Research Statement

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Research Interests

I am broadly interested in computing numerical analysis for solving partial differential equations drawn from problems in fluid dynamics, electromagnetism and plasma physics.

The study of fluid flow has a wide range of applications in many scientific and engineering fields such as aerodynamics, weather predictions, astrophysics, traffic engineering, petroleum engineering and modeling ocean currents. For these problems, the determination of forces and moments on aircrafts, prediction of weather patterns, understanding of nebulae in interstellar space, and estimating the mass flow rate of petroleum through pipelines, are critically important.

The Navier-Stokes equations (NSE) are the basis for simulating flows in computational modeling, and are widely believed to be the accurate physical model. Even though a large number of mathematicians and scientists have been investigating these equations for 160 years, understanding their fundamental solution properties remains elusive and is a \$1 million Clay Prize Problem [1]. To obtain an accurate numerical simulation of a velocity field for a flow with high Reynolds number, an extremely large number of degrees of freedom (dof) are needed, which is one of the main hurdles when computing solution. Even more complex situations arise in simulating magnetohydrodynamics (MHD) flow and weather forecasting, since these systems contain additional often nonlinear equations for different physical processes.

Recent advances in algorithms, large scale computing, and understanding of fluid flow phenomena has made it possible to begin considering the simulation of multiphysics flow problems which couple the NSE to conservation laws and constitutive equations for other physical phenomena. The objective of my research is to develop, improve accuracy and efficiency in such simulations. This includes numerical method development and analysis, as well as large scale parallel implementation and simulation.

Philosophy on collaboration: I like to build and maintain collaborative relationships with people across fields and disciplines whenever possible believing that working with collaborator is one of the best way to learn, broaden my views and take a fresh perspectives in a short time. I have worked with Dr. Leo Rebholz (Clemson University), Dr. Nan Jiang (Florida State University), Dr. Timo Heister (Clemson University), Dr. Songul Kaya (Middle East Technical University), Dr. Catalin Trenchea (University of Pittsburgh) and Dr. Traian Iliescu (Virginia Tech), they have helped me to work in advance numerical methods for MHD and NSE.

Research Experience

1.1 Efficient Numerical Methods for MHD Flow Simulation:

In recent years, the study of MHD flows has become important due to its various applications in, e.g. astrophysics and geophysics [13, 21, 11, 10, 4, 6], liquid metal cooling in nuclear reactors [3, 12, 22], and process metallurgy [8]. The governing equations for MHD are

$$u_t + (u \cdot \nabla)u - s(B \cdot \nabla)B - \nu\Delta u + \nabla p = f, \tag{1.1}$$

$$\nabla \cdot u = 0, \ \nabla \cdot B = 0, \tag{1.2}$$

$$B_t + (u \cdot \nabla)B - (B \cdot \nabla)u - \nu_m \Delta B + \nabla \lambda = \nabla \times g. \tag{1.3}$$

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Here, u is velocity, B is magnetic field, p is a modified pressure, f is body force, $\nabla \times g$ is a forcing on the magnetic field, s is the coupling number, ν is the kinematic viscosity, ν_m is the magnetic diffusivity and λ is a Lagrange parameter. At each time step, to solve the fully coupled systems will generally be computationally infeasible. The standard timestepping methods that decouple the equations are prone to unstable behavior without excessively small timestep sizes. A breakthrough for efficient MHD algorithms was recently made by C. Trenchea [23], when he showed that if MHD is first written in Elsässer variables instead of primitive variables (see below), then the MHD system can be decoupled into two Oseen problems at every time step in a first order timestepping method, in an unconditionally stable way. We explored this idea computationally, and it was shown to work very well. To describe the method, we first reformulate the MHD system into Elsässer variables: define $v := u + \sqrt{s}B$, $w := u - \sqrt{s}B$, $f_1 := f + \sqrt{s}\nabla \times g$, $f_2 := f - \sqrt{s}\nabla \times g$, $g_2 := g + \sqrt{s}\lambda$ and $g_2 := g_1 + \sqrt{s}\lambda$ and $g_2 := g_2 + \sqrt{s}\lambda$. Now, equation (1.1)-(1.3) produces

