RESEARCH STATEMENT

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1 Introduction

My research interests are in the areas of *Numerical analysis and Scientific computing*, *Computational and Applied Mathematics*. My expertise are in the numerical analysis of partial differential equations, derivation of error estimates and implementation of efficient high order numerical methods for partial differential equations (PDEs). High order methods (in my work this mostly refers to Discontinuous Galerkin methods (DG)) play a fundamental role in the simulation of processes in science and engineering for a several reasons. High order methods can capture small structures on relatively coarse grids. As a result for a given error tolerance, high order methods are computationally more efficient compared to low order methods. In addition, conservation of physical quantities such as mass or energy is an important requirement for most physical processes, attaining this requires high accuracy in both space and time, something which high order methods can deliver. DG methods can also be used on general geometries and triangulations and easily handle boundary conditions, this makes them suitable for many applications in science and engineering. In addition their compactness make them favorable to parallel implementation. Parallel computing is an important aspect in demonstrating the feasibility of these methods on practical applications. In view of this, high performance computing is also an important component of my work. My current work is on problems in computational fluid flow and radiotherapy treatment in medical applications.

2 Current research projects

2.1 Discontinuous Galerkin methods for moment methods for radiative transfer

One of the methods of modern cancer treatment is high energy ionizing radiation using photons. The success of radiative therapy depends on the application of maximum dosage to the tumor region while simultaneously protecting organs and tissue around the tumor that may be damaged by excessive radiation. The problem of determining the exact dosage distribution in a patient's body is very important. A general form of the radiative transport equation is:

$$\frac{1}{c}\partial_t\psi + \Omega\nabla\cdot\psi + \sigma_t\psi = \frac{\sigma_s}{4\pi}\int_{S_2}\psi(x,t,\Omega')\,\mathrm{d}\Omega' + Q, \tag{1}$$

were c is the speed of light, $\psi(x,t,\Omega)$ denotes the particle distribution at time t, at position x travelling in the direction Ω and Q denotes external sources. The interaction between particles is expressed by $\sigma_s(x), \sigma_a(x)$ characterizing scattering and absorption with $\sigma_t(x) = \sigma_a(x) + \sigma_s(x)$. The equation (1) is a model for photons traveling at the same speed. The large phase space of (1) makes it computationally expensive to solve directly. Considerable effort has been placed into finding approximate solution techniques that are faster and yet accurate enough for a given application.

Moment methods are one common way to approximate the full radiative transfer equation by averaging over the directional components and thus replacing them by a finite number of moments. The moment method results in moment closure problems which range from simple linear moment closure problems that result in linear hyperbolic systems to more complicated closures for example the minimum entropy closure that gives non-linear hyperbolic systems. Our goal is to develop and implement high order numerical methods to solve the moment closure problems approximating the full radiative transfer problem to determine the dosage distribution. In addition, we also want to compare different closures for the radiative transfer problem.

Our implementation of the DG method is well suited for this application due to the following challenges. First, the scattering and absorption parameters $\sigma_s(x), \sigma_a(x)$ can have sharp discontinuities as they reflect properties of different parts of the human body. We are able to capture the critical features of the flow of photons due to these discontinuities with relatively coarse grids. The DG method also allows for arbitrarily high order approximations on complex domains with unstructured meshes and easily handles boundary conditions. These properties are highly advantageous considering the potential complexities in modeling parts of the human anatomy.

in [6, 5, 4, 3, 7]. A common benchmark test in the radiative transfer community is a reactor core simulation

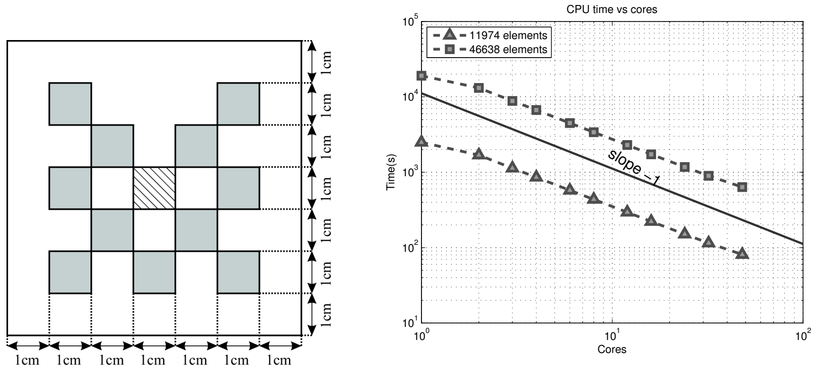

Figure 1: Computational domain resembles a reactor core structure with a central radiation source (left) and CPU times vs cores (right)

showin in Figure 1, the red and white regions are highly scattering and the blue regions are absorbing. Figure 2 shows the numerical solution from a linear moment closure at some sample times after the source is turned on in the white region. We observe the variation of the density of the particles reflects the underlying properties of the domain. We have tested the code on other benchmark problems common in the radiative transfer community

