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# Multiscale modeling of flow and geomechanics

**Abstract:** Numerical methods for subsurface modeling are currently being extended to account for geomechanical effects. These include locally mass conservative discretizations such as mixed and multipoint flux finite elements, discontinuous Galerkin finite elements, and multiscale mortar finite elements. Advanced techniques are also being applied such as a posteriori error estimation, physics-based preconditioners, and stochastic modeling. This paper describes the authors' work centered around the research simulator Integrated Parallel Accurate Reservoir Simulator, including key points of previous work and current developments.

**Keywords:** Multiscale, Mixed Finite Element, Mortar Finite Element, Multipoint Flux, Discontinuous Galerkin, Porous Media Flow, Geomechanics.

**Mathematics Subject Classifications 2010:** 65M55, 65M60, 76S05

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## 1 Introduction

Algorithms are currently in development that will enable scientists and engineers to readily model complex flow processes in porous media taking into account the accompanying deformations of the porous solids. Fluid motion and solid deformation are inherently coupled, but current major commercial packages for multiphase flow in porous media only model porous flow while solid deformation is normally integrated into a study in an ad hoc manner or must be included through complex iterations between one software package that models fluid flow and a separate package that models solid deformations. There are numerous field applications that would benefit from a better understanding and integration of porous flow and solid deformation. Important applications in the geosciences include environmental cleanup, petroleum production, solid waste disposal, and carbon sequestration, while similar issues also

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arise in the biosciences and chemical sciences. Examples of field applications include surface subsidence, pore collapse, cavity generation, hydraulic fracturing, thermal fracturing, wellbore collapse, sand production, fault activation, and disposal of drill cuttings. The aforementioned phenomena entail both economic as well as environmental concerns. For example, surface subsidence related to both consolidation of surface layers and fluid withdrawals from oil and gas reservoirs have had a significant impact on the greater Houston area over the last century and have resulted in the destruction of infrastructure, buildings, and private homes. Subsidence caused by oil and gas production also has been an issue of substantial economic importance in the North Sea oil fields. In some cases multibillion dollar adjustments to production platforms have been required due to the response to unexpected subsidence of the sea floor driven by oil production.

Another important related class of problems involves CO<sub>2</sub> sequestration, which is proposed as a key strategy for mitigating climate change driven by the high levels of anthropogenic CO<sub>2</sub> being added to the atmosphere. In a CO<sub>2</sub> sequestration project, fluid is injected into a deep subsurface reservoir (rather than being produced or extracted), so that inflation of the reservoir leads to uplift displacement of the overlying surface. As long as a CO<sub>2</sub> sequestration site is removed from faults, this uplift is several centimeters, while its wavelength is in tens of kilometers, so that the uplift poses little danger to buildings and infrastructure. Nevertheless the uplift displacements are of great interest for nonintrusive monitoring of CO<sub>2</sub> sequestration. Indeed, uplift can be measured with a submillimeter precision using Interferometric Synthetic Aperture Radar (InSAR) technology [148]. The feasibility of this approach has been established by measuring the uplift displacements over the first commercial scale CO<sub>2</sub> sequestration project conducted by BP in In Salah Algeria [130, 148]. In contrast, intrusive monitoring via drill holes bored into the reservoir is expensive, with costs of several million dollars per well. Furthermore, such wells are the most likely pathway for future leakage of sequestered CO<sub>2</sub> back into the atmosphere. Of course, if a CO<sub>2</sub> sequestration site is close to a fault, one should be concerned about triggering instability leading to large surface displacements that may result in significant losses.

Numerical methods for subsurface modeling are currently being extended to account for geomechanical effects. These include local mass conservative discretizations such as mixed and multipoint flux finite elements, discontinuous Galerkin (DG) finite elements, and multiscale mortar finite elements. Advanced techniques are also being applied such as a posteriori error estimation, physics-based preconditioners, and stochastic modeling. This chapter describes the authors' work centered around the research simulator Integrated Parallel Accurate Reservoir Simulator (IPARS), including key points of previous work and current developments.

The outline of this chapter is as follows. In Section 2, we give background on the multidomain methodology, discretization methods, and coupled flow and geomechanics. In Section 3, we describe multiscale multiphysics discretizations for flow and geomechanics. In Section 4, we describe multiscale domain decomposition solvers

and preconditioners. In Section 5, we describe a posteriori error estimation and time-stepping. In Section 6, we describe uncertainty quantification, verification, and validation. In Section 7, we describe several applications, including compositional modeling of multiphase flow, fixed stress iterative coupling scheme, and plasticity modeling. In Section 8, we give a summary and some conclusions. In Appendix 8, we give a list of nomenclature used throughout the chapter.

## 2 Background

In this section, we give a brief overview of the modeling and computational techniques that will be discussed in further sections.

### 2.1 Multidomain methodology

Most geological systems consist of different regions or subdomains, where different physical processes may occur. These relevant processes may occur on different spatial and temporal scales, and may require different models and data. Furthermore, these processes may interact, so that coupling mechanisms must be employed in a mathematically and physically meaningful fashion in order to obtain a global solution. The multidomain methodology [8, 119, 120, 161] has been developed to address these issues in an accurate and efficient fashion. The spatial physical domain is decomposed (i.e. decoupled) into different blocks (subdomains). The governing equations hold locally in each subdomain and physically driven matching conditions are imposed weakly on interfaces in a numerically stable and accurate way, through the use of mortar finite element spaces [8, 10].

Some computational advantages of the multidomain approach are: (1) *multiphysics*, different physical processes or mathematical models in different parts of the domain may be coupled in a single simulation (e.g. coupling single-phase, two-phase, and three-phase flows); (2) *multinumerics*, different numerical techniques may be employed on different subdomains (e.g. coupling mixed finite element (MFE) and DG methods or coupling explicit, adaptive implicit, and fully implicit formulations); (3) *multiscale resolution and adaptivity*, highly refined regions or fine scale models may be coupled with more coarsely discretized regions, and dynamic grid adaptivity may be performed locally on each block; and (4) *multidomains*, highly irregular domains may be described as unions of more regular and locally discretized subdomains with the possibility of having interfaces with nonmatching grids. The latter allows for the construction of grids that follow large-scale geological features such as faults, heterogeneous layers, and other internal boundaries. This grid construction is critical for discretization accuracy. In addition, the appropriate choice of physical models and numerical methods can substantially reduce the computational cost with

no loss of accuracy. The multidomain approach leads to a naturally parallelizable algorithm of the domain decomposition type. As a result, it may be combined with different uncertainty assessment and model reduction techniques and, moreover, implemented efficiently on massively parallel computers with near optimal computational load balance and minimal communication overhead.

### 2.1.1 Parallel multiphysics simulator

Parallel capability is essential because field applications involving simultaneous flow and deformation require considerable computing resources. Our current work in this area is building upon the IPARS developed at UT Austin by researchers at the Center for Subsurface Modeling [156] in collaboration with University of Pittsburgh. IPARS was designed to enable students to learn about subsurface simulation, to develop physical models of subsurface processes, and to implement them easily in high-performance parallel computing environments. IPARS provides multiscale and multiphysics capabilities to model multiphase and multicomponent (compositional) flow in porous media [154] coupled with reactive transport [7]. The reactive transport model can handle multiple components, multiple flowing and stationary phases, and can treat general biogeochemistry including adsorption, ion-exchange, precipitation, dissolution, bioremediation, and radionuclide decay. The multiscale and multiphysics capabilities are achieved through the software Seine/MACE [112, 176], which provides a dynamic geometry-based shared space model to support parallel coupled, multi-block simulations and scalable realizations. IPARS solvers are based on state-of-the-art techniques for nonlinear and linear problems including Newton–Krylov methods enhanced with algebraic multigrid, two-stage, and physics-based preconditioners [94, 95]. IPARS has also been used to solve optimization and parameter estimation problems in reservoir management [91]. Software exists to perform global stochastic optimization via the simultaneous perturbation stochastic approximation and the very fast simulated annealing approaches. The coupling of this software with IPARS uses Discover/AutoMate [111], which is an autonomic Grid middleware that enables dynamic and interactive computational work-flows supporting discovery and interactions between computational components to achieve application objectives. As opposed to commercial simulators, the IPARS source code is fully available to researchers.

Currently, IPARS includes classical elasticity as the solid mechanics model [60, 61]. However, modeling of compaction and subsidence requires solid mechanics models that take into account creep, plasticity, damage accumulation, and possibly other microstructural changes. These models must be properly coupled to the flow models. This is a significant issue because characteristic times associated with deforming solids undergoing microstructural changes are typically much longer than those associated with flow. Specific details will be discussed below.

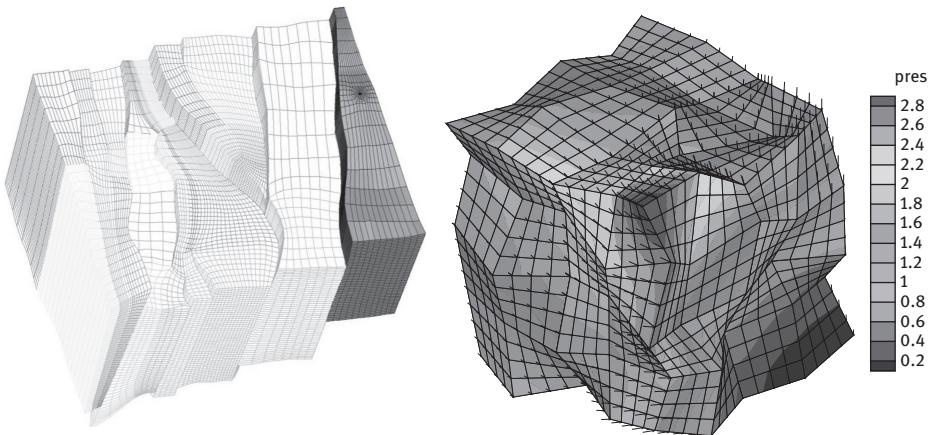
## 2.2 Discretization methods

We focus on flow discretizations based on variants of MFE and DG methods that provide local mass conservation and accurate treatment of irregular grids and rough coefficients.

### 2.2.1 Mixed finite element (MFE) and related methods

MFE discretizations [27] are variational methods that approximate accurately both the scalar variable and the flux. They are locally mass conservative with continuous fluxes. Lack of these properties may lead to nonphysical behavior such as spurious mass sources and discontinuous streamlines [87]. Applications of MFE methods to flow in porous media can be traced back to [48, 49]. Mixed methods have been successfully applied to many applications, including multiphase flow in porous media [119, 161], Stokes flow [27], and electromagnetics [46].

