RESEARCH STATEMENT IN: NUMERICAL ANALYSIS

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My research interests include the areas of numerical methods for hyperbolic conservation laws, shallow water flows, fluid dynamics, flows in porous media and multi-phase flows. Here I explain the contributions I have made to **numerical analysis**, in collaboration with Professor Smadar Karni. However, I also enjoy working on **semiclassical analysis**, which has been a parallel project in my doctoral dissertation. In collaboration with Professor Alejandro Uribe, we have made contributions to the quantization of some symplectic manifolds with boundary, and developed a symbolic calculus for pseudodifferential operators with singular symbols. This has applications to spectral theory and mathematical physics. My research statement of that area is available on my webpage:

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1. Introduction

Nonlinear hyperbolic conservation laws are equations of the form

$$W_t + F(W)_x = 0.$$

Here $W(x,t)$ is the vector of conserved quantities, $F(W)$ is the vector of flux functions, where the Jacobian $\frac{\partial F}{\partial x}$ has real eigenvalues and a complete set of eigenvectors.

Many physical phenomena can be modeled by this class of equations. The Euler equations and the shallow water equations with no topography are examples of such systems. Hyperbolic conservation laws are distinguished by the propagation of information along characteristics at finite speed. When faster information overtakes slower information, multi-valued solutions appear. Solutions are extended as weak weak solutions, which are piecewise smooth. This yields the so-called **jump conditions** $[F(W)] = s[W]$, where s is the the speed of the shock, and $[\cdot]$ denotes the jump. Weak solutions are not unique, even in the scalar case. Among all the possible candidates, the entropy condition selects a unique solution. See [13, 15] for details. This allows us to study the **Riemann problem**, where the initial data is piecewise constant. Besides shock waves, a typical solution for the Riemann problem may also contain rarefaction fans, which are characterized by quantities that remain constant across the fan, also known as **Riemann invariants**.

Due to the non-linearity of $F(W)$, exact solutions are rarely available. Solving those systems then relies on the construction of numerical methods. One property of these systems is the formation of shock waves (discontinuities) in finite time. Naive discretizations gives numerical methods that produce satisfactory results in smooth regions, but may be completely erroneous near shock waves. As a consequence, numerical results may converge to a non-physical weak solution. Even when exact solutions may be unattainable, much is known about the general mathematical structure of the solutions. Numerical methods may be carefully built according to the structure and properties of the given system. For example, **conservative methods** have the general form

$$W_j^{n+1} = W_j^n - \frac{\Delta t}{\Delta x}\left(F_{j+1/2} - F_{j-1/2}\right),$$

where $F_{j+1/2}$ is the numerical flux function. In this case, the **Lax-Wendroff theorem** ensures that if the numerical solution converges to some function as the grid is refined, the function has to be a weak solution of the conservation law.

I am particularly interested in conservation laws with source terms, also called **balance laws**, which are of the form

$$W_t + F(W)_x = S(x, W). \tag{1.1}$$

They model a wide variety of physical phenomena, where the source terms S generally describe geometrical effects, and do not involve the derivatives of the solution. Examples include source terms that describe the bottom topography of a domain, the geometry of a channel, or the effect of a non-cartesian geometry in the Euler equations. If the source terms are bounded, they do not affect the jump conditions and weak solutions are obtained analogously. A first numerical approach for this kind of equations is an operator splitting algorithm, where the problem is divided into two subproblems, where the solution is first updated by the transport equation followed by an ODE integration to account for the source terms. However, these equations often have steady-state solutions when a delicate balance between the flux gradient and the source terms is present. In those cases, splitting techniques perform poorly, as they fail to maintain such a balance. In [14], a f-wave algorithm for balance laws is described. Other techniques will be described in the next section.

The first project in my doctoral dissertation pertains to the shallow water equations, and is summarized as follows.

Project 1. Considering shallow water flows through channels of arbitrary geometry, we design a Roe-type upwind scheme that is conservative and respect the balance between the flux gradient and the source terms, recognizing the steady-state solutions. Numerical results are displayed to show the merits of the scheme.

Things get more complicated if the terms of the right-hand side in equation (1.1) involve derivatives of the solution itself, $S = S(x, W, W_x)$, which are referred to as **nonconservative products**. Both theoretical and computational complications arise in this case. On the theory side, the jump conditions are not defined, yielding theoretical issues about weak solutions. Numerical complications appear when both splitting and non-splitting algorithms fail to give satisfactory results and are sometimes disastrous, even if you solve the system with the conservative formulation. The second project of my doctoral dissertation is summarized as follows.

