RESEARCH STATEMENT

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1. INTRODUCTION

My research focuses primarily on the design and implementation of high-resolution, non-oscillatory numerical schemes for hyperbolic system of conservation laws and related problems. In particular, I am interested in the design of efficient algorithms that address the mathematical and computational challenges posed by nonlinear systems of conservation laws, such as the onset and propagation of discontinuous solutions, the enforcement of additional constraints, or the proper discretization of source terms in non-homogeneous systems.

My early research activity focused on the equations of *Ideal Magnetohydrodynamics* (MHD), a hyperbolic model which describes the dynamics of electrically conducting fluids in the presence of a magnetic field. Our implementation of several schemes based on central differencing demonstrated the remarkable ability of these to efficiently approximate the discontinuous solutions of the system without having to modify the base scheme for hyperbolic systems to enforce the constraint $\nabla \cdot \mathbf{B} = 0$ on the magnetic field $\mathbf{B}$.

More recently, my work has focused on non-homogeneous hyperbolic systems, such as the shallow water equations, commonly used to model flows in rivers and costal areas, and the Euler-Poisson equations describing the macroscopic behavior of two-spicies plasmas. In the first of these systems, the proper discretization of the source terms arising from the bottom topography and the varying width of the channel, is crucial for capturing steady-state solutions of the system accurately. In the second one, the source term couples the two hydrodynamical models describing each species present in the plasma.

In addition to the results already published and the ongoing research, the successful implementation of central schemes for MHD equations, led us into the development of CENTPACK: a software package capable of approximating the solution of hyperbolic system of conservation laws in one- and two-space dimensions with minimal input from the user. The first stage of this project –the release of the first stable version of the software– was completed in July of 2006. Presently, we continue working on improving this software by providing users with additional central solvers and extending its functionality to non-homogeneous hyperbolic systems.

2. BACKGROUND – HYPERBOLIC SYSTEMS OF CONSERVATION LAWS

Hyperbolic systems of conservation laws are of paramount importance in science and engineering as they govern a broad spectrum of physical phenomena such as compressible fluid dynamics, acoustics, optics, or nonlinear material science (see, for example, [11, 20]). Mathematically, these laws are described by the system of time dependent partial differential equations (PDEs)

$$\frac{\partial}{\partial t}\,\mathbf{u}(\mathbf{x},t) + \nabla_{\mathbf{x}} \cdot \mathbf{F}(\mathbf{u}(\mathbf{x},t)) = \mathbf{S}(\mathbf{u},\mathbf{x},t), \quad \mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}) \tag{1}$$

where t is the time variable, $\mathbf{x}$ a vector of d spatial variables, $\mathbf{u}(\mathbf{x},t)$ is a vector of m conserved quantities (e.g., mass, momentum, energy, etc.), $\mathbf{F}(\mathbf{u})$ is a matrix of size $d \times m$ whose rows, $\mathbf{f}_k(\mathbf{u}), k = 1, 2, \ldots, d$, are *nonlinear* flux functions, and $\mathbf{S}(\mathbf{u},\mathbf{x},t)$ stands for a vector of source terms. The system is said to be hyperbolic if the Jacobian matrices of the flux functions, $\frac{d\mathbf{f}_k}{d\mathbf{u}}$, have real eigen values and a complete set of m linearly independent eigen vectors.

The solutions of *nonlinear* conservation laws are characterized by the loss of smoothness in finite time, [19], requiring the use of so called *shock capturing* schemes capable of detecting and resolving accurately these discontinuous solutions as time evolves. Commonly, this type of numerical schemes rely upon very detailed information about the local structure of the solution which, in turn, results in complex and computationally expensive algorithms. Numerical schemes based on central differencing offer a simple –yet robust– approach to calculate the discontinuous solutions of hyperbolic conservation laws. By using only a minimal amount of characteristic information –an estimate of the maximum speed of propagation of the discontinuities, central schemes avoid costly (approximate) Riemann solvers, resulting in robust, efficient, and simple to implement numerical algorithms for nonlinear hyperbolic systems.

The challenges posed by hyperbolic conservation laws, often extend beyond the already delicate task of detecting and evolving discontinuous solutions. Many relevant systems of conservation laws include non-homogeneous terms –*e.g.*, shallow water equations– or are augmented by side constraints –*e.g.*, MHD equations– that pose additional challenges in themselves for the design of numerical schemes. To this end, the high adaptivity of central schemes –in the sense that they are not tied to the characteristic structure of the underlying system of PDEs– has allowed for the extension of existing schemes and the design of new ones for systems posing added difficulties, see, for example, [15, 26].

