}$$

in order for us to derive the basis for $RT_{[k]}(E)$.

Now, we can establish the way to derive the basis.

e_0 :

$$(\mathbf{v} \cdot \mathbf{n}_0, \ell_I(y))_{e_0} = \sum_{i=0}^{k+1} \alpha_{J_0(i,I)} \frac{(-1)^{i+1}}{2I+1}, \quad I = 0, 1, \dots, k \quad \text{at position } (I, J_0(i, I))$$

e_1 :

$$(\mathbf{v} \cdot \mathbf{n}_1, \ell_I(y))_{e_1} = \sum_{i=0}^{k+1} \alpha_{J_0(i,I)} \frac{(-1)^I}{2I+1}, \quad I = 0, 1, \dots, k \quad \text{at position } (I, J_0(i, I))$$

e_2 :

$$(\mathbf{v} \cdot \mathbf{n}_2, \ell_I(x))_{e_2} = \sum_{j=0}^{k+1} \alpha_{J_1(I,j)} \frac{(-1)^{j+I+1}}{2I+1}, \quad I = 0, 1, \dots, k \text{ at position } (I, J_1(I, j))$$

e_3 :

$$(\mathbf{v} \cdot \mathbf{n}_3, \ell_I(x))_{e_3} = \sum_{j=0}^{k+1} \alpha_{J_1(I,j)} \frac{1}{2I+1}, \quad I = 0, 1, \dots, k \text{ at position } (I, J_1(I, j))$$

E :

$$(\mathbf{v}, \mathbf{e}_0 \ell_i(x) \ell_j(y))_E = \alpha_{J_0(i,j)} \frac{1}{2i+1} \frac{1}{2j+1}, \quad i = 0, \dots, k-1, j = 0, \dots, k$$

at position $(I_0(i, j), J_0(i, I))$.

$$(\mathbf{v}, \mathbf{e}_1 \ell_i(x) \ell_j(y))_E = \alpha_{J_1(i,j)} \frac{1}{2i+1} \frac{1}{2j+1}, \quad i = 0, \dots, k, j = 0, \dots, k-1$$

at position $(I_1(i, j), J_1(i, I))$. with

$$I_0(i, j) = i(k+1) + j, \text{ and } I_1(i, j) = ik + j + k(k+1)$$

$$J_0(i, j) = i(k+1) + j, \text{ and } J_1(i, j) = i(k+2) + j + (k+1)(k+2)$$

Once the DOF matrix $\mathbf{A}$ is assembled we can construct the basis by solving $\mathbf{A}\alpha = \mathbf{e}_i$ with $i = 0, \dots, 2(k+1)(k+2)$

I was able to implemented such construction in DUNE and is now available at:

<http://cgkit.dune-project.org/repositories/dune-localfunctions>

Properties of Sobolev spaces

In appendix B, I supply some useful properties of functions in Sobolev space related to approximation theory.

The first result has to do with using smooth functions to approximate the functions in Sobolev spaces.

B.1 Approximation theories in Sobolev spaces

Lemma B.1.1. *The space $W_p^l(\Omega) \cap C^\infty(\Omega)$ is dense in $W_p^l(\Omega)$.*

This is very useful result to pass smooth function into weak formulation. The proof the result can be found in page 9 of [105].

Next result has to do with L^2 -orthogonal projection.

Lemma B.1.2. *Let $\mathcal{E}_h$ be the mesh sequence of the domain Ω . Let*

$$\pi_h^k : H^s(\Omega) \rightarrow \mathcal{P}_k(\mathcal{E}_h)$$

be the L^2 projection onto the piecewise polynomial space. Then, for $s = 0, \dots, k+1$ and all

$f \in H^s(E)$ with $E \in \mathcal{E}_h$, we have

$$|f - \pi_h^k f|_{H^m(E)} \leq C'_{app} h_E^{s-m} |f|_{H^s(E)}$$

This result can be found in [74].

Now, I shall present result of the convergence of the L^2 projection for the function in Sobolev space with minimal regularity.

Lemma B.1.3. *Let $f \in L^2(\Omega)$ and π_h^k be the L^2 projection define as previous lemma, then we have for all*

$$\pi_h^k f \rightarrow f \text{ strongly in } L^2(\Omega)$$

Proof. Let $\epsilon > 0$ be given, by the density argument in lemma B.1.1, we know there exist $\hat{f} \in C^\infty(\Omega) \cap L^2(\Omega)$ such that

$$\|\hat{f} - f\|_{L^2(\Omega)} \leq \epsilon$$

Thus, we have

$$\|\pi_h^k f - f\|_{L^2(\Omega)} \leq \|\pi_h^k f - \pi_h^k \hat{f}\|_{L^2(\Omega)} + \|\pi_h^k \hat{f} - \hat{f}\|_{L^2(\Omega)} + \|\hat{f} - f\|_{L^2(\Omega)}$$

For the first term we have by Cauchy-Schwartz inequality,

$$\begin{aligned} \|\pi_h^k f - \pi_h^k \hat{f}\|_{L^2(\Omega)}^2 &= \langle \pi_h^k f - \pi_h^k \hat{f}, \pi_h^k f - \pi_h^k \hat{f} \rangle = \langle \pi_h^k f - \pi_h^k \hat{f}, f - \hat{f} \rangle \\ &\leq \|\pi_h^k f - \pi_h^k \hat{f}\|_{L^2(\Omega)} \|f - \hat{f}\|_{L^2(\Omega)} \end{aligned}$$

So, the first term

$$\|\pi_h^k f - \pi_h^k \hat{f}\|_{L^2(\Omega)} \leq \epsilon$$

For the second term, according to the result in Lemma B.1.2, we know that

$$\pi_h^k \hat{f} \rightarrow \hat{f} \text{ strongly in } L^2(\Omega)$$

Therefore, $\pi_h^k f \rightarrow f$ strongly in $L^2(\Omega)$. □

Remark, in this case, we have only convergence for the L^2 projection without knowing the convergence rate.

As a corollary, we have following result in terms of the using piecewise constant approximation.

Corollary B.1.4. *Let $\bar{f}$ be the element-wise averaging approximation for $f \in L^2(\Omega)$ over the mesh sequence $\mathcal{E}_h$, then we have*

$$\bar{f} \rightarrow f \text{ strongly in } L^2(\Omega).$$

Proof. It is clear that

$$\langle \bar{f}, 1 \rangle_E = \langle f, 1 \rangle_E.$$

Thus, $\bar{f} = \pi_h^0 f$ is L^2 projection of the function f onto piecewise constant polynomial space.

By Lemma B.1.3, we can establish the result. □

B.2 Preliminary results

B.2.1 Basic inequalities

I begin by stating several well-known inequalities that will be used to obtain some useful results in the setting concerning the numerical scheme. In following analysis, I require the mesh for the numerical method to be a regular mesh, i.e. there are positive constant $a_\circ, a^\circ$,

$b_\circ$ and b° independent of h such that:

$$\begin{aligned} a_\circ |e|^{\frac{d}{d-1}} &\leq |E| \leq a^\circ |e|^{\frac{d}{d-1}} \\ b_\circ |e|^{\frac{1}{d-1}} &\leq h \leq b^\circ |e|^{\frac{1}{d-1}} \end{aligned}$$

where E is a mesh element and its measure $|E|$, e is a face and its measure $|e|$. We use the notation " $\lesssim$ " to denote the fact that the constant is independent of e, E and h . The properties above can be written as:

$$\begin{aligned} |e|^{\frac{d}{d-1}} &\lesssim |E| \text{ and } |E| \lesssim |e|^{\frac{d}{d-1}} \\ |e|^{\frac{1}{d-1}} &\lesssim h \text{ and } h \lesssim |e|^{\frac{1}{d-1}} \end{aligned}$$

If it satisfies the properties as above, we use the notation " $\approx$ " to describe the relationships. i.e.

$$|E| \approx |e|^{\frac{d}{d-1}}, h \approx |e|^{\frac{1}{d-1}} \text{ and } \frac{|E|}{|e|} \approx h \quad (\text{B.1})$$

I shall now state the inverse inequality as follow.