Geological applications present a significant challenge for numerical methods, since irregular geometries and heterogeneities such as faults and layers require methods to handle highly distorted grids and discontinuous coefficients, see Figure 6.1 (left). It has been established in recent years that some other locally conservative methods that work well on rough grids and coefficients, such as the mimetic finite difference (MFD) methods [20, 81, 82], the control-volume mixed finite element (CVMFE) methods [28, 37, 38], and the multipoint flux approximations (MPFA) [3] are closely related to MFE methods. Superconvergence for MFD and CVMFE has been established using these relations [22, 129]. Motivated by the MPFA, a new method, the multipoint flux mixed finite element (MFMFE) method has been recently developed [83, 164]. The method is more efficient than and comparable in accuracy to MFE, MFD, and CVMFE methods on irregular grids and rough coefficients. Moreover, since it leads to a harmonically averaged coefficients, the method is more accurate on rough grids and coefficients than existing cell-centered MFE methods [9, 11, 128, 155]. The method is based on the Brezzi–Douglas–Marini (BDM) [26] spaces in 2D or the Brezzi–Douglas–Duran–Fortin (BDDF) [25] spaces in 3D on simplicial, quadrilaterals, or hexahedral grids. A special quadrature rule allows for local elimination of the velocity that reduces the method to a cell-centered positive definite system for the pressure. Most recently a nonsymmetric MFMFE method has been developed that performs better than the symmetric MFMFE method on highly distorted hexahedra [160]. The method has been implemented in the parallel Stokes–Darcy simulator SDF developed jointly at University of Pittsburgh and The University of Texas at Austin for single-phase flow, see Figure 6.1 (right), and IPARS for multiphase flow.



**Figure 6.1:** Left: hexahedral mesh for a geological domain with faults and layers. Right: single-phase flow computation on rough hexahedral mesh using the MFMFE method.

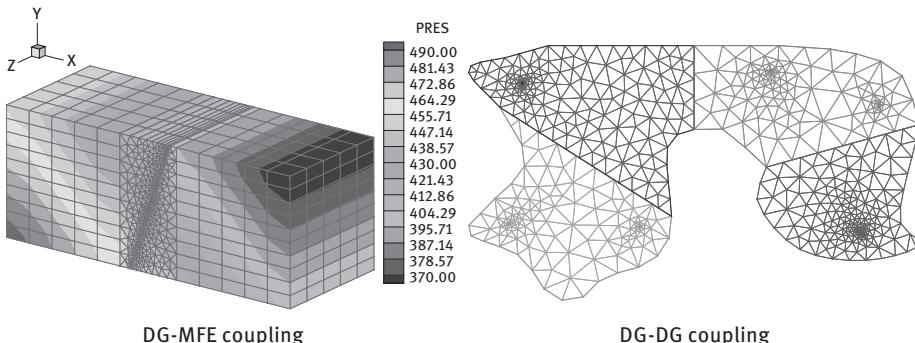
### 2.2.2 Discontinuous Galerkin (DG) methods

DG methods are finite element methods that use discontinuous approximations. Examples of these schemes include the Bassi and Rebay method [19], the local discontinuous Galerkin (LDG) [4, 41] methods, the Oden, Babuska, Bauman [110] method, and interior penalty Galerkin methods [44, 125, 126, 166]. Application of these methods to a wide variety of problems may be found in [40]. DG methods have a number of attractive features, e.g. they are locally mass conservative, provide robust high-order approximations on unstructured grids, and can deliver exponential rates of convergence on adaptively refined meshes.

DG methods are very effective for reactive transport and hyperbolic equations [127]. In [142], dynamic mesh adaptation is utilized to resolve time-dependent transport adequately without slope limiting. It is important to note that DG schemes retain local mass conservation during dynamic mesh adaptation. An LDG method is employed in [149] for contaminant transport in coupled subsurface-surface hydrological systems. The method is robust and accurate even for small or no diffusion. In IPARS, a DG method is employed to solve the saturation/concentrations equations in multiphase/compositional flows [145].

### 2.2.3 Multiscale mortar methods

Mortar MFE methods [8, 104, 120, 157] have been used successfully to impose matching conditions on interfaces in multidomain formulations. Mortar couplings allow for nonmatching grids across interfaces, including coupling highly refined with coarse regions. A posteriori error estimates have been developed to guide adaptive refinement of mortar and subdomain grids [10, 114, 163]. Mortar methods can also be

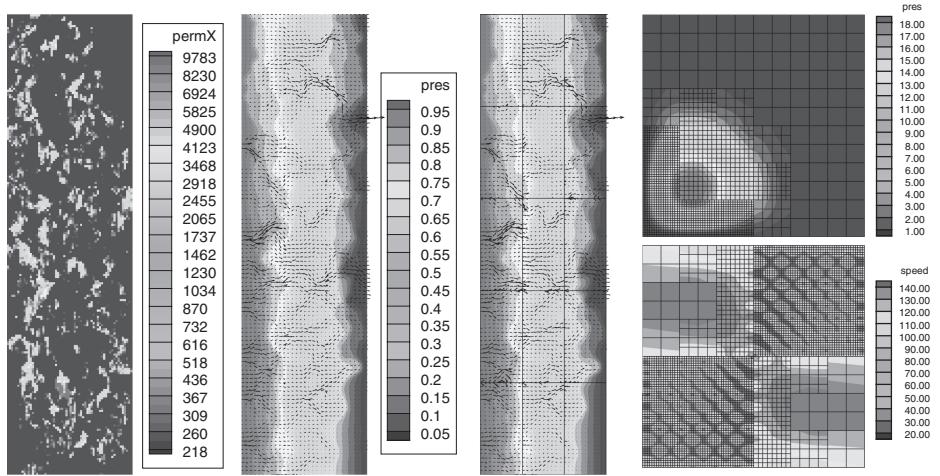


**Figure 6.2:** Left: pressure field from a coupled DG-MFE simulation of an aquifer with a fault. Right: grid partitioning across processors for a DG domain decomposition simulation of a reservoir with wells.

used to couple different discretization methods. For example, DG-MFE couplings have been developed in [72]. It is shown there that introducing mortar spaces for DG discretizations leads to a natural domain decomposition framework for DG; see Figure 6.2 for examples of DG–MFE and DG–DG couplings for reservoir simulation. The left plot in Figure 6.2 illustrates the flexibility of the mortar approach: an unstructured DG discretization around a fault is coupled with a structured MFE method in the rest of the domain. Mortar couplings between a pore scale flow model and a continuum Darcy’s flow model have also been developed [16].

Mortar methods also lead to efficient and accurate multiscale discretizations. The need for such methods arises since full fine scale resolution of flow in highly heterogeneous media is often computationally intractable. To effectively address this problem, the variational multiscale method [78, 79] and multiscale finite elements methods [2, 5, 6, 36, 52, 77, 84] have been developed.

The multiscale mortar MFE method [10] is based on both domain decomposition [73] and mortar finite elements. The porous media is divided into a series of small subdomains (or coarse elements), over which the original problem is posed. These subproblems are coupled together using a low degree-of-freedom mortar space defined on a coarse scale mortar grid. The implementation of the method is based on a nonoverlapping domain decomposition algorithm that reduces the global fine scale problem to a coarse grid interface problem. The mortar provides a natural Dirichlet pressure boundary condition for the subdomain problems, which can be solved easily because of their relatively small size. The (weak) velocity flux mismatch provides a criterion for updating the mortar pressure, and iterations are carried out until convergence is achieved. Moreover, as shown in [10], the use of higher order mortar approximation allows for compensating for the coarseness of the grid scale and maintaining good (fine scale) overall accuracy. The multiscale mortar approach has also been analyzed for DG–DG and DG–MFE couplings [72], as well as for slightly compressible single-phase flow [90].



**Figure 6.3:** Left: Permeability field (left), fine scale solution (middle), and multiscale solution with  $3 \times 5$  subdomains and a single linear mortar per interface (right). Right: Adaptive multiscale mortar MFE computations; top: pressure with boundary layer; bottom: velocity magnitude with highly oscillating permeability in certain regions.

An efficient implementation of the multiscale mortar mixed finite element method based on a multiscale flux basis has been described in [66]. The basis is precomputed by solving fine scale Dirichlet subdomain problems for each coarse scale mortar degree of freedom. The total cost is solving fixed number of local fine scale problems and a coarse scale interface problem. This is comparable to other existing multiscale methods. However, the multiscale mortar MFE method is more flexible than the variational multiscale method and multiscale finite elements, because one can improve global accuracy by refining the local mortar grid where needed. Furthermore, the multiscale basis stores only interface information, which requires significantly less memory. The efficiency and accuracy of the multiscale mortar MFE method are illustrated in Figure 6.3 (left) for a comparison between the pressure and velocity computed on a fine  $60 \times 220$  grid and the solution computed with the multiscale mortar method on a coarse  $3 \times 5$  grid for flow in a fluvial reservoir (the permeability data was taken from layer 85 of the 10th SPE Comparative Project [39]). Clearly, there is little disagreement between the two solutions. The cost of the multiscale solution is 26 fine scale subdomain solves, compared to 130 for the fine scale solution.

### 2.3 Coupled flow and geomechanics

Numerical simulation of coupled flow and geomechanics has great potential to answer many questions in energy and environmental research. In stress-sensitive reservoirs, variation of the effective stress resulting from fluid production may induce rock

deformation, causing permeability reduction and thereby compromising expected productivity. In other applications, when CO<sub>2</sub> is injected in saline aquifers, the impact on uplifting is still not completely understood.

A comprehensive survey of the reservoir engineering literature for coupling geomechanical effects with multiphase flow on the basin scale can be found in [60], Section 1.3.2. These simulations have a time scale of several decades and a desired resolution of about 1m. Coupled flow and geomechanics has also been concurrently investigated for purposes of sedimentary basin simulation in such works as [134]. Here the simulations have a time scale of millions of years, with simplified mechanics and an emphasis on other types of physics such as rock deposition and hydrocarbon formation.

Computational frameworks for solving poroelasticity problems for the Biot system have been proposed in [121, 122]. The formulation is based on a mixed method for flow equation and the CG method for solid equations. Theoretical convergence error estimates were derived for a strictly positive constrained specific storage coefficient. Further work addressed the problem of eliminating locking or removal of nonphysical pressure oscillations via the use of DG for elasticity [123]. Furthermore, in [17] the numerical solution of a coupled geomechanics and flow in a stress-sensitive porous media reservoir flow model was considered. In this model, the variation of the effective stress resulting from fluid production may induce deformation of the rocks and cause permeability reduction. This effect may significantly reduce expected productivity. Convergence was established in the  $L^2$ -norm for the pressure, in the average fluid velocity, as well as in the  $H^1$ -norm for the deformation.