3. Completed Research: Central Schemes for Ideal MHD Equations

A common simplification of the *full* MHD model follows from assuming the perfect conductivity (no resistivity) of the fluid. The simplified model provides a good description for plasmas where the effects of the diffusion of the magnetic field over time can be neglected, such as those present in active solar regions where *sunspots* are formed, [8]. This assumption results in the equations of ideal MHD, a nonlinear hyperbolic system of conservation laws that we write in vector form as,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{2a}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot [\rho \mathbf{v}\mathbf{v}^\top + (p + \frac{1}{2}B^2) I_{3\times 3} - \mathbf{B}\mathbf{B}^\top] = 0, \tag{2b}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \Big[\big(\frac{\gamma}{\gamma - 1} p + \frac{1}{2}\rho v^2\big)\mathbf{v} - (\mathbf{v} \times \mathbf{B}) \times \mathbf{B} \Big] = 0, \tag{2c}$$

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0, \tag{2d}$$

which is equivalent to, (1) with **S**(**u**,x,t) = **0**. The first three equations express, respectively, the *conservation* of mass per unit volume, ρ, momentum, $\rho\mathbf{v}$, and total energy per unit volume, e, and (2d) is the induction equation of the magnetic field, $\mathbf{B}$. The pressure, p, is coupled to the energy by the equation of state, $e = \frac{1}{2}\rho v^2 + \frac{1}{2}B^2 + p/(\gamma - 1)$, where γ is the (fixed) ratio of specific heats. The system is augmented by the *solenoidal* constraint,

$$\nabla \cdot \mathbf{B} = 0; \tag{3}$$

that is, if the condition $\nabla \cdot \mathbf{B} = 0$ is satisfied initially at $t = 0$, then by (2d) it remains invariant in time. While this constraint is implicitly satisfied by any exact solution of (2), the majority of numerical schemes commonly employed to approximate these solutions require additional techniques to guarantee it, (see, e.g., [25, 28]).

The solutions of this system develop discontinuities as time evolves requiring numerical schemes capable of detecting discontinuities and resolving them by identifying the direction and speed at which they propagate to approximate them. *Upwind* schemes rely in the spectral decomposition of the Jacobian matrices, $\frac{d\mathbf{f}_\mathbf{k}}{d\mathbf{u}}$, of the underlying system of PDEs, (1), to construct Riemann solvers that can determine those features. This

approach, accurate as it results, carries a high computational cost with it, especially when solving large systems of equations. In [1, 5], Tadmor, Wu, and I utilized the family of second- and third-order, nonoscillatory central schemes introduced by Tadmor and his collaborators in [12, 21, 22] to approximate the solution of several prototype problems for the equations of ideal MHD in one- and two-space dimension. When implemented over *staggered* grids, central differencing schemes eliminate the need for any detailed knowledge of the eigen structure of the Jacobian matrices of the system, avoid dimensional splitting in multidimensional settings, and allow for the use of simple quadrature formulae to realize the time evolution of cell averages –neither exact, nor approximate Riemann solvers are needed. This results in efficient, easy to implement black-box type numerical solvers.

While the solutions to (2) presented in [5] demonstrate the simplicity and robustness of central schemes, they also reveal certain limitations of the fully-discrete schemes. In particular, the staggered formulation requires the use of smaller time steps and, in some instances, make the formulation of boundary conditions difficult. In [1, 2, 4] we extended our results using the more versatile semi-discrete formulation introduced by Kurganov and Tadmor in [17]. By incorporating a minimal amount of characteristic information – an estimate of the maximum local speed of propagation of discontinuities, this formulation retains the simplicity of the original fully-discrete algorithms while avoiding the use of staggered grids. The resulting family of central schemes enjoys some additional advantages: larger time steps can be used without compromising the stability of the solution, a reduced amount of dissipation allows for better resolution of sharp profiles near discontinuities, and the actual computer implementation can be easily adapted to obtain higher-order schemes or to execute the algorithm with different numerical methods (e.g., time evolution can be carried out with Runge-Kutta or multi-step methods depending on their suitability for a particular problem).

For some of the two-dimensional prototype problems we solved, the initial configuration of the magnetic and velocity fields guarantees the solenoidal constraint, (3). For other problems (e.g., Orszag–Tang vortex system, [23]), however, this constraint is not necessarily guaranteed by the approximated values of the magnetic field. When the computed magnetic field fails to satisfy the solenoidal constraint, the numerical error accumulates from one time step to the next (due to the underlying characteristic structure of the system of PDEs), rendering the solution unstable. While most of the numerical schemes employed for MHD often require additional techniques to enforce this constraint, [28], our results indicate that central schemes do not require any modification (from their original formulation). In the case of fully discrete schemes, we observed that any increase in the value of $\nabla \cdot \mathbf{B}$ from one time step to the next, may only arise from the nonoscillatory reconstruction of point values from the computed –staggered– cell averages, and not from the evolution step, [4]. Our calculations, however, indicate that the value of $\nabla \cdot \mathbf{B}$ remains *small* (in the order of 10^{-13}) throughout the calculations. A similar behavior is observed for semi-discrete schemes.