Lemma B.2.1 (Inverse Inequality [91]). *Let $\rho h \leq \text{diam}(E) \leq h$, where $0 < h \leq 1$, and $\mathcal{P}$ be finite dimensional subspace of $W_{\ell,p}(E) \cap W_{m,q}(E)$, where $1 \leq p \leq \infty$, $1 \leq q \leq \infty$ and $0 \leq m \leq \ell$. Then there exists $C = C(\hat{\mathcal{P}}, \hat{E}, \ell, p, q, \rho)$ then*

$$\forall v \in \mathcal{P}, \|v\|_{W_{\ell,p}(E)} \leq C h^{m-\ell+\frac{d}{p}-\frac{d}{q}} \|v\|_{W_{m,q}(E)} \quad (\text{B.2})$$

Another inequality that will be used frequently is a simplified version of Jensen's inequality, stated as

Lemma B.2.2 (Jensen's Inequality [106]). *Let p, q , and n be positive integers. If $1 \leq q \leq$*

$p \leq \infty$, then

$$\left(\sum_{i=1}^n |a_i|^p \right)^{1/p} \leq \left(\sum_{i=1}^n |a_i|^q \right)^{1/q}, \forall a_i \in \mathbb{R} \quad (\text{B.3})$$

Also, the trace inequality is extremely useful when one needs to translate the property of element from edge to the interior of the element.

Lemma B.2.3 (Trace Inequality [83]). *If $v \in \mathcal{P}$, where $\mathcal{P}$ is a finite dimensional subspace, then*

$$\|v\|_{L^2(e)} \leq Ch^{-1/2} \|v\|_{L^2(E)} \quad (\text{B.4})$$

$$\|v\|_{L^4(e)} \leq Ch^{-1/4} \|v\|_{L^4(E)} \quad (\text{B.5})$$

where C is positive and independent of e and E .

B.2.2 Bounds for stabilization terms

In this section, we inspect the interior face terms $([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}\})_{\Gamma_h}$ and $([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}\})_{\Gamma_h}$ for the DG discretization for the concentration. The goal in this section is to establish the bound for these terms as stated in Proposition B.2.16. First, we obtain several inequalities that are proved to be useful for our analysis.

B.2.3 Properties of $\mathbb{D}(\mathbf{u})$

First, from (3.4), we deduce that

$$(\mathbb{D}(\mathbf{v}) \boldsymbol{\xi}, \boldsymbol{\xi}) \geq d_0(1 + |\mathbf{v}|_2) |\boldsymbol{\xi}|_2^2.$$

Hence

$$|\mathbb{D}^{-1/2}(\mathbf{v})|_2 \leq \frac{1}{(d_0(1 + |\mathbf{v}|_2))^{1/2}} \leq \frac{1}{d_0^{1/2}}. \quad (\text{B.6})$$

Similarly

$$|\mathbb{D}^{1/2}(\mathbf{v})|_2 \leq (d_1(1 + |\mathbf{v}|_2))^{1/2}. \quad (\text{B.7})$$

Furthermore

$$\{|\mathbb{D}^{1/2}(\mathbf{v})|_2\} \leq (d_1(1 + \{|\mathbf{v}|_2\}))^{1/2}. \quad (\text{B.8})$$

In the following lemmas, we estimate this right-hand side in $L^2(E)$ and $L^2(e)$ for any element E of $\mathcal{E}_h$ and face e of Γ_h .

Lemma B.2.4. *Let L be the Lipschitz constant of $\mathbb{D}$ and $\mathbf{v}$ any function in $L^2(\Omega)^d$. Then, for any E in $\mathcal{E}_h$,*

$$\|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)} \leq 2L\|\mathbf{v} - \mathbf{u}_h\|_{L^2(E)} + \|\mathbb{D}(\mathbf{v}) - \pi_h(\mathbb{D}(\mathbf{v}))\|_{L^2(E)}. \quad (\text{B.9})$$

Proof. By inserting $\mathbb{D}(\mathbf{v})$, we write

$$\begin{aligned} \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)} &\leq \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}(\mathbf{v})\|_{L^2(E)} + \|\mathbb{D}(\mathbf{v}) - \pi_h(\mathbb{D}(\mathbf{v}))\|_{L^2(E)} \\ &\quad + \|\pi_h(\mathbb{D}(\mathbf{v}) - \mathbb{D}(\mathbf{u}_h))\|_{L^2(E)}. \end{aligned}$$

Then (B.9) follows from the fact that π_h is a projection in $L^2(E)$ and from the Lipschitz continuity of $\mathbb{D}$. $\square$

Lemma B.2.5. *We retain the notation of Lemma B.2.4. Let e be any face of Γ_h and E an element of $\mathcal{E}_h$ adjacent to e . Then*

$$\begin{aligned} \|\mathbb{D}(\mathbf{u}_h)|_E - \pi_h(\mathbb{D}(\mathbf{u}_h))|_E\|_{L^2(e)} &\leq \left(\frac{|e|}{|E|}\right)^{1/2} \left(\hat{C} L \|\mathbf{u}_h - \pi_h(\mathbf{v})\|_{L^2(E)} \right. \\ &\quad \left. + L \|\pi_h(\mathbf{v}) - \mathbf{v}\|_{L^2(E)} + L \|\mathbf{u}_h - \mathbf{v}\|_{L^2(E)} + \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)} \right), \end{aligned} \quad (\text{B.10})$$

where $\hat{C}$ is a constant that depends only on the reference element and the degree of the polynomials.

Proof. To simplify the notation, we drop the index specifying restriction to E . The proof is not totally straightforward because to pass from e to E , we need either an equivalence of norms or a trace theorem and neither of them is applicable to $\mathbb{D}(\mathbf{u}_h)$, which is neither finite-dimensional nor sufficiently smooth. In order to argue in finite dimension, we insert $\pi_h(\mathbf{v})$ and write

$$\begin{aligned} \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)} &\leq \|\mathbb{D}(\mathbf{u}_h) - \mathbb{D}(\pi_h(\mathbf{v}))\|_{L^2(e)} + \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)} \\ &\leq L\|\mathbf{u}_h - \pi_h(\mathbf{v})\|_{L^2(e)} + \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)}, \end{aligned}$$

from the Lipschitz-continuity of $\mathbb{D}$. Now, as $\mathbf{u}_h - \pi_h(\mathbf{v})$ belongs to a finite-dimensional space, a standard equivalence of norms yields

$$\|\mathbf{u}_h - \pi_h(\mathbf{v})\|_{L^2(e)} \leq \hat{C} \left(\frac{|e|}{|E|} \right)^{1/2} \|\mathbf{u}_h - \pi_h(\mathbf{v})\|_{L^2(E)}.$$

Next, since $\mathbb{D}(\pi_h(\mathbf{v}))$ and $\pi_h(\mathbb{D}(\mathbf{u}_h))$ are both matrices with constant coefficients, we can write

$$\begin{aligned} \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)} &= |e|^{1/2} \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_2 \\ &= \left(\frac{|e|}{|E|} \right)^{1/2} \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)}. \end{aligned}$$

Then by inserting $\mathbb{D}(\mathbf{v})$ and using the Lipschitz-continuity of $\mathbb{D}$, we immediately derive

$$\begin{aligned} \|\mathbb{D}(\pi_h(\mathbf{v})) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)} &\leq L(\|\pi_h(\mathbf{v}) - \mathbf{v}\|_{L^2(E)} + \|\mathbf{v} - \mathbf{u}_h\|_{L^2(E)}) \\ &\quad + \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(E)}, \end{aligned}$$

whence (B.10). □

These two lemmas have the following consequences.