Project 2. Consider the Baer-Nunziato two-phase flow model, which describes the flow of compressible gas in a porous bed. They form a hyperbolic system with nonconservative products. I am interested in the corresponding Riemann problem, where the porosity changes across the **compaction wave**, also known as the interface. Conservative formulations fail to give satisfactory results near the interface (see [16]) as it is unable to maintain constant the Riemann invariants of this wave. We propose a hybrid strategy that substantially improves the numerical results. Comparisons are done to show the improvement.

2. Shallow Water Flows in Channels with Arbitrary cross-section

The shallow water equations model a variety of atmospherical and geophysical flows. They may be derived from the Euler equations by cross sectional averaging, and describe flows that are nearly horizontal. The source terms here represent the topography and geometry constraining the flow. Recent years have seen a rapidly growing interest in the development of numerical methods for shallow water systems in various numerical frameworks [19, 14, 17, 12, 2]. Most relevant to the present work are papers involving shallow water flows in variable geometry [21, 3, 11].

We are concerned with shallow water flows through channels with variable cross section. For simplicity, we write the equations here for the case where the channel has rectangular cross section, with variable (in x) width $\sigma(x)$.

$$\begin{pmatrix} \sigma h \\ \sigma h u \end{pmatrix}_t + \begin{pmatrix} \sigma h u \\ \sigma h u^2 + \frac{1}{2} g \sigma h^2 \end{pmatrix}_x = \begin{pmatrix} 0 \\ -g\sigma h B'(x) + \frac{1}{2} g h^2 \sigma'(x) \end{pmatrix}$$

where h and u denote the layer's depth and (average) velocity, $B(x)$ and $\sigma(x)$ denote the bottom topography and channel geometry, and g is the gravitational constant. Smooth steady-state solutions satisfy $Q = Au = const$ (where $A = \sigma h$ is the wet area), and E=$\frac{1}{2}u^2 + g(h+B) = const$. Discontinuous steady states have piecewise constant energy.

The hyperbolicity of the system enables us to use a Roe-type upwind scheme where the flux Jacobian is linearized in the interface of each pair of cells, and the contribution to each grid cell comes from waves moving into that cell (see [18]). The wave strength for each wave also contains the contribution of the source terms (see [19]). We can now impose conditions on the linearization to make the wave strengths zero in steady states, enabling the scheme to recognize those states. This mechanism enables the scheme to compute very accurately flows that are near steady-states.

We have found a linearization that makes the scheme conservative, respects steady-states of rest, and by imposing an entropy fix, we were able to handle near dry states. We tested the scheme in a range of different examples, including perturbation and convergence to steady states, and drainage problems. The work in rectangular channels appears in [11], and has been extended to channels with arbitrary cross-section in [5]. In both references, examples with shock waves are provided, showing that the scheme computes them very accurately. When we compute convergence to steady states, numerical schemes show their merits with their computed equilibrium variables Q and E being in good agreement with the exact constant (or piecewise constant) values. Figure 1 shows the numerical (dotted line) and exact (solid line) solution and the errors (bottom) for the convergence to steady-states in a channel with arbitrary cross-section. We notice that numerical and exact solutions are in excellent agreement. Figure 2 shows the geometry of the channel and a 3D view of the flow.

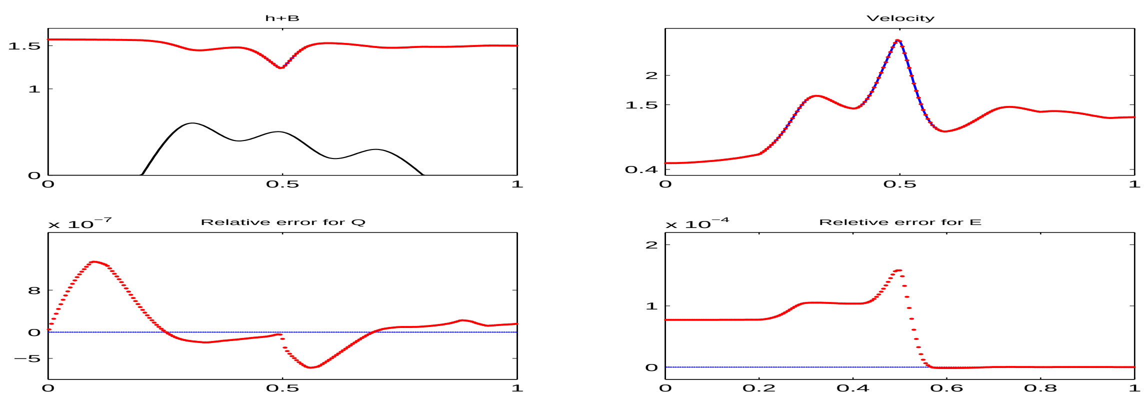

Figure 1. Convergence to a subcritical flow. Exact and numerical solutions are plotted with excellent agreement.