Solutions of several one- and two-dimensional MHD prototype problems obtained with these fully- and semi-discrete central schemes were presented in [1, 2, 4, 5]. They are qualitatively comparable to those obtained previously with upwind schemes by Brio and Wu, [6] and by Jiang and Wu, [13]. These results also complement those obtained by Del Zanna $et.\ al.$ in [9, 10] for relativistic MHD and those of a large scale, multidimensional MHD simulation by Wu and Chang, [30], and demonstrate the ability and efficiency of central schemes to detect and resolve accurately the relevant features of the solutions of MHD problems.

4. Current Research: Central Schemes for Non-homogeneous Hyperbolic Conservation Laws

My current line of research focuses on non-homogeneous hyperbolic systems. These non-homogeneous terms often account for important physical properties of the model, thus they must be taken into account when designing numerical schemes for approximating their solutions. Such is the case for numerical schemes for shallow water equations, where the proper discretization of the source terms is crucial for

the calculation of steady state solutions, [7, 14, 15, 29]; or the Euler-Poisson model for two-species plasmas which consists of two hyperbolic systems coupled by non-homogeneous terms whose calculation involves the solution of Poisson's equation, an elliptic PDE.

In the case of shallow water flows, the results presented in [15, 16, 27] demonstrate the ability of central schemes to incorporate simple *well balanced* discretizations of the source terms –no need to project them along the characteristic fields of the Jacobian matrices of the flux functions, $\partial \mathbf{f}_k / \partial \mathbf{u}$. These results suggest the design of new central schemes to handle additional source terms arising from more complex flows, such as flows along channels with irregular geometry, or flows involving multiple fluid layers. The motivation for designing central schemes for Euler-Poisson equations arises from the interest in comparing microscopic and macroscopic models for two-species plasmas so as to asses their validity and/or suitability for specific applications (see, for example, [18]).

4.1 **Shallow Water Equations.** Hydrodynamical flows along channels, river beds and coastal areas are commonly modeled by the shallow water equations. In the first part of our work on this topic (under review), we introduce a central scheme for on one-dimensional flows along channels with a bottom topography and varying rectangular cross-sections. This type of flows are described by a hyperbolic system of the form (1) above with,

$$\mathbf{u} = \begin{pmatrix} A \\ Q \end{pmatrix}, \quad \mathbf{f}(\mathbf{u}) = \begin{pmatrix} Q \\ \frac{Q^2}{A} + \frac{1}{2} g \sigma h^2 \end{pmatrix}, \quad \text{and} \quad \mathbf{S}(\mathbf{u}, x, t) = \begin{pmatrix} 0 \\ \frac{1}{2} g \sigma' h^2 - g \sigma B' \end{pmatrix}, \tag{4}$$

expressing the conservation of the wet cross-section, $A = \sigma h$, and the *discharge*, $Q = Av$, where h stands for the height of the water above the bottom of the channel, $B(x)$, $\sigma(x)$ is the width of the rectangular cross sections, v represents the fluid velocity, and g the acceleration of gravity.

In addition to the accurate approximation of discontinuous solutions, numerical schemes for shallow water flows must take into consideration the properties of steady state solutions, where the non-zero gradient of the flux function, $\mathbf{f}(\mathbf{u})$, must be exactly balanced by the source term, $\mathbf{S}(\mathbf{u}, x, t)$, that accounts for the effects that the bottom topography and the varying width of the channel have on the flow.

Our new central scheme for shallow water flows introduces three new features for flows along channels with irregular geometries:

- The polynomial reconstruction of the interface point values of the wet area, $A^{\pm}_{j\pm1/2}(t) \approx A(x^{\pm}_{j\pm1/2}, t)$, takes into account the *exact* information at these interfaces, $\sigma(x_{j\pm1/2})$ and $B(x_{j\pm1/2})$, and the value of the total height of the water, $w = h + B$, at the corresponding values at mid-cell points, x_j. This helps to further control the spurious oscillations normally observed in the approximation of discontinuous solutions and to achieve the balance between fluxes and source terms.
- A simple discretization of the source terms –no need for its projection along characteristic fields– accounting for the effects of the bottom topography and changing width of the channel that balances exactly the nonlinear fluxes for the steady-state solution of rest ($h + B \equiv const., v \equiv 0$).

