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Research Statement

I have always enjoyed modeling physical situations. It is this joy that guided me to study mathematics and physics as an undergraduate and to focus my graduate studies on numerical analysis and computational mathematics. Scientific computing, provides a researcher limitless opportunities to gain insight into real world problems. Computational mathematics and numerical analysis are the heart of mathematical modeling; because of this, my research centers in these areas.

When modeling physical applications the approximating systems are not always of a single type. Thus, the system of modeling equations may not be easily classified as elliptic, hyperbolic, or parabolic. If the approximating system is of mixed types, then different computational strategies are applicable to different portions of the system. In my career as a researcher, my primary focus has been on decomposition techniques for mixed systems of time dependent partial differential equations (PDEs). Decomposition techniques can have several advantages when used to solve PDEs. First, decomposition methods allow appropriate approximation techniques to be applied to each of the different types of equations within a modeling system. Second, depending on the physical situation being studied decomposition techniques have the potential to decouple unknowns into distinct solves and even linearize nonlinear systems.

I have studied decomposition techniques by considering their application to fluid flow problems. This research can be classified using three main modeling systems: the convection-diffusion equation, the viscoelastic fluid flow equations, and the modeling equations for two-phase flow in porous media. In my dissertation research, I have focused on the application of a fractional step θ-method to both convection-diffusion and viscoelasticity. In my discussion below, I outline this operator splitting technique and describe the modeling systems I have considered. I also discuss the groundwater flow equations that I have studied during my summer internships.

Fractional Step θ-method

The fractional step θ-method was introduced, and its temporal approximation accuracy studied for a symmetric, positive definite spatial operator, by Glowinski and Périaux in [8]. To illustrate the θ-method consider the partial differential equation given by

$$\frac{\partial u}{\partial t} + F(u,x,t) = 0 \text{ in } \Omega \times (0,T] \tag{1}$$

If we additively split the operator $F(u,x,t)$ into

$$F(u,x,t) = {}^1F(u,x,t) + {}^2F(u,x,t), \tag{2}$$

the general expression for the fractional step θ-method is obtained by dividing the time step Δt into three pieces, and advancing the solution from $n\Delta t$ to $(n+1)\Delta t$ in the following manner:

$$\text{Sub-step 1.} \qquad \frac{u_h^{(n+\theta)} - u_h^{(n)}}{\theta \Delta t} + {}^1F^{(n+\theta)} = -{}^2F^{(n)} \tag{3}$$

$$\text{Sub-step 2.} \qquad \frac{u_h^{(n+1-\theta)} - u_h^{(n+\theta)}}{(1-2\theta)\,\Delta t} + {}^2F^{(n+1-\theta)} = -{}^1F^{(n+\theta)} \tag{4}$$

$$\text{Sub-step 3.} \qquad \frac{u_h^{(n+1)} - u_h^{(n+1-\theta)}}{\theta \Delta t} + {}^1F^{(n+1)} = -{}^2F^{(n+1-\theta)} \tag{5}$$

For the optimal value of $\theta = 1 - \sqrt{2}/2$ the fractional step θ-method has both the second order temporal convergence of the Crank-Nicolson method and the strong A-stability of the implicit Euler method [16]. The θ-method is widely used for the accurate approximation of the Navier-Stokes equations (NSE) [16], [9]. In [11], Klouček and Rys showed, assuming a unique solution existed, that the θ-method approximation converged to the solution of the NSE as the spatial and mesh parameters went to zero ($h,\, \Delta t \rightarrow 0_+$). The temporal discretization error for the θ-method for the NSE was studied by Müller-Urbaniak in [12] and was shown to be second order. In [13, 14, 15] numerical implementations of the θ-method applied to viscoelastic fluid flow were considered; however, no error analysis of the method was done. I have implemented and analyzed the fractional step θ-method for both the time dependent convection-diffusion equation (6)-(8), as well as for the equations of viscoelastic fluid flow (9)-(14).

