

Research Statement

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Introduction: My research focuses on numerical analysis, scientific computing and mathematical modeling for temporal and spatial multi-scale problems in physics and engineering. Problems that interest me can be broadly classified as multi-scale fluids. These include plasmas, free surface problems with external forces, flow in micro/nano tubes, etc. As a class of problems, these types of fluids display a very rich and complex range of behavior; both analysis and simulation are needed to further understand these fluids. In the following paragraphs, I will provide a brief overview of some of the algorithms I have been developing. My current goal is to extended direct methods for multi-scale problems as far as possible before considering model reduction. To achieve this goal, I have been focusing on high order methods, i.e., methods that achieve the same accuracy on a coarse mesh compared with low order method computed on a fine mesh, but with greater efficiency than the low order methods.

My long term goal is to develop a simulation package for stiff plasma problems; a quintessential example of interest to me is plasma assisted combustion. This involves the development of (i) algorithms for advanced platforms, a current example being General Purpose Graphics Processing Units (240 cores per GPGPU for a single 4GiB block of memory in a distributed computing framework), (ii) automated model reduction and (iii) incorporation of mathematical tools that perform automated verification and validation. Such a simulation framework will have wide applicability in the study of basic plasma physics.

In the following sections, I will an overview of my most recent work on parallel time integrators, which promises to increase the efficiency of Lagrangian methods by at least a factor of 10 in wall clock time over standard Runge-Kutta methods. I will then provide a discussion of our progress on novel Strang split semi-Lagrangian methods for PDEs with structure similar to the Vlasov equation. These new Strang split semi-Lagrangian methods are the first to obtain higher than 3rd order in space, for dimensions greater than two, and still be conservative. Related work not discussed here include: model reduction [1], gridless Monte Carlo methods which avoid mesh based artifacts [2], semi-Lagrangian methods based on phase space contour mapping [3, 4, 5], the development of sparse mesh recovery theory for PDE's based on the statical sampling methods (*in preparation*), the development of WENO AMR (*in preparation*) and the development ultra fast spectral solvers based on compressive sensing methods tailored to the GPGPU systems (*in preparation*).

In my work, I have had the invaluable opportunity to co-advise four graduate students, one from mathematics, two from aerospace Engineering and one from physics. Further, I have co-advise two undergraduate students, one REU student and one student whom I supported long term on an AFOSR grant. I am currently advising three mathematics Ph.D. students and co-advising one Ph.D. student from environmental engineering. It has been an enriching experience and I have greatly enjoyed working with these students. Where applicable, I mention my students in the following sections. I have attached an appendix that details my collaborations and my student interactions.

Parallel Time Integrators Based on Defect Correction: In this work, the approach is to construct arbitrary order time integrators based on defect correction [6, 7]. In collaboration with my student (Ms. Maureen Morton) and my current and former post doc's (Dr. Ben Ong and Dr. Jing-Mei Qiu), we have developed Integral Defect Correction (IDC)[8, 9, 10], an extension of Spectral Deferred Correction (SDC)[6, 11, 12, 13, 14, 15]. IDC differs from traditional defect correction in that the integral from of the residual is used in the formulation

of the solution, instead of the differential form of the residual. On multi-core architectures, defect correction methods become extremely attractive because each correction step can be decoupled from the prediction and prior correction steps. In so doing, the methods are able to achieve high order accuracy in the wall clock time equivalent to that of the prediction step, provided multiple cores are used for the computation. We first present IDC followed by a discuss Revisionist IDC (RIDC), which allow for the corrections to be computed in parallel. **The parallel integrator we have developed is the first integrator to leverage multi-core cpus such that the method achieves p^{th} order in the wall clock time equal to that of a single forward Euler step.**

Consider a system of ODES and initial conditions,

$$y'(t) = f(t, y), \quad y(a) = \alpha, \quad t \in [a, b].$$

Given an approximate solution $\eta(t)$ to the exact solution $y(t)$, the error of the approximate solution is $e(t) = y(t) - \eta(t)$. If we define the residual as $\epsilon(t) = \eta'(t) - f(t, \eta(t))$, then the derivative of the error satisfies

$$e'(t) = y'(t) - \eta'(t) = f(t, y(t)) - f(t, \eta(t)) - \epsilon(t).$$

The integral form of the error equation can then be obtained,

$$\left[e(t) + \int_0^t \epsilon(\tau) d\tau \right]' = f(t, \eta(t) + e(t)) - f(t, \eta(t)).$$

