Research Statement

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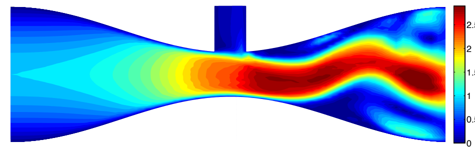
My research is interdisciplinary, combining mathematical analysis, numerical analysis and scientific computing. My main research accomplishments are in the analysis and the numerical computation of models that emerge from physical and life sciences, with specific attention to direct and inverse problems (optimal control / parameter identification) in connection with uncertainty quantification, fluid dynamics, magnetohydrodynamics, large eddy simulation of turbulent flows, and mathematical biology.

My expertise lies in the mathematical and numerical analysis of continuous, semi-discrete and fully-discrete space-time discretizations of deterministic and stochastic partial differential equations, convergence, error estimates, and the development of stable and accurate numerical algorithms. The mathematical areas and tools I use include: calculus of variations, adjoint-based methods for optimal control, finite differences and the finite element method, collocation and sparse grids for stochastic partial differential equations, semigroup theory, functional analysis, convex analysis, numerical analysis for stiff, nonstiff and symplectic ordinary differential equations, and differential equations in Hilbert spaces.

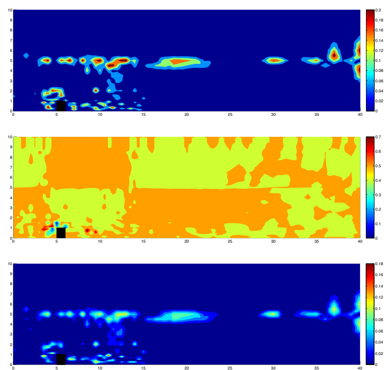
Modular Algorithms in multi-domain, multi-physics. Many important applications require the accurate solution of multi-domain [34, 38], multi-physics coupling [38, 41, 52, 53]. Among the examples which occur in my recent research are fluid-structure interaction, such as in blood flow [5, 6, 45], electrically conductive fluids and magnetic field, such as plasmas [18, 19, 21, 22, 33, 35, 36, 42, 54, 58], fluid-fluid interaction, such as ocean-atmosphere, groundwater and surface-water interaction [9, 10, 34, 53, 55], and reaction-diffusion systems [7, 8, 11–16, 43]. The essential problems of estimation of the penetration of a plume of pollution into groundwater and remediation after such a penetration are that (i) the coupled problems in both sub-regions are inherently time dependent, (ii) the different physical processes suggest that codes separately optimized for each sub-process need to be used for solution of the coupled problem and (iii) the large domains plus the need to compute for several turn-over times for reliable statistics require calculations over long time intervals. One approach, for which numerical analysis and test problems are relatively easy, is monolithic discretization by an implicit method followed by iterative solution of the system with subregion uncoupling in the preconditioner. In practical computing, partitioned schemes (and associated IMEX methods) have been used extensively in the computational practice of multi-domain, multiphysics applications. However, before my work, there was very little rigorous theory of stability, convergence etc. of partitioned methods. They are often motivated by available codes for subproblems and allow parallel, non-iterative uncoupling into independent sub-physics system per time step. This modularity capability is paramount since it enables, with the minimal extra cost of a script function, the exploitation of highly optimized (up-to-date, continuously upgraded as our understanding of physical processes improves, national laboratory supported) legacy codes. The partitioned methods, which require one (per sub domain) solve per time step, are also very attractive from the viewpoint of computational complexity compared to monolithic methods (requiring one coupled, non-symmetric system of roughly double size). I have developed new methods and a theoretical foundation for partitioned methods. They address the stability of modular computational algorithms for fluid-structure interaction modeling blood flow [6, 45], the groundwater and surface water coupling [34, 38], the fluid and magnetic field interaction [35, 54], and the general case of evolution equations with a skew symmetric coupling [38, 53].

Large eddy simulations in hydrodynamics and magnetohydrodynamics flows. Turbulence is an omnipresent phenomenon: when fluids are set into motion, turbulence tends to develop. When the fluid is electrically conducting, the turbulent motions are accompanied by magnetic fluctuations. Terrestrial conducting fluids include liquid metals and the flow of liquid sodium in the cooling ducts of a fastbreeder reactor. The extraterrestrial world abounds in plasma (99% of all material is plasma-ionized gas). For MagnetoHydroDynamics (MHD) turbulence, numerical simulations play a greater role than they play for hydrodynamic turbulence, since laboratory experiments are practically impossible and astrophysical systems (solar-wind turbulence, the most important system of high-Reynolds-number MHD accessible to *in situ* measurements) are too complex to be comparable with theoretical results.