$$v_t + w \cdot \nabla v + \nabla q - \frac{\nu + \nu_m}{2} \Delta v - \frac{\nu - \nu_m}{2} \Delta w = f_1, \tag{1.4}$$

$$\nabla \cdot v = 0, \quad \nabla \cdot w = 0, \tag{1.5}$$

$$w_t + v \cdot \nabla w + \nabla r - \frac{\nu + \nu_m}{2} \Delta w - \frac{\nu - \nu_m}{2} \Delta v = f_2. \tag{1.6}$$

The decoupled and unconditionally stable first order timestepping method has the form

$$\frac{1}{\Delta t}(v^{n+1}-v^n)+w^n\cdot\nabla v^{n+1}+\nabla q^{n+1}-\frac{\nu+\nu_m}{2}\Delta v^{n+1}-\frac{\nu-\nu_m}{2}\Delta w^n = f_1^{n+1},$$

$$\nabla\cdot v^{n+1}=0, \ \nabla\cdot w^{n+1}=0,$$

$$\frac{1}{\Delta t}(w^{n+1}-w^n)+v^n\cdot\nabla w^{n+1}+\nabla r^{n+1}-\frac{\nu+\nu_m}{2}\Delta w^{n+1}-\frac{\nu-\nu_m}{2}\Delta v^n=f_2^{n+1}.$$

Although a successful breakthrough idea, a drawback to the scheme is that it is limited to first order temporal accuracy. In a follow up work, a second order BDF2 extension is studied [17]; and found it was stable only under the data restriction $\frac{1}{2} < \frac{\nu}{\nu_m} < 2$. This restriction was shown to be sharp in [2], and such a restriction generally does not hold in practice. We propose and study a decoupled, unconditionally stable and higher order accurate scheme that has no restriction on ν and ν_m . By careful consideration of the analysis, we identify the 'problem terms' that lead to the restriction on $\frac{\nu}{\nu_m}$ in the second order method. We propose the following θ -method, which decouples the system and has no restriction on the data:

$$\begin{split} \frac{1}{2\Delta t}(3v^{n+1}-4v^n+v^{n-1}) + (2w^n-w^{n-1})\cdot\nabla v^{n+1} + \nabla q^{n+1} \\ -\frac{\nu+\nu_m}{2}\Delta v^{n+1} - \theta\frac{\nu-\nu_m}{2}\Delta(2w^n-w^{n-1}) - (1-\theta)\frac{\nu-\nu_m}{2}\Delta w^n &= f_1^{n+1}, \\ \nabla\cdot v^{n+1} &= 0, \ \nabla\cdot w^{n+1} &= 0, \\ \frac{1}{2\Delta t}(3w^{n+1}-4w^n+w^{n-1}) + (2v^n-v^{n-1})\cdot\nabla w^{n+1} + \nabla r^{n+1} \\ -\frac{\nu+\nu_m}{2}\Delta w^{n+1} - \theta\frac{\nu-\nu_m}{2}\Delta(2v^n-v^{n-1}) - (1-\theta)\frac{\nu-\nu_m}{2}\Delta v^n &= f_2^{n+1}. \end{split}$$

For this decoupled method, we proved unconditional stability of the method for any ν and ν_m , provided θ is chosen to satisfy $\frac{\theta}{1+\theta} < \frac{\nu}{\nu_m} < \frac{1+\theta}{\theta}, \, 0 \leq \theta \leq 1$. We also prove this scheme has temporal accuracy $O(\Delta t^2 + (1-\theta)|\nu - \nu_m|\Delta t)$. Even though the method is not second order, since in practice

 ν and ν_m are typically small, the method will typically behave like a second order method. This algorithm is potentially an enabling tool for future MHD simulations, and opens the door for many more types of investigating for MHD flow including MHD turbulence simulation which I plan to design studying very soon.

