Research Statement

by Akil Narayan

`akil@brown.edu`

Summary

My primary area of research is in the development of algorithms for the numerical solution of partial differential equations. I have studied the application of discontinuous Galerkin (DG) finite-element methods to hyperbolic partial differential equations (PDE), specifically in the context of Maxwell's equations. In addition, I have developed a novel orthogonal basis for approximation of functions over semi-infinite and infinite intervals. The main thrust of my current research involves optimizing adaptivity for hybrid Eulerian-Lagrangian schemes. The impetus for these research areas comes primarily from an application to plasma physics simulation, but the methods I have developed are applicable to a wide variety of fields and results I have obtained show promise for future work.

Plasma Physics

The numerical computations of plasma physics problems, of concern to those considering space and laboratory plasmas, poses a great number of challenges. The governing system of PDEs for the collisionless evolution of the density function for a charged particle species is the Vlasov (collisionless Boltzmann) equation coupled with Maxwell's equations of electromagnetism. Computing an explicit solution to the governing evolution PDE is often unfeasible in this case when there are six independent spatial dimensions; to make matters worse, three of those dimensions are infinite domains, where traditional approximation methods begin to stumble. A popular and computationally effective alternative is to replace the Eulerian description of a particle density with that of a Lagrangian characterization, thereby eliminating the Eulerian solve of the Vlasov equation. In other words, we essentially collapse the three spatially infinite dimensions and model the resultant loss of information by imposing some initial stochastic uncertainty in the form of many macroscopic, mobile particles. This results in a hybrid solver (Eulerian for Maxwell's equations and Lagrangian for the Vlasov equation), that goes by various names, including Lagrangian solvers, cloud-in-cell, and particle-in-cell (PIC) simulations. We shall use PIC to refer to all of these. The seminal compilation by Birdsall and Langdon [1] helped catalyze the research field of computational plasma physics using PIC. Despite this, PIC has notable disadvantages including noise inherited from its quasi-stochastic nature and relatively low accuracy compared to classical Eulerian solvers. Ideally, PIC algorithms would exhibit highly accurate characteristics similar to those of the *hp*-refinable finite-element methods. Unfortunately, the hybrid-scheme nature of PIC often precludes such rosy results in practice.

My research has focused on methods to mitigate precisely the aforementioned shortcomings of PIC algorithms. I have addressed reducing noise levels and improving accuracy. To this end, there are two main areas I have investigated:

- Development of a fast and accurate Eulerian solver for the full Vlasov-Maxwell system to serve as a 'truth solution' for comparison when performing PIC simulations
- Optimization (accuracy and computational effort) of the Lagrangian nature of the hybrid solver

The DG finite-element method has been shown to have very attractive properties for solving hyperbolic PDEs including efficiency, adaptivity, and accuracy [2]. Maxwell's equations and the Vlasov equation are both hyperbolic PDEs, and thus the DG finite-element scheme has proved to be competitive with traditional numerical schemes for this problem, both in terms of efficiency and accuracy. However, application of the DG method to PIC has only appeared recently [3]. My research has focused on using DG as a key component in the Maxwell and Eulerian Vlasov solver because of its superiority to conventional finite-difference or finite-elements methods in the convection-dominated regime. With the solid DG solver as the base, I have explored the two areas described above.

Eulerian solvers on unbounded domains

Many standard methods for solving differential equations on (semi-)infinite domains exist. However, all the current methods are handicapped by resolution properties, strict requirements on the function to be approximated, and non-optimal computational effort. Three of the Vlasov equation's spatial dimensions are infinite. In order to develop a fast and accurate Eulerian solver for the Vlasov-Maxwell system, I have pioneered work in generalizing an orthogonal rational function basis over the real line originally due to Wiener [4]. The original basis functions exhibit a linear polynomial decay rate, but the generalized basis set admits a parameter than can be tuned to yield functions of polynomial decay x^{-s} for any $s > \frac{1}{2}$ [5]. This generalized basis retains orthogonality with a weight function independent of s, the functions are easily computed via recurrence relations derived from orthogonal polynomials, and computation of the modal coefficients from nodal evaluations (and vice versa) can be accomplished very quickly with the fast Fourier transform (FFT) for integral values of the parameter s.