Contour plot of the speed of the stabilized coarse discretization solutions for the Navier-Stokes velocity solution at T=4 ([25]).

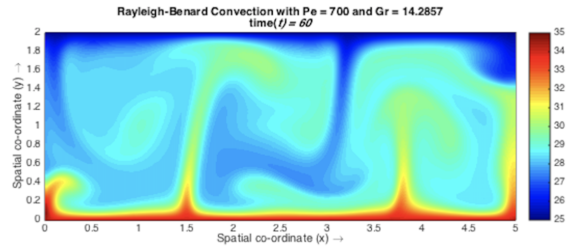
Turbulence in fluid dynamics. Turbulent flows consist of complex, interacting three dimensional eddies of various sizes down to the Kolmogorov microscale, $\eta = O(Re^{-3/4})$ in $3d$. A direct numerical simulation of the persistent eddies in a $3d$ flow thus requires roughly $O(Re^{+9/4})$ mesh points in space per time step. Therefore, direct numerical simulation of turbulent flows is often not computationally economical or even feasible. On the other hand, the largest structures in the flow (containing most of the flow's energy) are responsible for much of the mixing and most of the flow's momentum transport. This led us to various numerical regularizations [4, 17, 27–32, 37]; one of these is Large Eddy Simulation (LES). It is based on the idea that the flow can be represented by a collection of scales with different sizes, and instead of trying to approximate all of them down to the smallest, one defines a filter width $\delta > 0$ and computes only the scales of size bigger than δ (large scales), while the effect of the small scales on the large scales is modelled. This reduces the number of degrees of freedom in a simulation and represents accurately the large structures in the flow. If the LES model does not dissipate enough energy, there can be an accumulation of energy around the smallest resolved scales (i.e., wiggles in the computed velocity). The energy dissipation rates in various LES models are adjusted in various ways, such as using mixed models (i.e., adding eddy viscosity) and picking the parameters introduced to match the model's time averaged energy dissipation rate to that of homogeneous, isotropic turbulence. Parameter-free (not mixed) models have many advantages, and understanding their important statistics, such as their energy dissipation rate, is critical to advancing their reliability. I successfully used Approximate Deconvolution Models in many simulations of turbulent flows [27, 28, 33]. They are among the most accurate of turbulence models, and one of the few turbulence models for which a mathematical confirmation of their effectiveness is known.



Contour plots of the Vreman Filter (top), Q-Filter (middle) and VQ-Filter (bottom) [31].

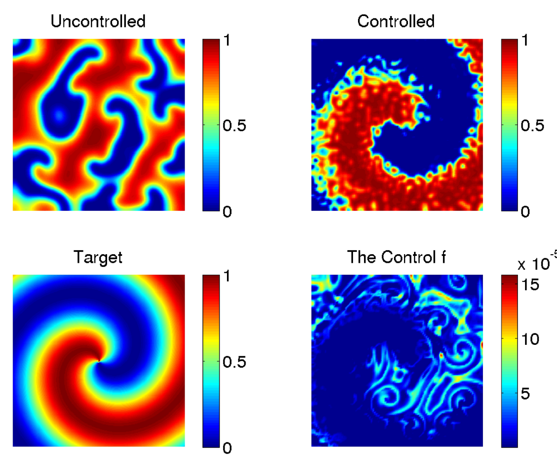
Magnetohydrodynamic turbulence. In many electrically and magnetically conducting fluids, turbulent MHD (magnetohydrodynamics [1]) flows are typical [18, 19, 21, 22, 28, 29, 34, 54]. The difficulties of accurately modelling and simulating turbulent flows are magnified many times over in the MHD case. They are evinced by the more complex dynamics of the flow due to the coupling of Navier-Stokes and Maxwell equations via the Lorentz force and Ohm's law. The MHD turbulent flow has many more parameter regimes and more uncertainties about basic physical mechanisms than turbulent flow of a non-conducting fluid. There are self-organization processes in MHD turbulence that have no hydrodynamic counterpart, originating from the existence of several ideal invariants with different decay rates, Alfvèn waves. The conservation of *cross-helicity* leads to highly aligned states, while the conservation of *magnetic helicity* yields the formation of force-free magnetic configurations, an inverse cascade of the magnetic helicity, and excitation of increasingly larger magnetic scales. There are several other important flow statistics, among which are the time averaged *energy*, the *magnetic* and the *cross helicity* dissipation rates [28, 29, 33]. The experience in turbulence models suggests that one critical factor for a reliable model is that it contains sufficient model dissipation for the required scale truncation without over-dissipation of critical structures and important dynamics. The added complexities, length scales, dynamics and the extra variables needed for MHD flows make accurate simulation of MHD turbulence still more challenging. Because of these (and other) factors, the development of accurate and reliable models for MHD turbulence is correspondingly more important than for ordinary turbulent flows and correspondingly less well developed.

