RESEARCH STATEMENT
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Areas of interest:
Singularly perturbed problems, Asymptotic methods, Numerical methods, Aggregation Kinetics, Charge Transport

Overview

Many important problems in applied mathematics can only be solved by a clever combination of analytical tools and numerical methods. These problems are fundamentally challenging in the sense that neither can they be solved–or even fully understood–analytically, nor can numerical methods be blindly applied to them. In order to gain an understanding to the problem and its solution one must adapt an appropriate numerical method to the underlying structure of the problem. Such adaptation may include an initial analysis of the problem using analytical tools such as **asymptotic expansions**, **multiple scales**, or **similarity solutions**. On the numerical side, it is advantageous if a numerical method mimics important characteristics of the equation has, for example, by conserving the same properties as the equation.

Important examples of such problems in my own research are **shape-optimization** in elastic theory [1, 2], **The hanging thin rod** [3], my PhD thesis on **aggregation kinetics** [4], and my ongoing research on **charge-transport in a superlattice**. In this vein, my **particle method for conservation laws** develops a better solver for hyperbolic conservation laws; one that not only respects the conservation law, but also maintains its second-order accuracy at the resulting shocks.

My work **shape-optimization** encompassed two problems in elastic theory [1, 2], the Shape of the Tallest Column, and the Shape of the Optimal Javelin. The structure of the two problems is similar: Starting from an optimization problem, an differential eigenvalue problem is formulated. This non-linear problem has **singular boundary-conditions** that make it difficult to solve using either numerical or analytical methods. Using a **similarity solution**, the system can be reduced in dimension and the singularity removed from the boundary. The resulting dynamical system *can* be solved using a numerical method. In a graduate-level modeling class I gave in UC3M (Madrid, Spain), the students solved several similar problems in this way, demonstrating that the **approach is general**.

I have recently returned to study a similar type of problem, albeit one that required a very different set of asymptotic methods to solve: **The hanging thin rod** [3]. Physically, the problem arises in a simple model for a fluttering flag [5]. Mathematically, the problem involves a **singularly perturbed** fourth-order ODE: A wave equation with a linearly increasing wave velocity that is perturbed by a small amount of bending rigidity. Here, again, numerical methods alone could not solve the problem due to a singularity at the boundary. After finding the correct **boundary layer scalings** the problem succumbed both to a specifically tailored numerical solution (which incorporates these scaling) and to an **asymptotic-expansion** solution. While the numerical solution provides a solution which is as accurate as we care to compute, the asymptotic solution provides an explicit dependence on the perturbation parameter, leading to a deeper understanding of the solution.

For my PhD thesis [4], I derived a physical model that can be reduced into two previously accepted, but seemingly contradictory models of cluster growth. I solved the resulting equations using **distinguished limits** that correspond to three phases of the solution. Modeling **homogeneous aggregation** and solving the resulting equations has both interesting mathematical content and important industrial motivations and applications, from the deposition of mono-layers on silicon wafers to the precipitation of acid from flue gases in furnaces, to name but two examples. Currently I am writing up my recent results pertaining to **nucleation and growth during a thermal quench**.

B. Seibold and myself recently derived a **new particle-based numerical method** for solving conservation PDE [6]. One novel aspect of this method is that it uses a similarity solution to interpolate between the particles. So the

motion of the particles mimics the advection while the use of similarity solution guarantees that the resulting numerical solution has the same conservation property that the analytic solution has. Unlike Godunov-type methods, however, the method is exact away from shocks and the only error is due to the initial sampling.

Recently, I have been looking at model for **charge-transport** of electrons in the conduction band of a semiconductor super-lattice. A super-lattice is an (artificially produced), one-dimensional crystal formed of layers belonging to two different semiconductors [7]. They have interesting physical properties, and important applications in the **semiconductor industry** (such as high-frequency devices) and yet, are still quite poorly understood. Even a simple problem, such as describing the time-dependence of the current when a constant voltage is applied across a sample is not easy to solve. And the results are far from trivial: Results (in the labs and numerically) show that a **rapidly oscillating** current can result. Mathematically, the equation is a non-linear advection equation in two-dimensions with a non-local collision term, coupled with a Poisson equation for the electrical field. The non-linearity of the problem makes solving analytically very difficult, while the different properties of the constituent parts makes the choice of a numerical solution not obvious. I have found that using **moments** in one of the dimensions greatly simplified the problem into a one-dimensional system of conservation laws, and allows for the parabolic Poission problem to be solved using finite elements. This guarantees the conservation of charge, while allowing for computation effort to be used more efficiently. Additionally the approach is flexible enough to be applied to a generalized model (for example, one that includes a second mini-band, or an oscillating bias voltage.)

In the following sections I elaborate on the aforementioned research projects.