Coupled flow and geomechanics simulations are large-scale problems, bringing a great challenge for solvers. In [60, 61], an iterative coupling procedure for coupled multiphase fluid flow and linear elasticity for a deformable porous solid was studied, and showed scalability on up to 512 processors. The pressure solutions from solving the fluid flow equation are fed into a linear elasticity solver as an additional body force for solid skeletons. The computed displacements are used to solve for an updated flow field. One can iterate between the two solvers until the mass balance satisfies a desired tolerance. Multilevel domain decomposition preconditioners using super-coarsening multigrid and displacement decomposition have been utilized to accelerate the iteration [62, 141]. In these works the iterative coupling approach was shown to provide improved stability and material balance compared to explicit formulations, while outperforming fully coupled formulations. The iterative coupling approach and efficient parallel implementation have become a practical, fast, and accurate computational tool for the evaluation of ground surface subsidence due to water and oil extraction.

In [71], a parallel domain decomposition method for solving a linear elasticity system was developed. Data across subdomains are transmitted by jumps, as in DG,

using mortar finite elements. The global system is reduced to a mortar interface problem and solved in parallel. In [70] this work was extended to couple a time-dependent poroelastic model in a localized region with an elastic model in adjacent regions. Each model was discretized independently on nonmatching grids and the systems were coupled using DG jumps and mortars. At each time step, an interface problem is solved, with subdomain solves performed in parallel. An algorithm was also proposed where the computation of the displacement is time lagged. In each case, the matrix of the interface problem is positive definite. Error estimates were established.

In order to handle irregular geometries and heterogeneities in the porous media for modeling subsurface flow in subsiding rock, the MFMFE flow model in IPARS has been coupled with the geomechanics simulator. The analysis of this coupled model is presented in [116]. Ongoing work currently involves simulations with linear elasticity coupled with fully compositional flow. Results for these simulations can be found in Section 7.1.

Numerical stability is an important concern for multiphysics problems. For example, Figure 6.5 (right)(a) shows a nonphysical oscillatory temperature profile near an injection oil well obtained from a continuous Galerkin (CG) finite element method when solving a convection-dominated thermo-poro-elasto-plasticity problem. This undesired effect was eliminated in Figure 6.5 (right)(b) using DG methods. The three coupled fields, i.e. the displacement of solid skeleton, pore pressure of fluid flow, and temperature of heat conduction and convection, were approximated by equal-order discontinuous spaces, and upwinding was incorporated on element interfaces to handle the convection effect [98, 100].

To improve the efficiency of the method, coupled CG-DG formulations were proposed in [101], where DG elements are used only in subdomains with large pressure gradients [101]. To facilitate the application of DG methods for solid mechanics problems, a nodal-based implementation for DG methods was developed in [99], where DG methods were naturally embedded in a popular CG finite element program through simply breaking continuous elements and adding interface stiffness.

Numerical formulations based on CG methods for solving classic plasticity problems are mature [138]. Quadratic convergence rates for the nonlinear Newton iteration are predominantly achieved by deriving local material integrators [80, 139] in commercial CG finite element codes. In [102], a consistent incomplete interior penalty DG formulation for modeling plasticity problems was presented, proving rigorous stability and quadratic convergence rates. These formulations used classic  $J_2$  plasticity and geomechanics Drucker–Prager plasticity models. Most importantly, this work demonstrated that DG methods could provide more accurate material yielding profiles than CG methods, using stresses on element surface quadrature points instead of interior points. More information about the plasticity models can be found in Section 7.3.

### 3 Multiscale multiphysics discretizations for flow and geomechanics

Using the domain decomposition approach, it is possible to formulate systems with complex multiphysics coupling, where subdomains may have mechanics-only models, or models with coupled mechanics and flow. Such an approach would generalize the preliminary elastic–poroelastic coupling approach described in [70], and is currently being integrated into the robust reservoir simulator IPARS. The admissible types of mechanics include both elasticity and plasticity, and the different types of flow may include varying numbers of phases and components. Appropriate models can be placed throughout the domain, given a priori knowledge about the behavior of problems, motivated by EOR and CO<sub>2</sub> sequestration applications. The relations used to couple these models require the formulation of well-posed and physically meaningful interface conditions. In practice, mortar finite elements are used to decouple computation, and allow each subdomain to use the solver and time step that works best for its model. The interface problem itself can be efficiently implemented using the multiscale preconditioner approach [65, 159].

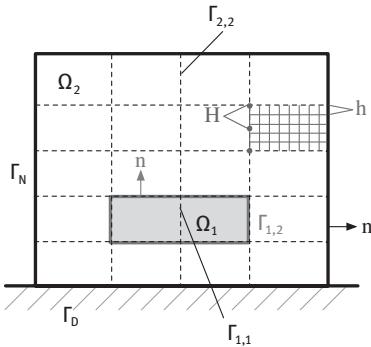
We illustrate our approach for the following model problem. Let  $\Omega = \Omega_1 \cup \Omega_2$  be the simulation domain, where  $\Omega_1$  is the coupled flow-geomechanics domain, often referred to as the pay-zone, and  $\Omega_2$  is a domain surrounding  $\Omega_1$ , the nonpay-zone, where we model only rock deformation. In Biot's consolidation mathematical model, solid deformation is quasi-statically coupled with single-phase flow in porous media by

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{f} \quad \text{in } \Omega, \quad (6.1)$$

$$\mathbf{z} = -\mathbf{K}(\nabla p - \rho \mathbf{g}) \quad \text{in } \Omega_1, \quad (6.2)$$

$$\frac{\partial}{\partial t}(c_0 p + \alpha \nabla \cdot \mathbf{u}) + \nabla \cdot \mathbf{z} = q \quad \text{in } \Omega_1, \quad (6.3)$$

where  $\boldsymbol{\sigma}$  is the Cauchy (total) stress tensor,  $\mathbf{u}$  is the displacement of the porous rock,  $p$  is the fluid pressure,  $\mathbf{z}$  is the Darcy velocity,  $\mathbf{K}$  is a symmetric and uniformly positive definite tensor representing the rock permeability divided by the fluid viscosity,  $\rho$  is the fluid density,  $\mathbf{g}$  is the gravity vector,  $\mathbf{f}$  is the body force,  $q$  is the source or sink term,  $c_0$  is the specific storage coefficient, and  $\alpha$  is the Biot–Willis constant. We assume that  $\Omega_1$  and  $\Omega_2$  are further decomposed into a union of subdomains,  $\Omega_1 = \cup \Omega_{1,i}$ ,  $\Omega_2 = \cup \Omega_{2,i}$ . The rock deformation in each subdomain  $\Omega_{1,i}$  is governed either by a linear elasticity or a plasticity model. We denote the elasticity and the plasticity regions in  $\Omega_1$  by  $\Omega_1^e$  and  $\Omega_1^p$ , respectively. We assume linear elasticity in the nonpay-zone  $\Omega_2$ . The plasticity model is a nonlinear geomechanics model for subsidence of ground surface, sand production, and oil well failure due to fluid extraction or injection. The permanent deformation of solid skeletons is modeled using rate-independent plasticity theories. The long-term effect on deformation is addressed by material creep



**Figure 6.4:** Multiscale mortar modeling methodology for poroelasticity–elasticity coupling.

theories. Thermal variations may also affect the strain. More precisely, we have

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} - \alpha p \mathbf{I} \quad \text{in } \Omega_1, \quad \boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} \quad \text{in } \Omega_2, \quad (6.4)$$

where  $\tilde{\boldsymbol{\sigma}}$  is the effective stress satisfying

$$\tilde{\boldsymbol{\sigma}} = \mathbf{D}(\boldsymbol{\epsilon}) \quad \text{in } \Omega_1^e \cup \Omega_2, \quad \tilde{\boldsymbol{\sigma}} = \mathbf{D}(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^p - \boldsymbol{\epsilon}^c - \boldsymbol{\epsilon}^T) \quad \text{in } \Omega_1^p. \quad (6.5)$$

In the above,  $\boldsymbol{\epsilon}$ ,  $\boldsymbol{\epsilon}^p$ ,  $\boldsymbol{\epsilon}^c$ , and  $\boldsymbol{\epsilon}^T$  are the total strain, plastic strain, creep strain, and thermal strain, respectively, and  $\mathbf{D}$  is the fourth-order elasticity tensor. The total strain is the symmetric gradient of the displacement,  $\boldsymbol{\epsilon} = 1/2(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ . The plastic strain is given later in equation (6.18), and the creep strain and thermal strain can be found in works on thermo-elasto-plasticity, such as [98]. Details on modeling the nonlinear stresses, including fractures, are given in Section 7.3.

As shown in Figure 6.4, the following conditions are imposed on subdomain interfaces.

Continuity of medium:	$[\mathbf{u}] = \mathbf{0}$	on $\Gamma_{1,1}, \Gamma_{1,2}, \Gamma_{2,2}$
Continuity of normal stress:	$[\boldsymbol{\sigma} \mathbf{n}] = \mathbf{0}$	on $\Gamma_{1,1}, \Gamma_{1,2}, \Gamma_{2,2}$
No-flow outside pay-zone:	$\mathbf{z} \cdot \mathbf{n} = \mathbf{0}$	on $\Gamma_{1,2}$
Continuity of pressure:	$[p] = 0$	on $\Gamma_{1,1}$
Continuity of normal flux:	$[\mathbf{z} \cdot \mathbf{n}] = 0$	on $\Gamma_{1,1}$

Here,  $\Gamma_{1,1} = \bigcup_{i < j} \partial\Omega_{1,i} \cap \partial\Omega_{1,j}$ ,  $\Gamma_{2,2} = \bigcup_{i < j} \partial\Omega_{2,i} \cap \partial\Omega_{2,j}$ , and  $\Gamma_{1,2} = \partial\Omega_1 \cap \partial\Omega_2$ . One can further consider multiphysics flow models in  $\Omega_1$ , where the flow on each subdomain  $\Omega_{1,i}$  can be either single phase, two phase, black oil, or compositional, as described in Section 7.2. All of these flow models have been implemented in IPARS.

