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14. ABSTRACT
January 2011:
During this quarter, NumerEx and its associated research institutions worked on
1. Consideration of the EMPIC numerical grid heating problem from the point of view of renormalization group analysis. This work included a literature survey and presentations at conferences at the University of Wisconsin and Stanford (Caflisch, UCLA).
2. An analysis of the effect of the Coulombic collision operator on a bump on the tail of a Maxwellian distribution and its application to stabilization of cathode flicker. This work included a draft manuscript on the 1-d evolution of bump, and another on non-adiabatic evolution via extremal statistics of stochastic ODE¿s (Promislow, MSU).
3. Formulation of a geometric optics approach to the perturbation analysis of the Child-Langmuir-Jaffe virtual cathode problem. A manuscript was begun on this approach, and another on the stable and unstable modes of this problem (Caflisch, UCLA).

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(STTR PHASE II) “DEVELOPMENT OF A RENORMALIZATION GROUP APPROACH TO MULTI-SCALE PLASMA PHYSICS COMPUTATION”

by

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to

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Small Business Technology Transfer (STTR) Program
Proposal Cover Sheet

				Date Submitted:	
Proposal Number: F2-4459		**Agency:**	**Air Force**	DUNS:	612410605
Phase I Proposal Number:	**F074-022-0286**			CAGE:	0XLG7
Topic Number:	**AF07-T022**	Command:	AFO		
Proposal Title:	Development of a Renormalization Group Approach to Multi-Scale Plasma Physics Computation				

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Percentage of work: 40 %	

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Percentage of work: 40 %	

Proposed Cost:	367172	Phase: II		Duration:	12

Business Certification: (Check all that apply)

Are you a small business as described in paragraph 2.3 (note: wholly owned subsidiaries are not eligible)?	**YES**
Number of employees including all affiliates (average for preceding 12 months):	**12**
Is the INSTITUTION a research institute as defined in section 2.4? paragraph 2.4?	**YES**
University	
Are you a socially or economically disadvantaged business as defined in paragraph 2.5 ?	**NO**
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Are you a certified HUBZone small business concern as described in paragraph 2.12 ?	**NO**
Are you a service-disabled veteran-owned small business as described in paragraph 2.13 ?	**NO**
Are you a veteran-owned small business as described in paragraph 2.14 ?	**NO**
Is more than 50 percent of your firm owned or managed by a corporate entity?	**NO**
Are you proposing to use foreign nationals as defined in paragraph 2.18 for work under the proposed effort?	**NO**
Is primary employment of the principal investigator (identified below) with your firm as described in paragraph 1.3?	**YES**
Is a Historically Black College or University or Minority Institution (HBCU/MI) participating in this effort as a teaming partner or subcontractor?	**NO**
If yes, name of HBCU/MI:	
Has a proposal for essentially equivalent work been submitted to other US government agencies or DoD components?	**NO**

If yes, list the name(s) of the agency or component and Topic Number in the space below.

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Technical Abstract (Limit your abstract to 200 words with no classified or proprietary information)

NumerEx/UCLA propose advanced theoretical and computational research in the application of the renormalization group (RG) to speed the development of advanced methods to simulate dense plasmas exhibiting critical kinetic phenomena. These dense plasmas combine a wealth of length and time scales by virtue of their high plasma frequencies and short Debye lengths, while still requiring long length/time scale simulation due to the large size of plasma, and the evolution of the critical system physics. Starting with an analytic approach to a fundamental plasma process, namely that of electrostatic shielding, we will demonstrate how short length scale behavior can be incorporated in coarse representations. This naturally leads to a numerical weighting approach that can be used in conjunction with kinetic methods to systematically handle dense plasmas in a kinetic framework. Additionally, we propose extending temporal renormalization group methods to investigate the role of the collision operator in dense plasma situations. This complements our spatial RG approach by suggesting the means to ensure the fidelity of multi-scale numerical methods dynamically. These two approaches will be combined to provide for a multi-dimensional plasma physics tool based on RG methods.

Anticipated Benefits/Potential Commercial Applications of the Research or Development. (No classified or proprietary information)

Renormalization Group (RG) methods will dramatically increase the capability to accurately and efficiently model multi-scale phenomena in plasma physics. A wide range of devices from directed energy sources of electromagnetic energy, spacecraft thrusters, plasma processing devices, to fusion reactors all exhibit behavior where short length/time scale events influence the system-level performance of the device. RG-based modeling tools naturally capture multi-scale physics, leading to both improved modeling codes and novel high technology devices. Potential applications include first-principles modeling software based on RG methods for fundamental research, parametric tools with well-characterized domains of application to aid the development of plasma-based technology, and engineering services leading to improved experimental hardware in the fusion science, directed energy, and thruster arenas.

List a maximum of 8 Key Words or phrases, separated by commas, that describe the Project.