For the purposes of function approximation, I have demonstrated that this generalized basis is as good as, and in many cases superior to, domain truncation or using other existing basis sets on unbounded intervals. Hermite and Laguerre polynomial/function basis sets are either unbounded at infinity (the polynomials) or decay exponentially quickly (the functions), making approximation in the pointwise sense difficult for a large class of functions. This problem is mitigated by the new basis set because the rate of decay can be tuned accordingly. I have also shown that the computational advantage of the FFT is large, often yielding a computational savings of an order of magnitude for large problems; in contrast, computation with the FFT is entirely unavailable for Hermite and Laguerre expansions.

When solving differential equations, the generalized Wiener basis also admits sparse Galerkin matrices for differentation, and for certain values of the decay parameter s the product of two basis functions is a sparse combination of basis functions. This allows for fast Galerkin solutions of linear differential equations, and in certain cases even nonlinear ones. Furthermore a combination Galerkin-collocation solver (e.g. for nonlinear problems with linear differential terms) can be solved quickly with aid from the FFT.

Although I have developed this basis set intending to use it as an application for plasma physics, it has numerous applications in a variety of other areas. Some areas that I anticipate exploring are applications to the Schrödinger equation of quantum mechanics [6] and infinite-element finite element methods for outgoing radiation waves [7].

There have been many by-products of my research in this area: notably, I have determined that the FFT can be used for expansions in a wide variety of Jacobi polynomial families [8], where previously such a result was only manifest for the four families of Chebyshev polynomials. Furthermore, building on work by Hesthaven [9], I have shown that nearly-optimal Lebesgue constants for polynomial interpolation can be obtained by considering the appropriate Gauss or Gauss-Lobatto quadrature nodes for non-Chebyshev families of Jacobi polynomials [10]. The scope of potential applications for and extension of these findings is wide. Jacobi polynomials are building blocks for the resolution of the Gibbs phenomenon [11]; expansions in spherical harmonics (the eigenmodes of the spherical Laplacian) are partly expansions in modified Jacobi polynomials and are ubiquitous in geophysics and electromagnetism; also, data compression for electrocardiogram measurements using Jacobi polynomials [12] has been competitive with standard wavelet compression. All of my findings for increasing the speed and accuracy of Jacobi polynomial expansions can be employed to yield contributions for the above applications.

Hybrid scheme adaptivity

Because the dynamics of a plasma simulation can have significantly different properties in different spatial regimes, one should consider locally adapting the numerical method to suit the requirements in each regime. With this goal, I have considered using a three-pronged strategy: optimizing the particle-to-density reconstruction (kernel estimation), using the Lagrangian formulation only when necessary (perturbation methods), and allowing the particle properties to evolve (particle adaptivity).

One of the basic elements of PIC algorithm is the reconstruction of the density function given a distribution of particle samples; this is also often the least accurate portion of the PIC solver. The PIC algorithm method of choice for density estimation is usually kernel density estimation, wherein one endows each particle with a shape function, i.e. a macroscopic size and radius-dependent strength of influence. In studies I have performed I have concluded that the reconstruction of the density from the particles is not the only problem to resolve: in addition to judicious choices of shape function and particle size, we must also reconcile our reconstruction with the underlying finite-element mesh of the discretization. Juggling all of these is a highly nontrivial task and I am currently in the process of exploring mathematically rigorous metrics to judge the quality of the reconstructions, and computationally efficient methods of carrying out these reconstructions.

The disadvantages of traditional Monte-Carlo-type sampling algorithms are clear: the noise level can be unacceptably large if too few samples are used and even a very large number of samples will only yield slow convergence to the desired density. Because of this, many alternatives have been proposed to mitigate this problem. One particular method I believe has merit is the delta-f method [13]. Often times the noise resulting from a Lagrangian representation dominates the temporal fluctuations of the total density function. To alleviate this, the delta-f method proposes to model only the perturbations with a Lagrangian representation, instead of the entire function. The result is that the particle representation captures the perturbations to a much greater degree of accuracy than if we were to simply to represent the entire function.

The last ingredient in a potential adaptive algorithm is the ability for the particle properties to evolve. This includes shape functions, weights, and number of particles. With regard to the number of particles, recently there has been some work on fragmenting and merging particles [14] ,[15] and also promising results for efficiently implementing the fragment/merge criteria [16]. Augmenting the shape functions and weights has also been explored [15], although to a much lesser extent. Each of these methods has its advantages, but also its limitations. I will investigate whether a balanced mix of them can produce an approximation that is superior to employing only one option.

The three main tools I envision in a successful adaptive particle code are the ability to prescribe an accurate reconstruction procedure, proper use of Lagrangian representations only on evolving parts of the solution, and optimizing the types and numbers of particles present with respect to the dynamics. Each of these methods has shown its utility in the literature, and I believe a judicious synthesis of them will yield a highly accurate and efficient PIC algorithm.