The discretization of the above multidomain multiphysics system involves two main components – subdomain discretizations for (6.1)–(6.3) and interface discretizations for the coupling conditions. For the numerical approximation of the flow equa-

tions (6.2) and (6.3) the focus is on discretizations that preserve the physical principles that (1) mass is conserved locally and, in the case of multiphase or compositional flow, (2) diffusion or dispersion cannot produce local maxima or minima in the concentrations. Numerical approximation schemes that fail to preserve these principles may lead to erroneous results. Moreover, current discretizations with rectangular or brick-like elements in 3d are being improved so that the computational mesh follows the geometrically irregular geologic strata, and allows local refinement to increase resolution in regions where the PDE solution varies greatly, as near wells or faults [115, 158]. Further investigations are planned for the MFMFE methods [83, 160, 164], MFD methods [21, 22, 81, 97], and DG methods [72, 124] for solving the pressure equation on general hexahedral meshes. DG and LDG methods will be used for transport processes [115, 127, 142], since they provide conservative nonoscillatory approximations of advection dominated and hyperbolic systems and accommodate irregular and nonconforming meshes. All of the considered methods exhibit local mass conservation. For the discretization of the geomechanics equation (6.1) DG methods that avoid locking and nonphysical pressure oscillations can be employed [123].

The interface conditions are discretized via coarse scale mortar finite elements consisting of either discontinuous or continuous polynomials of a certain degree on the interface mesh. This approach leads to efficient and accurate multiscale approximations. More precisely, for the elasticity interface conditions formulations using DG jumps and mortars [70–72] as well as direct mortar orthogonality can be utilized. Both approaches allow to decouple the subdomains, resulting in a domain decomposition algorithm suitable for parallel implementation. For the flow interface conditions one can employ mortar finite elements for MFMFE [165], MFD [21], and DG [72] methods. In multiphysics flow models, only continuity of flux of the phases present in the neighboring subdomains is imposed, leading to different number of mortar variables on different interfaces [120, 174]. All of these papers contain many examples where mortar discretizations have been applied.

## 4 Multiscale domain decomposition solvers and preconditioners

The numerical simulation of flow requires physics-based linear and nonlinear solvers that can efficiently cope with a wide range of geometrical complexities and scales involved in the porous medium. In our work we emphasize nonoverlapping domain decomposition algorithms [8, 10, 73, 118, 161]. The global system is reduced to an interface (mortar) problem, which is solved by an iterative method. Each interface iteration requires solving subdomain problems that may be based on different physical, mathematical, and/or numerical models. The balancing preconditioner [10, 42, 105, 118] and interface multigrid [162] provide efficient ways to speed up the interface

iterations for problems with large jumps in material coefficients across interfaces. In these problems, the actions of subdomain operators are needed. These subdomains have full fine scale heterogeneity, without any simplification. The accuracy of the method is entirely determined by the number of mortar degrees of freedom on the interface.

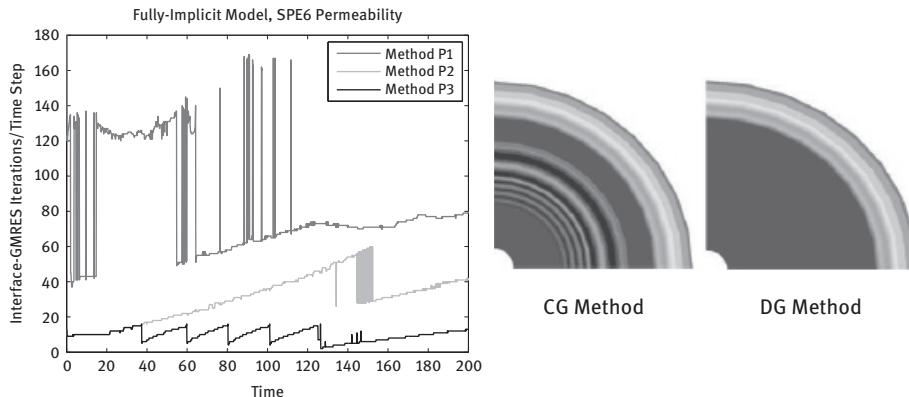
Recognizing that these subdomain problems represent the dominant computational cost in large-scale interface problems, research into a new implementation has shown to greatly improve computational efficiency by precomputing a multiscale flux basis before the interface iteration begins [66]. This basis contains discrete Green's functions corresponding to the degrees of freedom along the subdomain interfaces. Taking linear combinations of multiscale basis functions replaces the need to solve additional subdomain problems during the interface iteration. Since the number of mortar degrees of freedom is a controllable quantity, one may bound the number of linear systems required during the interface iteration, leading to a significant and measurable decrease in run-time.

For linear elliptic problems, the multiscale basis implementation has been shown to be competitive or superior to a state of the art balancing preconditioner [66]. Moreover, multiscale basis techniques can be combined with various preconditioners in order to further optimize the interface problem. As the multiscale basis implementation promises to allow greater scalability and tractability, a significant amount of effort has been invested into implementing these techniques into the parallel flow simulators SDF and IPARS in anticipation of future ways to utilize this approach.

The construction of a multiscale basis for the mortar mixed finite element method in [66] has led to the development of an efficient multiscale preconditioner [159]. The general idea is to compute the multiscale basis using a carefully selected training operator and to apply this multiscale basis as a preconditioner for subsequent test operators. The choice of the training operator is based entirely on the physics, and may be recomputed if the difference between the training and test operators becomes significant. Given the multiscale basis for the training operator, the preconditioner can be applied efficiently in a distributed parallel environment. Furthermore, theoretical and numerical results demonstrate that the number of iterations required for the preconditioned system to converge is independent of the subdomain mesh size, the number of subdomains, the mortar mesh size, or the mortar and subdomain approximation spaces.

Additional levels of difficulty arise when the problem to solve on the interface is nonlinear, which is the case for multiphase flow [120, 174]. Multilevel nonlinear interface solvers with Newton–GMRES smoothing and Neumann–Neumann preconditioners (based on inexact Neumann subdomain solves) for interface GMRES iterations have been developed for multiphysics couplings of single-phase, two-phase, and three-phase flow in porous media [173–175].

Another technique known as the multiscale flux basis provides even more robust and efficient preconditioner for the nonlinear problem [63, 65]. The Newton–Krylov



**Figure 6.5:** Left: Interface-GMRES iterations versus time without preconditioning (method P1), with a single multiscale preconditioner (method P2), and with periodic recomputation of the multiscale preconditioner (method P3). Right: Temperature profiles predicted by CG and DG methods for fluid injection problems with graded mesh.

interface iteration leads to a sequence of linear problems. The spectral properties of the Jacobian can be observed to change gradually throughout the nonlinear iteration. The preconditioner is formed by computing a multiscale basis for a fixed state of the variables, which could be the state at the beginning of the nonlinear iteration or the state at the initial time in the case of time-dependent problems. It is then used to compute the action of a preconditioner for the coarse scale interface iteration by solving a secondary interface iteration, which can be done efficiently in a distributed parallel environment. The basis can be recomputed if a specified number of GMRES iterations is reached. Computational experiments for modeling multiphase flow in porous media show dramatic reduction in the number of interface iterations and robustness with respect to the subdomain and mortar mesh size, and the number of subdomains [63, 65]. Figure 6.5 (left) illustrates this effect in a two-phase benchmark problem, where a multiscale preconditioner is computed once at the initial time step versus periodic recomputation throughout the simulation [63]. In this example, the average number of GMRES iterations per time step was reduced from 82.8 for the un-preconditioned case to 9.7, thereby reducing the run-time error from 322.2 to 67.3 min.

A critical component of the solver methodology is developing efficient subdomain solvers. In the nonlinear case Krylov–Secant updates [43] or algebraic multigrid [95] may be used to accelerate Newton or quasi-Newton iterations. In the arena of algebraic multigrid and multilevel methods, there have been advances to include coarsening heuristics that may extract particular physical or algebraic features from the problem [12, 23, 24, 93, 141]. The effectiveness of these methods is tied to the degree of ellipticity of the algebraic operators. The main feature of these solvers is to automate the complete process of creating a multilevel hierarchy. Based only on the

concept of strength of connectivity between variables these methods mimic the capability of geometric multigrid in a “black-box” fashion. Therefore, these methods are particularly attractive as building blocks for designing multiple stages for solver or preconditioning strategies [93, 141].

Nonoverlapping domain decomposition algorithms are being developed for the parallel solution of the algebraic system arising from the multiscale multiphysics discretizations described earlier. In this setting, the coupled global problem is reduced to solving an interface problem in the coarse scale mortar space for the unknown interface pressure and normal stress. The interface problem imposes continuity of normal velocity and displacement on the interfaces. It is solved by an iterative Krylov space method, where the action of the interface operator at each iteration is computed by solving subdomain problems with specified mortar data as a boundary condition. The interface problem is linear in the simplest case of single-phase flow and linear elasticity, but is nonlinear for multiphase flow or nonlinear elasticity models, as discussed in the previous section.

The previously developed interface solvers for porous media flow can be extended to the coupled flow-geomechanics models. In particular, a multiscale basis formulation and implementation is possible, which involves precomputing local fine scale subdomain responses (fluxes and stresses) for each mortar coarse scale basis function (pressures and displacements). Note that only the resulting interface responses need to be stored. Ongoing efforts involve both the use of the multiscale basis as a solver, where subdomain solves are replaced by linear combinations of the basis functions [66], and as a preconditioner, where the basis is employed to compute the action of an efficient interface preconditioner for speeding up the interface iteration [65, 159]. Based on our previous results for flow, the multiscale basis is expected to give a significantly improved performance for coupled flow and geomechanics.

The development of accurate, efficient and robust solvers for the large subdomain nonlinear systems represents a formidable challenge. General-purpose solver technology is inadequate for the complexity of the multiphysics and multiscale systems arising in the applications of interest, such as CO<sub>2</sub> injection for enhanced oil recovery (CO<sub>2</sub>-EOR) or CO<sub>2</sub> sequestration. Significantly faster run-times can be achieved by tailoring the solvers to the application, providing reasonable turnaround time for engineering and risk analysis [33]. In the related area of field of sedimentary basis simulation, [133] presented work using two stage preconditioners and algebraic multigrid. In this paper’s topic of reservoir simulation, investigations on algorithms for linear and nonlinear solvers are given in [92–95, 117, 161]. These flow solvers as well as others such as SAMG [141, 172] and Hypre [1], have been employed for coupled flow and geomechanics with field scale simulations.

