RESEARCH STATEMENT

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Introduction

My research interests are in the areas of *Numerical analysis and Scientific computing*, *Computational and Applied Mathematics*. My focus is on developing efficient numerical schemes for solving partial differential equations (PDEs) arising in applications in science and engineering. I have worked on problems in fluid flow, transport and flow in porous media and particle transport in radiotherapy treatment medical applications. Another component of my work is on high performance computing in an effort to produce numerical schemes fast enough to efficiently solve problems of practical significance.

Current research projects

Discontinuous Galerkin methods for moment methods for radiative transfer

My recent work has been on developing efficient numerical schemes for solving the radiative particle transport equation. Solving this problem has important applications to Radiotherapy treatment. In this treatment technique radiation produced by external sources in the form of photons or other heavy ions is used to destroy infected cancer cells. An important part of this treatment process involves devising a treatment plan to determine the dosage distribution that maximizes the destruction of bad cells but minimizes any damage to healthy ones. In collaborative work [5] involving Temple University and Aachen University in Germany we model the transport of radiation particles using the Radiative Transfer Equation (RTE):

$$\partial_t \psi + \Omega \cdot \nabla_x \psi + (\sigma_s + \sigma_a)\psi = \frac{\sigma_s}{4\pi} \int_{S^2} \int_0^\infty k(x, \epsilon, \epsilon', \Omega \cdot \Omega')\psi(x, t, \epsilon', \Omega')\, d\epsilon' d\Omega' + Q. \tag{1}$$

The variables x, t, ϵ and Ω denote the spacial, time, energy and angle of flight respectively. The Radiative Transfer equation (1) describes the time evolution of the distribution of particles $\psi(x, t, \epsilon, \Omega)$, which represents the number of particles at position x, time t, with energy ϵ, moving in a direction Ω. The major difficulty in solving the Radiative Transfer equation is that it is a high dimensional problem. In particular we have three spacial dimensions, one time dimension, and three angular dimensions, a total of 8 dimensions. As a result it is computationally expensive to solve, for instance to approximate (1) on a uniform grid with 100 cells on each dimension would require a grid with 100^8 cells which is computationally intractable.

We use moment methods to derive approximate systems of lower dimension to approximate (1). This is a new line of research into deterministic approaches to solving (1) that is a possible alternative to traditional Monte-Carlo methods that are computationally expensive. The resulting systems are deterministic lower dimensional hyperbolic systems with the average distribution and radiative flux of the particles as the unknowns. These systems are are smaller and computationally less expensive to solve compared to (1). However, these systems can be highly nonlinear and need to be solved on highly heterogeneous domain (the human body) consisting of material of varying properties. For example the speed of propagation of particles in lung tissues will be different from that in bone tissue. In addition the solution needs to be highly accurate in the areas of the tumor and vital organs that may fail if exposed to high levels of harmful radiation. This makes obtaining an accurate numerical scheme a very challenging problem. In view of these challenges we use the discontinuous Galerkin method (DG) to

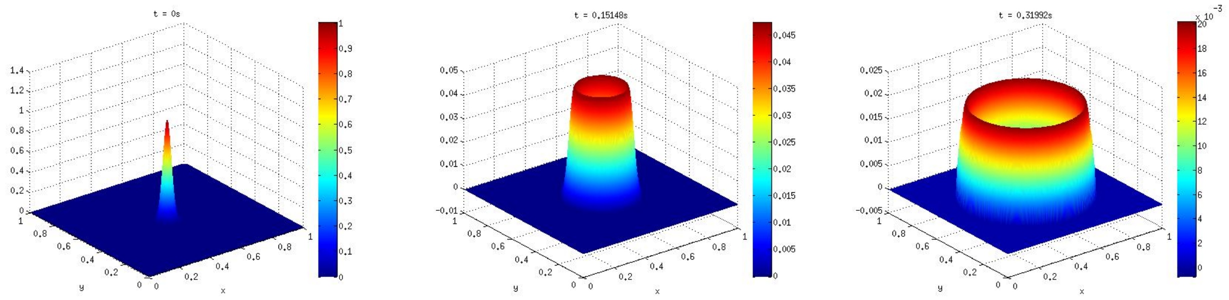

Figure 1: Time evolution of radiative particle distribution.