Convection-diffusion

The convection-diffusion equation

$$\begin{aligned} \frac{\partial u}{\partial t} - \triangle u + \mathbf{b} \cdot \nabla u + c\, u &= f \quad \text{in} \quad \Omega \times (0,T], && (6) \\ u(x,t) &= 0, \quad x \in \partial\Omega \times (0,T], && (7) \\ u(x,0) &= u_0(x), \quad x \in \Omega, && (8) \end{aligned}$$

models the concentration of a specimen u on a domain Ω, where $\mathbf{b} = [b_1(x,t), b_2(x,t)]^T$ is an incompressible velocity field (i.e $\nabla \cdot \mathbf{b} = 0$), $c(x,t) \geq c_0$ is an absorption coefficient, and $f(x,t)$ is a given body force. The model in (6) has two characteristic parts: parabolic diffusion in the term $\triangle u$, and a hyperbolic transport piece given by $\mathbf{b} \cdot \nabla u$. It was ideal to examine convection diffusion prior to the study viscoelastic flow, as the modeling system for viscoelasticity involves a parabolic momentum conservation equation coupled to a hyperbolic constitutive equation. The analysis and implementation of the θ-method for convection-diffusion can be found in [4] and [5]. For our implementation we completely separate the convection operator from the diffusion operator, and stabilize the hyperbolic convective solve using a streamline upwinded Petrov-Galerkin (SUPG) method. Main results in [4] and [5] are:

- A description of a θ-method for the time dependent convection-diffusion problem.
- Proof of existence and uniqueness of the θ-method approximation to (6)-(8).
- Proof of second order accurate temporal a priori error estimates for the θ-method approximation to (6)-(8).
- Numerical results verifying the optimal value of θ, and supporting the established a priori error estimate.

Viscoelastic Fluids

Mathematical models of viscoelastic fluids are commonly found in industrial and biological settings where they are used to investigate materials that exhibit properties of both elastic solids and Newtonian fluids (i.e polymers, paint, blood). The non-dimensional modeling equations for a viscoelastic fluid in a given domain $\Omega \subset \mathbb{R}^{\acute{d}}$ ($\acute{d} = 2, 3$) using a Johnson-Segalman constitutive equation are written as:

$$\begin{aligned}
\boldsymbol{\sigma} + \lambda\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{\sigma} + g_a(\boldsymbol{\sigma}, \nabla\boldsymbol{u})\right) - 2\alpha\mathbf{d}(\boldsymbol{u}) &= \mathbf{0} \quad \text{in } \Omega, && (9)\\
Re\left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{u}\right) + \nabla p - 2(1-\alpha)\nabla\cdot\mathbf{d}(\boldsymbol{u}) - \nabla\cdot\boldsymbol{\sigma} &= \mathbf{f} \quad \text{in } \Omega, && (10)\\
\nabla\cdot\boldsymbol{u} &= 0 \quad \text{in } \Omega, && (11)\\
\boldsymbol{u} &= \mathbf{0} \quad \text{on } \partial\Omega, && (12)\\
\boldsymbol{u}(0,x) &= \boldsymbol{u}_0(x) \text{ in } \Omega, && (13)\\
\boldsymbol{\sigma}(0,x) &= \boldsymbol{\sigma}_0(x) \text{ in } \Omega. && (14)
\end{aligned}$$

Here (9) is the constitutive equation relating the fluids velocity $\boldsymbol{u}$ to the elastic stress $\boldsymbol{\sigma}$, and (10) and (11) are the conservation of momentum and conservation of mass equations. The fluids pressure is denoted by p. The Weissenberg number λ is a dimensionless constant defined as the product of a characteristic strain rate and the fluid's relaxation time [1]. *Re* denotes the fluids Reynolds number, $\mathbf{f}$ are the body forces acting on the fluid, and $\alpha \in (0, 1)$ represents the proportion of the total viscosity that is considered to be viscoelastic [7].