## 5 A posteriori error estimation and time-stepping

In numerical simulations, errors due to mesh discretization, function approximation, and temporal discretization can lead to inaccurate results. Without some guidance on where to appropriately place the mesh and change the polynomial order of approximation, the reliability of computed quantities is questionable. Moreover, one would like to compute a reliably accurate solution with minimal degrees of freedom; this is especially important when studying multiple stochastic realizations. While standard a priori error estimates demonstrate convergence of the solution with fine enough resolution, these error bounds are in general not computable, as they involve knowledge of the analytic solution. A posteriori error estimators/indicators may be used to assess the accuracy of a computed solution [76, 167] and signify where modifications in discretization parameters need to be made. By effectively estimating error, one can control the entire computational process through adaptive algorithms. A posteriori error estimates for mortar MFE methods and algorithms for adapting the mortar and subdomain grids have been developed in [10, 114, 163]; see Figure 6.3 (right) for an illustration of the method’s ability to capture boundary layers and treat coefficients that oscillate on different scales in different parts of the domain.

From time discretization standpoint, there are basically two different ways to solve nonlinear flow and transport problems: (1) fully implicit, which implies solving the nonlinear coupled system of algebraic equations; and (2) time splitting, which implies decoupling the discretized set of equations and solving them separately. The former is expensive to compute and requires the implementation of very robust nonlinear and linear solvers. The latter is computationally less expensive but may introduce numerical errors that compromise the size of the time step [13, 74].

Effective time-stepping schemes are essential for modeling reactive transport and multiphase flow. In reactive transport, it is not clear a priori how tightly different types of physics are coupled together [30, 31, 88]. In such cases an adaptive fully implicit and time splitting approach is highly desirable for both single domain and multiple domain simulations. However, this imposes extreme challenges for preserving mass and volumes across space-time boundaries, and may also affect the time step [62].

Effective error estimation and control is critical for resolving the multiscale features of the physical processes at a reasonable cost. In modeling subsurface flows, various numerical errors contribute to the total error between the computed and the exact solutions. The sources of errors arise from the following:

- spatial discretization
- time discretization (backward Euler or other time stepping schemes)
- linearization error (Newton linearization or other linearizations)
- iterative linear solver.

It is important to derive rigorous error estimators for these different sources of errors. These estimators must be fully and easily computable and give guaranteed upper bounds. By distinguishing different sources of errors, the iterative procedure at given time level can be terminated when the individual errors are sufficiently small and do not affect significantly the overall error. For a given mesh, one can use spatial error information in order to not over or under solve the nonlinear and linear algebraic problems. In addition, the spatial and temporal discretization errors can be adjusted so that they are of similar size. Thus computing error estimators provide an adaptive strategy to control both time step size and spatial mesh based on desired computational tolerances.

The benefits of such a procedure are twofold. First, the overall error is controlled and strategies for obtaining a user-given final precision at the end of the simulation can be devised. Second, it is likely to lead to substantial computational savings such as reducing an excessive number of unnecessary linearization/iterative coupling/linear solver iterations.

Ongoing research is following [114, 150, 163], where a posteriori error estimates for mortar MFE discretizations of steady-state single-phase flow have been developed, as well as [53] for time-dependent problems. These ideas are being extended to estimators for both fully implicit and iteratively coupled two-phase and black-oil models. The work in [114, 150] provides a unified approach for a wide class of locally mass conservative spatial discretizations, including MFMFE and DG methods on general grids. The effect of the algebraic error and stopping criteria for the linear and non-linear iterative solvers will also be incorporated, utilizing techniques from [86]. Some preliminary work is described in [151]. Further developments will include a posteriori error estimates for the poroelasticity system, combining our mortar MFE error estimates [114, 163] with techniques for residual-type estimates for coupled elliptic-parabolic systems [54] and the space-time potential and flux reconstruction approach from [53]. This will result in efficient, reliable, and fully computable a posteriori error estimates for the flow-geomechanics system.

Explicit time stepping is inadequate for CO<sub>2</sub> injection, since the various physics modules simulate complex nonlinearities at multiple spatial and temporal scales. Fully implicit methods are too computationally expensive. Iterative coupling methods [103] are a possible way to overcome these difficulties, and have been shown to produce stable schemes when coupling reservoir simulation with geomechanics [89, 147]. Flexible approaches are being implemented that involve iterative coupling and adaptive time stepping based on error estimators discussed earlier. The simulator IPARS is being used for testing these concepts, including designing effective time stepping strategies, and appropriately terminating the nonlinear/linear iterations.

## 6 Uncertainty quantification, verification, and validation

High fidelity deterministic simulations of subsurface models are computationally intensive, and performing comprehensive uncertainty analysis exponentially increases these demands. Moreover, in many cases stochastic distributions may vary wildly throughout the whole domain (at different physics and scales), making the uncertainty assessment a very challenging task.

Stochastic subsurface modeling methods can be roughly classified as sampling (nonintrusive) and nonsampling (intrusive) methods. A typical example in the latter category is the stochastic finite element method [15, 45, 69, 153], which discretizes simultaneously a large dimensional problem involving both physical and stochastic variables. The method provides accurate approximations based on polynomial interpolation in stochastic space. However, the resulting system is significantly large, may be difficult to set up, and the solution algorithm does not easily lend itself to parallelization.

An alternative is to use finite elements in the physical domain, and to sample the stochastic space only at certain points. The Monte Carlo method [56] is the most popular of these sampling techniques. The advantage of this approach is that the resulting deterministic FEM problems are completely uncoupled, and may be solved in parallel. The disadvantage of the Monte Carlo method is that the convergence rate with respect to the stochastic space is slow.

The stochastic collocation method is another nonintrusive approach that improves upon the Monte Carlo method by sampling at specially chosen collocation points in order to form a polynomial interpolant in the stochastic space. Different varieties of stochastic collocation arise by considering different sets of collocation points. Collocation methods converge much faster than Monte Carlo in cases where the dependence on the stochastic parameters is smooth, which is oftentimes the case in reservoir simulation [14, 64, 169, 170]. However, the simplest approach based on a full tensor product grid of collocation points suffers from the so-called curse of dimensionality: increasing the number of stochastic dimensions exponentially increases the number of collocation points. To cope with this problem, more advanced collocation techniques are possible such as the so-called probabilistic collocation method [96] and the Smolyak sparse grids [108, 109, 169]. Sparse grids grow at a rate that is much slower than tensor grids with respect to dimension, rendering much higher dimensional simulations tractable with the sparse grid.

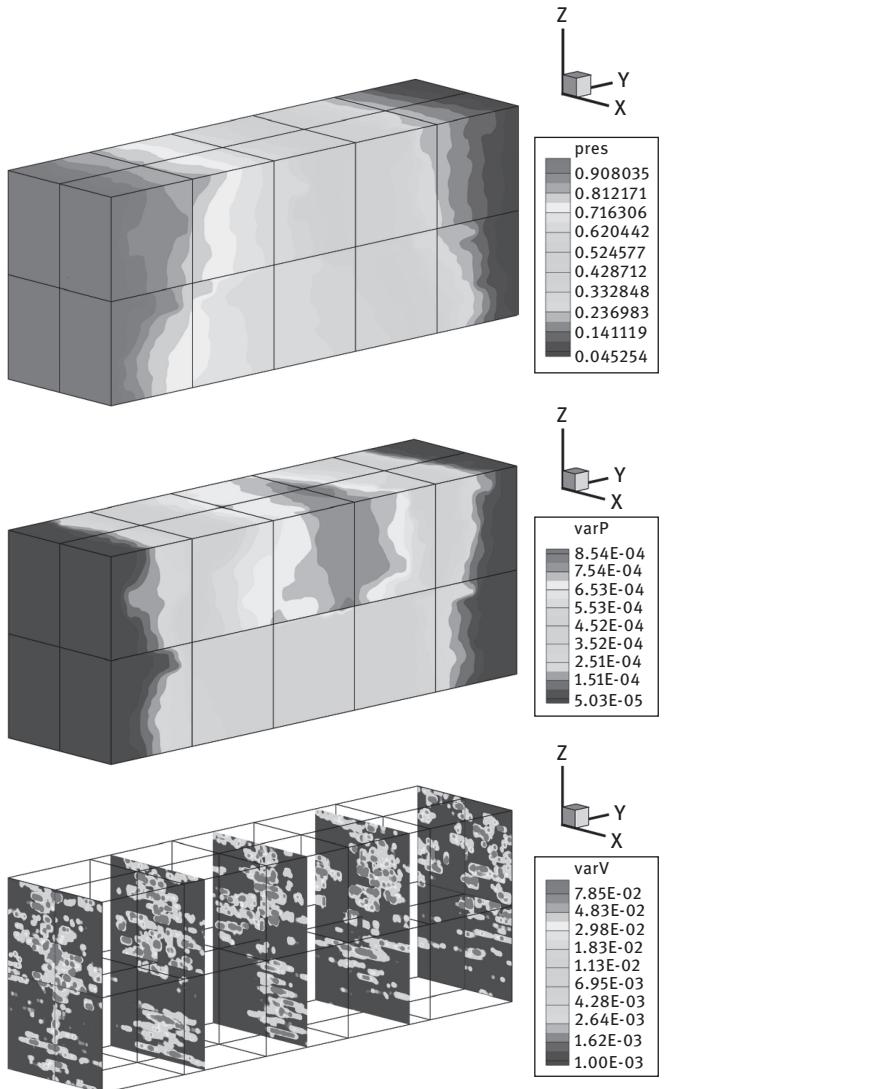
Stochastic modeling of multiple rock types has been investigated by applying different statistics to different subdomains [67], resulting in UQ problems with a high dimension in stochastic space. In particular, a multiscale mortar MFE stochastic collocation method has been developed for the nonstationary problem. It is efficiently implemented by forming a stochastic analog of the multiscale basis. It is reused not

only throughout the interface iteration for a single stochastic realization, but also for many realizations that do not change the local permeability field. This approach has been shown to substantially increase the efficiency of the algorithm by orders of magnitude. Furthermore, comparisons with Monte Carlo simulations indicate that comparable accuracy can be achieved with orders of magnitude fewer realizations.

The above algorithm requires recomputing the multiscale flux basis for each realization of the local stochastic expansion. This cost can further be reduced by using multiscale preconditioner [159]. In particular, a multiscale mortar basis is computed for the mean permeability and used as a preconditioner for each stochastic realization. The use of the multiscale preconditioner leads to a significant improvement in the number of interface (coarse scale) iterations and in the total solution time [159].

A crucial task is to build confidence in the results of the numerical simulations and to understand how sensitive different models and numerical approaches are with respect to given parameters. The work of [67] demonstrated how domain decomposition can be coupled with stochastic collocation using a multiscale basis in order to efficiently perform uncertainty quantification in stochastic flow problems. Similar studies are being performed to develop efficient stochastic algorithms for coupled geomechanics-flow models in order to investigate the propagation of uncertainties in these types of systems.