solve the systems approximating the RTE. The DG method is a high order method that allows us to capture fine structures on relatively coarse meshes. In addition, the DG method works on unstructured meshes which means we are able to highly refine the computational mesh in the areas of interest which saves computational cost. This computational technique is also highly parallelizable. However, the use of high order methods results in spurious oscillations of the numerical scheme which may cause the particle distribution to become negative and thus unphysical. In [5] we implemented a parallel numerical scheme to solve (1) and demonstrated optimal convergence as well as tested on benchmark problems that are relevant to the radiative transfer community for different kinds of moment methods that approximate the RTE. For example Figure 1 shows the evolution of the particle distribution with time starting from an initial line source in the center of the domain.

In [6] we are working on a numerical scheme that preserves the physical characteristics of the solution for the nonlinear moment models that are prone to shocks and oscillations but tend to produce more physical results.

Goals and future work on radiative transfer

1. *To develop a parallel and fully scalable 3D research code that could be used to estimate dosage. Preliminary results from our parallel 2D codes show that the numerical schemes are scalable on a shared memory platform and numerical tests on benchmark problems in the radiative transfer community show expected results.*

2. *Coupling the radiative transport equation with an energy equation for the particles and using data from CT scans provided by our colleagues at the center for Computational Engineering Science at Aachen University.*

Numerical solutions for time-dependent incompressible viscous flows

The other direction of my work focusses on accurate numerical approximations of incompressible flow modelled by the Navier-Stokes equations. I am particularly interested in applications to fluid-structure interactions that require accurate computation of stresses and forces at the boundary and therefore require high order accurate solutions near the boundary. This has important applications in computing stresses at the boundary for example in modelling the movement of objects in a fluid for example in aerospace and mechanical engineering as well as some biological applications. These applications require accurate approximations of the gradient of the velocity and pressure. The difficulty in the numerical computation of incompressible flow is how to implement incompressibility or equivalently: how to recover pressure from the velocity.

In collaborative work involving collaborators from MIT and McGill University, we apply the finite element method to Pressure Poisson Equation (PPE) reformulations of the time dependent Navier-Stokes equations. The PPE reformulations are similar to projection methods. However, they do not suffer from boundary layer effects that are present in projection approaches due to ambiguities in the boundary conditions. They are also not limited in order due to splitting errors that are present in classical projection methods making them ideal for this application. We have derived the weak formulation for the PPE reformulation introduced in [3]. Starting with the Navier-Stokes equations (NSE):

$$\begin{aligned} \boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} &= \nu \Delta \boldsymbol{u} - \nabla p + \boldsymbol{f} \quad \text{for } \boldsymbol{x} \in \Omega, && (2)\\ \nabla \cdot \boldsymbol{u} &= 0 \quad \text{for } \boldsymbol{x} \in \Omega, && (3)\\ \boldsymbol{u} &= \boldsymbol{g} \quad \text{for } \boldsymbol{x} \in \partial\Omega. && (4) \end{aligned}$$

The variables $\boldsymbol{u}$, p, and ν are the fluid velocity, pressure and viscosity respectively. The NSE equations are replaced by an equivalent system of equations in the same variables (The PPE reformulation):

$$\begin{cases} \boldsymbol{u}_t - \nu \Delta \boldsymbol{u} = -\nabla p - (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \boldsymbol{f} & \text{for } \boldsymbol{x} \in \Omega, \\ \boldsymbol{n} \times (\boldsymbol{u} - \boldsymbol{g}) = 0 & \text{for } \boldsymbol{x} \in \partial\Omega, \\ \nabla \cdot \boldsymbol{u} = 0 & \text{for } \boldsymbol{x} \in \partial\Omega, \end{cases} \tag{5}$$

$$\begin{cases} \Delta p = -\nabla \cdot ((\boldsymbol{u} \cdot \nabla u) + \nabla \cdot \boldsymbol{f} & \text{for } \boldsymbol{x} \in \Omega, \\ \boldsymbol{n} \cdot \nabla p = \boldsymbol{n} \cdot (\boldsymbol{f} - \boldsymbol{g}_t + \nu \Delta \boldsymbol{u} - (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} & \text{for } \boldsymbol{x} \in \partial\Omega. \end{cases} \tag{6}$$

Finding a numerical approximation to the system (5) and (6) is challenging due to the complicated boundary conditions and the complex geometries that arise in the relevant applications. We have derived a numerical scheme for this system and verified convergence for a first order semi-explicit numerical scheme.