An iteration scheme is implemented to generate successively more accurate approximations,

$$\left[\eta^{(k)}(t) - \int_0^t f(\tau, \eta^{(k-1)}(\tau)) d\tau \right]' = f(t, \eta^{(k)}(t)) - f(t, \eta^{(k-1)}(t)). \quad (1)$$

In fact, it can be shown that each correction loop increases the *order of accuracy* of the approximation. In references [9] and [10], we established that for high order explicit, implicit and semi-implicit methods embedded in IDC, we have established the following theorem,

THM Let $y(t)$ be the solution to IVP with at least S ($S \geq M + 2$) degrees of smoothness in the continuous sense. Consider IDC applied to the time interval $t \in I_j$, constructed using uniformly spaced quadrature nodes on the sub-interval, an $(r_0)^{th}$ order RK method in the prediction step and $(r_1, r_2, \dots, r_{kloop})^{th}$ order RK methods in $kloop$ correction loops of IDC. Define the cumulative order $s_k = \sum_{j=0}^k r_j$. If $s_{kloop} \leq M + 1$, then the local truncation error on I_j is of order $\mathcal{O}(h^{(s_{kloop}+1)})$.

It is possible to simultaneously compute updates from each correction loop if multiple computing cores are available [16]. Consequently, high-order accurate results are obtained in just slightly more wall-clock time than a base scheme computation on a single core computer.

Let the time domain is discretized as $t_m = m\Delta t = m \left(\frac{b-a}{M} \right)$, $m = 0, 1, \dots, M$. Computing an l^{th} order approximation to $\int_{t_{i-1}}^{t_i} f(\tau, \eta^{(k-1)}(\tau)) d\tau$ requires the values $\eta_i^{(k-1)}, \eta_{i-1}^{(k-1)}, \dots, \eta_{i-l}^{(k-1)}$. Figure 1a shows a schematic sketch of the information needed to compute $\eta_m^{[2]}$ for a fourth-order RIDC method after initial start up costs.

To test the efficiency, RIDC schemes were applied to a particle formulation of the Vlasov–Poisson equations, which describe the dynamics of collisionless plasmas. RIDC schemes using

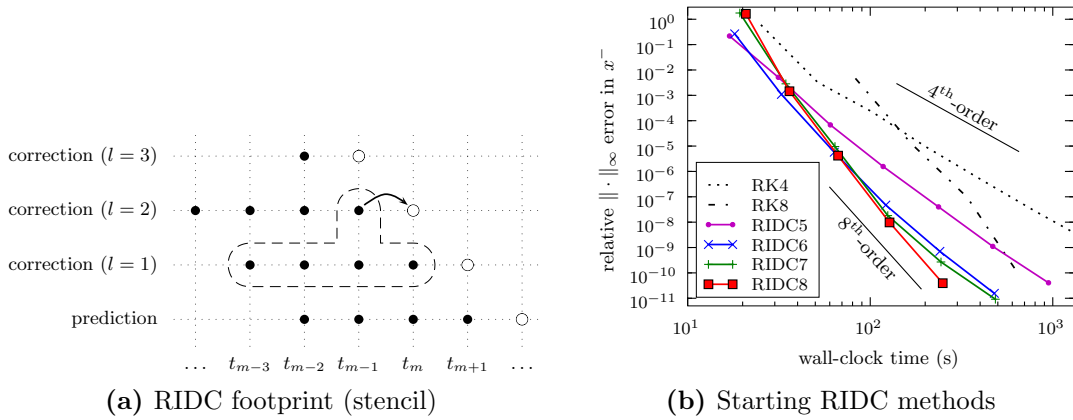


Figure 1: (a) The stencil needed to compute $\eta_m^{[2]}$ is shown in the dashed region for a fourth-order RIDC method. Additionally, this figure shows the minimum memory “foot print” if special care is taken to minimize the amount of data that has to be stored, shown as black dots. Central to our algorithm, is the realization that the prediction and each of the three corrections can be computed simultaneously and independently. After all four computations have completed, the oldest value at each level can be discarded. (b) Convergence study using high-order RIDC5, RIDC6, RIDC7 and RIDC8 (using five, six, seven, and eight cores respectively) and reduced stencils. The panel depicts the wall-clock time for each method and it shows that the RIDC significantly outperform high-order RK schemes.

multiple cores significantly outperform high order RK schemes. In Figure 1b, we show that RIDC methods significantly outperforms high-order RK schemes, in terms of wall clock time, provided sufficient cores are available.