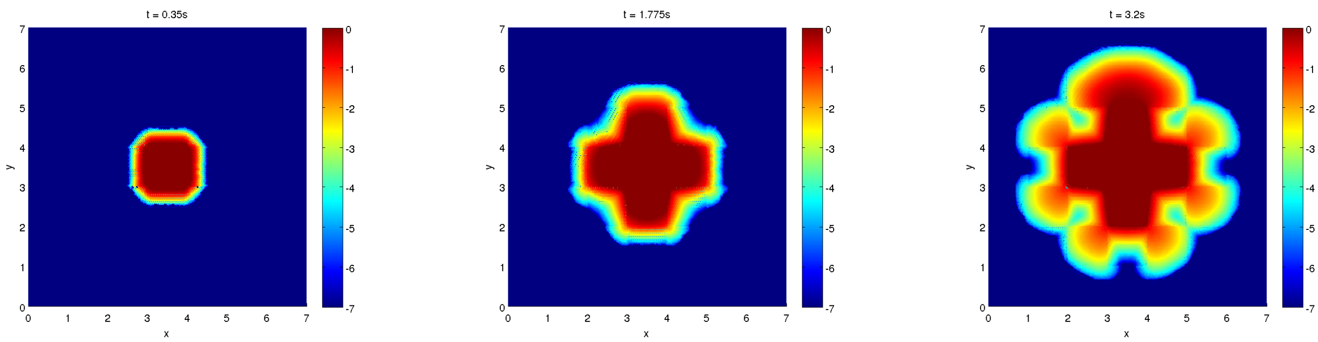

Figure 2: Computed radiation intensity (Log scale) at sample times after source is turned on.

and verified optimal convergence rates.

Our implementation of the DG method is robust as shown by results from benchmark test, parallel and scales almost perfectly as illustrated in Figure 1). It is clear that the computational time decreases as we increase the number of cores. This work is ongoing [11].

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. Work in the immediate future includes adding more physics to the general model and testing on more practical problems in order to compare with experimental results from medical researchers in the field.

We have recently started a collaboration with a team at Jefferson University to enable us to start working towards simulating experiments we can compare with medical data.

3. High order methods suffer from spurious oscillations, limiting is therefore required for the solution. In addition we want limiting that preserves the physics of the solution. To our knowledge this has not been fully studied for moment closure problems for radiative transfer equations.

2.2 High order numerical methods for transient Navier-Stokes equations

Pressure Poisson Equation (PPE) reformulations of the time dependent incompressible Navier-Stokes equations are similar to projection approaches. 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. This means that PPE reformulations provide a framework for arbitrary order approximations in space and time. Our goal in this project is to look at fluid-structure interactions that require computation of stresses and forces at the boundary and therefore require a high order accurate solution near the boundary.

In the PPE reformulations the incompressibility constraint $\nabla \cdot u$ is replaced by a Poisson equation for the pressure. This allows for the addition of an extra boundary condition that must be selected so that incompressibility is maintained in the new system. This process leads to systems which (for sufficiently smooth solutions) are equivalent to the Navier-Stokes equations, but have explicit boundary conditions for the pressure. The pressure can be recovered from the velocity without ambiguity up to an additive constant by solving a Poisson problem with explicit boundary conditions. The PPE reformulations we consider have been analyzed in [9].

Goals and future work on PPE reformulations

1. The goal of this project is to solve the PPE reformulations using a finite element approach. PPE reformulations allow for arbitrary order in time methods. Discontinuous Galerkin methods allow for arbitrary high order approximations in space, therefore it is an attractive choice for this project.

2. Mathematical analysis of the weak solution for the PPE reformulation and error analysis.

3. Implementation of high order schemes in 3D.

3 Completed research projects

3.1 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 geosciences (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:

3.1.1 Analysis of Weak Solution and Error Analysis

In collaboration with B. Rivière in [13], I analyzed the weak formulation of the coupled free flow and porous media flow problem. We have shown existence and uniqueness of a weak solution and proved a priori error estimates for the coupled problem.

One of the difficulties in understanding the coupling 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 [2], 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. The work completed in [13] provides numerical examples to test the two models. The solutions obtained by the two models differ under low viscosity.