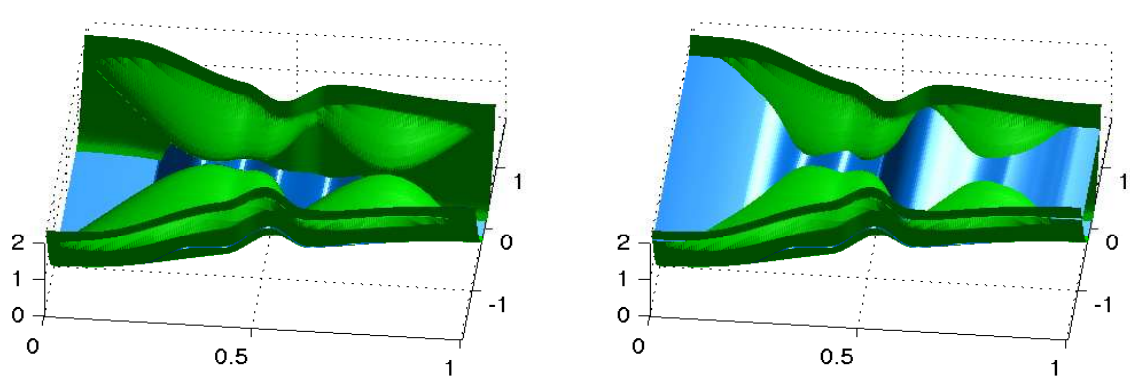

Figure 2. Convergence to a subcritical flow. 3-D View of the channel geometry and the flow.

3. A Hybrid Algorithm for Two-Phase Flows in Porous Media

The Baer-Nunziato model describe the flow of compressible gas in a porous bed. The equations are given by

$$(\phi_g\rho_g)_t + (\phi_g\rho_g u_g)_x = 0 \qquad (\phi_s\rho_s)_t + (\phi_s\rho_s u_s)_x = 0$$

$$(\phi_g\rho_g u_g)_t + (\phi_g\rho_g u_g^2 + \phi_g p_g)_x = p_g(\phi_g)_x \qquad (\phi_s\rho_s u_s)_t + (\phi_s\rho_s u_s^2 + \phi_s p_s)_x = p_g(\phi_s)_x$$

$$(\phi_g E_g)_t + (u_g(\phi_g E_g + \phi_g p_g))_x = p_g u_s(\phi_g)_x \qquad (\phi_s E_s)_t + (u_s(\phi_s E_s + \phi_s p_s))_x = p_g u_s(\phi_s)_x$$

$$(\phi_s)_t + u_s(\phi_s)_x = 0$$

Here the subscript $(\ )_{g,s}$ denote gas and solid phases respectively, $\rho,\ u,\ p$ and E denote the density, velocity, pressure and energy of the respective phases, both assumed ideal fluids and satisfying the Equation of State $E = \frac{1}{2}\rho u^2 + \frac{p}{\gamma-1}$, where γ is the ratio of specific heats, and ϕ is the porosity, satisfying $\phi_g + \phi_s = 1$.

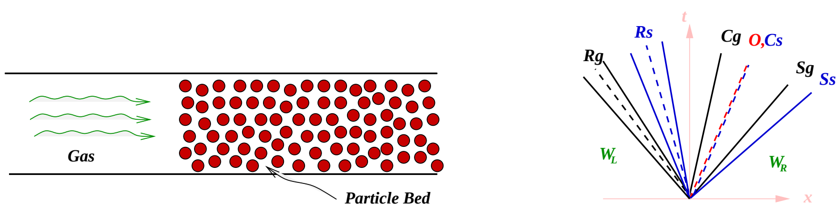

Figure 3. A schematic (left) and typical weak solution (right) for the Riemann problem.