1 Particle methods for Conservation Laws

Conservation PDEs are natural models for physical quantities. They can describe shocks and rarefaction behavior while preserving the relevant physical quantity. One dimensional scalar conservation laws exhibit presence of similarity solutions, and the existence of characteristic curves.

B. Seibold (Temple U.) and myself developed a particle-based numerical method for solving one-dimensional, scalar conservation PDE of the form

$$u_t + f(u(x))_x = 0, \tag{1}$$

for a broad class of flux functions, f[1] Like many other particle-based methods, the data is located on a cloud of points, the "particles", which move with a characteristic velocity, $f'(u(x))$. One novel aspect of our method is that it uses an interpolation based on a *similarity solution* of the original problem to add or remove particles when needed. The use of this particular interpolation guarantees that the modification of the solution is done in a locally conservative way. The result is a method which is variation diminishing, entropy non-increasing, and, naturally, exactly conservative. Additionally, it has second-order accuracy and remains so even after shocks are formed, and this accuracy measure *includes* the shock regions.

An example of how a flexible numerical method can be taylored to solve a specific physical problem is our solution of the stiff reaction kinetics problem [8]:

$$u_t + uu_x = \frac{1}{\tau}u(u-1)(\beta-u), \qquad \tau \ll 1, 0 < \beta < 1, \tag{2}$$

in which τ emerges as the size of a reaction front connecting a region of $u = 0$ (on the left) with a region of $u = 1$ on the right. In order to correctly resolve the front velocity (β), other numerical methods must accurately resolve the front, which usually implies an unacceptably small grid-size, or a complicated adaptive grid. Using our particle-method, we were able to resolve the correct speed and front shape using much less particles, and thereby, much smaller computational cost.

The application to reaction kinetics demonstrates how our method can be applied to specific physical problem, solving them without having to resolve the specific internal dynamics.

[1] Specifically, f must be either concave or convex, though we have found some ways to work with an inflection point as well.

1.1 Burger's equation with a convolution term

The equation

$$u_t + uu_x = u * \sin x, \quad x \in [0, 2\pi] \tag{3}$$

with periodic boundary conditions is a simple model for weakly non-linear pressure waves in a thin tapered tube. It conserves u ("mass") locally, and u^2 ("entropy") is conserved away from shocks. R. Rosales (MIT) has conjectured that the stable solutions of equation (3) form a *fractal set* as in KAM theory. Numerical evidence for this could be found by examining the stability of solutions along different segments of function space, However to do this, the numerical method must conserve both mass and entropy. Since the conservation of entropy is global, not local, previously existing method cannot reproduce it numerically. While exactly conservative numerical methods that can deal with shocks exist, they often introduce numerical dissipation unless the mesh is unacceptably small. Furthermore, there is no way to conserve the entropy in these methods.

The structure of our numerical method (specifically, the existence of a natural interpolation between the particles) allows us to generalize it so that it accounts for the source term while conserving entropy as the solution does, making it uniquely suitable for examining the long-term of (3). Using our method, we are examining the long-time behavior of a family of initial conditions, looking for a fractal structure in the family of solutions.

1.2 The Relativistic Burgers' Equation

The equation

$$u_t + \partial_x \left(\frac{u^2}{1 + \sqrt{(1 + u^2)}} \right) = 0, \tag{4}$$

is a scalar, non-linear asymptotic approximation to the ***Relativistic*** Navier-Stokes' equations. It is applicable when the characteristic speeds of the problem are very close to c, the speed of light. When for such large speeds ($u \gg 1$ in our notation), the characteristics become nearly parallel, which poses a difficulty for most numerical methods. Analytically, the problem is just a conservation law with a convex flux-function, which is why our particle method can resolve the solution with little computational effort while both fronts and shocks remain sharp despite the nearly parallel characteristics that pose a challenge to other numerical solvers. We are comparing the results to those found by other solvers and examining relevant applications where the solution can be compared to a solution of the original relativistic Navier-Stokes' equation. This research is pursued in collaboration with A. Marquina from UV, Spain.

1.3 Traffic Networks

Traffic flow is a globally important problem that has remained without a satisfying solution for a long time. it is even difficult to solve the first order equations for traffic flow when one is looking for a solution on a large network of roads, for example, the network of high-ways in the United States, or Europe. A good predictive solution is crucial for example for infrastructure development as well as for planning good emergency response. To model the traffic flow correctly, most methods require a fine grid so that detailed structure of the traffic density can be captured. This causes an unacceptable computational cost when the solution needs to be found on the whole network at once. While the cost of a single computation might seem to be acceptable, this problem is likely to be part of an optimization or control problem and so one would expect it be solved repeatedly, and subsequently a requirement be a possibility to solve the whole network as a small cost.