With my collaborators I investigate the mathematical properties of several models for the simulation of the large eddies in turbulent viscous, incompressible flows, electrically conducting flows and new numerical models that permit long-time simulations. This includes the mathematical and numerical analysis of new models for turbulent flows and MHD flows [27–29, 33], e.g., stability and error estimation [30, 55], time-stepping schemes [30, 35, 54], spatial filtering and spectral eddy-viscosity models [17, 32], modular linear and nonlinear filters [4, 30, 31], commutators, filtering through the wall [37], computational algorithms, and the development of new filters specific to MHD turbulence.



Optimal control, parameter estimation, uncertainty quantification. Predictions based on computational simulations are central not only to science and engineering, but also to risk assessment and decision-making in economics, public policy and many other venues. In all cases, the information used by engineers for design purposes and by those formulating decisions is uncertain in the sense that one cannot unequivocally state that it is correct; the best one can hope to do is to quantify the uncertainty in the information, e.g., by providing confidence intervals or error bars. One of the central objectives of the scientific community is to investigate and resolve several important mathematical, algorithmic and practical issues related to the efficient, accurate, and robust computational determination of quantities of interest, i.e., the information used by engineers and decision makers, that are determined from solutions of (stochastic) partial differential equations.

Optimal control theory is a mathematical technique used to determine control variables that maximize a performance criterion subject to constraints (state equations). It continues to be an active area of research with applications in many areas. The inverse problems are intrinsically ill-posed in the Hadamard sense, meaning that a solution might not exist, or if it exists is not unique, or does not depend continuously on data. Even if the continuous inverse problem is well posed, when discretization in time and/or space is performed, the approximating inverse problem could become ill-posed. This means lack of smoothness in the solutions with respect to the parameters, which requires regularization techniques and extra effort (such as the Brezzi-Rappaz-Raviart and Fink-Rheinboldt theories) to prove error estimates and the convergence of the regularized (discrete) problem to the primary (continuous) problem [19, 20]. I successfully solved optimal control and parameter identification problems associated with reaction-diffusion equations and pattern formation [11–13, 15], the time-periodic elliptic equations [50], the wave equation [44, 49], the Euler-Bernoulli equation [51], the Boussinesq equations [52], the Navier-Stokes equations [3, 37], and the magnetohydrodynamic (MHD) equations [18, 19, 21, 22].



The uncontrolled and the optimally controlled states (top), the target states and the control (bottom) [11].

Motivation for stochastic models. Many applications (especially those predicting future events) are affected by a relatively large amount of uncertainty in the input data such as model coefficients, forcing terms, boundary conditions, geometry, etc. An example includes forecasting financial markets where this may depend on the number of economic factors, number of underlying assets or the number of time points/time steps, human behaviors, etc. Important examples include the enhancement of reliability of smart energy grids, development of renewable energy technologies, vulnerability analysis of water and power supplies, understanding complex biological networks, climate change estimation and design and licensing of current and future nuclear energy reactors.

Stochastic models give quantitative information about uncertainty. In practice it is necessary to address the following types of uncertainties: aleatoric and epistemic. The aleatoric (random) uncertainty is due to the intrinsic/irreducible variability in the system, e.g. turbulent fluctuations of a flow field around an airplane wing, permeability in an aquifer, etc. The epistemic uncertainty is due to incomplete knowledge, and can be reduced by additional experimentation, improvements in measuring devices, etc., e.g. mechanical properties of many bio-materials, polymeric fluids, highly heterogeneous or composite materials, the action of wind or seismic vibrations on civil structures, etc.