3.1.2 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. My implementation of 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.

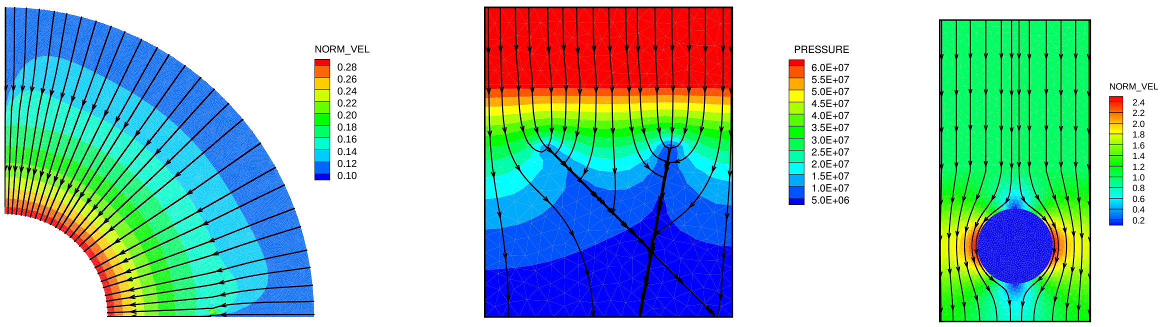

Figure 3: Computed velocity and pressure field for different flow test cases (details can be found in our paper [14])

3.1.3 Simulation of coupled flow problem

In order to test the numerical scheme we have proposed in [13], I have implemented different combinations of the continuous finite element and discontinuous Galerkin methods for the coupled model using the *C* programming language aided by the PETSc toolkit [1]. The purpose of the numerical examples is to illustrate the robustness of the scheme under different situations that arise in physical situations. 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. In a paper [14] with B. Rivière we present numerical examples for different physical phenomenon illustrating the coupled flow problem and tables showing optimal convergence rates.

3.2 Coupling complex flow with transport equation

Monitoring the effects of contamination of groundwater 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. The model is shown below: 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 [10]. In this work we used an improved discontinuous Galerkin method by upwinding the fluxes.

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

In a paper [15] with B. Rivière, I applied 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 [16]. In this approach the coupled problem is solved on a coarse mesh. The second step is to decouple the problem on the fine mesh and use the solution from the coarse mesh as data for the interface variables when solving the problem in each domain. One advantage of this technique is that we can then solve the two larger problems in parallel once we have solved the smaller problem on the coarse mesh. This technique will reduce the computational time as it will allow for a parallel implementation of the current solver.

3.4 Coupling Discontinuous Galerkin Method with Finite Volume Method for Elliptic Problem

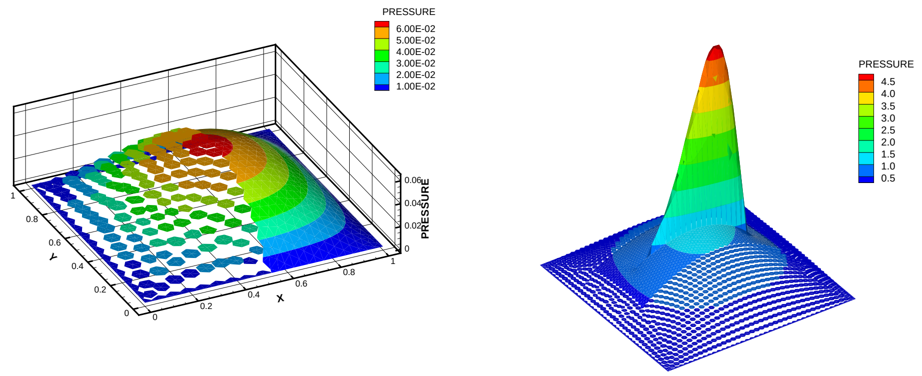

Figure 4: Computed pressure field for coupled finite volume with DG scheme (details can be found in [12])

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. In [12] we couple the two methods so that in parts of the domain where higher order approximations are useful the discontinuous Galerkin method can be used. 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 subset of the domain.

3.5 Future work on multi-numerics and coupled flow problems

1. *Coupling Free flow with Multiscale Darcy*
The main motivation behind my work has been to model the interaction between groundwater 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 [8]. 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 inline with my goal of developing software that will have capabilities of solving large scale problems.

2. *Implementation of 3D Numerical Coupled Flow Simulator*
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 groundwater sources.

3. *Adaptive refinement techniques*
   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 contribution.

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