Stochastic permeability can be modeled with a finite Karhunen–Loëve (KL) expansion, leading to a stochastic poroelasticity system. The mortar multiscale spatial discretizations described earlier will be coupled with sparse grid stochastic collocation for efficient and accurate approximation in high-dimensional stochastic spaces. A priori error estimates for the coupled physical–stochastic discrete system can be derived, extending our analysis from [67] to poroelasticity. Furthermore, the efficiency of the poroelastic multiscale basis implementation can be obtained for modeling non-stationary poroelastic media. Results for Darcy flow indicate a substantial speedup due to the use of the multiscale basis, which is further increased by its reuse for multiple stochastic realizations. We have been able to perform a comprehensive uncertainty analysis for flow in the full 3D domain of the 10th SPE Comparative Project [39]. In [67], we report computational results for media with 20 stochastic regions, with expansions having 12 KL terms, for a total of 240 stochastic dimensions, as shown in Figure 6.6. These simulations use a covariance function for a Gaussian kernel. For level 1 sparse grid collocation with 481 global realizations, the traditional domain decomposition implementation requires 101 826 linear systems per processor, while the multiscale basis implementation requires 8658. This is even further reduced to only 1362 by storing and reusing the multiscale basis in multiple stochastic realizations. In addition to a priori error analysis, a posteriori error analysis and adaptive algorithms can be formulated to control the error due to the spatiotemporal discretization, the stochastic collocation, and the truncation of the KL expansion. Spatial estimators



**Figure 6.6:** Pressure mean (top), pressure variance (middle), and cross-sections of the  $y$ -velocity variance (bottom).

described earlier will be coupled with stochastic estimators of the Richardson extrapolation type, designed to provide efficient multilevel approximations in stochastic space. Both isotropic and anisotropic (with varying polynomial degrees in different stochastic dimensions) tensor product and sparse grid approximations are being investigated [108, 109]. Anisotropic approximations are especially useful for problems with large correlation lengths [108].

Verification and validation studies should be performed on new models and their implementations. One possibility is to compare simulation results with existing commercial simulators such as ECLIPSE and CMG. One can further perform benchmark studies against research codes such as the UTCOMP simulator [34] with advanced physics and many years of careful validations. Possible scenarios include large-scale simulations of synthetic reservoirs, CO<sub>2</sub> injection strategies, well placements, and mobility control methods.

## 7 Applications

The existing computational framework IPARS is being used for the development of new geomechanical applications [94, 144, 145, 156]. In addition to enhancing the IPARS software with high fidelity algorithms, new models of specific physical processes are being developed. These include (i) compositional modeling of multiphase flow (namely, development of appropriate phase behavior and fluid property modules for compositional flow, e.g. CO<sub>2</sub>-EOR and sequestration), (ii) a fixed-stress iterative coupling scheme for flow and geomechanics, and (iii) classical Druker–Prager plasticity models. Let us now discuss the specific details for each of these three areas of study.

### 7.1 Compositional modeling of multiphase flow

The compositional flow model in IPARS is a multicomponent, three-phase equation of state compositional model coupled to several other models for types of physics: thermal energy balance, transport, and chemical reactions [146]. For simplicity, we provide a formulation for the isothermal fluid flow with no chemical reactions between fluid components and solid medium. Let  $i$  and  $\alpha$  represent component and phase indices respectively. We assume that there are  $n_c$  components with the convention of  $i = 1$  denoting the water component. Component mass balances for components  $i = 1, \dots, n_c$  are then given by

$$\frac{\partial(\phi N_i)}{\partial t} + \nabla \cdot \sum_{\alpha} (\rho_{\alpha} \xi_i^{\alpha} \mathbf{u}_{\alpha}) = q_i, \quad (6.6)$$

$$\mathbf{u}_{\alpha} = -\frac{k_{r\alpha} \mathbf{K}}{\mu_{\alpha}} (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}), \quad (6.7)$$

coupled with the constitutive equations

$$\phi = \phi_0[1 + c_r(p - p_0)] \quad (6.8)$$

$$p_{\alpha} = p + p_{c\alpha}(S_{\alpha}) \quad (6.9)$$

$$\xi_i^\alpha = \xi_i^\alpha(p, T, N_i) \quad (6.10)$$

$$\mu_\alpha = \mu_\alpha(p, T, \xi_i^\alpha) \quad (6.11)$$

$$S_\alpha = S_\alpha(p, N_i, \xi_i^\alpha, T) \quad (6.12)$$

$$\rho_\alpha = \rho_\alpha(p, T, \xi_i^\alpha) \quad (6.13)$$

$$k_{r\alpha} = k_{r\alpha}(S_\alpha) \quad (6.14)$$

$$f_i^\alpha = \Phi_i^\alpha \xi_i^\alpha p \quad (6.15)$$

$$\Phi_i^\alpha = \Phi_i^\alpha(p, T, \xi_i^\alpha, N_i) \quad (6.16)$$

In the fluid flow mass conservation law (6.6),  $\phi$  is the porosity,  $N_i$  is the molar concentration of component  $i$ ,  $\rho_\alpha$  is the molar density of phase  $\alpha$ ,  $\xi_i^\alpha$  is the molar fraction of component  $i$  in phase  $\alpha$ , and  $q_i$  is the molar rate of component  $i$  injected or produced per reservoir unit volume. The phase velocity  $\mathbf{u}_\alpha$  is given by Darcy's law in (6.7), where  $k_{r\alpha}$  is the relative permeability of phase  $\alpha$ ,  $\mu_\alpha$  is the viscosity of phase  $\alpha$ ,  $\mathbf{K}$  is the absolute permeability tensor, and  $\mathbf{g}$  is the gravitational acceleration vector.

Without geomechanical coupling, equation (6.8) gives a linear relation for porosity  $\phi$  depending upon initial conditions, rock compressibility constant  $c_r$ , and a chosen reference pressure  $p$ , typically taken to be the oil phase pressure  $p_o$ .

In the remaining constitutive equations,  $S_\alpha$  is the saturation of phase  $\alpha$ , temperature  $T$  is a constant,  $p_{c\alpha}$  is the capillary pressure of phase  $\alpha$ ,  $f_i^\alpha$  is fugacity of component  $i$  in phase  $\alpha$ , and  $\Phi_i^\alpha$  is the fugacity coefficient of component  $i$  in phase  $\alpha$ .

The solution of the compositional flow equation is based on applying an IMPEC implicit pressure, explicit concentration algorithm [146]. IMPEC was chosen for ease in implementation, and to apply specialized preconditioners for different types of physics. The time step is not overly restricted when taking multiple concentration steps for each pressure step. The mass balance equations are discretized using a MFE method in space and backward Euler in time. In the IMPEC scheme, the discrete mass balance equations are summed to obtain an equation for the reference pressure  $p$ . The phase pressures  $p_\alpha$  are eliminated in terms of  $p$  using capillary pressure relationships. The resulting nonlinear equation for the reference pressure is solved implicitly using the Newton–Raphson method. Applying several small fractional time steps,  $n_c - 1$  concentrations  $N_i$  are next computed explicitly. This is followed by a flash calculation based to determine the overall composition of each grid block: this means solving a coupled system of nonlinear equations for the Rachford–Rice, mixing rule, Peng–Robinson cubic equation of state, and fugacity coefficient equations. The result of this computation will be component mole fractions. Using the updated phase saturations, and composition, new phase pressures can be computed, and the process repeats until the sum of the saturations is within a tolerance of one, i.e. a volumetric balance constraint is achieved.

## 7.2 Fixed stress iterative coupling scheme

In Section 3, we discussed multiscale and multiphysics coupling of single-phase flow and linear elasticity. This formulation can be extended to the compositional model by replacing equations (6.2) and (6.3) with the compositional model (6.6)–(6.16), and redefining the porosity as

$$\phi^* = \phi_0 + \frac{1}{M}(p - p_0) + \alpha \nabla \cdot (\mathbf{u} - \mathbf{u}_0), \quad (6.17)$$

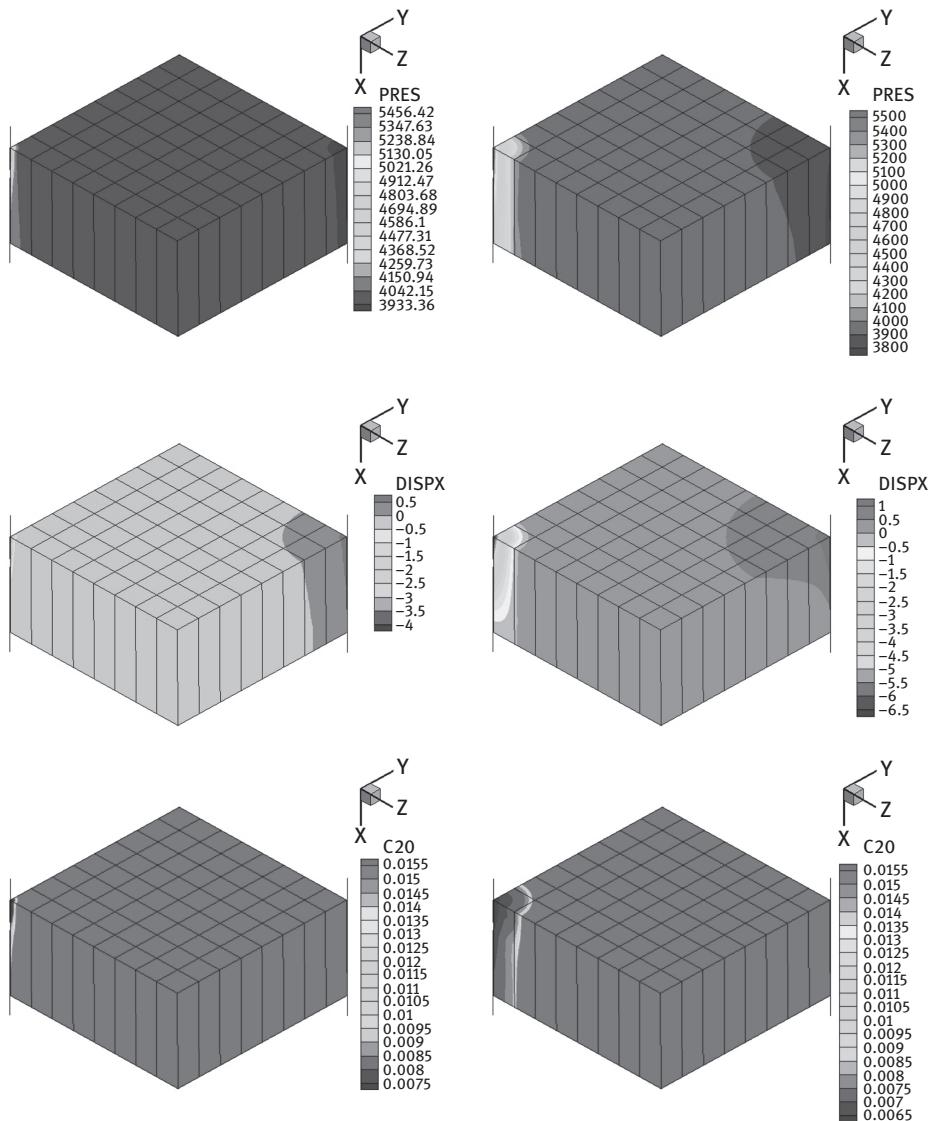
where  $\phi_0$ ,  $p_0$ , and  $\mathbf{u}_0$  are initial conditions for porosity, reference pressure, and solid displacement, respectively. The Biot coefficients  $M$  and  $\alpha$  have been derived in [60] for multiphase flow and [35] for single phase slightly compressible flow. It should be noted that the porosity model is coupled to the compositional flow model through the reference pressure. The coupled compositional flow and linear poroelasticity equations for reference pore pressure  $p$ , component molar concentrations  $N_i$ , and solid phase displacement vector  $\mathbf{u}$  is a computationally expensive system to solve simultaneously. While fluid and solid unknowns cannot be completely decoupled, it is possible to develop iteratively coupled schemes.