Corollary B.2.6. *We suppose that*

$$\lim_{h \rightarrow 0} \|\mathbf{u}_h - \mathbf{u}\|_{L^2(0,T;L^2(\Omega)^d)} = 0.$$

Then

$$\lim_{h \rightarrow 0} \|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)\|_{L^2(0,T;L^2(\Omega)^d)} = 0$$

where

$$\mathbb{D}_h(\mathbf{u}_h) = \mathbb{D}(\bar{\mathbf{u}}_h).$$

Proof. Let L be the Lipschitz constant of $\mathbb{D}$ that for any $\mathbf{v}$ in $L^2(\Omega)^d$,

$$\|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)\|_{L^2(\Omega)} \leq 2L\|\mathbf{u}_h - \mathbf{v}\|_{L^2(\Omega)} + \|\mathbb{D}(\mathbf{v}) - \pi_h(\mathbb{D}(\mathbf{v}))\|_{L^2(\Omega)}.$$

Take $\mathbf{v} = \mathbf{u}$. Then the first term in the above right-hand side tends to zero. For the second term, by Lemma B.1.3 we have

$$\lim_{h \rightarrow 0} \|\mathbb{D}(\mathbf{u}) - \pi_h(\mathbb{D}(\mathbf{u}))\|_{L^2(0,T;L^2(\Omega)^d)} = 0. \quad (\text{B.11})$$

□

Proposition B.2.7. *We suppose that the mesh $\mathcal{E}_h$ is regular. Then, there exists a constant C , depending only on the reference element, the degree of the polynomials, the Lipschitz constants of $\mathbb{D}$, and the regularity of the mesh, such that*

$$\begin{aligned} \sum_{e \in \Gamma_h} h_e \|\{\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)\}_2\|_{L^2(e)}^2 &\leq C \left(\|\mathbf{u}_h - \mathbf{v}\|_{L^2(\Omega)}^2 + \|\mathbf{v} - \pi_h(\mathbf{v})\|_{L^2(\Omega)}^2 \right. \\ &\quad \left. + \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(\Omega)}^2 \right). \end{aligned} \quad (\text{B.12})$$

Proof. We have

$$\|\{|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)|_2\}\|_{L^2(e)}^2 \leq \{\|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)\|_{L^2(e)}^2\}.$$

As in Corollary B.2.6,

$$\|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)\|_{L^2(e)}^2 \leq \|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)}^2.$$

Therefore, we must bound

$$\sum_{e \in \Gamma_h} h_e \{\|\mathbb{D}(\mathbf{u}_h) - \pi_h(\mathbb{D}(\mathbf{u}_h))\|_{L^2(e)}^2\}.$$

By applying (B.10) and substituting (B.9), we see that each term in the sum over e is multiplied by $\frac{h_e|e|}{|E|}$, where E are the elements sharing e . The other factors are constants that depend on m, g_1, L , on the reference element and on the degree of the polynomials. But the regularity of the mesh implies that

$$\frac{h_e|e|}{|E|} \leq C,$$

with a constant C independent of e , E , and h . This yields (B.12). $\square$

By choosing $\mathbf{v} = \mathbf{u}$ and using (B.11), an immediate argument proves the following corollary:

Corollary B.2.8. *In addition to the assumptions of Proposition B.2.7, we suppose that*

$$\lim_{h \rightarrow 0} \|\mathbf{u}_h - \mathbf{u}\|_{L^2(0,T;L^2(\Omega)^d)} = 0.$$

Then

$$\lim_{h \rightarrow 0} \left(\int_0^T \sum_{e \in \Gamma_h} h_e \|\{|\mathbb{D}_h(\mathbf{u}_h) - \mathbb{D}(\mathbf{u}_h)|_2\}\|_{L^2(e)}^2 \right)^{1/2} = 0.$$

The result we obtain for the diffusion-dispersion tensor $\mathbb{D}(\mathbf{u})$, also apply to the tensor

$\mathbb{K}(c)$ which is more regular than the diffusion-dispersion tensor. Therefore, we simply state following result.

Corollary B.2.9. *In addition to the assumptions of Proposition B.2.7, we suppose that*

$$\lim_{h \rightarrow 0} \|c_h - c\|_{L^2(0,T;L^2(\Omega)^d)} = 0.$$

Then

$$\lim_{h \rightarrow 0} \left(\int_0^T \sum_{e \in \Gamma_h} h_e \|\{\|\mathbb{K}_h(c_h) - \mathbb{K}(c_h)|_2\}\|_{L^2(e)}^2 \right)^{1/2} = 0$$

and

$$\lim_{h \rightarrow 0} \|\mathbb{K}_h(c_h) - \mathbb{K}(c_h)\|_{L^2(0,T;L^2(\Omega)^d)} = 0$$

where

$$\mathbb{K}_h(c_h) = \mathbb{K}(\bar{c}_h).$$

B.2.4 Properties of the interior face terms

Lemma B.2.10. *Let e be a given face of an arbitrary mesh element E . If $\mathbf{w} \in \mathcal{P}^d$ where $\mathbf{w}$ is a vector function and $\mathcal{P}$ is a finite dimensional subspace, then*

$$\|\mathbf{w}\|_{L^2(e)} \lesssim h^{-1/2} \|\mathbf{w}\|_{L^2(E)}$$

Proof. We write the definition of L^2 norm:

$$\|\mathbf{w}\|_{L^2(e)} = \left(\sum_{i=1}^d \int_e w_i^2 \right)^{1/2} = \left(\sum_{i=1}^d \|w_i\|_{L^2(e)}^2 \right)^{1/2}$$

Hence, applying the Trace Inequality in Lemma B.2.3 we have

$$\|\mathbf{w}\|_{L^2(e)} \lesssim \left(\sum_{i=1}^d h^{-1} \|w_i\|_{L^2(E)}^2 \right)^{1/2} \lesssim h^{-1/2} \left(\sum_{i=1}^d \int_E w_i^2 \right)^{1/2} \lesssim h^{-1/2} \|\mathbf{w}\|_{L^2(E)}$$

□

With the help of this inverse estimate, the following inequalities can be obtained.

Lemma B.2.11. *Given $w_h \in \mathcal{P}$ and $\mathbf{u}_h \in \mathcal{P}^d$ then for a fixed element E and a face $e \in \partial E$,*

$$\|\nabla w_h\|_{L^2(e)} \lesssim h^{-1/2} \|\nabla w_h\|_{L^2(E)} \text{ and } \|\mathbf{u}_h|_E\|^{1/2} \|\nabla w_h\|_{L^2(e)} \lesssim h^{-1/2} \|\mathbf{u}_h\|^{1/2} \|\nabla w_h\|_{L^2(E)}.$$

Proof. The first inequality directly follows from Lemma B.2.10.