Goals and future work on PPE reformulations

1. *The goal of this project is to demonstrate that PPE reformulations can result in arbitrarily high order approximations to the Navier-Stokes equations. We are also currently working on the analysis of the weak problem as well as stability and convergence results for the numerical scheme.*
2. *Implementation of a 3D scheme for testing practical problems.*

Completed research projects

In my Ph.D dissertation and the first year of my post-doc, I completed the following projects. This work was motivated by the problem that arises in environmental studies of pollution of ground water due to surface pollution. This is a critical problem because a lot of people depend on ground water for drinking and increasing industrial activity poses a threat to clean water when contaminates are allowed to percolate into the subsurface. In tackling this problem we developed a coupled model of free flow with porous media flow and then coupled this with a transport equation to track pollutants. This is a very challenging problem both from both the mathematical and numerical point of view because we considered all three different models in one system.

Coupling free flow with porous media flow

The coupling of free flow and porous media flow has a wide range of applications for example in Geo-sciences (modeling interaction between rivers and ground flow) and biology (modeling interaction between organs and blood flow). In my Ph.D thesis I completed the mathematical and numerical analysis of a coupled model with the Navier-Stokes equations modeling free flow and Darcy's law modeling flow in the porous medium. In this work the challenges are resolving accurately the flow in the porous medium which may have discontinuities in the permeability field due to varying rock structures, fractures or cracks. This project also combined two different physics models of flow, which also presents challenges on how to properly combine them. My work on the coupled model comprised of the following:

Analysis of Weak Solution and Error Analysis

In [8] we analyze the weak formulation of the coupled free flow and porous media flow problem using the Navier-Stokes and Darcy equations. We have shown existence and uniqueness of a weak solution and proved a priori error estimates for the coupled problem. The difficulty in coupling the two flows arises on the interface because of the different orders of magnitude of velocity that exist in the free flow and porous media domain. There is no consensus on the right interface conditions to use. We propose to impose at the interface, the continuity of the normal component of velocity, the Beavers-Joseph-Saffman law [1], and the balance of forces. The later condition has been presented it in two ways: one including the inertial forces and another without. The condition including inertial forces is better mathematically suited as it yields stronger existence and uniqueness results. The other condition is the usual condition applied in the case of the linear Stokes coupled with Darcy problem. Our Numerical experiments in [8] show that both conditions give physically reasonable flow simulations.

Multi-numerics scheme

Modelling flow in a porous medium is a challenging problem due to complex geometries such as cracks and faults and discontinuities in permeability fields. We use high order discontinuous Galerkin methods overcome this difficulty in the porous medium. We are able to resolve the critical features of the flow using relatively coarse meshes. We prove and numerically verify optimal convergence of this numerical scheme in [8].

Simulation of coupled flow problem

Computing an accurate numerical scheme to the coupled problem poses a challenge due to the heterogeneity of the porous medium and the different length scales of velocity in the free flow region compared to the porous medium were flow moves at a slower pace. In order to test the numerical scheme we have proposed in [8], we proposed a numerical scheme combining the continuous finite element and discontinuous Galerkin method. We have shown through numerical examples that the combination of the continuous finite element method with the discontinuous Galerkin method gives the most efficient solver for the coupled problem. Figure 3 shows computed pressure and velocity streamlines for a coupled simulation with a fault structure. In [9] we present numerical examples for different physical phenomenon illustrating the coupled flow problem and tables showing optimal convergence rates.