The properties and adequate behavior of the scheme are verified with a number of numerical tests that include the comparison of computed solutions against several nontrivial steady-state exact solutions, [24], and other prototype problems for shallow water flows (*e.g.*, dam breaks and small perturbations from rest).

4.2 **Euler-Poisson Equations.** In this project we are interested in problems arising from plasma physics such as laser-plasma interaction or fusion plasmas. These type of phenomena are modeled by the Boltzman-Maxwell equations and by other simplified models such as the Vlasov-Poisson equations,

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \nabla_{\mathbf{x}} \cdot f_i + \mu_i E \nabla_{\mathbf{v}} \cdot f_i = 0, \tag{5}$$

where $f_i(\mathbf{x}, \mathbf{v}, t)$, $i = 1, 2$ represents the particle distribution of each species in phase space and μ_i its signed charge/mass ratio. The equations for the two species are coupled through the electric field $E(\mathbf{x}, t)$, given by Poisson's equation,

$$\nabla \cdot E = \frac{e}{\epsilon_0} \int_{\mathbb{R}^3} (Z f_2 - f_1)\, d\mathbf{v}, \tag{6}$$

Here e is the (unsigned) charge of the electron, Z stands for the atomic number of the second species (assuming $i = 1$ corresponds to electrons), and ϵ_0 is the permittivity of free space.

This system provides a rather accurate microscopic description of collisionless plasmas, however, numerical simulations require the discretization of each component of the velocity field as one more variable in phase space which, in turn, demands considerable computer time and power. Alternatively, one can consider the Euler-Poisson equations, which can be expressed in conservation form, (1). We write them in one-space dimension with,

$$\mathbf{u} = \begin{pmatrix} n_i \\ j_i \\ w_i \end{pmatrix}, \quad \mathbf{f}(\mathbf{u}) = \begin{pmatrix} j_i \\ \frac{j_i^2}{n_i} + p \\ (w_i + p_i)\frac{j_i}{n_i} \end{pmatrix}, \quad \mathbf{S}(\mathbf{u}, x, t) = \begin{pmatrix} 0 \\ \mu_i n_i E \\ \mu_i j_i E \end{pmatrix}, \quad i = 1, 2, \tag{7}$$

a macroscopic model resulting from taking the first three moments of equation (5). The coupled Euler-Poisson systems express the conservation of density, n_i, current, j_i, and kinematic energy, w_i of each species, where their pressures, p_i, are given by two equations of state, $p_i = p_i(n_i)$.

While this formulation is not as accurate as its microscopic counterpart (5), it is still adequate for many plasma simulations and considerable less computationally expensive to simulate, [18, 26]. In [26] fully-discrete central schemes are presented for two Euler-Poisson models for semiconductors, we propose to extend these results by developing new high-resolution semi-discrete central schemes for the system (7).

5. Development of Software for Scientific Problems

The successful implementation of central schemes for MHD equations led us to the development of CentPack: a collection of C++ libraries that implement several high order central schemes for hyperbolic conservation laws in one- and two-space space dimensions, [3]. The software exploits the simplicity and ease of implementation of central schemes, requiring from the user only a small number of subroutines specific to the hyperbolic model, (1), to be solved, namely, a description of the flux functions $\mathbf{f}_k$, boundary and initial conditions, and an estimate of the maximum speed of propagation of the discontinuous waves. The software also enjoys the high adaptability of central schemes, allowing for the implementation of other versions of central schemes, or their extension to more complex models with minor changes in the existing code.

At the present, we continue working on the development and distribution of CentPack, adding new features and capabilities to the central schemes the package implements and incorporating the new central schemes that result from our ongoing research.

6. Other Areas of Interest for Future Research

My main area of interest is the design of numerical schemes for physical models. In particular, there are three topics I am interested in investigating:

- Extension of central schemes for shallow water flows for more complex channel geometries and multilayer fluids in one and two space dimensions. The results obtained so far with central schemes suggest their extension to handle these more complex flows whose source terms include non-conservative

products of the conserved variables accounting for the exchange of momenta across layers. These type of schemes can also be adapted to other systems of conservation laws with source terms.

- Completion and extension of the project described in §4.2 above. This project is on its initial stages, but preliminary numerical results indicate the suitability of central schemes to approximate the solutions of two-species plasma models and their extension to concrete applications in physics and engineering.
- The design of numerical schemes for relativistic flows. The mathematical theory for relativistic models is not as well developed as that of non-relativistic ones. In addition to the possibility of simulating of relativistic flows, the design of robust numerical schemes for these models may also shed light about the properties of their solutions.

Other areas of interest for future research include spectral and wavelets methods for PDEs and related fields such as image processing.

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