Renormalization group, plasma physics, multi-scale computation, kinetic methods, dense plasmas, Debye shielding

Summary

NumerEx and the University of California at Los Angeles are pleased to propose advanced theoretical and computational research in the application of the renormalization group (RG) to speed the development of advanced methods to simulate *dense plasmas exhibiting critical kinetic phenomena*. These dense plasmas combine a wealth of length and time scales by virtue of their high plasma frequencies and short Debye lengths, while still requiring long length/time scale simulation techniques due to the large size of plasma, and the evolution of the critical system physics. Building on our Phase I STTR successes, we will show how the renormalization group provides rigorous separation of physical phenomena based on their length/time scales. Starting with an analytic approach to a fundamental plasma process, namely that of electrostatic shielding, we will demonstrate how short length scale behavior can be incorporated in coarse representations. This naturally leads to a numerical approach that can be used in conjunction with kinetic methods to systematically handle dense plasmas in a kinetic framework, where numerical issues like grid heating typically harm fidelity. Additionally, we propose extending the temporal renormalization group methods to investigate the role of the collision operator in dense plasma situations. This complements our spatial RG approach by suggesting the means to track the fidelity of a numerical method dynamically, where the temporal RG allows re-projection of the physics onto a manifold with sufficient accuracy to model critical kinetic behavior. These two approaches will be combined to provide for a multi-dimensional plasma physics code based on RG methods. Perhaps even more important, the team has shown, through its Phase I effort, that in addition to numerical algorithms, RG provides a systematic means to develop multi-scale test problems for verification and validation of these advanced algorithms and provide sensible re-scaling techniques to enhance the usefulness and fidelity of existing legacy techniques.

Identification and Significance of Problem or Opportunity

Technology is a critical component to the Department of Defense's efforts to safeguard national security. Advanced computation and virtual prototyping can enable and support the capability to rapidly develop novel technology to support the warfighter. Examples abound in the DoD, but include such diverse areas as computational fluid dynamics for aircraft design, multi-scale simulations of nanotubes and quantum structures, and coupled environmental weather prediction [CHIPS – The Department of the Navy Information Technology Magazine, Spring 2003]. Despite these advanced computational capabilities, however, more challenges exist. Recently, the former director of operational testing and evaluation Phillip E. Coyle [*National Defense*, p.20, May 2006] and the former director of defense research and engineering John Young [*Defense News*, p.8 29 Jan 2007] have both stated that the Department of Defense needs to do a better job of rapidly prototyping new technology and applying modeling and simulation to speed the development and deployment of high technology to the field while keeping development costs sufficiently low that they can be supported by the country.

This challenge is not unique to the Department of Defense. Virtually all science and technology efforts, in the government as well as in private industry, are realizing the role of computational science in solving challenging technical problems. While virtual prototyping has advanced via the improvement in computer hardware, as summarized by the ubiquitous Moore's Law, and the advent of parallel algorithms to take advantage of high performance computing assets, there is always a pressing need for state-of-the-art algorithm development. Perhaps nowhere is this truer than in the domain of multiple scale lengths scientific computation. Consider, for example, directed energy technology: The Air Force Office of Scientific Research and the DoD High Performance Computing Modernization Office has had on-going efforts in both hardware and software producing a state-of-the-art capability for the modeling and simulation of directed energy technology embodied in the massively parallel particle-in-cell plasma physics software ICEPIC. Particle-in-Cell combines classical time-domain electromagnetics with relativistic Newton-Lorentz force laws to provide a kinetic description of plasma, self-consistently including the nonlinear self-forces. Developed by the Air Force Research Laboratory, ICEPIC has performed a wide variety of important simulations, and by exploiting its parallel nature, researchers have been able to perform fully three-dimensional simulations with realistic timescales that approach those exhibited by laboratory devices. This has led to virtual testing and evaluation of various high power microwave concepts and devices before cutting the metal necessary for laboratory experimentation as well assistance in interpretation and understanding of laboratory phenomena. The ICEPIC effort in the directed energy arena is a case study on how experiment and simulation can work in concert to rapidly advanced high technology.

Despite these advances, however, the nature of computational physics is to demand ever-higher fidelity. Continuing with the directed energy example, there are critical quantum mechanical phenomena in the emission of electrons into the device. Since these electrons are the source of kinetic energy that is converted to high power microwaves, it is clear that this physics must be treated correctly. At the other extreme, the kinetic nature of the plasma electrons co-exists with dense plasma that forms on the boundaries of the source. This plasma is sufficiently dense that it exhibits fluid-like phenomena, despite the critical co-existence with the kinetic electrons that produce the coherent electromagnetic radiation. Attempting to break this problem into two pieces, dense plasma algorithms that handle fluid behavior with kinetic methods to study the details of phase space are fraught with difficulty. First, there is no natural way to separate these populations as they intermingle in space and time. Second, the questions of fidelity and consistency between algorithms require strict test problems for verification and validation. Even brute force approaches, such as using high performance computing assets to simulate the fluid phenomena with kinetic methods leads to numerical artifacts, such as grid heating, due to the mismatch between physics and algorithm. These challenges drive the scientist to ever more complex discretizations that eventually overwhelm even massively parallel supercomputers.

Luckily, however, there are a variety of advances leading to true multiple scale methods. One of the most promising is the renormalization group (RG). RG methods constitute a broad class of techniques that explicitly find the important scales that exist in a problem. With this identification of scale, high fidelity analytic test problems, novel numerical methods, and fresh sets of equations suddenly become feasible. As we will show in this proposal, UCLA and NumerEx, with the strong assistance of our subcontractors, have assembled a team of highly trained experts in plasma physics, applied mathematics, numerical methods, and software engineering to exploit the renormalization group for the simulation of *kinetic dense plasmas*, where we must explicitly treat both discrete and continuum physics in a self-consistent manner. RG provides the means to develop both high fidelity and fast methods for simulations of these challenging problems. But most importantly to our minds, the RG technique allows for explicit inclusion of kinetic effects in fluid algorithms, correction for dense plasma shielding in legacy kinetic methods, and the clear plus rigorous means to understand the impact of the approximations introduced by numerical and analytic techniques.