Much work remains to be undertaken in this area. In particular, the big open question is what properties of the base schema will IDC or RIDC method inherit. For example, if a RIDC method is constructed using symplectic integrators, can we ensure that the method is symplectic for all successive orders. If not, can we estimate the number of correction steps that can be taken before the method loses its energy conserving property? In hyperbolic PDEs, the strong stability preserving property is desirable. Is it possible to build an RIDC method that has the SSP property? etc. . .

Vlasov Solvers: Plasmas exhibit a range of complex dynamics, i.e., they can form boundary and internal layers, develop instabilities, setup nonlinear oscillations, exhibit rigid body like behavior, etc. This very rich set of multi-scale behaviors which make them difficult to simulate using traditional fixed mesh methods. For these systems, the most complete model would be to describe each species in the system using a kinetic model. However, kinetic descriptions are very computationally expensive, so it is common to use kinetic descriptions for as few species as possible. For example, if it is known that kinetic phenomenon of a particular species can be neglected, it is more efficient to model that species as a fluid. There are many options for numerically solving the coupled system of kinetic equations [3, 17, 18, 19, 20, 21, 22, 23, 24].

My goal in this work is to develop robust grid-free Lagrangian and mesh based semi-Lagrangian numerical methods for simulating hybrid plasma models. The methods could be exported to other grid-free simulations. I have invested substantial effort in the development of grid-free Lagrangian methods that combine fast summation, kernel regularization

and boundary integral methods [25, 26]. I have analyzed the error associated with kernel regularization and its interplay with errors boundary integral methods[?]. I have applied these methods to a range of problems [27, 26, 28], including the rigid rotation on Penning traps [27, 28]. More recently, I have been focusing on Strang split semi-Lagrangian numerical methods. In particular, we have developed the first Strang split semi-Lagrangian Vlasov solver that is capable of being conservative as well as arbitrary high order in phase space for dimension greater than 2. This new method has clearly demonstrated that high order spatial integrators are far more critical than high order time discretizations[29]. The 9th order version of the method is five times more efficient for the same accuracy as the 3rd order version of the method [29]. Below, I will talk about high order semi-Lagrangian Vlasov solver. The method offers perfect parallelizability in a GPGPU setting, which we expect will translate into a factor of 100 speed up over non-GPGPU computing.

High Order Semi-Lagrangian Vlasov Solver: Consider the Vlasov-Poisson (VP) system which describes collisionless plasmas,

$$\partial_t f_j + \mathbf{v}_j \cdot \nabla_{\mathbf{x}} f_j + \frac{\mathbf{F}_j}{m_j} \cdot \nabla_{\mathbf{v}} f_j = 0 \quad (2)$$

$$\nabla_{\mathbf{x}}^2 \Phi(\mathbf{x}) = -\frac{\rho_t(\mathbf{x})}{\epsilon_o} \quad (3)$$

$$\rho_t(\mathbf{x}) = \sum_j q_j \int f_j(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}, \quad \mathbf{F}_j = -q_j \nabla \Phi,$$

where $f_j(t, \mathbf{x}, \mathbf{v})$ is a probability distribution function describing the probability of a particle being at position \mathbf{x} with velocity \mathbf{v} at time t , the subscript j refers to the various charged species, Φ is the electrostatic potential, q_j is the charge on species j , ρ_t is the total charge density at time t , ϵ_o is the permittivity of free space and \mathbf{F}_j is the force.

We start with the standard dimensionally split semi-implicit Vlasov equation and developed a conservative formulation based on fluxes. This formulation easily lends itself to arbitrary high order WENO reconstruction, providing a good mechanism for maintaining phase space resolution on coarse meshes. In addition, we have rigorously established that the formulation is conservative. The key to all of this is that the dimensionally split Vlasov equation is a 1D hyperbolic problem in each direction of the form,

$$\partial_t f + v \partial_x f = 0.$$

As an example, we present third order reconstruction of the exact solution for the semi-implicit formulation. We denote $x_{i+\frac{1}{2}} = (x_i + x_{i+1})/2$, cell $I_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ and cell $I_{i+\frac{1}{2}} = [x_i, x_{i+1}]$. Let $xshift = v \frac{\Delta t}{\Delta x}$, and f_i^n be the point value of the numerical solution at $x = x_i$ and $t = t^n := n\Delta t$. The first case we consider is the development of a conservative reconstruction when $xshift \in [0, \frac{1}{2}]$. The algorithm for the first order case is as follows:

1. To compute the solution at t^{n+1} , we start with a reconstruction of the true function at t^n using a piecewise cubic approximation, $f^n(x) \sim \tilde{f}^n(x)$. Its projection on cell $I_{i-\frac{1}{2}}$ is $\tilde{f}_{i-\frac{1}{2}}^n(\xi)$, which is reconstructed from the stencil $\{f_{i-2}^n, f_{i-1}^n, f_i^n, f_{i+1}^n\}$. In matrix notation,

$$\tilde{f}_{i-\frac{1}{2}}^n(\xi) = (f_{i-2}^n, f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot A_3^L \cdot (1, \xi, \xi^2, \xi^3)', \quad (4)$$

where $\xi(x) = \frac{x-x_i}{x_{i-1}-x_i} \in [0, 1]$, $x \in I_{i-\frac{1}{2}}$. The interpolating matrix and two related matrices are:

$$A_3^L = \begin{pmatrix} 0 & -\frac{1}{6} & 0 & \frac{1}{6} \\ 0 & 1 & \frac{1}{2} & -\frac{1}{2} \\ 1 & -\frac{1}{2} & -1 & \frac{1}{2} \\ 0 & -\frac{1}{3} & \frac{1}{2} & -\frac{1}{6} \end{pmatrix}, \quad B_3^L = \begin{pmatrix} \frac{1}{6} & 0 & -\frac{1}{6} \\ -1 & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 1 & -\frac{1}{2} \\ \frac{1}{3} & -\frac{1}{2} & \frac{1}{6} \end{pmatrix}, \quad \text{and } C_3^L = \begin{pmatrix} -\frac{1}{6} & 0 & \frac{1}{6} \\ \frac{5}{6} & \frac{1}{2} & -\frac{1}{3} \\ \frac{1}{3} & -\frac{1}{2} & \frac{1}{6} \end{pmatrix}$$

2. An update for the function at the point value x_i at time level t^{n+1} (i.e. f_i^{n+1}) can be obtained by tracing the characteristic back to $\xi = \xi_0$ and evaluating $\tilde{f}_{i-\frac{1}{2}}^n(x)$ at $\xi = \xi_0$,

$$f_i^{n+1} = \tilde{f}_{i-\frac{1}{2}}^n(\xi = \xi_0). \quad (5)$$

3. Next we observe that the update for f_i^{n+1} in equation (5) with (4) can be written in a conservative form,

$$f_i^{n+1} = f_i^n - \xi_0((f_{i-2}^n, f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot B_3^L \cdot (1, \xi_0, \xi_0^2)') \quad (6)$$

$$= f_i^n - \xi_0((f_{i-2}^n, f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot \left(\begin{pmatrix} \vec{0} \\ C_3^L \end{pmatrix} - \begin{pmatrix} C_3^L \\ 0 \end{pmatrix} \right) \cdot (1, \xi_0, \xi_0^2)') \quad (7)$$

$$= f_i^n - \xi_0((f_{i-1}^n, f_i^n, f_{i+1}^n) \cdot C_3^L - (f_{i-2}^n, f_{i-1}^n, f_i^n) \cdot C_3^L) \cdot (1, \xi_0, \xi_0^2)'. \quad (7)$$

4. Finally, we define the flux function $\hat{f}_{i+\frac{1}{2}}^n(\xi) = f_i^n$,

$$\hat{f}_{i-\frac{1}{2}}^n(\xi) = (f_{i-2}^n, f_{i-1}^n, f_i^n) \cdot C_3^L \cdot (1, \xi, \xi^2)', \quad (8)$$

so that equation (7) can be written as

$$f_i^{n+1} = f_i^n - \xi_0(\hat{f}_{i+\frac{1}{2}}^n(\xi_0) - \hat{f}_{i-\frac{1}{2}}^n(\xi_0)). \quad (9)$$

Reconstruction when $xshift \in [-\frac{1}{2}, 0)$ uses the same idea and $|xshift| > \frac{1}{2}$ is handed by whole cell shifts followed by either of the first two cases. Finally, we make use of WENO to reconstruct the fluxes in a non-oscillatory fashion for this conservative formulation. We have found that high order reconstruction in phase space makes a significant difference in the quality of our solution generated by the Strang split system. This work is in collaboration in my former post doc Dr. Jing-Mei Qiu, now an Assistant Prof. at Colorado School of Mines [29]. I am working with my student, Ms. Morton, on extending IDC to correct for the second order time splitting error. We are also working to extend this split framework to Maxwell's equations, then to combined these efforts to make a multi-D Vlasov Maxwell solver.