To solve the coupled compositional flow and mechanics system, we apply a fixed stress iterative coupling procedure [89, 147]. By assuming constant mean total stress during a flow step, we can iterate sequentially between flow and mechanics, such that each system can leverage existing software specifically tailored for each type of specifics. More specifically, we use the IMPEC scheme for compositional flow described in Section 7.1 and we use a continuous Galerkin scheme for the quasi-static linear elasticity system.

### 7.2.1 Numerical example

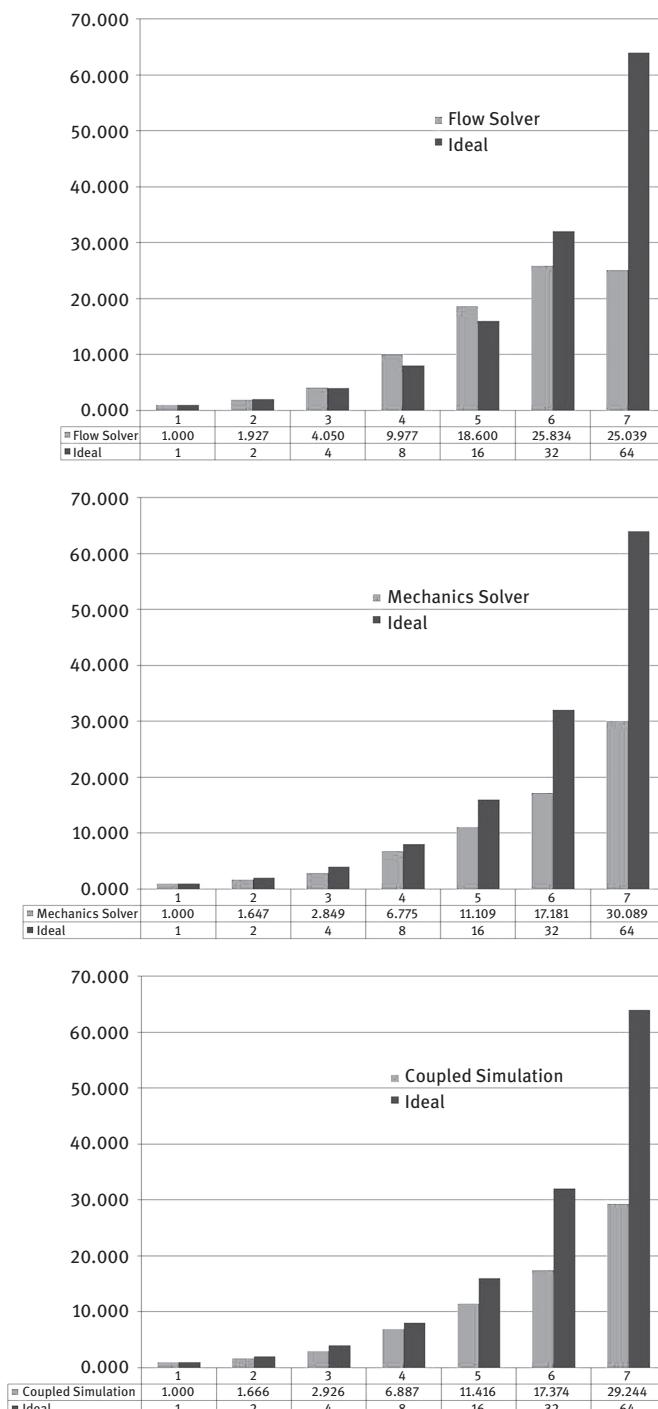
The following numerical example demonstrates a parallel compositional poroelastic problem with a quarter five-spot reservoir model. The dimension of the reservoir is  $100 \times 3600 \times 3600$  (ft) with a uniform grid of  $6 \times 144 \times 144$  elements. There are  $n_c = 7$  chemical components, which are  $\text{H}_2\text{O}$ ,  $\text{C}_1$ ,  $\text{C}_3$ ,  $\text{C}_6$ ,  $\text{C}_{10}$ ,  $\text{C}_{15}$ , and  $\text{C}_{20}$ . These parameters make the total number of degrees of freedom 870 912 for compositional flow and 441 525 for linear poroelasticity.

The length of the simulation is 91 (days) with 22 time steps. The rates of both injection and production wells are set to equal (50 000 B/day). Boundary conditions are no-flow, zero normal displacement and zero shear tractions on all faces except the top, and a compressive traction of 4200 psi on the top face. Initial stresses are  $(\sigma_{xx}, \sigma_{yy}, \sigma_{zz}) = (-4200, 4000, 4000)$  psi at the top of the reservoir, with an in-situ stress gradient of  $(-1.0231, 0, 0)$  psi/ft. Oleic phase pressure, vertical displacement, and  $\text{C}_{20}$  concentration distribution (using 64 processors) at the end of day 1 and day 91 are shown in Figure 6.7. Solid lines indicate the processor partitioning for



**Figure 6.7:** Oil pressure at day 1 (top left) and day 91 (top right), vertical displacement at day 1 (middle left) and day 91 (middle right), and concentration of component C<sub>20</sub> at day 1 (bottom left) and day 91 (bottom right).

the parallel computation. The compositional flow model uses BCGS as a solver with a multigrid preconditioner and several LSOR smoothing steps; for the linear poroelasticity model, GMRES is used as solver with AMG as a preconditioner, using the HYPRE library. [1]



**Figure 6.8:** Parallel efficiency of flow solver (top), mechanics solver (middle), and iteratively coupled poromechanics solver (bottom) for the compositional example.

Figure 6.8 shows the speed up results from 1 to 64 processors for flow solver, poromechanics solver, and coupled flow and poromechanics model. The flow solver has speed up very close to the ideal up to 16 processors. At 64 processors, the speed up deteriorates because the size of the problem is not large enough to offset the increase in communication overhead. For the poromechanics solver, the speed up for 64 processors is far from ideal. This evidence supports the claim that better preconditioners are necessary for the mechanics equations to properly balance the parallel performance of the flow solver. The final graph shows that the parallel performance of the coupled flow and poromechanics system is dominated by the performance of the poromechanics solver in the iteratively coupled model.

### 7.3 Plasticity modeling

Here we present details on modeling the nonlinear stresses in (6.5). We also discuss modeling of fractured media.

The rate of change of the plastic strain  $\epsilon^p$  is modeled by the material yielding function  $Y$  and the flow potential  $F$ :

$$Y(\tilde{\sigma}, \epsilon^p) = 0, \quad \frac{d}{dt} \epsilon^p = \lambda \frac{\partial F(\tilde{\sigma}, \epsilon^p)}{\partial \tilde{\sigma}}. \quad (6.18)$$

Specifically, the Druker–Prager theory [50], a pressure-dependent plasticity model is popular in modeling geomaterials. For compaction-dominated rock deformation due to fluid extraction, the Sandler and Rubin cap plasticity model [131, 132] has been developed. Moreover, to overcome the numerical difficulty resulting from the nonsmoothness of the yielding surface of the Sandler and Rubin cap model, Pelessone [113] and Desai [47] developed cap models with smooth yielding and flow surfaces. The Pelessone cap model is also called the National Lab cap model [57, 58].

Sand production results from well drilling and reservoir pressure drawdown [152]. During the drilling process, sand grains detach from damaged rock skeletons, which is mainly due to large plastic shear deformation of solid skeleton. With oil extraction from reservoirs, following pressure drawdown, stresses in the rock solid skeletons increase, which is the reservoir compaction phenomenon. In this case, rock failure is directly related to a critical plastic volume strain of the rock skeleton matrix. The inelastic strain including both plastic strain and creeping strain in (6.5) can be used as a key rock damage index to evaluate the volume of sand production during drilling and reservoir production.