The NumerEx/UCLA team builds on a successful Phase I STTR effort. Herein, we show the advances that RG provides for the solution of discrete effects in continuum descriptions, verification and validation of these solutions, potential savings in simulation costs associated with understand these solutions, and algorithmic enhancements to legacy PIC models to better handle dense plasma effects. Further, we will show the potential of the TRG framework as a numerical tool for rigorously determining when a plasma can be treated as a fluid and when it must be treated as something more complex. This will eventually lead to hybrid codes where the minimal description of the distribution function is employed, i.e., if the distribution is primarily Maxwellian, it would be treated as a fluid model. These examples will show our conviction that RG-based plasma simulation tools offer new analytic methods, new computational methods, and new tools for verification and validation in the study of plasmas exhibiting multiple scales.

Phase II Technical Objectives

We have four broad goals for this Phase II STTR, all of which are tied to improving the simulation of dense plasmas that still require some description of the plasmas' phase space for accurate reproduction of natural phenomena. These four goals offer an interlocking plan of attack to reach a full featured, multi-dimensional plasma code that can model dense kinetic plasmas with either higher accuracy or faster computation times than legacy particle-in-cell methods while maintaining aggressive verification and validation of the multiple scale physics. The team feels that this last point is a critical advance that RG provides over alternative options to capture this wide range of physics. Our Phase II goals are:

- Develop better test problems – Building on our Phase I work on the Debye problem, incorporate testing for multi-scale effects into our algorithms
- Develop methods for better coupling between continuum and kinetic descriptions, including the effects of fluctuations – Use RG to provide kinetic information to fluid descriptions and vice-versa
- Develop better algorithms – Using a RG approach, we look to provide the capability to simulate dense plasmas by incorporating physical knowledge of the Debye length into numerical particle weighting schemes
- Develop novel equations – Use RG to link Boltzmann style approach to continuum via better collision operators

These goals build on our Phase I efforts. The first two goals show that our approach to RG is designed to be flexible and exploit problem specific information, so that we know when to use a specific technique, and when we should rely on fully kinetic models. With this choice between levels of fidelity, verification and validation is perhaps *the* important question for these multi-scale models. With these problem-specific examples, we generalize to numerical algorithms with flexibility to handle a more wide-ranging plasma via control of (a) the particle weighting or "shape" in a kinetic context, resulting in macro-particles having higher information content, and (b) the collision operator to directly provide coupling between discrete and continuum scales via on-going assessment of the quality of the solution for a given RG scale.

Phase II Work Plan

To achieve these technical goals, we propose a set of technical tasks. The level of effort for this STTR program is $750,000.00 dollars over a two-year period of performance. The details of this effort are presented in our budget. To place the work plan in context, we start with some background on the renormalization group and our results from Phase I. The work plan follows directly after this description.

Renormalization Group for Plasma Dynamics

Multiple length and time scales as well as multiple physics are present in many plasma problems, and they present a formidable challenge to simulation of plasma dynamics. Examples include kinetic scales associated with particle velocities and collisions, continuum scales from fluid dynamic phenomena and fluid-particle interaction scales as in Landau damping. Each of these different phenomena can produce small scale fluctuations that are difficult to effectively simulate in a full scale computation, typically because of the conflicting requirements of fine resolution of the scales while simultaneous studying a sufficiently large problem to capture the long wavelength phenomena. A primary goal of this proposal is the development of Renormalization Group (RG) methods and a connection between RG and computations, as a method for robust treatment of fluctuations in plasmas.

RG is a method for describing the coarse-grained effect of small scale fluctuations. It goes beyond traditional perturbation expansion methods in that it allows for a continuum of length scales with no clear separation between macroscopic and microscopic scales. For plasma dynamics, RG has been used by Chang [T. Chang, S.W.Y. Tan and C.C. Wu "Complexity induced anisotropic bimodal intermittent turbulence in space plasmas" Phys. Plasmas. 11 (2004) 1287-1299.] to describe phenomena such as the scaling of the power spectrum in turbulent space plasmas, and by Nevins [W.M. Nevins et. al., "Discrete particle noise in PIC simulations of plasma micro-turbulence" Phys. Plasmas. 12(2005) 122305] to study the impact of turbulence in large-scale fusion plasmas.

As described in the Technical Objectives section, we are developing RG for plasmas dynamics through new application of RG to problems of scientific and technological importance, use of RG to derive new plasma kinetic models and development of computational strategies that incorporate RG. As an example consider the quasi-neutral shield distance, in plasmas, namely the Debye length. Under ongoing support from Phase 1, we have successfully applied RG to the Debye problem and connected that approach to a particle-in-cell computational method, found a solution method for small-scale fluctuations in the cathode flicker problem, and developed a strategy for using RG to derive better continuum equations that incorporate kinetic effects.

RG for the Debye Problem

Debye shielding is a basic phenomena of great importance for electromagnetic systems, including plasmas. Whereas the original derivation of Debye was based on a continuum description, RG has been used for determination of the Debye length from more basic physics, including quantum field and statistical mechanics effects. In the spirit of the original derivation by Debye, we have used a classical continuum description and applied RG to describe the influence of continuum fluctuations on the Debye length. In our analysis, the source of fluctuations has been the background ion density or the electron temperature. To the best of our knowledge, this is the first analysis of these effects. We also plan to generalize this to include kinetic fluctuations. When considered for a computational perspective, this problem is especially challenging as we include short wavelengths in our analysis that require fine resolution while considering a problem where the shielding exists on a macroscopic level.