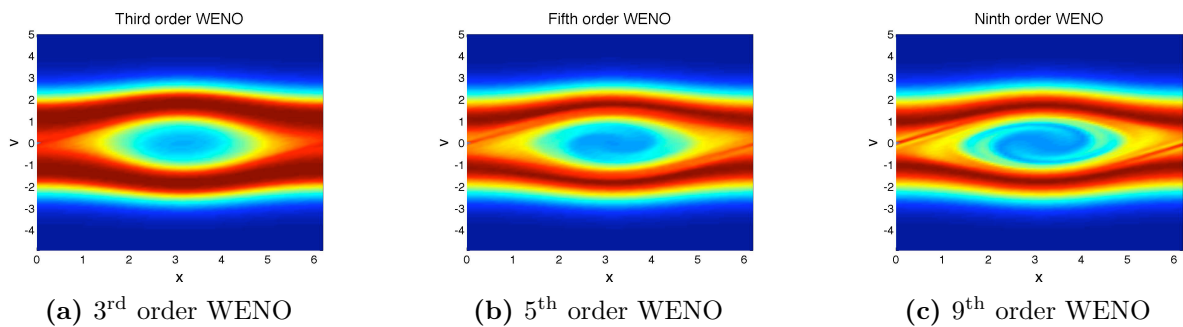


Figure 2: Two stream instability $T = 53$, mesh 64×128 . a) 3rd, b) 5th, and c) 9th order.

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Appendix

Senior Collaborators

- Iain Boyd (Department of Aerospace Engineering, University of Michigan). Projects: Simulation of micro-scale gas flows, grid-free simulations of ion optics and simulation of droplet formation in electrostatic fluids.
- David Bortz (Department of Applied Mathematics, University of Colorado – Boulder). Projects: Sparse mesh recovery theory (SMRT). Identifying the optimal mesh for numerical solving a PDE. (AFOSR-Computational Math)
- Russel Caflisch (Department of Mathematics, University of California – Los Angeles). Projects: Renormalization group as a numerical tool in plasma physics. Use RG to identify an analytic metric to identify if a plasma may be treated using a fluid approximation or if it must be modeled kinetically. (Part of an AFOSR-STTR)
- Jean-Luc Cambier (AFRL: Edward’s Air Force Base). Projects: Grid-free laser plasma simulations and development of reduced phase space models for electrons.
- Keith Cartwright (AFRL: Kirtland Air Force Base). Projects: Sub-grid models for extending the accuracy of traditional mesh based particle codes. (Related to my IPA with Kirtland)
- Nick Hitchon (Department of Electrical and Computer Engineering, University of Wisconsin). Projects: Development of semi-Lagrangian methods for simulating problems in both gas and plasma dynamics.
- Eric Keiter (Sandia National Laboratories). Project: Development of semi-Lagrangian Methods for the simulation of plasma dynamics problems.
- Robert Krasny (Department of Mathematics, University of Michigan). Projects: Development of grid-free numerical methods for problems in plasma physics, e.g., simulation of the two stream instability and the simulation of the Penning trap using dynamic point insertion.
- John Luginsland (NumerEx). Projects: Renormalization group as a numerical tool in plasma physics. Use RG to develop particle methods that can span a much large range of densities. (Part of an AFOSR-STTR)
- Keith Promislow (Department of Mathematics, Michigan State University). Projects: Renormalization group as a numerical tool in plasma physics. Use RG to identify analytic metric to identify if a plasma may be treated using a fluid approximation or if it must be modeled kinetically. (Part of an AFOSR-STTR)
- Georg Raithel (Department of Physics, University of Michigan). Project: Simulation of an apparatus designed to generate a continuous Bose–Einstein condensate.
- James Rossmann (Department of Mathematics, University of Wisconsin). Project: Development and validation of simplified models for flows in thin channels.