The g_a term and deformation tensor $\mathbf{d}(\boldsymbol{u})$ are defined as:

$$g_a(\boldsymbol{\sigma}, \nabla\boldsymbol{u}) := \frac{1-a}{2}\left(\boldsymbol{\sigma}\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\boldsymbol{\sigma}\right) - \frac{1+a}{2}\left(\nabla\boldsymbol{u}\boldsymbol{\sigma} + \boldsymbol{\sigma}(\nabla\boldsymbol{u})^T\right)$$

and

$$\mathbf{d}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right).$$

The gradient of $\boldsymbol{u}$ is defined such that $(\nabla\boldsymbol{u})_{i,j} = \partial u_i/\partial x_j$.

Accurate numerical methods for modeling viscoelastic fluid flow are difficult for a variety of reasons. The modeling equations (assuming *slow* flow, where $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$ in (10) is neglected) represent a "Stokes system" for the conservation of mass and momentum equations, coupled with a non-linear hyperbolic equation describing the constitutive equation for the stress. The numerical approximation requires the determination of the fluid's velocity, pressure and stress (a symmetric tensor). For an accurate approximation a direct approximation technique requires the solution of a very large non-linear system of equations at each time step. The fractional step θ-method decouples the approximation of velocity and pressure from the approximation of the stress, thereby reducing the size of the algebraic systems which have to be solved at each sub-step. An added benefit of the θ-method is that the algebraic systems to be solved at each sub-step are linear.

We have investigated numerical implementations of the θ-method for viscoelastic fluid flow in [3], [2], and [6] using a SUPG approximation to stabilize the hyperbolic constitutive equation. Our analysis of the θ-method is accomplished in two main parts. One part of the analysis, in [2] and [6], follows the method of proof used in [5] to establish error estimates for the θ-method applied to the "Stokes system" assuming a known stress. Also in [2] and [6], the θ-method is applied to the constitutive equation assuming known velocity and pressure. Highlights of the research presented in [2], and [6] are

- A description of a θ-method for the time dependent viscoelastic fluid flow using a Johnson-Segalman constitutive relationship.
- Proof of a second order accurate temporal a priori error estimate for the θ-method approximation of the constitutive equation assuming known velocity and pressure.
- Proof of a second order accurate temporal a priori error estimate for the θ-method approximation of the "Stokes system" assuming a known value for stress.
- Numerical results verifying the optimal value of θ, and supporting the established a priori error estimates.

My current work on the analysis for the fractional step θ-method applied to viscoelasticity in [3] couples error estimates similar to those obtained in [6] and [2] for the θ-method applied to the constitutive equation with known velocity and pressure, and the "Stokes system" with known stress. Ultimately, a second order accurate temporal a priori error estimate for the θ-method applied to (9)-(11) will be established.

Two-phase flow in porous media

Over the past two summers I have had the opportunity to collaborate with researchers at the U.S. Army Corps of Engineers Engineering Research and Development Center (ERDC) in Vicksburg, Mississippi. My research during my first summer at ERDC focused on stabilization and shock capturing techniques for nonlinear advection-diffusion equations. In summer 2007, one of the key components of my research consisted of implementing an IMPES (implicit pressure, explicit saturation) scheme to approximate two-phase air water flow in a heterogeneous porous media. The modeling equations for a mixture of two mobile, immiscible fluid phases (labeled non-wetting, n, and wetting w) are:

$$
\begin{aligned}
\frac{\partial(\omega s_w \rho_w)}{\partial t} + \nabla \cdot \vec{q}_w + c_w &= 0 && (15)\\
\frac{\partial(\omega s_n \rho_n)}{\partial t} + \nabla \cdot \vec{q}_n + c_n &= 0 && (16)\\
\vec{q}_w &= -\frac{\rho_w \bar{k}_i \bar{k}_{rw}}{\mu_w}(\nabla p_w - \rho_w \vec{g}) && (17)\\
\vec{q}_n &= -\frac{\rho_n \bar{k}_i \bar{k}_{rn}}{\mu_n}(\nabla p_n - \rho_n \vec{g}) && (18)\\
s_n &= 1 - s_w && (19)\\
p_n - p_w &= p_c(\vec{x}, s_w) && (20)\\
\bar{k}_{r\alpha} &= \bar{k}_{r\alpha}(\vec{x}, s_w) && (21)\\
\bar{k}_i &= \bar{k}_i(\vec{x}) && (22)\\
\rho_\alpha &= \rho_\alpha(p_\alpha) && (23)\\
\omega &= \omega(\vec{x}, p_n, p_w) && (24)
\end{aligned}
$$