B. Seibold and myself are extending our particle method to a network of one-dimensional domains, on each of which the traffic flow problem is solved. Since our method can adjust (by adding or removing particles) to the solution, it can be used to solve large networks to high accuracy without requiring much computational power.

Furthermore, it seems that the result will be easily parallelizable, so that splitting the network into different computational domains will require only minimal communication between the different nodes. This can greatly increase the speed at which the problem can be solved.

The behavior of traffic at the intersections is modeled by "junction rules" that inform how traffic merges or splits in a junction. These "junction rules" must be integrated into our particle method, that is, we must provide a particle management scheme at the boundaries of each edge that resects the junction rules. The difficulties arise due to the change in flux function across the boundary. This implies that our similarity solution approximation on one side becomes a function that is (generally) not a similarity solution. Finding a way to project this function onto our space of solutions, while maintaining both conservation properties and TVD (whenever possible) is our goal.

2 Homogeneous Aggregation

The coalescence of small particles (monomers) into large aggregates (clusters) is a fundamental natural process. First-order phase transitions associated with condensation in a gas/liquid system [9, 10], solidification of melts, and precipitation out of a liquid solution [11, 12, 13, 14] are basic examples. Important examples of applications in which aggregation and growth of clusters have a major role include the precipitation of liquid drops out of the gases in energy plants, industrial production of semi-conductors, cloud formation, among many others.

In my PhD thesis [4], I derived a physical model that encompasses both the Becker-Döring model of cluster growth (which is based on surface reactions) and the Lifshitz-Slyozov growth rate (which is based on diffusion limited growth). The model is based on accepting the sensible arguments in each model (mass-action law for BD, and diffusion-limited growth for LS), while rejecting the arbitrary and imprecise assumptions (both models assume a wrong value for the monomer density at the cluster's boundary). From the combined model a natural cluster sizes emerges, it separates the domain of small clusters for which the model reduces to the BD model, and large clusters for which it reduces to the LS model.

Under the relevant scaling for nucleation the resulting equations for the cluster size density can be approximated as an advection PDE with an integral term:

$$\partial_t r + \partial_n(\eta n^{\frac{1}{3}} - 1)r = 0 \text{ in } n > 0, \qquad \eta n^{\frac{1}{3}} r \to \mathrm{e}^{-\frac{1}{\eta^2}} \text{ as } n \to 0^+, \tag{5}$$

$$\eta(t) = \eta(0) - \int_0^\infty n r(n,t)\,\mathrm{d}n. \tag{6}$$

For the sake of clarity, all the physical constants and numerical factors have been set to 1. Remaining are the important variables: $r(n,\, t)$ is the density of clusters of size n at time t, and $\eta(t)$ is the super-saturation, a measure of instability of the system. The usual model is only valid for small values of η, and this smallness is used extensively in the asymptotic solution.

In the rest of my thesis I solved equations (5 6) asymptotically (in the initial value of η) using three distinguished limits which correspond to three "eras" of the solution: *creation*, during which most of the clusters are formed [15]; *growth*, wherein the clusters all grow in a narrow distribution of sizes and no new clusters form; and lastly *coarsening*, in which the larger clusters grow at the expense of the smaller ones and the distribution converges to a specific member [16] of a family of similarity solutions.

2.1 Homogeneous aggregation in a thermal quench

Usually the literature includes studies of the evolution of a system with a positive super-saturation. Rarely is is asked how did the system get to be supersaturated? Clusters start forming (at a exponentially low rate) once the super-saturation is positive, so a system comprising only monomers and a positive supersaturation is not entirely feasible.

I am interested in studying the evolution of a system *while the temperature is being lowered* (aka a quench). Preliminary results [17] show that after a time-lag, a short burst of nucleation lowers the super-saturation, which has risen due to the cooling. In response to further cooling these clusters grow however *no new ones form*. The speed of the quench control the amount of clusters created.

2.2 Condensation on a Cold Wall

The solution of the quenched system may provide insight for another interesting problem: aggregation in the flow of hot, humid gas onto a cold surface. This problem is inspired by the creation of Na_4SO_2 droplets in the flue gas of coal-fired power stations [18, 19, 20]. One goal of this project is to find the amount of condensation that lands on the cold surface by the combined effects of direct condensation and droplet transport. In the boundary layer near the surface, droplets nucleate and grow, removing monomers from the vapor. A solution would involve examining the thermal and viscous boundary-layer near the stagnation point and solving the coupled problem for flow speed, temperature, super-saturation and cluster size. I am co-advising (with L. L. Bonilla) M. D. Camejo who is working on this problem as part of his PhD thesis at UC3M.