For the second inequality,

$$\begin{aligned} \|\mathbf{u}_h\|^{1/2} \|\nabla w_h\|_{L^2(e)} &\lesssim |e|^{1/4} \left(\int_e |\mathbf{u}_h|^2 |\nabla w_h|^4 \right)^{1/4} \lesssim |e|^{1/4} \left(\sum_{i,j=1}^d \int_e u_{h,i}^2 \left(\frac{\partial w_h}{\partial x_j} \right)^4 \right)^{1/4} \\ &\lesssim |e|^{1/4} \left(\sum_{i,j=1}^d \|u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2\|_{L^2(e)}^2 \right)^{1/4} \end{aligned}$$

As the consequence of Trace Inequality from Lemma B.2.3,

$$\|u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2\|_{L^2(e)} \lesssim h^{-1/2} \|u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2\|_{L^2(E)}$$

Hence, we related the face to the interior of the element E ,

$$\|\mathbf{u}_h\|^{1/2} \|\nabla w_h\|_{L^2(e)} \lesssim |e|^{1/4} \left(h^{-1} \sum_{i,j=1}^d \|u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2\|_{L^2(E)}^2 \right)^{1/4}$$

By the Inverse Inequality from Lemma B.2.1,

$$\left\| u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2 \right\|_{L^2(E)} \lesssim h^{-d/2} \| u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2 \|_{L^1(E)}$$

Therefore, we can conclude

$$\begin{aligned} |||\mathbf{u}_h|^{1/2} |\nabla w_h| |||_{L^2(E)} &\lesssim |e|^{1/4} \left(h^{-1} h^{-d} \sum_{i,j=1}^d \| u_{h,i} \left(\frac{\partial w_h}{\partial x_j} \right)^2 \|_{L^1(E)}^2 \right)^{1/4} \\ &\lesssim h^{-1/2} \left(\sum_{i,j=1}^d \left(\int_E |u_{h,i}| \left(\frac{\partial w_h}{\partial x_j} \right)^2 \right)^2 \right)^{1/4} \\ &\lesssim h^{-1/2} \left(\int_E \sum_{i=1}^d |u_{h,i}| |\nabla w_h|^2 \right)^{1/2} \\ &\lesssim h^{-1/2} \left(\int_E |\mathbf{u}_h| |\nabla w_h|^2 \right)^{1/2} \\ &\lesssim h^{-1/2} |||\mathbf{u}_h|^{1/2} |\nabla w_h| |||_{L^2(E)} \end{aligned}$$

□

Lemma B.2.12. *If $w_h \in \mathcal{P}$, then we have*

$$\|\nabla w_h\|_{L^2(\mathcal{E}_h)} \lesssim \|\nabla w_h\|_{L^4(\mathcal{E}_h)}$$

Proof. We apply Cauchy-Schwarz inequality,

$$\begin{aligned} \left(\sum_{E \in \mathcal{E}_h} \|\nabla w_h\|_{L^2(E)}^2 \right)^{1/2} &\leq \left(\sum_{E \in \mathcal{E}_h} |E|^{1/2} \left(\int_E |\nabla w_h|^4 \right)^{1/2} \right)^{1/2} \\ &\leq \left(\sum_{E \in \mathcal{E}_h} |E| \right)^{1/4} \left(\sum_{E \in \mathcal{E}_h} \int_E |\nabla w_h|^4 \right)^{1/4} \lesssim \|\nabla w_h\|_{L^4(\mathcal{E}_h)} \end{aligned}$$

□

Lemma B.2.13. *Let $\mathbf{u}_h \in \mathcal{P}^d$ and $c_h \in \mathcal{P}$, then for an element E and one of its face e ,*

$$\|\mathbb{D}^{1/2}(\mathbf{u}_h|_E)\nabla c_h\|_{L^2(e)} \lesssim h^{-1/2}\|\mathbb{D}^{1/2}(\mathbf{u}_h)\nabla c_h\|_{L^2(E)}$$

and

$$\|\mathbb{D}^{1/2}(\mathbf{u}_h|_E)\nabla c_h\|_{L^2(e)} \lesssim h^{-1/2} \left(\|\nabla c_h\|_{L^2(E)} + \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|\nabla c_h\|_{L^4(E)} \right)$$

Proof. Recall the property of diffusivity tensor in (3.4), we have

$$d_0(1 + |\mathbf{u}_h|) |\nabla c_h|^2 \leq \nabla c_h^T \mathbb{D}(\mathbf{u}_h) \nabla c_h \leq d_1(1 + |\mathbf{u}_h|) |\nabla c_h|^2$$

We therefore obtain the inequality,

$$\begin{aligned} \left(\int_e \mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \nabla c_h \right)^{1/2} &\lesssim \left(\int_e (1 + |\mathbf{u}_h|) |\nabla c_h|^2 \right)^{1/2} \\ &\lesssim \left(\|\nabla c_h\|_{L^2(e)}^2 + \| |\mathbf{u}_h|^{1/2} |\nabla c_h| \|_{L^2(e)}^2 \right)^{1/2} \end{aligned}$$

According to Lemma B.2.11, we have

$$\begin{aligned} \left(\int_e \mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \nabla c_h \right)^{1/2} &\lesssim h^{-1/2} \left(\|\nabla c_h\|_{L^2(E)}^2 + \| |\mathbf{u}_h|^{1/2} |\nabla c_h| \|_{L^2(E)}^2 \right)^{1/2} \\ &\lesssim h^{-1/2} \left(\int_E (1 + |\mathbf{u}_h|) |\nabla c_h|^2 \right)^{1/2} \end{aligned}$$

Therefore, we obtain the first inequality using the property (3.4),

$$\|\mathbb{D}^{1/2}(\mathbf{u}_h)\nabla c_h\|_{L^2(e)} \lesssim h^{-1/2}\|\mathbb{D}^{1/2}(\mathbf{u}_h)\nabla c_h\|_{L^2(E)}$$

Also, by Lemma B.2.2

$$\begin{aligned}
\left(\int_E (1 + |\mathbf{u}_h|) |\nabla c_h|^2 \right)^{1/2} &= \left(\int_E |\nabla c_h|^2 + \int_E |\mathbf{u}_h| |\nabla c_h|^2 \right)^{1/2} \\
&\leq \left(\int_E |\nabla c_h|^2 \right)^{1/2} + \left(\int_E |\mathbf{u}_h| |\nabla c_h|^2 \right)^{1/2} \\
&\leq \|\nabla c_h\|_{L^2(E)} + \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|\nabla c_h\|_{L^4(E)}
\end{aligned}$$

Therefore, we have

$$\|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(e)} \lesssim h^{-1/2} \left(\|\nabla c_h\|_{L^2(E)} + \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|\nabla c_h\|_{L^4(E)} \right)$$

□

With all the helpful inequalities attained so far, we can now bound the terms $([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_e$ and $([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e$ in our scheme.

For the next result, let E_+^e and E_-^e be the mesh elements that share the face e . We define the average to be:

$$\{\|w\|_{L^p(E^e)}\} = \frac{1}{2} \left(\|w\|_{L^p(E_+^e)} + \|w\|_{L^p(E_-^e)} \right)$$

likewise,

$$\{\|w\|_{L^p(E^e)} \|v\|_{L^q(E^e)}\} = \frac{1}{2} \left(\|w\|_{L^p(E_+^e)} \|v\|_{L^q(E_+^e)} + \|w\|_{L^p(E_-^e)} \|v\|_{L^q(E_-^e)} \right)$$

we also use the notations

$$w^+ = w|_{E_+^e} \text{ and } w^- = w|_{E_-^e}$$

In the rest of the analysis, we will use the notations P_h , $\mathbf{U}_h$ and C_h corresponding to the finite element spaces for the numerical scheme. But, those results hold for all the piecewise polynomials.