Uncertainty quantification (UQ) attempts to quantitatively assess the impact of uncertain data on simulation outputs. In the stochastic context, the forward problem consists in determining, for known probability distribution functions (PDF) of coefficients, the PDF of the (uncertain) outputs of the system. The inverse problem consists in determining statistical moments of the input random fields, given a set of measurements that correspond to some statistical quantities of interest (e.g. moments, inverse CDF, etc.) corresponding to the solution of the stochastic partial differential equation (SPDE). One approach is by minimization of appropriately formulated cost functionals. In the recent works [20, 47, 48] we introduced several identification objectives that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate L^p norm, where the distributed parameters/control can be both deterministic or stochastic. For a given objective we prove the existence of an optimal solution, establish the validity of the Lagrange multiplier rule and obtain a stochastic optimality system of equations. The modeling process may describe the solution in terms of high dimensional spaces, particularly in the case when the input data (coefficients, forcing terms, boundary conditions, geometry, etc) are affected by a large amount of uncertainty. For higher accuracy, the computer simulation must increase the number of random variables (dimensions), and expend more effort approximating the quantity of interest in each individual dimension. Hence, we introduced a novel stochastic parameter identification algorithm that integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM approach. This allows for decoupled, moderately high dimensional, parameterized computations of the stochastic optimality system, where at each collocation point, deterministic analysis and techniques can be utilized. The advantage of our approach is that it allows for the optimal identification of statistical moments (mean value, variance, covariance, etc.) or even the whole probability distribution of the input random fields, given the probability distribution of some responses of the system (quantities of physical interest). We rigorously derived error estimates, for the fully discrete problems, and used them to compare the efficiency of the method with several other techniques. Numerical examples in [20, 47] illustrate the theoretical results and demonstrate the distinctions between the various stochastic identification objectives and the efficacy of our approach.

Collaborations

I am collaborating with researchers at Notre Dame University, University of Connecticut, University of Alberta, Florida State University, Oak Ridge National Laboratory, Clemson University, Air Force Institute of Technology, University of Guelph, University of Iasi Romania, Istituto per Applicazioni del Calcolo "M.Picone" Bari Italy, University of Reading and Oxford University.

Research Grants

My work was partially supported by grants from the Air Force Office of Scientific Research, National Science Foundation, University of Pittsburgh, and the Romanian Department of Education and Research.

An important part of my charge is seeking scientific funding. Currently, I am preparing a series of proposals on work related to partitioning of fluid-structure interaction for blood-flow on moving domains, ocean-atmosphere, and coupling of groundwater-surface water with transport/contamination.

1. Research highlights.

- [6] "**BOundary Update via Resolvent for fluid-structure interaction**".
In this work we built upon the understanding of the fluid and thin-structure interaction, which we developed in a recent work [45], and construct a novel unconditionally stable second-order partitioned method. Currently, we are extending this study in different directions: to a variable-step algorithm, to using a spatial filtering in the fluid domain, and to a partitioned scheme for the fluid-structure interaction in moving/compliant vessels for blood flow.
We propose a BOundary Update using Resolvent (BOUR) partitioned method, second-order accurate in time, unconditionally stable, for the interaction between a viscous, incompressible fluid and a thin structure. The method is algorithmically similar to the sequential Backward Euler - Forward Euler implementation of the midpoint/Crank-Nicolson discretization scheme. (i) The structure and fluid sub-problems are first solved using a Backward Euler scheme, (ii) the velocities of fluid and structure are updated on the boundary via a second-order consistent resolvent operator, and then (iii) the structure and fluid sub-problems are solved again, using a Forward Euler scheme. The stability analysis based on energy estimates shows that the scheme is unconditionally stable. Error analysis of the semi-discrete problem yields second-order convergence in time. The two numerical examples confirm the theoretical convergence analysis results and show an excellent agreement of the proposed partitioned scheme with the monolithic scheme, making BOUR an appealing alternative to the monolithic scheme.
- [10] "**Partitioned penalty methods for the transport equation in the evolutionary Stokes-Darcy-transport problem**".
This is part of a series of collaborations on partitioning fluid-fluid [5, 9, 34, 38, 53] coupling problems.
There has been a surge of work on models for coupling surface-water with groundwater flows which is at its core the Stokes-Darcy problem, as well as methods for uncoupling the problem into subdomain, subphysics solves. The resulting (Stokes-Darcy) fluid velocity is important because the flow transports contaminants. The numerical analysis and algorithm development for the evolutionary transport problem has, however, focused on a quasi-static Stokes-Darcy model and a single domain (fully coupled) formulation of the transport equation. This report presents the first numerical analysis of a partitioned method for contaminant transport for the fully evolutionary system. The algorithm studied is unconditionally stable with one subdomain solve per step. Numerical experiments are given using the proposed algorithm that investigates the effects of the penalty parameters on the convergence of the approximations.
- [23] "**The Williams step increases the stability and accuracy of the hoRA time filter**". This work is part of a study on time filters used in weather predictions [24, 39, 40].
The explicit weakly-stable second-order accurate leapfrog scheme is widely used in the numerical models of weather and climate, in conjunction with the Robert-Asselin (RA) and Robert-Asselin-Williams (RAW) time filters. The RA and RAW filters successfully suppress the spurious computational mode associated with the leapfrog method, but also weakly damp the physical mode and degrade the numerical accuracy to first-order. The recent higher-order Robert-Asselin (hoRA) time filter reduces the undesired numerical damping of the RA and RAW filters and increases the accuracy to second up to third-order. We prove that the combination of leapfrog-hoRA and Williams' step increases the stability by 25%, improves the accuracy of the amplitude of the physical mode up to two significant digits, effectively suppresses the computational modes, and further diminishes the numerical damping of the hoRA filter.
- [42] "**Partitioned second order method for magnetohydrodynamics in Elsässer variables**".
This builds on my previous work [54] on partitioning methods for magnetohydrodynamics, where I proved, for the first time, that the full evolutionary MHD equations at high Reynolds numbers, can be discretized and decoupled in an unconditional scheme, allowing for larger computations by halving the number of variables on each processor. We later on extended the first-order method to second-order [33], using deferred correction. In here we used a backward differentiation formula BDF-2 and proved unconditional stability.
Magnetohydrodynamics (MHD) studies the dynamics of electrically conducting fluids, involving Navier-Stokes equations coupled with Maxwell equations via Lorentz force and Ohm's law. Monolithic methods, which solve fully coupled MHD systems, are computationally expensive. Partitioned methods, on the other hand, decouple the full system and solve subproblems in parallel, and thus reduce the computational cost. This paper is devoted to the design and analysis of a partitioned method for the MHD system in the Elsässer variables. The stability analysis shows that for magnetic Prandtl number of order unity, the method is unconditionally stable. We prove the error estimates and present computational tests that support the theory.