We are concerned with flows in which the porosity changes discontinuously across the compaction wave, and consider the related Riemann problem. A schematic is given in Figure 3 (left). Exact weak solutions were studied and obtained in [1] for the Riemann problem. Figure 3 (right) shows a typical solution with two rarefaction waves (R_g, R_s), two gas and solid contact discontinuities (C_g, C_s), and two solid and gas shock waves (S_g, S_s), traveling at speeds $u-c, u, u+c$ respectively. Here $c = \sqrt{\gamma p/\rho}$ is the speed of sound. The two Euler subsystems are linked through the compaction wave O, which is traveling at the same speed as C_s, making u_s a double eigenvalue. The Riemann invariants across a compaction wave are found in [1, 16]. Given a left and a right state in a Riemann problem, finding the weak solutions necessitates a rootfinding algorithm. We are using the algorithm proposed in [20].

Due to the formation of shock waves, conservative formulations are essential for computations. However, a recent study in [16] showed that conservative methods may fail to give accurate approximations near the compaction wave, as they are unable to compute the right jump conditions in the interface. As observed in [16], Figure 4 (left) shows that for the shock-tube problem conservative formulations fail to keep the gas entropy $\eta_g = p_g/{\rho_g}^{\gamma_g}$, an invariant across the compaction wave, constant. Notice that the entropy satisfies the following equation:

$$(\eta_g)_t + u_g(\eta_g)_x = 0,$$

and so replacing the momentum equation by this one will give a numerical method that respects constant entropy near the compaction wave, provided we have a consistent discretization. Of course this is not a conservative formulation. We propose to use a hybrid formulation, where we use the the conservative variables $W^C = (\phi_g\rho_g, \phi_g\rho_g u_g, \phi_g E_g)$ away from the compaction wave (where shock waves may appear), and the variables $W^R = (\phi_g\rho_g, \eta_g, \phi_g E_g)$ near the interface. This hybridization was done by implementing a mechanism that detects when we are close to a compaction wave. Similar hybridization has been done in other contexts (see for example [6], [7]). Figure 4 compares the conservative (left) and the hybrid (right) formulation, We observe that the hybrid formulation gives more accurate and clean solutions, recognizing that the entropy is constant across the interface.

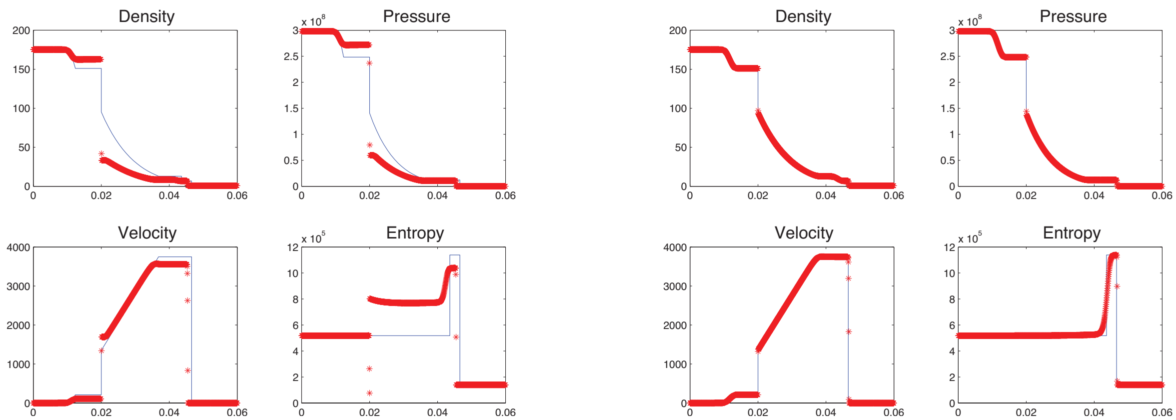

FIGURE 4. Computed and exact solution by the conservative (left) and hybrid (right) formulations.

In [9], we are concerned with the simplified model where the solid bed is assumed stationary and incompressible. In [10], we focus on the full system, where we use all of the Riemann invariants as variables near the compaction wave. We observe that compared to standard splitting and non-splitting methods, the hybrid formulation gives much cleaner results. Tests were done in a variety of different cases with special challenges.

4. FUTURE WORK

Our numerical method in shallow water flows has proven to be very robust near dry states. In future work, we would like to modify it so that it strictly preserves positivity. On the other hand, imposing positivity in central schemes is sometimes more natural due to their structure. In future work, we will also consider those schemes in channels with arbitrary geometries.

Hyperbolicity in *two layer* shallow water flows is conditional and obtaining good numerical methods is challenging, even when the channel has vertical walls. Generalizing it to channels with arbitrary cross section is even more challenging, and hybrid strategies may be used here. We will also work in the future along this direction.

Finally, other problems I am interested in include shallow water flows with moving topography, multi-layer flows, and flows in a pipe, where the geometry consists of a circular tube. This is one more direction where we will focus on.

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