Lemma B.2.14. *Let e be a given face of an arbitrary mesh element E . Given $c_h, w_h \in C_h$, $\mathbf{u}_h \in \mathbf{U}_h$ and $\mathbb{D}$ the diffusion dispersion matrix satisfying the property (3.4), then we have*

$$([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \times \left\{ \|\nabla w_h\|_{L^2(E^e)} + \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \right\}$$

Proof. We begin by expanding and bounding the terms using Cauchy-Schwarz's inequality,

$$\begin{aligned} ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e &\lesssim ([c_h], \mathbb{D}(\mathbf{u}_h^+) \nabla w_h^+ \cdot \mathbf{n}_e)_e + ([c_h], \mathbb{D}(\mathbf{u}_h^-) \nabla w_h^- \cdot \mathbf{n}_e)_e \\ &\lesssim \left\{ \int_e |\mathbb{D}^{1/2}(\mathbf{u}_h) \mathbf{n}_e|^2 [c_h]^2 \right\}^{1/2} \left\{ \int_e |\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h|^2 \right\}^{1/2} \\ &\lesssim \left\{ \left(\int_e |\mathbb{D}^{1/2}(\mathbf{u}_h) \mathbf{n}_e|^2 [c_h]^2 \right)^{1/2} \left(\int_e |\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h|^2 \right)^{1/2} \right\} \\ &\lesssim \left(\int_e \{|\mathbb{D}^{1/2}(\mathbf{u}_h) \mathbf{n}_e|\}^2 [c_h]^2 \right)^{1/2} \left\{ \left(\int_e |\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h|^2 \right)^{1/2} \right\} \end{aligned}$$

By the property (3.4), we obtain

$$([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(e)} \} \quad (\text{B.13})$$

By Lemma B.2.13, therefore, we have

$$([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \times \left\{ \|\nabla w_h\|_{L^2(E^e)} + \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \right\}$$

□

Lemma B.2.15. *Given c_h, w_h , $\mathbf{u}_h$ and $\mathbb{D}$ as in Lemma B.2.14, then*

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E^e)} \}$$

Proof. From (B.13), we have

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(e)} \}$$

And according to Lemma B.2.13,

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_e \lesssim \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E^e)} \}$$

□

We now sum up the contributions over all the interior edge and establish the following proposition.

Proposition B.2.16. *Let c_h, w_h be in C_h and $\mathbf{u}_h$ be in $\mathbf{U}_h$. We have*

$$([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim J(c_h, c_h; \mathbf{u}_h)^{1/2} (\|\nabla w_h\|_{L^2(\mathcal{E}_h)} + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|\nabla w_h\|_{L^4(\mathcal{E}_h)}) \quad (\text{B.14})$$

and

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim R(w_h; \mathbf{u}_h) \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)} \quad (\text{B.15})$$

with

$$J(c_h, c_h; \mathbf{u}_h) = \sum_{e \in \Gamma_h} h^{-1} \int_e (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \quad (\text{B.16})$$

and

$$R(w_h; \mathbf{u}_h) = \left(1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \right) \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4} \quad (\text{B.17})$$

Proof. To sum up over all the interior edges, by Lemma B.2.14 one would have

$$\begin{aligned}
([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} &= \sum_{e \in \Gamma_h} ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e \\
&\lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \{ \|\nabla w_h\|_{L^2(E^e)} + \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \} \\
&\lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \left(\{ \|\nabla w_h\|_{L^2(E^e)} \} + \{ \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \} \right) \\
&\lesssim J(c_h, c_h; \mathbf{u}_h)^{1/2} \left(\left(\sum_{e \in \Gamma_h} \{ \|\nabla w_h\|_{L^2(E^e)} \}^2 \right)^{1/2} + \left(\sum_{e \in \Gamma_h} \{ \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \}^2 \right)^{1/2} \right)
\end{aligned}$$

For the term,

$$\left(\sum_{e \in \Gamma_h} \{ \|\nabla w_h\|_{L^2(E^e)} \}^2 \right)^{1/2}$$

we have

$$\left(\sum_{e \in \Gamma_h} \{ \|\nabla w_h\|_{L^2(E^e)} \}^2 \right)^{1/2} \lesssim \left(\sum_{e \in \Gamma_h} \left(\|\nabla w_h\|_{L^2(E_+^e)}^2 + \|\nabla w_h\|_{L^2(E_-^e)}^2 \right) \right)^{1/2} \lesssim \|\nabla w_h\|_{L^2(\mathcal{E}_h)}$$

Likewise, we can obtain

$$\begin{aligned}
\left(\sum_{e \in \Gamma_h} \{ \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \}^2 \right)^{1/2} &\lesssim \left(\sum_{E \in \mathcal{E}_h} \|\mathbf{u}_h\|_{L^2(E)} \|\nabla w_h\|_{L^4(E)}^2 \right)^{1/2} \\
&\lesssim \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|\nabla w_h\|_{L^4(\mathcal{E}_h)}
\end{aligned}$$

Therefore, for the term $([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h}$ we have

$$([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim J(c_h, c_h; \mathbf{u}_h)^{1/2} (\|\nabla w_h\|_{L^2(\mathcal{E}_h)} + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|\nabla w_h\|_{L^4(\mathcal{E}_h)})$$

For the term $([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h}$ using Lemma B.2.15 we have,

$$\begin{aligned}
([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} &= \sum_{e \in \Gamma_h} ([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_e \\
&\lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E^e)} \} \\
&\lesssim J(w_h, w_h; \mathbf{u}_h)^{1/2} \left(\sum_{e \in \Gamma_h} \{ \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E^e)} \}^2 \right)^{1/2} \\
&\lesssim J(w_h, w_h; \mathbf{u}_h)^{1/2} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)}
\end{aligned}$$

Thus,

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim J(w_h, w_h; \mathbf{u}_h)^{1/2} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)} \quad (\text{B.18})$$

For $J(w_h, w_h; \mathbf{u}_h)^{1/2}$, we can establish the inequality,

$$\begin{aligned}
J(w_h, w_h; \mathbf{u}_h)^{1/2} &= \left(\sum_{e \in \Gamma_h} \int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \\
&\lesssim \left(\sum_{e \in \Gamma_h} \int_e h^{-1} [w_h]^2 \right)^{1/2} + \left(\sum_{e \in \Gamma_h} \int_e h^{-1} \{|\mathbf{u}_h|\} [w_h]^2 \right)^{1/2}
\end{aligned}$$

For the first term we have,

$$\begin{aligned}
\left(\sum_{e \in \Gamma_h} \int_e h^{-1} [w_h]^2 \right)^{1/2} &\lesssim \left(\sum_{e \in \Gamma_h} h^{-1} |e|^{1/2} \left(\int_e [w_h]^4 \right)^{1/2} \right)^{1/2} \\
&\lesssim \left(\sum_{e \in \Gamma_h} |E| \right)^{1/4} \left(\sum_{e \in \Gamma_h} h^{-2} \frac{|e|}{|E|} \int_e [w_h]^4 \right)^{1/4}
\end{aligned}$$

Using the property of regular mesh in (B.1), we have

$$\left(\sum_{e \in \Gamma_h} h^{-2} \frac{|e|}{|E|} \int_e [w_h]^4 \right)^{1/4} \lesssim \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4}$$

For the second term we notice,

$$\begin{aligned} \left(\sum_{e \in \Gamma_h} \int_e h^{-1} |\mathbf{u}_h^+| [w_h]^2 \right)^{1/2} &\lesssim \left(\sum_{e \in \Gamma_h} h^{-1} \left(\int_e |\mathbf{u}_h^+|^2 \right)^{1/2} \left(\int_e [w_h]^4 \right)^{1/2} \right)^{1/2} \\ &\lesssim \left(\sum_{e \in \Gamma_h} \|\mathbf{u}_h^+\|_{L^2(e)}^2 \right)^{1/4} \left(\sum_{e \in \Gamma_h} h^{-2} \int_e [w_h]^4 \right)^{1/4} \\ &\lesssim \left(\sum_{e \in \Gamma_h} h^{-1} \|\mathbf{u}_h\|_{L^2(E_+^e)}^2 \right)^{1/4} \left(\sum_{e \in \Gamma_h} h^{-2} \int_e [w_h]^4 \right)^{1/4} \\ &\lesssim \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4} \end{aligned}$$