- [41] "**Existence and ergodicity for the two-dimensional stochastic Boussinesq equation**". The existence of solutions to the Boussinesq system driven by random exterior forcing terms both in the velocity field and the temperature is proven using a semigroup approach. We also obtain the existence and uniqueness of an invariant measure via coupling methods.
- [8] "**Analysis of a second-order in time implicit-symplectic scheme for predator-prey systems**". We analyze a second-order accurate implicit-symplectic (IMSP) scheme for reaction-diffusion systems modeling spatio-temporal dynamics of predator-prey populations. We prove stability, errors estimates and positivity of the the semi-discrete in time approximations. The numerical simulations confirm the theoretically derived rates of convergence, and show, at same computational cost, an improved accuracy in the second-order IMSP in comparison with the first-order IMSP.
- [45] "**A Second-Order in Time Approximation of Fluid-Structure Interaction Problem**". We propose and analyze a novel, second-order in time, partitioned method for the interaction between an incompressible, viscous fluid and a thin, elastic structure. The proposed numerical method is based on the Crank–Nicolson discretization scheme, which is used to decouple the system into a fluid subproblem and a structure subproblem. The scheme is loosely coupled, and therefore at every time step, each subproblem is solved only once. Energy and error estimates for a fully discretized scheme using finite element spatial discretization are derived. We prove that the scheme is stable under a CFL condition, second-order convergent in time, and optimally convergent in space. Numerical examples support the theoretically obtained results and demonstrate the applicability of the method to realistic simulations of blood flow.
- [7] "**Numerical analysis of a first-order in time implicit-symplectic scheme for predator–prey systems**". The numerical solution of reaction-diffusion systems modelling predator-prey dynamics using implicit-symplectic (IMSP) schemes is relatively new. When applied to problems with chaotic dynamics they perform well, both in terms of computational effort and accuracy. However, until the current paper, a rigorous numerical analysis was lacking. We analyse the semi-discrete in time approximations of a first-order IMSP scheme applied to spatially extended predator-prey systems. We rigorously establish semi-discrete a priori bounds that guarantee positive and stable solutions, and prove an optimal a priori error estimate. This analysis is an improvement on previous theoretical results using standard implicit-explicit (IMEX) schemes. The theoretical results are illustrated via numerical experiments in one and two space dimensions using fully-discrete finite element approximations.
- [43] "**Analysis of stability and error estimates for three methods approximating a nonlinear reaction-diffusion equation**". We present the error analysis of three time-stepping schemes used in the discretization of a nonlinear reaction-diffusion equation with Neumann boundary conditions, relevant in phase transition. We prove L^∞ stability by maximum principle arguments, and derive error estimates using energy methods for the implicit Euler, and two implicit-explicit approaches, a linearized scheme and a fractional step method. A numerical experiment validates the theoretical results, comparing the accuracy of the methods.
- [25] "**An optimally accurate discrete regularization for second order timestepping methods for Navier-Stokes equations**".
  This work applies my general IMEX treatment methodology for local/nonlocal effects [55] to the case of Navier-Stokes equations.
  We propose a new, optimally accurate numerical regularization/stabilization for (a family of) second order timestepping methods for the Navier-Stokes equations (NSE). The method combines a linear treatment of the advection term, together with stabilization terms that are proportional to discrete curvature of the solutions in both velocity and pressure. We rigorously prove that the entire new family of methods are unconditionally stable and $\mathcal{O}(\Delta t^2)$ accurate. The idea of 'curvature stabilization' is new to CFD and is intended as an improvement over the commonly used 'speed stabilization', which is only first-order accurate in time and can have an adverse effect on important flow quantities such as drag coefficients. Numerical examples verify the predicted convergence rate and show the stabilization term clearly improves the stability and accuracy of the tested flows.
- [47] "**Optimal Control of Systems Governed by PDEs with Random Parameter Fields**". In here we build on the work [20] done in collaboration with Max Gunzburger (Florida State University) and Clayton Webster (Oak Ridge National Laboratory). Namely, we introduce and analyze a general methodology for quantifying uncertainty and robust computational determination of quantities of interest. We present methods for the optimal control / parameter identification of systems governed by partial