Future Work

Although much of the research I have done has been in reaction to the problems of computational plasma physics, the applications of the developed methods are diverse. in the future, I envision new studies in the following areas:

- Applications
    - Proof-of-concept studies showing the advantage of using the FFT for classical Jacobi polynomial expansions. Additionally this serves to show how taking the Lebesgue constant into account produces a quanitatively superior interpolant.
    - Using the generalized Wiener basis set for solving PDEs arising in e.g. quantum mechanics, electromagnetics, and oceanic processes.
- Further mathematical research I intend to pursue:
    - Refining the generalized Wiener basis: salient open questions include e.g. the ability to efficiently tune the decay parameter s mid-computation and nested Gauss-Kronrod-type quadrature rules for efficient error estimation.

- Continuing my exploration of hybrid scheme adaptivity. The end goal is a computationally efficient and accurate Eulerian-Lagrangian scheme; I suspect that this can be achieved by combining existing results from density estimation, perturbation methods, and particle adaptivity.

- Investigation of other methods of density estimation for PIC simulations. This applies not only to novel kernel estimation techniques, but also more general methods, such as clustering methods for lattice-Boltzmann type models.

Bibliography

[1] C. Birdsall and A. Langdon, *Plasma Physics via Computer Simulation*. McGraw-Hill, 1985.

[2] J. Hesthaven and T. Warburton, *Nodal discontinuous Galerkin methods: algorithms, analysis, and applications*. Springer, 2007.

[3] G. Jacobs and J. Hesthaven, "High-order nodal discontinuous galerkin particle-in-cell method on unstructured grids," *Journal of Computational Physics*, vol. 214, pp. 96–121, 2006.

[4] N. Wiener, *Extrapolation, interpolation, and smoothing of stationary time series*. MIT Technology Press and John Wiley & Sons, 1949.

[5] A. Narayan and J. Hesthaven, "A generalization of the wiener rational basis over the infinite interval." In preparation.

[6] J. Boyd, C. Rangan, and P. Bucksbaum, "Pseudospectral methods on a semi-infinite interval with application to the hydrogen atom: a comparison of the mapped fourier-sine method with laguerre series and rational chebyshev expansions," *Journal of Computational Physics*, vol. 188, pp. 56–74, 2008.

[7] L. Kantha and C. Clayson, *Numerical Models of Oceans and Oceanic Processes*, vol. 66 of *International Geophysics Series*. Academic Press, 2000.

[8] A. Narayan and J. Hesthaven, "Application of the fast fourier transform to general jacobi polynomial expansions." In preparation.

[9] J. Hesthaven, "From electrostatics to almost optimal nodal sets for polynomial interpolation in a simplex," *SIAM Journal of Numerical Analysis*, vol. 35, no. 2, pp. 655–676, 1998.

[10] A. Narayan and J. Hesthaven, "Quasi-optimal lebesgue constants from gauss quadrature nodes for orthogonal polynomials." In preparation.

[11] D. Gottlieb and C.W.-Shu, "On the gibbs phenomenon and its resolution," *SIAM Review*, vol. 39, no. 4, pp. 644 – 668, 1997.

[12] D. Tchiotsop, D. Wolf, V. Louis-Dorr, and R. Husson, "Ecg data compression using jacobi polynomials," in *Proceedings of the 29th annual international conference of the IEEE EMBS*, pp. 1863 – 1867, 2007.

[13] R. Sydora, *Lecture notes in physics*, vol. 615, ch. Low Noise Electrostatic and Electromagnetic Delta-f Particle-in-Cell Simulation of Plasmas. Springer, 2003.

[14] D. Larson, "A coulomb collision model for pic plasma simulation," *Journal of Computational Physics*, vol. 188, pp. 123–138, 2003.

[15] D. Hewett, "Fragmentation, merging, and internal dynamics for pic simulation with finite particles," *Journal of Computational Physics*, vol. 189, pp. 390–426, 2003.

[16] D. Welch, T. Genoni, R. Clark, and D. Rose, "Adaptive particle management in a particle-in-cell code," *Journal of Computational Physics*, vol. 227, pp. 143–155, 2007.

Akil Narayan

Divison of Applied Mathematics
Brown University
182 George St., Box F
Providence, RI 02912
(401) 863-2230

`akil@brown.edu`

`http://www.dam.brown.edu/people/anaray`