In the same way we can establish,

$$\left(\sum_{e \in \Gamma_h} \int_e h^{-1} |\mathbf{u}_h^-| [w_h]^2 \right)^{1/2} \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4} \quad (\text{B.19})$$

To summarize we have,

$$\left(\sum_{e \in \Gamma_h} h^{-1} \int_e (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \lesssim (1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2}) \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4} \quad (\text{B.20})$$

Therefore, we conclude

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim R(w_h; \mathbf{u}_h) \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)}$$

□

Lemma B.2.17 (Continuity properties). *Let c_h and w_h be in C_h and let $\mathbf{u}_h$ be in $\mathbf{U}_h$.*

$$|B_d(c_h, w_h; \mathbf{u}_h)| \lesssim (1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2}) \|c_h\|_{C_h} \|w_h\|_{W^{1,4}(\mathcal{E}_h)}, \quad (\text{B.21})$$

$$\begin{aligned} |B_{cq}(c_h, w_h; \mathbf{u}_h)| &\lesssim \|w_h\|_{W^{1,4}(\mathcal{E}_h)} \\ &(\|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|c_h\|_{C_h} + (\|q^I + q^P\|_{L^2(\Omega)} + \|\mathbf{u}_h\|_{L^2(\Omega)}) \|c_h\|_{L^4(\Omega)}). \end{aligned} \quad (\text{B.22})$$

The proof of Lemma B.2.17 is now given.

Proof. The first term of $B_d(c_h, w_h; \mathbf{u}_h)$ is

$$(\mathbb{D}(\mathbf{u}_h) \nabla c_h, \nabla w_h)_{\mathcal{E}_h} \leq \sum_{E \in \mathcal{E}_h} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E)} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(E)}.$$

Notice that by (3.4),

$$\begin{aligned} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla w_h\|_{L^2(E)} &\lesssim \left(\int_E (1 + |\mathbf{u}_h|) |\nabla w_h|^2 \right)^{1/2} \lesssim \|\nabla w_h\|_{L^2(E)} + \left(\int_E |\mathbf{u}_h| |\nabla w_h|^2 \right)^{1/2} \\ &\lesssim \|\nabla w_h\|_{L^2(E)} + \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|\nabla w_h\|_{L^4(E)}. \end{aligned}$$

So, we have

$$\begin{aligned} (\mathbb{D}(\mathbf{u}_h) \nabla c_h, \nabla w_h)_{\mathcal{E}_h} &\lesssim \sum_{E \in \mathcal{E}_h} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E)} \left(\|\nabla w_h\|_{L^2(E)} + \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|\nabla w_h\|_{L^4(E)} \right) \\ &\lesssim \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)} \left(\|\nabla w_h\|_{L^2(\mathcal{E}_h)} + \left(\sum_{E \in \mathcal{E}_h} \|\mathbf{u}_h\|_{L^2(E)} \|\nabla w_h\|_{L^4(E)}^2 \right)^{1/2} \right) \\ &\lesssim \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)} \left(\|\nabla w_h\|_{L^2(\mathcal{E}_h)} + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|\nabla w_h\|_{L^4(\mathcal{E}_h)} \right). \end{aligned}$$

And consequently using the fact that

$$\|\nabla w_h\|_{L^2(\mathcal{E}_h)} \lesssim \|\nabla w_h\|_{L^4(\mathcal{E}_h)}, \quad (\text{B.23})$$

we have,

$$(\mathbb{D}(\mathbf{u}_h) \nabla c_h, \nabla w_h)_{\mathcal{E}_h} \lesssim \|c_h\|_{C_h} \left(1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2}\right) \|w_h\|_{W^{1,4}(\mathcal{E}_h)}. \quad (\text{B.24})$$

For the term $([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h}$ we have,

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)}. \quad (\text{B.25})$$

We have the following inequality:

$$\left(\sum_{e \in \Gamma_h} \int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \lesssim \left(\sum_{e \in \Gamma_h} \int_e h^{-1} [w_h]^2 \right)^{1/2} + \left(\sum_{e \in \Gamma_h} \int_e h^{-1} \{|\mathbf{u}_h|\} [w_h]^2 \right)^{1/2}.$$

Using Cauchy-Schwarz's inequality and the fact that $|e| \approx h^{d-1}$, we have

$$\sum_{e \in \Gamma_h} \int_e h^{-1} [w_h]^2 \lesssim \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/2} \left(\sum_{e \in \Gamma_h} h^d \right)^{1/2} \lesssim \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/2}. \quad (\text{B.26})$$

For the other term, we can write

$$\sum_{e \in \Gamma_h} \int_e h^{-1} \{|\mathbf{u}_h|\} [w_h]^2 \lesssim \sum_{e \in \Gamma_h} \int_e h^{-1} |\mathbf{u}_h^+| [w_h]^2 + \sum_{e \in \Gamma_h} \int_e h^{-1} |\mathbf{u}_h^-| [w_h]^2.$$

We treat each term separately, but in a similar fashion

$$\begin{aligned} \sum_{e \in \Gamma_h} \int_e h^{-1} |\mathbf{u}_h^+| [w_h]^2 &\lesssim \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/2} \left(\sum_{e \in \Gamma_h} h \int_e |\mathbf{u}_h^+|^2 \right)^{1/2} \\ &\lesssim \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/2} \left(\sum_{e \in \Gamma_h} \|\mathbf{u}_h\|_{L^2(E_+^e)}^2 \right)^{1/2}. \end{aligned}$$

Therefore we have

$$\sum_{e \in \Gamma_h} \int_e h^{-1} \{|\mathbf{u}_h|\} [w_h]^2 \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)} \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/2}. \quad (\text{B.27})$$

To summarize, from (B.26) and (B.27), we have,

$$\left(\sum_{e \in \Gamma_h} h^{-1} \int_e (1 + \{|\mathbf{u}_h|\}) [w_h]^2 \right)^{1/2} \lesssim \left(1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \right) \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4}, \quad (\text{B.28})$$

and thus,

$$([w_h], \{\mathbb{D}(\mathbf{u}_h) \nabla c_h \cdot \mathbf{n}_e\})_{\Gamma_h} \lesssim \left(1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \right) \|w_h\|_{W(\mathcal{E}_h)} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)}. \quad (\text{B.29})$$

For the third term of $B_d(c_h, w_h; \mathbf{u}_h)$, we use a trace inequality and a similar argument as in (B.13)

$$\begin{aligned} ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_{\Gamma_h} &= \sum_{e \in \Gamma_h} ([c_h], \{\mathbb{D}(\mathbf{u}_h) \nabla w_h \cdot \mathbf{n}_e\})_e \\ &\lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \{ \|\nabla w_h\|_{L^2(E^e)} + \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \} \\ &\lesssim \sum_{e \in \Gamma_h} \left(\int_e h^{-1} (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2} \left(\{ \|\nabla w_h\|_{L^2(E^e)} \} + \{ \|\mathbf{u}_h\|_{L^2(E^e)}^{1/2} \|\nabla w_h\|_{L^4(E^e)} \} \right) \\ &\lesssim \|c_h\|_{C_h} \left(\|\nabla w_h\|_{L^2(\mathcal{E}_h)} + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|\nabla w_h\|_{L^4(\mathcal{E}_h)} \right). \end{aligned} \quad (\text{B.30})$$

Using Cauchy-Schwarz's inequality and (B.28), the penalty term in $B_d(c_h, w_h; \mathbf{u}_h)$ can be

bounded as

$$\begin{aligned}
& (\sigma h^{-1}(1 + \{|\mathbf{u}_h|\})[c_h], [w_h])_{\Gamma_h} \\
& \lesssim \left(\sum_{e \in \Gamma_h} \int_e h^{-1}(1 + \{|\mathbf{u}_h|\})[c_h]^2 \right)^{1/2} \left(\sum_{e \in \Gamma_h} \int_e h^{-1}(1 + \{|\mathbf{u}_h|\})[w_h]^2 \right)^{1/2} \\
& \lesssim \|c_h\|_{C_h} \left(1 + \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \right) \|w_h\|_{W(\mathcal{E}_h)}. \tag{B.31}
\end{aligned}$$

Therefore the bound (B.21) is obtained by combining (B.23), (B.24), (B.29), (B.30) and (B.31).