We have developed two approaches to RG for the Debye problem to show the flexibility of the methods. The first approach is an interpretation of the classic method of Ma and Mazenko in terms of the Chapman-Enskog expansion. The results that are described in the following are written with more detail in our technical report [RE. Caflisch, A. Christlieb, J. Luginsland and D. Vvedensky. "Renormalization Group for the Debye Problem" UCLA CAM Report.].

The Debye problem describes the electrostatic potential φ due to a fixed test particle at $x=0$ surrounded by a uniform background of ions and electrons. The ions are assumed to have unit charge q. Because of their relatively large mass, they are also assumed to have a fixed density n_i. The electrons have charge $-q$ and density that varies as $n_e e^{q\varphi/kT_e}$. The potential satisfies the equation

$$\nabla^2\varphi = (q/\varepsilon_0)(\delta(x) + n_e e^{q\varphi/k_B T_e} - n_i) \tag{1}$$

in which ε_0 is the permittivity of free space.

We wish to derive the Debye length λ and its dependence on fluctuations ξ in T_e^{-1} and ζ in n_i (we have also considered fluctuations in the electron temperature, but we omit it here for brevity). Assume that

$$n_i = n_e + \zeta$$

in which n_e is constant. The noise satisfies

$$\langle \zeta \rangle = 0 \tag{2}$$

$$\begin{gathered}\langle \zeta(k)\zeta(k') \rangle = \sigma_{\zeta\zeta}(k)\delta_{kk'} \\ \sigma_{\zeta\zeta}(k) = \bar{\sigma}_{\zeta\zeta}k^{-n}\end{gathered} \tag{3}$$

We keep only constant, linear and quadratic terms in φ. This yields

$$\nabla^2\varphi = \lambda^{-2}\varphi + \alpha\delta + \beta\zeta + \gamma\varphi^2 \tag{4}$$

in which $\alpha = (q/\varepsilon_0)$

$$\begin{gathered}\lambda^{-2} = \lambda_D^{-2} = n_\varepsilon q^2(\varepsilon_0 k_B \bar{T}_e)^{-1} \\ \beta = -(q/\varepsilon_0) \\ \gamma = \frac{1}{2}q^3(n_e/\varepsilon_0)(k_B\bar{T}_e)^{-2}\end{gathered} \tag{5}$$

in which λ_D is the usual Debye length of classical plasma physics. Denote

$$\begin{gathered}L = \nabla^2 - \lambda^{-2} \\ G_0 = L^{-1} \\ \varphi_0 = G_0(\alpha\delta + \beta\zeta).\end{gathered} \tag{6}$$

The equation for φ is

$$\varphi = \varphi_0 + G_0(\gamma\varphi^2) \tag{7}$$

In the absence fluctuations and nonlinearities (i.e., $\beta = \gamma = \kappa = 0$), we recover the traditional solution of $\varphi = r^{-1}e^{-r/\lambda}$. The goal is to use renormalization group to find the effects of fluctuations on the Debye length λ.

Our renormalization group analysis follows the method of Ma & Mazenko [S.K. Ma and G.F Mazenko "Critical dynamics of ferromagnets in 6-ε dimensions: General discussion and detailed calculation" Phys. Rev. B 11 (1975) 4077-4100.]. It works in Fourier wavenumber variable k and consists of several steps. First we divide the potential φ into high and low wavenumbers

$\varphi^{>} = \varphi$ for wavenumbers k with Λ/b<|k|<Λ

$\varphi^{<} = \varphi$ for wavenumbers k with |k|<Λ/b.

corresponding to a cutoff Λ. The equations for $\varphi^{>}$ and $\varphi^{<}$ are

$$\varphi^{>} = \varphi_0^{>} + \gamma G_0^{>}(\varphi^{>2} + 2\varphi^{<}\varphi^{>} + \varphi^{<2}) \tag{8}$$

$$\varphi^{<} = \varphi_0^{<} + \gamma G_0^{<}(\varphi^{>2} + 2\varphi^{2}\varphi^{>} + \varphi^{<2}). \tag{9}$$

We solve for the high wavenumber component $\varphi^{>}$ as a function of the low wavenumber component $\varphi^{<}$, using an expansion for $\varphi^{>}$ in powers of the parameters α, β, and γ without expansion of $\varphi^{<}$. Then we expand the equation for $\varphi^{<}$, which results in a modification of the coefficients λ, α, β, and γ in the equation. The modifications are Fourier integrals that are easily evaluated.

This is analogous to the Chapman-Enskog expansion [S. Chapman and T.G. Cowling. *The Mathematical Theory of Nonuniform Gases*. Cambridge. 1952.] for the nonlinear Boltzmann equation of rarefied gas dynamics, in which the non-hydrodynamic modes are solved by an expansion method, then the hydrodynamic modes are found by an expansion of the equations for them. This yields the Euler equations at leading order and Navier-Stokes at the next order.