To model sand production, we will incorporate the Pelessone model into IPARS and couple it with multiphase flow. The yielding function of the Pelessone model is

written as follows:

$$Y(\tilde{\sigma}, X_0, \sigma_0) = \Gamma^2 J_2 - \left[ 1 - H(K_0 - I_1) \left( \frac{I_1 - K_0}{R Y_s(K_0, \sigma_0)} \right)^2 \right] Y_s^2(I_1, \sigma_0) \quad (6.19)$$

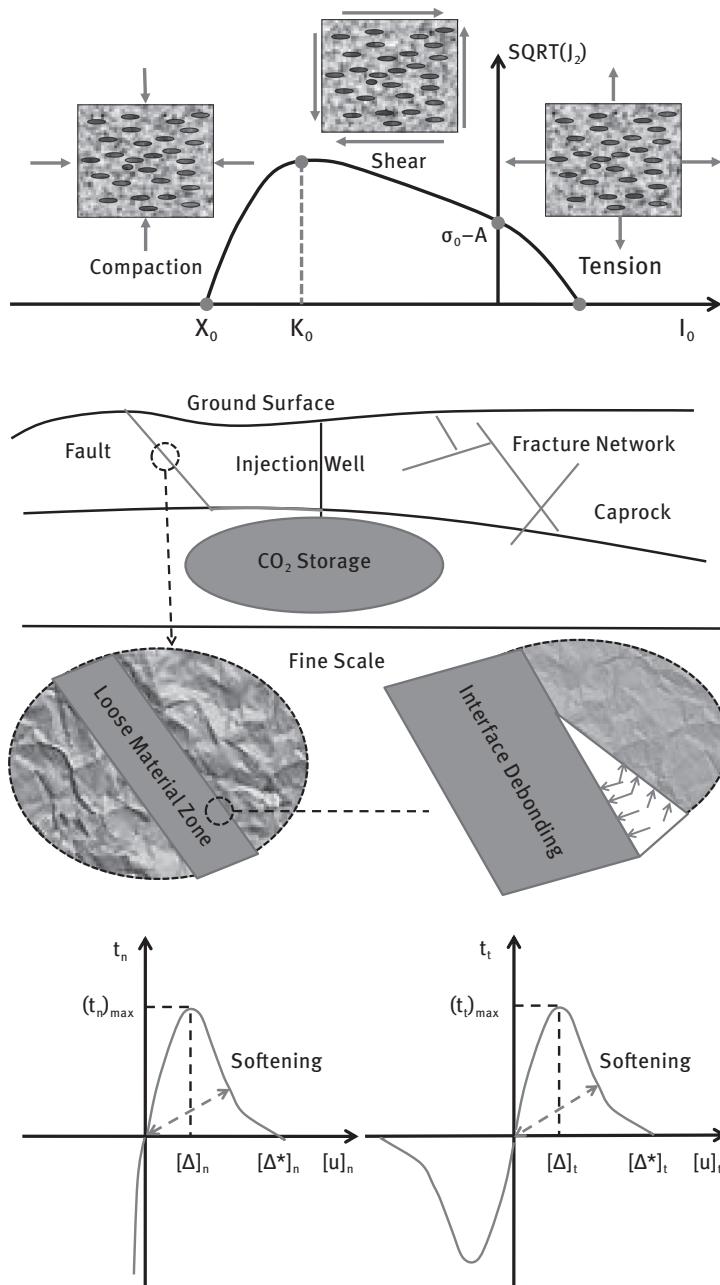
$$Y_s(I_1, \sigma_0) = \sigma_0 - A e^{Y I_1} - \alpha I_1 \quad (6.20)$$

$$\Gamma = \frac{1}{2}(1 + \sin(3\beta)) + \frac{1}{\Psi}(1 - \sin(3\beta)) \quad (6.21)$$

$$\beta = -\frac{1}{3} \sin^{-1} \left( \frac{3\sqrt{3}J_3}{2J_2^{3/2}} \right) \quad (6.22)$$

where  $I_1, J_2$ , and  $J_3$  are the three invariants of the effective Cauchy stress tensor,  $Y_s$  is the shear envelope yielding function,  $\sigma_0$ ,  $X_0$ , and  $K_0$  are the material shear-related strength, compaction strength, and the intersection coordinate of the shear and cap portions, respectively,  $\Psi$  is the ratio of tri-axial extension strength to compression strength,  $H$  is the Heaviside function, and the other parameters the model are constants related to the shapes of the shear envelope and cap portion. Figure 6.9 (left) shows the configuration of the Pelessone yielding surface decomposed into compaction, shear, and tension zones. Furthermore, nonassociated cap models are obtained by taking the flow potential to be different from the yielding function in equation (6.22). The hardening cap models are obtained through defining  $\sigma_0$  and  $X_0$  as functions of plastic strains.

Several second-order local material integrators have been formulated for cap plasticity models [59, 75, 135, 143, 168]. However, challenges still remain for numerical simulations using cap plasticity models. First, although the Pelessone cap model has a smooth yielding surface, current material integrators available in the literature may not converge for cap models with sharp transition zones. This issue is being investigated by developing new numerical schemes or procedures to improve the robustness of the material integrators for modeling compaction-dominated geomechanics problems with sharp transition zones. Second, simulations of many tension-dominated geomechanics problems often exhibit instabilities or nonconvergence. One reason is the relatively weak tension strength of the majority of geomaterials, which results in very large plastic strains. More precisely, the predicted deformation for the area under tension may be unrealistic because materials should fail or cracks should occur before the deformation goes that far. To overcome this issue, we will propose a tension-cutoff and switch to a crack opening method such as cohesion zone models (CZMs) that will be addressed below. Another problem is the serious element distortion due to large plastic strain. We propose multilevel re-meshing (fine mesh) for dividing a distorted element into a few sublevel elements with more regular shapes. We will investigate the convergence issues potentially resulting from re-meshing and also interpolating or mapping state variables from a coarse level to a fine level. Furthermore, plasticity models, due to their nonlinearity, present a challenge for parallel computation using domain decomposition methods. Scalable nonlinear domain de-



**Figure 6.9:** Top: Pelessone smooth cap plasticity model. Middle: Gas injection and potential gas leak path. Bottom: Exponential cohesive zone model.

composition algorithms for plasticity problems are being developed, building on our experience in similar methods for multiphase flow in porous media [65, 161, 173–175]. Dynamic load balancing schemes are also being investigated [85].

The long term and thermal effects of fluid extraction or injection on the subsidence or sand production are modeled through the creep and thermal strains in equation (6.5). The use of the flow functions for plasticity as the creep potentials is a convenient approach for taking into account creep strain [51]. Specifically, for cap models we will incorporate two creep functions, one for shear portion and the other for compaction portion. Shao et al. [136, 137] and Liu et al. [98, 100] have done convection-dominated thermal analysis for fluid injection problems, assuming that the injected fluids are the reservoir fluids. We will extend these formulations to the coupled multiphase flow with geomechanics through taking into account three fluid phases, i.e. water, oil, and gas. We will investigate the instability issue brought by the convection effect reported in [98, 100] and will develop more robust numerical schemes for handling the convection effect.

A major concern in CO<sub>2</sub>-EOR projects is gas leak through the existing fracture networks and faults. Fractures and faults, illustrated in Figure 6.9 (middle), are narrow regions and can be viewed as interfaces between subdomains. Gas leak involves failure, crack initiation, and crack propagation of these interfaces. These phenomena have been modeled by treating the narrow region as continuum with graded properties, separating thin surfaces by springs, or employing CZMs. CZM [18, 29, 68, 106, 107, 171] are based on micromechanical approaches and are powerful in modeling fracture and crack problems where the crack paths are known. We will investigate gas leak using CZM as the gas leak paths are mainly among the existing faults. Rather than applying stress–strain relationships, specific traction (stress-like)–separation (jumps on displacements) relations are used for the interfacial constitutive laws of the solid phase. We will incorporate Xu and Needleman’s exponential CZM model [171] into our multiscale finite element code through the variational formulation below:

$$\sum_i \int_{E_i} \boldsymbol{\sigma} : \delta \boldsymbol{\epsilon} + \sum_i \int_{S_i} \mathbf{t}([\mathbf{u}]) \cdot \delta \mathbf{v} = \sum_i \int_{\Gamma_i} \mathbf{t} \cdot \delta \mathbf{v} + \sum_i \int_{E_i} \mathbf{f} \cdot \delta \mathbf{v}, \quad (6.23)$$

where  $\mathbf{t}$  is the traction at the boundary (prescribed) and on the interior faces and  $[\mathbf{u}]$  is the displacement jump across the interface. The normal  $t_n$  and tangential  $t_\tau$  components of the interface traction are given by

$$t_n = \mathbf{t} \cdot \mathbf{n} = \frac{\partial \Phi}{\partial [u]_n}, \quad t_\tau = \| (II - \mathbf{n} \otimes \mathbf{n}) \boldsymbol{\tau} \|_2 = \frac{\partial \Phi}{\partial [u]_\tau}, \quad (6.24)$$

where  $II$  is the fourth order identity tensor and  $\Phi$  is the interfacial potential for the exponential CZM defined as

$$\Phi([u]_n, [u]_t) = \Psi_n + \Psi_n e^{-x} \left( (1 - \tilde{\alpha} + x)^{\frac{1-q}{\tilde{\alpha}-1}} - x \left( q + \frac{\tilde{\alpha}-q}{\tilde{\alpha}-1} \right) e^{-y^2} \right) \quad (6.25)$$

Here  $x = \frac{[u]_n}{[\Delta]_n}$ ,  $\gamma = \frac{[u]_t}{[\Delta]_t}$ ,  $q = \frac{\Psi_n}{\Psi_t}$ ,  $\tilde{\alpha} = \frac{[\Delta^*]_n}{[\Delta]_n}$ ,  $\Psi_n = e\sigma_{\max}[\Delta]_n$ ,  $\Psi_t = \sqrt{e/2}\tau_{\max}[\Delta]_t$ ,  $[u]_n = [\mathbf{u}] \cdot \mathbf{n}$ ,  $[u]_t = \|(\mathbf{I} - \mathbf{n} \otimes \mathbf{n})[\mathbf{u}]\|_2$ ,  $[\Delta^*]_n = [u]_n|_{t_n=0}$ , and  $[\Delta]_n$  and  $[\Delta]_t$  are, respectively, the normal and tangential displacement jumps at which the corresponding normal and tangential tractions reach their maximum values. Figure 6.9 (right) presents the traction–separation curves based on equations (6.24) and (6.25).

Our three major research directions in applying CZM for modeling potential gas leak problems are summarized below. First, as shown in Figure 6.9 (right), we note that CZM generally involve material softening behavior, which bring a challenge for numerical simulations. A few issues related to CZM stability and robustness due to material softening have been demonstrated through numerical examples in [32, 55, 140]. We will perform rigorous stability and accuracy analysis for CZM. We believe that such an analysis is crucial to understand why formulations sometimes lead to numerical nonconvergence and is also a guide for designing more robust algorithms for softening models. Second, CZM have been developed for problems with conforming meshes and have few applications for problems with nonmatching grids. On the other hand, for postseparation due to shear failure, special algorithms must be provided for handing the nonmatched grids. We will develop new mortar finite element methodologies to integrate the CZM models into our multiphysics, multiblock, and multiscale frameworks with nonmatching grids. Finally, very few studies have been reported for CZM applied to interfaces with fluid pressure loading. Particularly, as shown in Figure 6.9 (middle) fluids with high pressure penetrate and occupy debonded interfaces. We will develop new formulations to address these physical processes.

## 8 Summary and conclusions

This chapter summarizes many of the areas of active research on coupled flow and geomechanics, centered around the authors’ work and the research simulator IPARS. These topics are extremely diverse and cover many aspects of the numerical simulation including: multiscale discretizations, a posteriori error estimation, domain decomposition, time stepping, physics-based preconditioners, and stochastic modeling. Applications to compositional flows and plasticity modeling have been presented.

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