- Mark Sussman (Department of Mathematics, Florida State University): Simulation of droplet formation in electrostatic fluids.
- Peter Smereka (Department of Mathematics, University of Michigan): Project: Development and validation of simplified models for flows in thin channels.
- John Verboncoeur (Department of Nuclear Engineering, University of California-Berkley). Project: Comparison and validation of grid-free plasma simulations methods with mesh based approaches, e.g., virtual cathode and Penning trap simulations,

Post Doc Collaborators

- Current:
 - Benjamin Ong (Post Doc. - Department of Mathematics-MSU): Dr. Ong and I are collaborating on high order time stepping methods and the development fast summation methods for the integral form of Maxwells equations with moving point charges (**Work was/is supported by a grant from AFOSR-YIP**)
- Former:
 - Lyudmyla Barannyk (Assistant Professor - Department of Mathematics, University of Idaho): Dr. Barannyk collaborated with me on the development of reduced phase space models for plasma species near a known distribution. (**Work was supported by contract AFRL**)
 - Jing-Mei Qiu (Assistant Professor - Department of Mathematics, Colorado School of Mines): Dr. Qiu and I have collaborated, and continue to collaborate, on high order time stepping methods and the development of high order semi-Lagrangian solvers based on WENO. (**Work was/is supported by grants from AFOSR-YIP and NSF**)

Graduate Student Collaborators

- Current:
 - **Advisor: Lee VanGroningen**, PhD Student in Mathematics (Spring 2008-Present). Thesis Topic: Undecided, currently working on *Multi-Scale fluid models using implicit limiters in a Krylov Deferred Correction Framework*. I have started working with Mr. VanGroningen, meeting and discussing the extension of Krylov Deferred Correction by making use of high order corrections inside of the Deferred Correction Framework. Further, we are discussing how to formulate the limiters as an algebraic constraint, so that one might apply KDC to fluid simulations which develop shocks. An accurate implicit fluid solvers would be a critical advance in the simulation of temporal multi-scale plasma involving multi-species models.
 - **Advisor: David Lawlor**, PhD Student in Mathematics (Fall 2007-Present). Thesis Topic: *Statistical Fast Sampling Methods and the High Wave Number Problem*. Mr. Lawlor has made great progress over the past year. He has implemented and is the first to have optimized a deterministic fast sampling method that is

a derivative of the statical fast sampling methods. He has recently started looking into identifying the optimal $\log N$ points the theory predicts are needed for solving the problems on a sub-Nyquist grid.

- **Advisor: Maureen Morton**, PhD Student in Mathematics (Fall 2007-Present). Thesis Topic: *High Order Split Schemes and Integral Differed Correction*. Ms. Morton has extended the theory of Dr. Qiu, Dr. Ong and myself to both semi-implicit and implicit time stepping methods. We are currently working applying IDC to Strang split Vlasov solvers to make the method higher than 2^{nd} order in time. Ms. Morton is working with myself, Dr. Qiu and Dr. Ong. (**Work Supported by NSF**)
- Former:
 - **co-advisor** with Iain D. Boyd: **Jerry Emhoff**, PhD Aerospace Engineering (spring 2005). Thesis Title: *Simulation of Ion Optics Using Particle-In-Cell and Treecode Methods*. I advised Jerry regarding the development of grid-free plasma simulations for ion optics. Dr. Emhoff is now a research scientist at Johns Hopkins University Applied Physics Laboratory (APL) working on thruster design.
 - **co-advisor** with Iain D. Boyd: **Anton VanderWyst**, PhD Aerospace Engineering (spring 2006). Thesis Topic: Modeling the probability distribution function of droplet size for a field emission electric propulsion system. I advised Anton regarding the modeling and simulation of a free surface in electrostatic fluids. Dr. VanderWyst is now a research scientist at Raytheon (classified work).
 - **co-advisor** with Georg Raithel: **Spencer Olson**, PhD Physics (spring 2006). Thesis Topic: Numerical and experimental studies of novel techniques for the generation of a continuous Bose-Einstein condensate. I advised Spencer regarding the development of mesh-free Monte Carlo methods for rarefied gas flows. Dr. Olson is now a a research scientist AFRL-Kirtland RDHE working on our Gridless DSMC method.

Undergraduate Student Collaborators

- Current:
 - none
- Former:
 - Supervisor: **Benjamin Loseth**, Math/Physics, Professorial Assistant 2007-08. Project Title: *Numerical Methods and Dynamics Systems* Currently working with me on modeling point vortex interaction.
 - **co-supervisor** with Robert Krasny: **Benjamin E. Sondag**. Ben is a dual Math and Physic major. I advised Ben on the the development of point insertion methods for Lagrangian simulations of the Vlasov equation. (**Undergraduate research supported by AFOSR grant F012457**) Now a PhD Student in Applied Mathematics at Princeton.