1.2 Uncertainty Quantification for MHD Flow:

In numerical simulation of fluid flows, uncertainty may be due to either lack of precise data about the physical phenomenon, or the inherent irregularity of the physical process involved. In MHD flow simulations with incomplete data, uncertainty quantification plays an important role in validation of simulation methodologies which aims at developing rigorous methods to characterize the effect of variability on the velocity and magnetic fields. We can estimate the uncertainties in the result by calculating an ensemble of J solutions to increase the scope of predictability by taking mean of J solutions and to estimate solution sensitivities. For incompressible MHD flows of an electrically conducting and non-magnetic fluids such as salt water, liquid metals, hot ionised gases (plasma) and strong electrolytes [9] at high Reynolds numbers, incomplete date, quantification of uncertainty, increasing forecasting skill, estimation of flow sensitivities and other issues, e.g. [7, 20, 18, 15, 16, 19] lead to the problem of computing ensemble solutions u_j , B_j and p_j for the following system of evolution equations [14, 5, 9]

$$u_{j,t} + u_j \cdot \nabla u_j - sB_j \cdot \nabla B_j - \nu \Delta u_j + \nabla p_j = f_j(x,t), \text{ in } \Omega, j = 1, \dots J, \tag{1.7}$$

$$\nabla \cdot u_j = 0, u_j(x, 0) = u_j^0(x), \ \nabla \cdot B_j = 0, \ B_j(x, 0) = B_j^0(x) \text{ in } \Omega,$$
 (1.8)

$$B_{i,t} + u_i \cdot \nabla B_i - B_i \cdot \nabla u_i - \nu_m \Delta B_i + \nabla \lambda_i = \nabla \times g_i(x,t) \text{ in } \Omega, \quad j = 1, \dots, J, \tag{1.9}$$

$$u_j = B_j = 0 \text{ on } \partial\Omega.$$
 (1.10)

in $\Omega \times (0,T)$, where Ω is the domain of the fluid, J is the number of realizations. The following efficient algorithm is proposed and studied for computing flow ensembles of the above system under uncertainties in initial or boundary data.

$$\frac{v_{j}^{n+1} - v_{j}^{n}}{\Delta t} + \nabla q_{j}^{n+1} - \frac{\nu + \nu_{m}}{2} \Delta v_{j}^{n+1} - \frac{\nu - \nu_{m}}{2} \Delta w_{j}^{n} + \langle w \rangle^{n} \cdot \nabla v_{j}^{n+1} + (w_{j}^{n} - \langle w \rangle^{n}) \cdot \nabla v_{j}^{n}}{-\nabla \cdot (2\nu_{T}(w_{j}^{'}, t)\nabla v_{j}^{n+1}) = f_{1, j}^{n+1},$$

$$\frac{w_{j}^{n+1} - w_{j}^{n}}{\Delta t} + \nabla r_{j}^{n+1} - \frac{\nu + \nu_{m}}{2} \Delta w_{j}^{n+1} - \frac{\nu - \nu_{m}}{2} \Delta v_{j}^{n} + \langle v \rangle^{n} \cdot \nabla w_{j}^{n+1} + (v_{j}^{n} - \langle v \rangle^{n}) \cdot \nabla w_{j}^{n}}{-\nabla \cdot (2\nu_{T}(v_{j}^{'}, t)\nabla w_{j}^{n+1}) = f_{2, j}^{n+1}.$$

where $\nu_T(u_j',t) = \sqrt{2}\mu l_u \sqrt{k_u'}$, l_u is the mixing length of fluctuations which is either Δx or $|u_j'|\Delta t$, $k_u' = \frac{1}{2}|u_j'|^2$ is the kinetic energy in fluctuations and μ is a tuning parameter. The ensemble average of J realizations is approximated through the clever algorithm (adapted from a breakthrough idea of Jiang and Layton, 2014) that, at each time step, uses the same matrix for each of the J system solves. Hence, preconditioners need built only once per time step, and the algorithm can take advantage of block linear solvers. Additionally, an Elsasser variable formulation is used, which allows for a stable decoupling of each MHD system at each time step. We prove stability and convergence of the algorithm, and test it with numerical experiments.