The second step is to rescale the low wavenumber component $\varphi^{<}$ to a full function φ, based on the assumption of self-similarity. The resulting rescaled coefficients λ', α', β', and γ' are the image of the renormalization group action on the original coefficients λ, α, β, and γ. This group action is the discretization of a "flow" with respect to a variable ℓ that can be thought of as a length scale. The resulting flow has the form

$$\frac{d}{d\ell}(\lambda,\alpha,\beta,\gamma) = F(\lambda,\alpha,\beta,\gamma).$$

Fixed points at which F=0 are of primary interest. If the exponent n for decay of the power spectrum of the noise ζ is less than ½ we find a fixed point (λ_0, α_0, β_0, γ_0) with

$$\begin{aligned}\lambda_0 &= c(n)\Lambda^{-1} \\ \alpha_0 &= 0\end{aligned}.$$

Moreover the renormalized charge α approaches 0 at an exponential rate

$$\alpha \cong \bar{\alpha}e^{-a(n)\ell}.$$

Since $\lambda_0 > \lambda_D$, we find that the Debye length increases through the RG flow with fluctuations. The decrease in the renormalized charge is a second mechanism for impact of spatial noise on the plasma screening with the interpretation that the charge must be reduced to hold at a constant screening distance.

In addition to fixed points, the values away from fixed points may be applicable to systems with a specific length scale, as would be found in a numerical simulation. As part of Phase II, we will connect the length scale of a simulation problem to the RG results at that length scale, as determined through the solution of the RG flow equation. Further details for the solution described above can be found in [Caflisch et. al. "…Debye Problem." *ibid*.].

Computational Verification of the RG approach

In the interests of verification and validation, we developed a three-dimensional first-principles particle-in-cell model of the Debye shielding of a test particle with spatial fluctuations in the ion background. This is a challenging computational problem as it combines short wavelength noise in a large problem. For the simulations, we chose to initialize a baseline plasma with a temperature of 0.2 eV and 2 x 10^6 cm^{-3} density, resulting in 0.235cm Debye length. Our simulations were of a 2 cm cube with periodic boundary conditions to provide enough space for significant shielding to be exhibited. To avoid numerical grid heating associated with aliasing [A. Christlieb, and K. Cartwright, "Boundary Integral Corrected Particle-in-Cell, APS-DPP meeting 2007], our simulation had one millions cells and 8 million macroparticles. The Debye length was measured using curve fitting of the analytic Debye formulation and a novel use of a complex Fast Fourier Transform (FFT) to capture the damping due to shielding. Both methods compared well with the expected analytic Debye length in the absence of spatial ion noise, with the complex FFT offering more robustness in the face of the numerical particle noise. To our knowledge, this use of a complex FFT for measuring Debye length was a first in the literature.

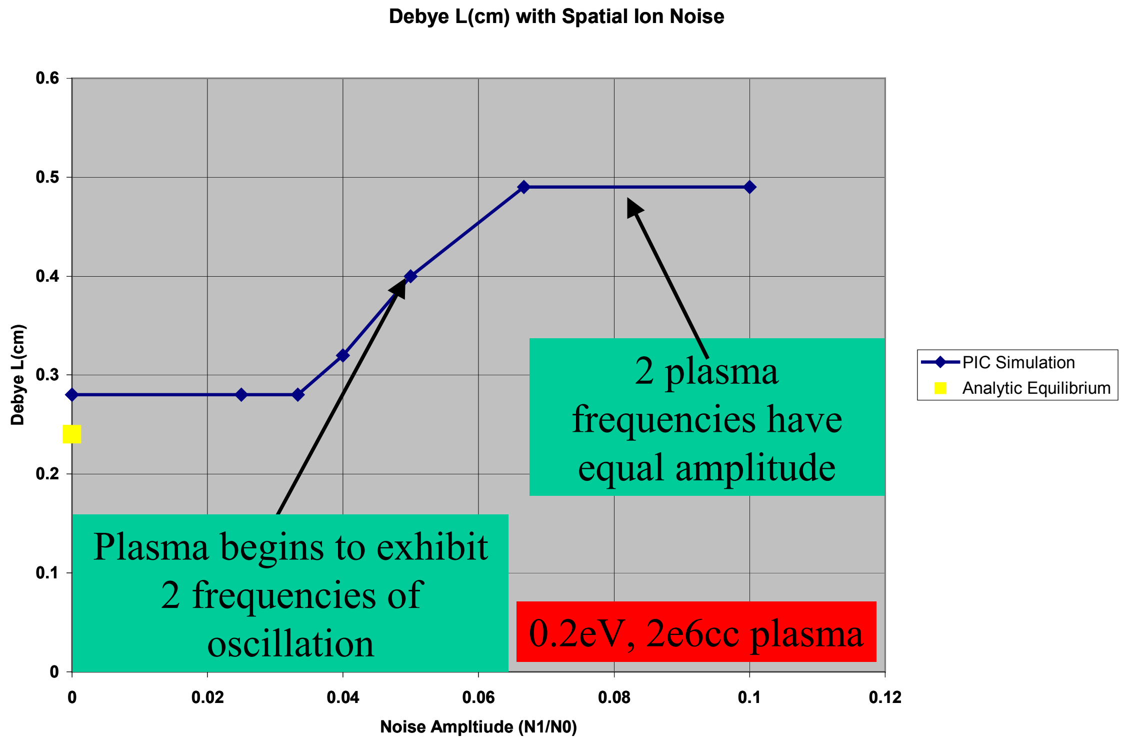

Figure 1. Dependence of Debye length on spatial ion noise.