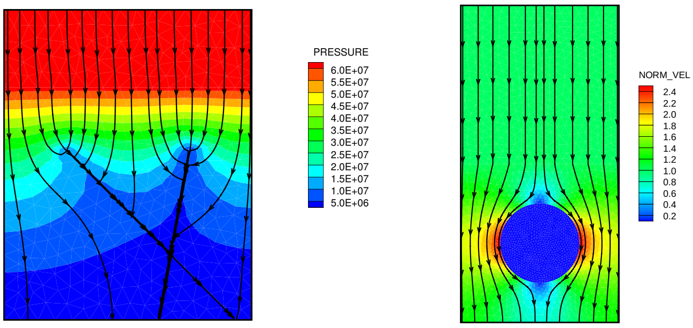

Figure 2: Computed velocity streamlines and pressure field for different flow test cases (details can be found in our paper [9])

Coupling complex flow with transport equation

Monitoring the effects of contamination of ground-water sources is an important environmental problem. This problem can be simulated by coupling the solution from the Navier-Stokes and Darcy flow with a transport equation. We have proved the well-posedness of the weak solution and error estimates for this problem and provided some numerical examples that simulate the flow [4]. In this work we used an improved discontinuous Galerkin method by upwinding the fluxes.

Two-grid method for coupled Navier-Stokes/Darcy coupling

In considering the coupled problem is was quickly clear that the matrices arising from the fully coupled problem were very large and difficult to solve. In [10] we solved this problem by applying a two grid approach to solve the coupled Navier-Stokes and Darcy problem. This technique has been applied to the steady state Navier-Stokes problem by Girault and Lions in [11]. In this approach the coupled problem is solved on a coarse mesh. The problem is then decoupled into the two problems in the free flow and porous media domains both using the solution from the coarse mesh as data for the interface variables. The advantage of this technique is that we can then solve two smaller linear systems in each domain and this can be done in parallel on the fine mesh.

Coupling Discontinuous Galerkin Method with Finite Volume Method for Elliptic Problem

Finite volume methods on Voronoi cells are widely used in engineering practice, in particular for reservoir simulations. However they do not allow for high order approximations but they approximate the flow very well in parts of the domain that have a permeability that homogeneous. In [7] we couple the two methods so that in parts of the domain where higher order approximations are useful (e.g areas with faults and fractures) the discontinuous Galerkin method can be used and the finite volume method everywhere else. This is an important contribution as it will improve accuracy of simulations and keep the computational cost down because the discontinuous Galerkin method will be used on a small subset of the domain.

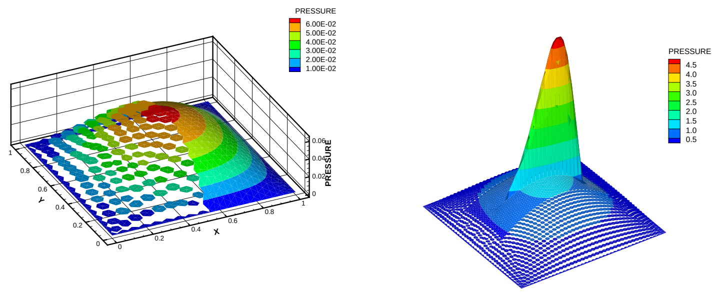

Figure 3: Computed pressure field for coupled finite volume with DG scheme (details can be found in [7])

Future directions on Complex Flows

The main motivation behind my work has been to model the interaction between ground-water and subsurface flow. This is a difficult problem because the permeability field in the porous medium has a wide range of scales over very large domains. The fine scale effects often have profound effects on the coarser scales and the resulting flow in general. Multiscale finite elements have been applied to the elliptic problem in the past [2]. Adding this technique to the current model will greatly improve the ability to effectively capture the large scale behavior of the flow in the porous medium without resolving the small scale effects. This is a natural step in line with my goal of developing software that will have capabilities of solving large scale problems. A 3D simulation of the coupled problem will provide greater insight for application purposes. This combined with Upscaling techniques will provide a model that can provide a better understanding of the effect of pollution on ground-water sources. For practical applications the coupled model describes flow in very large domain. As the problem grows larger, adaptive mesh refinement capabilities will make the code more efficient. Obtaining error estimators for mesh refinement techniques for this problem will be an important mathematical and practical contribution.

References

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