differential equations with random input data. We consider several identification objectives that either minimize the expectation of a tracking cost functional or minimize the difference of desired statistical quantities in the appropriate spatial-L^p norm (including higher order moments, hence allowing to match any statistics, e.g., the variance, skewness, kurtosis, etc.). A specific problem of parameter identification of a linear elliptic PDE that describes flow of a fluid in a porous medium with uncertain permeability field is examined. We present numerical results to study the consequences of the moment-tracking approximation and the efficiency of the method. The stochastic parameter identification algorithm integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation mixed-FEM approach. We also derive rigorous error estimates for fully discrete problems, using the Fink-Rheinboldt theory for the approximation of solutions of a class of nonlinear problems.

- [40] "**Analysis of time filters used with the leapfrog scheme**".
We present the linear analysis of recent time filters used in numerical weather prediction. We focus on the accuracy and the stability of the leapfrog scheme combined with the Robert-Asselin-Williams filter, the higher-order Robert-Asselin type time filter, the composite-tendency Robert-Asselin-Williams filter and a more discriminating filter.
- [48] "**A convergence analysis of stochastic collocation method for Navier-Stokes equations with random input data**".
Stochastic collocation has proved to be an efficient method and been widely applied to solve various partial differential equations with random input data, including Navier-Stokes equations. However, up to now, rigorous convergence analyses are limited to linear elliptic and parabolic equations; its performance for Navier-Stokes equations was demonstrated mostly by numerical experiments. In this paper, we present an error analysis of the stochastic collocation method for a semi-implicit Backward Euler discretization for NSE and prove the exponential decay of the interpolation error in the probability space. Our analysis indicates that due to the nonlinearity, as final time T increases and NSE solvers pile up, the accuracy may be reduced significantly. Subsequently, an illustrative computational test of time dependent fluid flow around a bluff body is provided.
- [58] "**High Accuracy Method for Magnetohydrodynamics System in Elsässer Variables**".
The MHD flows are governed by the Navier-Stokes equations coupled with the Maxwell equations through coupling terms. We prove the unconditional stability of a partitioned method for the evolutionary full MHD equations, at high magnetic Reynolds number, in the Elsässer variables. The method we propose is a defect correction second order scheme, and entails the implicit discretization of the subproblem terms and the explicit discretization of coupling terms.
- [24] "**Stability analysis of the Crank–Nicolson-Leapfrog method with the Robert–Asselin–Williams time filter**".
Geophysical flow simulations have evolved sophisticated Implicit-Explicit time stepping methods (based on fast slow wave splittings) followed by time filters to control any unstable models that result. These time filters are wonderfully elegant as algorithms, modular and embarrassingly parallel. Their effect on stability of the overall process has been tested in numerous simulations but never studied analytically. We do so herein.
- [36] "**Numerical analysis of two partitioned methods for uncoupling evolutionary MHD flows**".
We introduced two partitioned methods to solve evolutionary MHD equations in case of (terrestrial applications, which occur at) low magnetic Reynold numbers. The methods we study allow us at each time step to call NSE and Maxwell codes separately, each possibly optimized for the subproblem's respective physics.
- [39] "**A higher-order Robert-Asselin type time filter**".
In this work we built upon a recent work of Paul Williams [56,57] for time filters. The Robert-Asselin (RA) time filter combined with the leapfrog scheme is widely used in numerical models of weather and climate. It successfully suppresses the spurious computational mode associated with the leapfrog method, but it also weakly dampens the physical mode and degrades the numerical accuracy. The Robert-Asselin-Williams (RAW) time filter is a modification of the RA filter that reduces the undesired numerical damping of RA filter and increases the accuracy. We propose a higher-order RA (hoRA) type time filter which effectively suppresses the computational modes and achieves third-order accuracy with the same storage requirement as RAW filter. Like RA and RAW filters, the hoRA filter is non-intrusive, and so it would be easily implementable. The leapfrog scheme with hoRA filter is almost as accurate, stable and efficient as the intrusive third-order Adams-Bashforth (AB3) method.