2.3 Aggregation in a two-dimensional medium

Aggregation in 2-D is important for the silicon-industry (to name but one), and is interesting mathematically due to the logarithmic solutions to the 2-D diffusion equation. Experiments suggest that even when the "far field" super-saturation is kept constant, the growth of clusters stagnates long before the clusters encroach on one another [21, 22]. The logarithmic solutions (to the diffusion equation) that surround every cluster could explain the long-range interaction, and provide a path for solving this problem. Since these logarithmic solutions are not bounded at infinity, the solution would not have a steady-state form, and averaging over many such solution becomes difficult. These challenges are only the obvious ones on the way to a solution of this problem.

3 Charge Transport

Semiconductor super-lattices are artificial one-dimensional crystals formed by alternating layers of two different semiconductor materials [23]. The difference in the energy gaps of the component semiconductors causes the conduction band of the super-lattice to be a periodic succession of barriers and wells with typical periods of several nanometers. When an appropriate DC voltage is held between the ends of one such SL with finitely many periods, it is possible to obtain high-frequency, self-sustained oscillations of the current[23]. These oscillations are caused by repeated formation of electric field pulses at the injecting contact of the SL that move forward and disappear at the receiving contact. These oscillations have frequencies in the Gigahertz range and have been observed in experiments with GaAS/AlAs SL (and with other SL based on III-V semiconductors) since 1996 and are the basis of fast oscillator devices [24], which have important applications in industry.

Although mathematical models at the level of semi-classical kinetic theory go back to the 1970s [25], their analysis has been based on simplified reduced rate equations (ordinary differential equations) [26, 27] which typically ignore space-charge effects. Electron transport in a single-miniband SL can be described by a kinetic equation coupled to a Poisson equation approximately describing the electric potential due to the other electrons [28]. With all constant set to unity, electron density in the $x-k$ space (position and momentum) satisfies the non-linear, hyperbolic PDE:

$$f_t + \sin(k) f_x + F f_k = f(x,-k) + f^{\mathrm{FD}} - 2f(x,k), \tag{7}$$

Where F is the electric field,

$$\int_{-\pi}^{\pi} f(x,k)dk - 1 = F_x, \tag{8}$$

$$\varphi_x = F, \tag{9}$$

$$\varphi(0) = 0, \qquad \varphi(1) = V; \tag{10}$$

And f^{FD} is the Fermi-Dirac distribution which depends itself on the local electron density.

The collision term in the kinetic equation contains a relaxation term that dissipates energy and momentum, and a simple one-dimensional energy-conserving (but momentum-dissipating) term representing impurity collisions [26]. An important point is that the dispersion relation between miniband energy and momentum is periodic because this periodicity gives rise to a relation between electron drift velocity and electric field which has a maximum value [23]. Thus, the drift velocity decreases as the field increases for large field value and this, in turn, causes the self-sustained current oscillations (SSCO) for appropriate bias and contact boundary conditions [23]. These features are absent in the more usual Boltzmann-Poisson systems with parabolic band dispersion relations.

Recently, Cebrin et al [29] solved numerically the kinetic equation using a direct approach and showed that self-oscillations are among its solutions and also studied the relation between these solutions and those of the limiting drift-diffusion equation. Their numerical solution was based on a hybrid particle/fixed-grid method that used the particles to solve the advective terms and used the grid for calculating the solution to the Poisson problem and for evaluating the effect of the source term. This has several disadvantages: First, it adds a layer of complication as the solution needs to be continually projected back and forth from the particles to the grid; second, it seems to be slightly non-conservative, despite the conservative nature of the equations; lastly, it would be difficult to extend this solution method to allow for a non-DC bias voltage and for solving the fully non-classical equations.

I am solving this equation using moments (Fourier basis) in k. This has several advantages:

- The 2D PDE gets transformed into a conservative system of 1D conservation Laws (for the coefficients of the moments) which are solved using a standard method for conservation laws (upwind, Godonov method).
- The zero moment's (electron density) equation is conservative by itself, which makes guaranteeing a conservative solution much easier
- Since the total density is a known quantity, solving the Poisson equation is almost trivial
- The first moments (if one uses the Fourier basis) are simply the current and energy, which one would like to know for comparing with experiments.
- This approach can be extended to a more realistic model
- Due to the convergance-rate of fourier bases, I expect that the computational cost would be lower using this method

It is only fair to state at this point that this approach is not without its challenges:

- The use of moments means that it is difficult to guarantee positive electron density, something that is important physically
- It is most natural to give boundary conditions for positive k when $x = 0$ and for negative k when $x = 1$. The use of moments makes literal translation of such BC cumbersome, thus alternative ones must be devised. This can make direct comparison between the two result difficult

Overall, my view is that moment method is more appropriate for this problem, and that the advantages are greater than the disadvantages.

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