Next, we systematically varied amplitude of the ionic spatial fluctuations and the nature of the fluctuation's power spectrum. As shown in Figure 1, as the fluctuation amplitude increased, the shielding distance also increased in agreement with the RG theory presented above. Furthermore, RG correctly predicted the details of the noise spectrum under which the fixed point would disappear. When the spectrum fall-off in wavenumber k was modified to an exponent greater than ½, we observed a transition from quiescent plasma to time dependent structures as the plasma struggled to shield both the test particle and the spatial ion density non-uniformity. In both the high amplitude and critical spectrum cases, the plasma could be kept in a quiescent state by reducing the charge on the test particle, in agreement with the rescaling of test particle charge suggested by the RG solution. Thus, by re-scaling the test particle charge in a manner consistent with the RG solution, it is possible to construct a less computationally expensive simulation.

Functional Integral Formulation of Debye Screening

During the course of the numerical validation effort, it became clear that transition to numerical methods based on RG techniques required the inclusion of boundary conditions and grid effects. A functional integral approach shows how to include both finite grid size and the impact of periodic boundary conditions through the introduction of "cutoff" depending on the scales in the problem. This offers a toolkit to study the Debye problem as well as computational implementations thereof. Here, we present a flavor of these methods for comparison to the previous formulation of the Debye shielding. Both methods provide identical analytic solutions to the Debye problem.

Lattice Formulation

We begin by considering a d-dimensional Cartesian lattice whose lattice spacing is a and with a total volume of V. Charges $\pm e$ can occupy the sites i_k of this lattice and there is a Coulomb interaction between these charges. For $d = 3$, the lattice Coulomb potential between sites i and j is

$$U_{ij} = \frac{1}{4\pi a\,|i-j|}. \qquad (10)$$

There are two main reasons for putting the system on a lattice. First, the lattice avoids the singularity of the Coulomb potential at the origin, which would otherwise necessitate introducing a short-range cut-off. This issue will arise when we take the continuum limit, but for the moment there are no short-range singularities. The other advantage of a lattice formulation is that we can develop a field-theoretic formulation for the partition function in close analogy with that for the Ising model, which facilitates the identification of mean-field limits and perturbations thereof. The canonical partition function Z_N for N charges $q_k = \pm e$ at positions i_k, for $k = 1,\dots,N$, is

$$Z_N = \sum_{\substack{\{i_k\}\\ \{q_k=\pm e\}}} \frac{1}{N!}\exp\left[-\frac{\beta}{2}\sum_{\substack{j,k\\ 1\le j,k\le N}}{}' q_j U(i_j,i_k) q_k\right], \qquad (11)$$

where the factor $N!$ is to ensure correct Boltzmann counting, $\beta = 1/k_B T$, k_B is Boltzmann's constant, T is the absolute temperature, the prime on the summation indicates that the terms $j = k$ are excluded, and the factor of $\frac{1}{2}$ is to avoid double counting. The associated grand canonical partition function Ξ is

$$\Xi = \sum_{N=0}^{\infty} z^N \mu^{Nd} Z_N, \qquad (12)$$

where $z = e^{\beta\mu}$ is fugacity and μ is the chemical potential.

The Functional Integral

The evaluation of Ξ proceeds by using the Hubbard–Stratonovich transformation. After several standard manipulations that parallel those of the Ising model, we obtain the functional integral

$$\Xi = \int \exp\{\frac{1}{2}\int[\phi\nabla^2\phi + 4z\cos(\alpha\phi)]\,dx\}D[\phi], \qquad (13)$$

with $\alpha = e/\sqrt{k_B T}$.

There are several advantages to the functional integral representation of a statistical mechanical problem over other formulations:

1. A large class of problems can be represented as functional integrals, ranging from equilibrium statistical mechanics, as the Debye problem, to non-equilibrium statistical dynamics. The Ising model serves as the canonical example for this approach, and the expression obtained in Eq. (13) has several formal similarities with the functional integral for the Ising model.
2. Mean-field limits are straightforward to identify, for example, as Gaussian field

theories, corrections to which can be evaluated with various expansions. For the case at hand, the mean-field limit corresponds to the Debye–Hückel theory. This will shown explicitly in the next section.

3. Renormalization-group calculations can be carried out using either the Wilson or field-theoretic formalism. Time-dependence, vector fields, and other degrees of freedom enter such calculations simply as summations/integrals in the evaluation of individual terms. The structure of the RG expansion is determined by the polynomial terms in the functional integral.

Mean-Field Theory

The simplest evaluation of the functional integral (13) is to expand the cosine function and retain terms only to quadratic order:

$$\cos(\alpha\phi) = 1 - \frac{(\alpha\phi)^2}{2} + \cdots, \tag{14}$$

in which case we obtain a Gaussian field theory,

$$\Xi = e^{2zV} \int \exp[\frac{1}{2}\int(\phi\nabla^2\phi - \xi^{-2}\phi^2)\,dx]D[\phi], \tag{15}$$

where V is the volume of the system and $\xi^{-2} = 2z\alpha^2$. We will neglect the constant prefactor, since we are interested only in averages. Consider now the evaluation of the two-point correlation function $\left\langle \phi(q)\phi(q^{'})\right\rangle$ which, in the limit $V \to \infty$, is calculated as

$$\begin{aligned}\left\langle \phi(q)\phi(q^{'})\right\rangle &= \tfrac{1}{\Xi}\int D\phi(k)\phi(q)\phi(q^{'})\exp[-\int_0^{\Lambda}\tfrac{dk}{(2\pi)^d}(k^2+\xi^{-2})\,|\,\phi(k)\,|^2] \\ &= \frac{\delta(q+q^{'})}{q^2+\xi^{-2}}\end{aligned} \tag{16}$$

Performing the Fourier transform yields

$$\left\langle \varphi(r)\varphi(0)\right\rangle = \int \frac{dq}{(2\pi)^3}\frac{e^{-iq\cdot r}}{q^2+\xi^{-2}} = \frac{e^{-r/\xi}}{4\pi r}. \tag{17}$$

The quantity

$$\xi = (\frac{k_B T}{n_0 e^2})^{1/2}, \tag{18}$$

is the Debye length.