◦ [5] "**Analysis of partitioned methods for Biot system**".
We analyzed several partitioned methods for the coupling of flow and mechanics/poroelasticity. We derived energy estimates for each method for the fully discrete problem, and expressed the obtained stability conditions in terms of a key control parameter defined as a ratio of the coupling strength and the speed of propagation. Depending on the parameters in the problem, we provided the choice of the partitioned method which allows the largest time step.

◦ [9] "**On Limiting Behavior of Contaminant Transport Models in Coupled Surface and Groundwater Flows**".
There has been a surge of work on models for coupling surface-water with groundwater flows which is at its core the Stokes-Darcy problem. The resulting (Stokes-Darcy) fluid velocity is important because the flow transports contaminants. The analysis of models including the transport of contaminants has, however, focused on a quasi-static Stokes-Darcy model. Herein we consider the fully evolutionary system including contaminant transport and analyze its quasi-static limits.

◦ [20] "**A generalized stochastic collocation approach to constrained optimization for random data identification problems**".
We introduced a novel stochastic parameter identification algorithm that integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM approach. This allows for decoupled, moderately high dimensional, parameterized computations of the stochastic optimality system, where at each collocation point, deterministic analysis and techniques can be utilized. The advantage of our approach is that it allows for the optimal identification of statistical moments (mean value, variance, covariance, etc.) or even the whole probability distribution of the input random fields, given the probability distribution of some responses of the system (quantities of physical interest).

◦ [38] "**Stability of two IMEX methods, CNLF and BDF2-AB2, for uncoupling systems of evolution equations**".
We proved the stability of two partitioned methods for decoupling a multi-physics problem. <u>This answered the 1963 unsolved problem of stability of Crank-Nicolson leap-frog method</u>.

◦ [53] "**Stability of partitioned IMEX methods for systems of evolution equations with skew-symmetric coupling**".
Here I generalize the work [38], providing a novel proof for a whole family of second order IMEX methods that contains CNLF and BDF2-AB2.

◦ [54] "**Unconditional stability of a partitioned IMEX methods for magnetohydrodynamic flows**". Using the Elsässer variables I decoupled the full MHD equations at high magnetic Reynolds numbers into two subproblems of half the size, using the same solver for each variable.

◦ [35] "**Analysis of stability and errors of IMEX methods for magnetohydrodynamics flows at small magnetic Reynolds number**". We introduce an implicit-explicit method where the MHD equations can be evolved in time by calls to the NSE and Maxwell codes, each optimized for the subproblem's respective physics.

◦ [30] "**Numerical analysis of modular regularization methods for the BDF2 time discretization of the NSE**". We give a complete stability analysis and error estimates of an uncoupled, modular regularization algorithm for approximation of the Navier- Stokes equations.

◦ [34] "**Analysis of Long Time Stability and Errors of Two Partitioned Methods for Uncoupling Evolutionary Groundwater - Surface Water Flows**". We analyzed and tested two such partitioned (non-iterative, domain decomposition) methods for the fully evolutionary Stokes-Darcy problem, that model the multi-physics coupling of groundwater to surface water, allowing the use of the best groundwater and surface water codes.