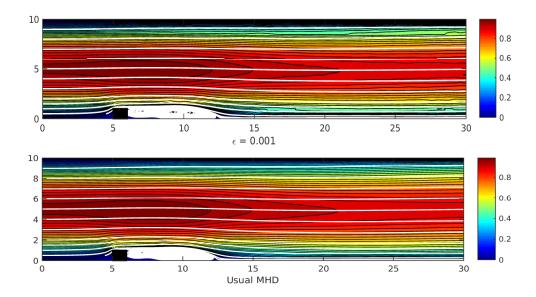


Figure 1: Shown above are T = 40, velocity ensemble solutions (shown as streamlines over speed contours) for MHD channel flow over a step with dt = 0.05, s = 0.01 and dof = 75222.

On going work and future plan

1.3 Effect of divergence-free snapshots on ROM-accuracy:

Currently, I am working on reduced-order modeling. We consider using ROM bases derived from strongly divergence-free (Scott-Vogelius) and weakly divergence-free (Taylor-Hood) finite element simulations of a 2D channel flow past a cylinder. We find that the strongly divergence-free bases provides more accurate predictions of lift and drag, in particular over longer time intervals.

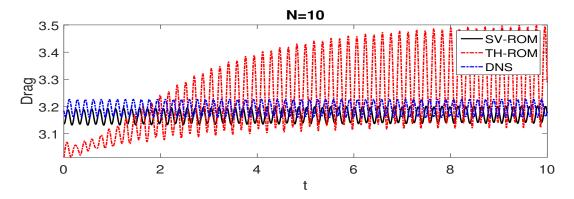


Figure 2: Plots of ROM solutions' drag, lift coefficients vs. time, for flow past a cylinder with Re=100, 23K with varying N=10 using linearized BDF2 scheme for SV vs. TH elements.

Efficient algebraic splitting methods for MHD:

I am also working on an efficient and accurate algebraic splitting methods for block saddle point problems arising in MHD. At each time step, we want to find (u, B, p, λ) for the following governing equations in a domain $\Omega \subset \mathbb{R}^d$ (d=2,3)

$$\frac{\alpha}{\Delta t}u + U.\nabla u - \nu \Delta u - sB^* \cdot \nabla B + \nabla p = \tilde{f}_1, \tag{1.11}$$

$$\nabla \cdot u = 0, \ \nabla \cdot B = 0, \tag{1.12}$$

$$\nabla \cdot u = 0, \ \nabla \cdot B = 0,$$

$$\frac{\alpha}{\Delta t} B + U \cdot \nabla B - B^* \cdot \nabla u - \nu_m \Delta B + \nabla \lambda = \tilde{f}_2.$$
(1.12)

where ν is the kinematic viscosity, ν_m is the magnetic diffusivity, Δt is a timestep size, U and B^* are given solenoidal vector fields (e.g. for BDF2 time stepping, $\alpha = \frac{3}{2}$, $U = 2u^n - u^{n-1}$, and $\tilde{f}_1 = f_1 + \frac{2}{\Delta t}u^n - \frac{1}{\Delta t}u^{n-1}$). After applying a finite element discretization to (1.11)-(1.13), a block linear system arises of the form

$$\begin{pmatrix} A_{11} & N_1 & C_1 & 0 \\ N_2 & A_{22} & 0 & C_1 \\ C_1^T & 0 & 0 & 0 \\ 0 & C_1^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{U} \\ \hat{B} \\ \hat{P} \\ \hat{\lambda} \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \\ 0 \\ 0 \end{pmatrix}$$
(1.14)

By applying the usual or pressure-corrected Yosida splitting techniques to the discretization, we want to show that the accuracy is increased by $O(\Delta t)$ without any additional cost in the respective methods. In the future, I plan to work on turbulence modeling for NSE and MHD, and improvement in linear solvers such as these will enable me to do so.