To obtain (B.22), we now bound each term in $B_{cq}(c_h, w_h; \mathbf{u}_h)$. For the first term, using (3.4), we have:

$$\begin{aligned}
(\mathbf{u}_h \nabla c_h, w_h)_{\mathcal{E}_h} & \leq \sum_{E \in \mathcal{E}_h} \left(\int_E |\mathbf{u}_h| |\nabla c_h|^2 \right)^{1/2} \left(\int_E |\mathbf{u}_h| w_h^2 \right)^{1/2} \\
& \lesssim \sum_{E \in \mathcal{E}_h} \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(E)} \|\mathbf{u}_h\|_{L^2(E)}^{1/2} \|w_h\|_{L^4(E)} \\
& \lesssim \|\mathbb{D}^{1/2}(\mathbf{u}_h) \nabla c_h\|_{L^2(\mathcal{E}_h)} \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|w_h\|_{L^4(\Omega)}. \tag{B.32}
\end{aligned}$$

Similarly we have

$$\begin{aligned}
(\mathbf{u}_h c_h, \nabla w_h)_{\mathcal{E}_h} & \leq \sum_{E \in \mathcal{E}_h} \|\mathbf{u}_h\|_{L^2(E)} \|c_h\|_{L^4(E)} \|\nabla w_h\|_{L^4(E)} \\
& \leq \|\nabla w_h\|_{L^4(\mathcal{E}_h)} \|\mathbf{u}_h\|_{L^2(\Omega)} \|c_h\|_{L^4(\Omega)}. \tag{B.33}
\end{aligned}$$

For the third term in $B_{cq}(c_h, w_h; \mathbf{u}_h)$ we easily obtain

$$((q^I + q^P)c_h, w_h) \leq \|q^I + q^P\|_{L^2(\Omega)} \|c_h\|_{L^4(\Omega)} \|w_h\|_{L^4(\Omega)}. \tag{B.34}$$

For the upwind term, we remark that

$$|c_h^{\text{up}}| \leq \max \{ |c_h^+|, |c_h^-| \} \leq |c_h^+| + |c_h^-|.$$

Therefore, using the fact that $\mathbf{u}_h^+ \cdot \mathbf{n}_e = \mathbf{u}_h^- \cdot \mathbf{n}_e$, we can write

$$(c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_e \leq \int_e |c_h^+| |\mathbf{u}_h^+| |[w_h]| + \int_e |c_h^-| |\mathbf{u}_h^-| |[w_h]|.$$

We treat each term separately but in a similar fashion. By Cauchy-Schwarz's inequality and trace inequalities, we have

$$\begin{aligned} \int_e |c_h^+| |\mathbf{u}_h^+| |[w_h]| &\leq \left(\int_e |\mathbf{u}_h^+|^2 |c_h^+|^2 \right)^{1/2} \left(\int_e |\mathbf{u}_h^+| [w_h]^2 \right)^{1/2} \\ &\lesssim \|\mathbf{u}_h\|_{L^2(E_+^e)}^{1/2} \|c_h\|_{L^4(E_+^e)} \left(h^{-1} \int_e \{|\mathbf{u}_h|\} [w_h]^2 \right)^{1/2}. \end{aligned}$$

Next, we sum up over all interior faces and obtain

$$\sum_{e \in \Gamma_h} (c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_e \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|c_h\|_{L^4(\Omega)} \left(\sum_{e \in \Gamma_h} h^{-1} \int_e \{|\mathbf{u}_h|\} [w_h]^2 \right)^{1/2}, \quad (\text{B.35})$$

which, with (B.27), yields

$$(c_h^{\text{up}} \mathbf{u}_h \cdot \mathbf{n}_e, [w_h])_{\Gamma_h} \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)} \|c_h\|_{L^4(\Omega)} \left(\sum_{e \in \Gamma_h} h^{-3} \int_e [w_h]^4 \right)^{1/4}. \quad (\text{B.36})$$

We apply the same idea as in (B.35) to the last term and have:

$$(w_h^{\text{down}} \mathbf{u}_h \cdot \mathbf{n}_e, [c_h])_{\Gamma_h} \lesssim \|\mathbf{u}_h\|_{L^2(\Omega)}^{1/2} \|w_h\|_{L^4(\Omega)} \left(\sum_{e \in \Gamma_h} h^{-1} \int_e (1 + \{|\mathbf{u}_h|\}) [c_h]^2 \right)^{1/2}. \quad (\text{B.37})$$

Therefore, the bound (B.22) is obtained by combining (B.32), (B.33), (B.34), (B.36) and (B.37). $\square$

Lemma B.2.18. *Let w_h be in C_h , then we have*

$$\|w_h\|_{W^{1,4}(\mathcal{E}_h)} \lesssim \left(\sum_{E \in \mathcal{E}_h} \|w_h\|_{H^2(E)}^2 \right)^{1/2}. \quad (\text{B.38})$$

Proof. By the inverse inequality, we have

$$\|w_h\|_{W^{1,4}(E)} \lesssim h^{1-\frac{d}{4}} \|w_h\|_{H^2(E)},$$

which implies

$$\|w_h\|_{L^4(E)}^4 + \|\nabla w_h\|_{L^4(E)}^4 \lesssim h^{4-d} \|w_h\|_{H^2(E)}^4.$$

For the jump term, we have according to the trace inequality,

$$\|[w_h]\|_{L^4(e)} \lesssim h^{-\frac{1}{4}} \|w_h\|_{L^4(E_e^+)} + h^{-\frac{1}{4}} \|w_h\|_{L^4(E_e^-)}.$$

So, based on inverse inequality,

$$\|[w_h]\|_{L^4(e)} \lesssim h^{2-\frac{1+d}{4}} \|w_h\|_{L^4(E_e^+)} + h^{2-\frac{1+d}{4}} \|w_h\|_{L^4(E_e^-)}.$$

We simply sum the terms and use Jensen's inequality,

$$\|w_h\|_{W^{1,4}(\mathcal{E}_h)} \lesssim \left(\sum_{E \in \mathcal{E}_h} h^{4-d} \|w_h\|_{H^2(E)}^4 \right)^{1/4} \lesssim \left(\sum_{E \in \mathcal{E}_h} \|w_h\|_{H^2(E)}^2 \right)^{1/2}$$

□

These results are used extensively in the analysis to come concerning the stability and compactness theorem. In our analysis, we use a rather unconventional jump term to bypass the difficulty of the low regularity condition.

User manual for the software

In this part of the appendix, I provide some descriptions about the software developed for the miscible displacement simulations.