◦ [55] "**Second order implicit for local effects and explicit for nonlocal effects is unconditionally stable**". The second order method considered is implicit in local and stabilizing terms in the underlying PDE and explicit in nonlocal and unstabilizing terms. Unconditional stability and convergence of the numerical IMEX scheme are proved by the energy method and by algebraic techniques. The stability result is surprising because usually when different methods are combined, the stability properties of the least stable method play a determining role in the combination. This is the first solution to the problem of finding a scheme that is (provably) unconditionally stable and treats the stabilizing term explicitly. First order schemes were known in [2, 26] and [26] gives a second order scheme stable provided all operators commute.

◦ ◦ [12], [15]. "**An efficient and robust numerical algorithm for estimating parameters in Turing**

systems". We introduce a general methodology for parameter identification in reaction-diffusion systems that display pattern formation via the mechanism of diffusion-driven instability.

- ◦ [31] "**Modular Nonlinear Filter Stabilization of Methods for Higher Reynolds Numbers Flow**". This is a breakthrough work: we develop nonlinear filter stabilizations which tune the amount and location of eddy viscosity to the local flow structures and whether the nonlinearity tends to break marginally resolved scales down to smaller scales or let the local structure persist.
- ◦ [4] "**Improved accuracy in regularization models of incompressible flow via adaptive nonlinear filtering**". We study adaptive nonlinear filtering in the Leray regularization model for incompressible, viscous Newtonian flow. The filtering radius is locally adjusted so that resolved flow regions and coherent flow structures are not 'filtered-out'. The method decouples the problem so that the filtering becomes linear at each timestep and is decoupled from the system.
- ◦ [37] "**The Das-Moser commutator closure for filtering through a boundary is well posed**". When filtering through a wall with constant averaging radius, in addition to the subfilter scale stresses, a non-closed commutator term arises. We consider a proposal of Das and Moser to close the commutator error term by embedding it in an optimization problem, and showed that this optimization based closure, with a small modification, leads to a well posed problem.
- ◦ ◦ [29] [28] "**Large eddy simulation for turbulent magnetohydrodynamic flows**". "**Approximate deconvolution models for magnetohydrodynamics**". We consider the family of approximate deconvolution models (ADM) and the zeroth order model (LES) for the simulation of the large eddies in turbulent viscous, incompressible, electrically conducting flows. We prove existence and uniqueness of solutions, we prove that the solutions to the ADM-MHD equations converge to the solution of the MHD equations in a weak sense as the averaging radii converge to zero, and we derive a bound on the modeling error. We prove that the energy and helicity of the models are conserved, and the models preserve the Alfvèn waves.
- ◦ [33] "**Bounds on Energy, Magnetic Helicity and Cross Helicity Dissipation Rates of Approximate Deconvolution Models of Turbulence for MHD Flows**". For body force driven turbulence, we prove directly from the model's equations of motion bounds on the model's time averaged energy dissipation rate, time averaged cross helicity dissipation rate and magnetic helicity dissipation rate.
- ◦ [17] "Analysis of Nonlinear Spectral Eddy-Viscosity Models of Turbulence".
- ◦ [27] "Mathematical Architecture of Approximate Deconvolution Models of Turbulence".
- ◦ [32] "Theory of the NS-$\overline{\omega}$ model: a complement to the NS-α model".
- ◦ [18] "The velocity tracking problem for MHD flows with distributed magnetic field controls".
- ◦ [11] "Optimal control of a 'nutrient-phytoplankton-zooplankton-fish' system".
- ◦ [13] "Finite element approximations of spatially extended predator-prey interactions with the Holling type II functional response".
- ◦ [16] "A second-order, three level finite element approximation of an experimental substrate inhibition model" [14] "Spatiotemporal dynamics of two generic predator-prey models".
- ◦ [22] "Analysis of an optimal control problem for the three-dimensional coupled modified Navier-Stokes and Maxwell equation". [19] "Analysis and Discretization of an Optimal Control Problem for the Time-Periodic MHD Equations". [50] "Optimal control of an elliptic equation under periodic conditions". [52] "Periodic optimal control of the Boussinesq equation". [3] "Noncooperative optimization of controls for time periodic Navier-Stokes systems with multiple solutions". [51] "Internal optimal control of the periodic Euler-Bernoulli equation". [49] "Optimal control of the periodic string equation with internal control". [44] "Identification for nonlinear periodic wave equation". [46] "Hamilton-Jacobi equation and optimality conditions for control systems governed by semilinear parabolic equations with boundary control".

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