Summary of the RG Approach to the Debye Problem

Our RG calculation accurately predicted the details of the simulations. Indeed, the accurate resolution of the ion noise was crucial to getting the correct physics. Considered from another perspective, this illustrates all aspects of our proposed use of RG – (1) develop new test problems to study multi-scale physics, (2) rescale existing calculation in light of RG theory to operate at reduced resolution, and (3) suggest that controlled rescaling of the test charge offers a means to include the physics of one scale in a coarser description.

Next we change gears and describe our other main result from Phase I, which again studies the coupling of fine scales into long wavelength phenomena in the context of space-charge limited flow – another traditional plasma physics phenomenon.

Cathode Flicker Problem

Through a clever solution of the stationary continuum equations for electron flux in a confined channel, Child [C.D. Child, “Discharge from Hot CAO" *Phys. Rev. Series I*, 32 (1911) 492-511] and Langmuir [I. Langmuir, “The effect of space charge and residual gases on thermionic currents in high vacuum" *Phys. Rev.*, 2 (1913) 450 - 486] found an expression for the maximal current between a cathode and anode for electrons having zero velocity as they leave the cathode. Jaffe [G. Jaffé, “On the currents carried by electrons of uniform initial velocity" *Phys. Rev.*, 65 (1944) 91-98] generalized their solution to allow for a nonzero electron velocity. Cathode flicker, i.e., temporal fluctuations in the electrons as they leave the cathode, has proved to be a difficult and important problem [D. Shiffler et. al., “Emission uniformity and shot-to-shot variation in cold field emission cathodes.” IEEE Trans. Plas. Sci., 32(2004) 1262-1266] that has defied definitive analytic treatment. We model the cathode flicker as temporal fluctuations in the electron velocity at the cathode, with the electron density held fixed at the cathode and the electrostatic potential held fixed at both cathode and anode. The results that are described in the following are written with more detail in our technical report [RE. Caflisch, J. Devita, X. Yu, A. Christlieb and J. Luginsland. “WKB Solution for the Cathode Flicker Problem” UCLA CAM Report].

The one-dimensional continuum equations for the flux of electrons from a cathode at x_0 to an anode at x_1 are

$$\begin{aligned} \rho_t + (\rho v)_x &= 0 \\ v_t + v v_x &= -\frac{q}{m}\varphi_x \\ \varphi_{xx} &= -\varepsilon_0^{-1}\rho \end{aligned} \tag{19}$$

in which ρ is the electron density, v is the electron velocity and φ is the electrostatic potential. Also q and m are the electron charge and mass and ε_0 is the free space electrical permittivity. The boundary conditions at the ends of the channel are

$$\left.\begin{aligned} \varphi &= \varphi_0(2) \\ v &= v_0(3) \\ \rho &= \rho_0 \end{aligned}\right\} \text{on} x = x_0 \tag{20}$$

$$\varphi = \varphi_1 \text{on} x = x_1 \tag{21}$$

We denote the Child-Langmuir-Jaffé solution as $(\rho, v, \varphi) = (\bar{\rho}, \bar{v}, \bar{\varphi})(x)$, and look for solutions of the form $(\rho, v, \varphi) = (\bar{\rho}, \bar{v}, \bar{\varphi}) + (\rho', v', \varphi')$ with ρ', v' and φ' solving the linearized equations

$$\begin{aligned} \rho'_t + (\bar{v}\rho' + \bar{\rho}v')_x &= 0 \\ v'_t + \bar{v}v'_x + \bar{v}_x v' &= -\frac{q}{m}\varphi'_x \\ \varphi'_{xx} &= -\varepsilon_0^{-1}\rho' \end{aligned} \tag{22}$$

We look for solutions in the WKB form $(\rho', v', \varphi') = (R, U, \Phi)e^{i\theta/\varepsilon}$ in which R,U, Φ, θ are functions of (x,t) and $\varepsilon \ll 1$. We find two WKB solutions, the first is a convective solution in which $\theta = \theta^c$ is carried with the fluid velocity (i.e., $\theta_t + \bar{u}\theta_x = 0$) and $(R, U, \Phi) = (R^c, \varepsilon U_1^c, \varepsilon^2 \Phi_2^c)$. In this solution, the values of R^c, U^c and θ^c (i.e., fluctuating values of ρ and v) can be specified on the cathode $x = x_0$.

The second WKB solution type is an edge solution in which $\theta_x = 0$. There are two such solutions associated with the left and right boundaries, denoted by $(\theta, R, U, \Phi) = (\theta^\ell, \varepsilon^2 R_2^\ell, \varepsilon U_1^\ell, \Phi^\ell)$ and $(\theta, R, U, \Phi) = (\theta^r, \varepsilon^2 R_2^r, \varepsilon U_1^r, \Phi^r)$. In these solutions, the values of R^ℓ, U^ℓ and θ^ℓ can be specified on the left boundary and the values of R^r, U^r and θ^r can be specified on the right boundary.