C.1 Installation and compilation

Since the code is based on DUNE and DUNE-PDELab, it is important to talk about the installation and compilation of the DUNE and DUNE-PDELab. The code is compatible only with the most current version of DUNE, namely DUNE 2.3.1. `gcc` 4.7 or greater is required for the compiler. On DaVinCI cluster, I load following modules

- `gcc/4.8.2`
- `openmpi/1.6.5-gcc`
- `cmake`

for compilations. For the code to be fully functional, additionally, we need external libraries listed as follows.

- `gmp`
- `metis`

- parmetis
- UGGrid
- OpenBLAS
- UMFPack
- SuperLU

They need to be compiled with the same compiler. After properly compiling the external libraries, we can create the root directory and extracting all the DUNE and DUNE-PDELab modules in the root directory. The folders are

- dune-common-2.3.1
- dune-geometry-2.3.1
- dune-grid-2.3.1
- dune-istl-2.3.1
- dune-localfunctions-2.3.1
- dune-typetree-2.3.1
- dune-pdelab-2.0.0
- dune-pdelab-howto-2.0.0

Then for a simple compilation, enter the DUNE root directory and type:

```
./dune-common-2.3.1/bin/dunecontrol all
```

This simple compilation is only for serial code without the external libraries. In order for us to run the miscible displacement simulation with DG discretization on structured and unstructured grid in parallel, we have to compile DUNE in following way:

```
./dune-common-2.3.1/bin/dunecontrol --opts=my.opts all
```

In my case, the option file `my.opts` is given as:

```
SHELL="bash"

GXX_WARNING_OPTS=" \
    -Wall \
    -Wunused \
    -Wmissing-include-dirs \
    -Wcast-align \
    -Wno-sign-compare \
    -Wno-packed-bitfield-compat \
    -Wno-unused-parameter"

GXX_OPTS=" \
    -fopenmp \
    -fno-strict-aliasing \
    -fstrict-overflow \
    -ffast-math \
    -fno-finite-math-only \
    -O3 \
    -march=native \
    -DNDEBUG=1"

LDFLAGS_OPTS=" \
    -Wl,-rpath \
    -Wl,/opt/apps/gcc/4.8.2/lib64
"

CONFIGURE_FLAGS=" \
    --enable-parallel \
    --enable-fieldvector-size-is-method \
```

```

--with-gmp=/home/jl48/local/external-new/gmp-gcc4.8 \
--with-superlu=/work/br1/jl48/external-new/SuperLU_4.3-gcc4.8 \
--with-superlu-dist=/work/br1/jl48/external-new/SuperLU_DIST_3.2 \
--with-alugrid=/work/br1/jl48/external-new/ALUGrid \
--with-ug=/work/br1/jl48/external-new/ug-3.11.0-gcc4.8 \
--with-metis=/work/br1/jl48/external-new/metis-gcc4.8 \
--with-parmetis=/work/br1/jl48/external-new/parmetis-gcc4.8 \
--with-umfpack-includedir=/home/jl48/local/external-new/UMFPACK-gcc4.8/
include \
--with-umfpack-libdir=/home/jl48/local/external-new/UMFPACK-gcc4.8/lib \
--with-blas="/work/br1/jl48/external-new/OpenBLAS-gcc4.8/lib/
libopenblas.a -pthread\"
"

```

and it should be placed in the root directory. The user should make changes in the option file for the path of the external libraries and compiler if they differ.

During the compilation, user might encounter compilation failure for `dune-istl`. Most likely, the problem is caused by the timer. To resolve the issue, simply add:

```

#ifndef TIMER_USE_STD_CLOCK
#define TIMER_USE_STD_CLOCK
#endif

```

at the beginning of the `timer.hh` header in the directory:

```

dune-common-2.3.1/dune/common/

```

Once the compilation is successful, user can extract `dune-miscible-flow` into the root directory. For compilation type:

```

./dune-common-2.3.1/bin/dunecontrol --opts=my.opts
--only=dune-miscible-flow all

```


When the compilation is completed, the user should have a miscible displacement simulation driver in the directory:

`dune-miscible-flow/src`

with the file name `dune-miscible-flow`. In the next section I introduce anatomy of the code for `dune-miscible-flow`.

C.2 Anatomy of dune-miscible-flow

In this section, I introduce components of simulator for users to get a better understanding of the content and capability of the research code. The source code are contained in the directory:

`dune-miscible-flow/src`

The content of the code is as follows,

- the driver

- `dune-miscible-flow.cc`:

- * problem setup
 - * grid setup
 - * finite element space setup
 - * discretization setup
 - * solver setup
 - * time loop
 - * input and output

- discretization routines:

- `diffusionccfv.hh`

- * cell-center finite volume (CCFV) discretization for Darcy's system
- `diffusiondg.hh`
 - * DG discretization for Darcy's system
- `convectiondiffusionccfv.hh`
 - * CCFV discretization for transport system
- `convectiondiffusiondg.hh`
 - * DG discretization for transport system
- Solver routine:
 - `cg_to_dg_prolongation.hh`
 - * subspace correction
 - `ovlp_amg_dg_backend.hh`
 - * AMG solver setup
- Post-processing routines:
 - `slope-limter.hh`
 - * slope-limiter
 - `utility.hh`
 - * flux reconstruction
 - * error estimate
 - * permeability generating
- Problem files:
 - `dune_miscible_flow-param-5spot-fingering.hh`
 - * radial flow viscous fingering simulation problem with diagonal grid

-
- `dune_miscible_flow-param-5spot-fingering-parallel.hh`
 - * radial flow viscous fingering simulation problem with parallel grid
 - `dune_miscible_flow-param-5spot.hh`
 - * quarter of 5-spot simulation problem
 - `dune_miscible_flow-param-analytical.hh`
 - * problem with analytical solution
 - `dune_miscible_flow-param-fingering-disc.hh`
 - * viscous fingering simulation problem on a disc
 - `dune_miscible_flow-param-fingering.hh`
 - * core flooding viscous fingering simulation problem
 - `dune_miscible_flow-param-lens.hh`
 - * miscible displacement problem with heterogeneous permeability on a square
 - `dune_miscible_flow-param-spe10.hh`
 - * flow problem with SPE10 permeability model with Dirichlet boundary condition
 - `dune_miscible_flow-param-spe10-well-injection.hh`
 - * flow problem with SPE10 permeability model with well injection

Users are also given following options:

- `#define USE_PURE_NEUMANN`: solve problem with no-flow boundary condition
- `#define USE_CN`: solve the problem using Crank-Nicolson method (implicit Euler by default)
- `#define USE_UGGRID`: use unstructured grid (quadrilateral mesh by default)

- `#define USE_SIMPLEX`: use triangular (2D) or tetrahedral mesh (3D) for unstructured grid

Once the users have the problem and options setup, to compile go to the directory:

```
dune-miscible-flow/src
```

and type:

```
make
```

The code is recompiled accordingly.

C.3 Running the simulation

In this section, I explain how to run the code. For users to run the code type:

```
mpiexec -n <#procs> dune-miscible <nx> <ny> <nz> <level> <tend>
<timestep> <sigma_p> <sigma_c> <addintorder>
```

The parameters are given as follows:

- `<#procs>`: number of processes
- `<nx>`: numbers of the cells in x directions
- `<ny>`: numbers of the cells in y directions
- `<nz>`: numbers of the cells in z directions
- `<level>`: level of bisection refinement
- `<tend>`: the final time of the simulation in sec
- `<timestep>`: time step size
- `<sigma_p>`: penalty parameter for Darcy's system

- `<sigma_c>`: penalty parameter for transport system
- `<addintorder>`: additional order for the numerical quadrature

By building the application on DUNE and DUNE-PDELab, I expect the code to be easily modifiable and maintainable by others to further the study and research in the area of numerical methods for porous media flows.

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