Equations (17) and (18) are the multiphase extensions of Darcy's law. The phase pressures, p_w and p_n, are porous medium scale pressures derived for each phase separately. Saturations, s_w and s_n, are the fractions of the pore space occupied by the fluid phases. The intrinsic permeability of the medium, $\bar{k}_i$, is the part of the proportionality constant in the extensions of Darcy's law that reflect the flow properties of the medium (the porosity and the connectivity of the pore space). The relative permeabilities, $\bar{k}_{rw}$ and $\bar{k}_{rn}$, are the fractions of the intrinsic permeability "available" to the fluids. Here μ_α is the dynamic viscosity of each phase. The porosity, ω, is the volumetric fraction of the porous medium that can transmit fluid. It is usually assumed to be a (spatially variable) constant or a weakly nonlinear function of phase pressures. The phase densities, ρ_w and ρ_n, are the mass per unit volume of each phase. Sources and sinks in each phase are represented by c_α. We use $\vec{g}$ as gravitational acceleration vector.

The IMPES scheme examined allowed for a complete decoupling of the pressure phase solution from the saturation phase. Our goal is to make a comparison between the two-phase flow equations for immiscible air/water flow using both fully coupled and IMPES formulations with Richards' equation for water flow in variably saturated porous media. Richards' equations neglects the effect of the viscous air phase. The results of our study will be presented in [10], and will contain numerical results for a set of physically realistic scenarios where Richards' equation is an accurate approximation as well as a set where it is not.

Ongoing and Future Work

There are many opportunities for future research. The following is a brief list of topics I wish to investigate further:

Convection-diffusion

- The θ-method implemented for convection-diffusion uses two approximations of the same equation (with different right hand sides) next to each other in the algorithm (i.e solve (5) in time step n followed by solve (3) in time step $n+1$). This hints at the possibility of creating a two step approximation method for the convection-diffusion equations that maintains all the benefits of the three step θ-method studied in [5].
- Often convection-diffusion problems contain spatial regions where one physical phenomenon dominates the other (i.e sharp advective-fronts in only portions of the problem domain). It would be interesting to investigate operator splitting methods based on a local Péclet number which expresses the ratio of convective to diffusive transport. This work could be extended to two-phase flow in porous media.

Viscoelastic Fluids

- After completing the a priori error estimates of the θ-method applied to viscoelastic fluid flow using SUPG stabilization for stress in [3], one possible research direction would be to consider the θ-method implementation using discontinuous Galerkin (DG) elements to resolve the stress. This would also allow for a comparison of the θ-method for viscoelastic fluid flow using SUPG and DG stabilization.
- The split used when setting up the θ-method for the viscoelastic fluid flow equations is not unique. Further examination may provided a better way to decouple the equations into explicit and implicit solves.

- I also plan to implement an operator splitting method for a coupled problem involving viscoelastic fluid flow and generalized Darcy flow in a porous media (i.e flow of a polymer through a filter).

Two-phase flow in porous media

- The first goal of this research will be to complete the numerical comparison of the two-phase flow with Richards equations.
- It would be interesting to investigate an implementation and analysis of a fractional step θ-method applied to groundwater modeling equations. The application of the fractional step θ-method to groundwater modeling equations is a natural extension of my dissertation work.

More information about my research including: papers, preprints, technical reports, and numerical examples can be found at *http://people.clemson.edu/∼jchrisp*.

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