References

- [1] http://www.claymath.org/millennium-problems/navier-stokes-equation.
- [2] M. Akbas, L. Rebholz, and F. Tone. A note on the importance of mass conservation in longtime stability of Navier-Stokes equations. Applied Mathematics Letters, 45:98–102, 2015.
- [3] L. Barleon, V. Casal, and L. Lenhart. MHD flow in liquid-metal-cooled blankets. Fusion Engineering and Design, 14:401–412, 1991.
- [4] J.D. Barrow, R. Maartens, and C.G. Tsagas. Cosmology with inhomogeneous magnetic fields. Phys. Rep., 449:131–171, 2007.
- [5] D. Biskamp. Magnetohydrodynamic Turbulence. Cambridge University Press, Cambridge, 2003.
- [6] P. Bodenheimer, G.P. Laughlin, M. Rozyczka, and H.W. Yorke. Numerical methods in astrophysics. Series in Astronomy and Astrophysics, Taylor & Francis, New York, 2007.
- [7] M. Carney, P. Cunningham, J. Dowling, and C. Lee. Predicting probability distributions for surf height using an ensemble of mixture density networks. International Conference on Machine Learning, pages 113 – 120, 2005.

- [8] P. A. Davidson. An introduction to magnetohydrodynamics. Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 2001.
- [9] P.A. Davidson. An Introduction to Magnetohydrodynamics. Cambridge University Press, 2001.
- [10] E. Dormy and A.M. Soward. Mathematical aspects of natural dynamos. Fluid Mechanics of Astrophysics and Geophysics, Grenoble Sciences. Universite Joseph Fourier, Grenoble, VI, 2007.
- [11] J. A. Font. Gerneral relativistic hydrodynamics and magnetohydrodynamics: hyperbolic system in relativistic astrophysics, in hyperbolic problems: theory, numerics, applications. *Springer*, *Berlin*, pages 3–17, 2008.
- [12] H. Hashizume. Numerical and experimental research to solve MHD problem in liquid blanket system. Fusion Engineering and Design, 81:1431–1438, 2006.
- [13] W. Hillebrandt and F. Kupka. Interdisciplinary aspects of turbulence. Lecture Notes in Physics, Springer-Verlag, Berlin, 756, 2009.
- [14] L.D. Landau and E.M. Lifshitz. *Electrodynamics of Continuous Media*. Pergamon Press, Oxford, 1960.
- [15] M. Leutbecher and T.N. Palmer. Ensemble forecasting. *Journal of Computational Physics*, 227:3515–3539, 2008.
- [16] J. M. Lewis. Roots of ensemble forecasting. Monthly Weather Review, 133:1865 1885, 2005.
- [17] Y. Li and C. Trenchea. Partitioned second order method for magnetohydrodynamics in Elsasser fields. *Submitted*, 2015.
- [18] O.P. Le Maître and O.M. Knio. Spectral methods for uncertainty quantification. Springer, 2010.
- [19] W.J. Martin and M. Xue. Sensitivity analysis of convection of the 24 May 2002 IHOP case using very large ensembles. *Monthly Weather Review*, 134:192–207, 2006.
- [20] J. D. Giraldo Osorio and S. G. Garcia Galiano. Building hazard maps of extreme daily rainy events from PDF ensemble, via REA method, on senegal river basin. *Hydrology and Earth System Sciences*, 15:3605 3615, 2011.
- [21] B. Punsly. Black hole gravitohydrodynamics. Astrophysics and Space Science Library, Springer-Verlag, Berlin, Second Edition, 355, 2008.
- [22] S. Smolentsev, R. Moreau, L. Buhler, and C. Mistrangelo. MHD thermofluid issues of liquid-metal blankets: Phenomena and advances. Fusion Engineering and Design, 85:1196–1205, 2010.
- [23] C. Trenchea. Unconditional stability of a partitioned IMEX method for magnetohydrodynamic flows. *Applied Mathematics Letters*, 27:97–100, 2014.