Denote the corresponding fluctuating WKB solutions as $(\rho^c, v^c, \varphi^c) = (R^c, U^c, \Phi^c)e^{i\theta^c/\varepsilon}$ with similar definitions for the right and left solutions with superscript ℓ and r. Then a fluctuating solution that has specified fluctuations in v on the left boundary with no fluctuations in ρ on the left boundary or in φ on either boundary, can be written in the form

$$(\rho', v', \varphi') = (\rho^c, v^c, \varphi^c) + (\rho^\ell, v^\ell, \varphi^\ell) + (\rho^r, v^r, \varphi^r).$$

More generally the method could be adapted to produce a solution with specified fluctuations in all of these boundary values. Further details for the solution described above can be found in [Caflisch et. al. "WKB Solution…", *ibid.*].

Next we plan to perform numerical computation for slowly varying coefficients in the WKB solutions. We will also extend the WKB solution to higher order in ε, at which resonance and secular terms will enter and may affect the maximal current that can flow through the channel. We believe that solution presented above is an essential ingredient in an RG analysis of the cathode flicker problem. It will provide a solution for the rapidly fluctuating modes in terms of the slowly fluctuating modes, which is the first step in an RG analysis. Furthermore, cathode flicker is the basis of our verification/validation efforts in the extensions to temporal RG, which play a critical role in the development of numerical methods for more general plasma problems. This will be discussed further in the tasks below.

Proposed Work for Phase II

The research completed so far in Phase I has demonstrated the viability and potential of RG methods in plasma physics. We have used RG to investigate physical phenomena and we have developed strategies for applying RG in the derivation of new multi-scale models and as a guide to simulation for complex phenomena. In Phase II, we propose to continue and extend these investigations and further develop RG for numerical modeling and simulation.

Task 1 - Applications of RG: The Debye and Cathode Flicker Problems

For the cathode flicker problem, we propose to use the WKB solution as a method for finding the rapid fluctuations in terms of the slow fluctuations. The WKB solution will play the role of the Green's function in the description of RG for the Debye problem. This is an essential first step in the RG method. We also plan to investigate the possibilities of resonance and secularity, as described above, in the solution. The result may have important effects on the maximal current. We also plan to extend the WKB solution to multi spatial dimensions, so that the texture of the cathode surface can be included in the model.

For both the Debye and cathode flicker problems, we plan to incorporate fluctuations due to kinetic effects into the RG analysis. This application requires a choice of the relevant RG map. One choice would be to use a Fourier basis in physical space and Hermite function basis in velocity. Another possibility would be to use waves in phase space as the primary solution modes, which would correspond to Fourier variables for both physical and velocity space.

This effort helps achieves the first technical goal of this effort by developing well-characterized solutions to problems with important physics at multiple scales. It also furthers the second technical goal by providing detailed information about how various scales communicate in these plasma problems.

Task 2 – Computational validation of RG-inspired methods for Debye and Flicker

Using an approach similar to that demonstrated in Phase I, we will use kinetic particle-in-cell methods, operating at high resolution, to develop a traditional kinetic approach to these problems. This will provide insights into the application of RG in plasmas, develop general coupling concepts between scales, and provide test cases to show the evolution of the critical scale due to the plasma dynamics. Tasks 1 and 2 provide the foundation of test problems for a general plasma code, as well as insight into the coupling between multiple scales. Furthermore, these efforts provide the basis for understanding how rescaling can be used to enhance legacy algorithms. These tasks support the first two technical goals.

Task 3 – Development of temporal RG for plasma physics

This task focuses on the development of new numerical methods for time-dependent plasma problems. Specifically, this effort focuses on the application of the temporal renormalization group (TRG) to problems exhibiting both continuum and discrete physics. This task directly supports the technical goals of developing better algorithms and better coupling equations. We first provide a description TRG, and then discuss how this task will develop numerical methods for plasma problems.

Temporal RG Reductions of Coherent Structure Plasma Flows

Temporal Renormalization Group (TRG) methods have recently made substantial progress in the rigorous reduction of systems of parabolic and hyperbolic PDEs to low dimensional flows associated to interacting coherent structures. We extend these methods to obtain a systematic reduction of collisional gas dynamics and ionized flows to multi-bumped Maxwellian and other quasi-equilibria solutions, substantially extending the scope and improving the accuracy of existing δf methods by employing the correct *spectral* decomposition of the flow into an adiabatic Maxwellian and kinetic portions whose evolution uncouples at leading order. This decomposition is couched in a rigorous TRG framework which provides a systematic self-check for the validity of the decomposition, indicating when the underlying quasi-equilibrium ansatz is no longer self-consistent and also when it loses stability to temporal resonance which is distinct from simple linear stability. The decomposition of the flow into thermalized and kinetic particles is amenable to a wide variety of versatile hybrid methods, which exploit efficient Monte-Carlo and Wild summation approaches. We first give a broad overview of the Temporal RG methods, and then present specific applications to the rarified gas dynamics and collisional ions flows.

Description of the Temporal RG method

Self-similarity verses Discrete spectrum

In the context of partial differential equations, renormalization group methods have successfully been applied to understand the long-time asymptotics of self-similar behavior. This is typically achieved by interweaving temporal evolution and rescaling the spatial domain. The easiest example is the self-similar nature of long term decay in the heat equation,

$$\begin{aligned} u_t &= u_{xx}, \\ u(x,1) &= u_1(x), \end{aligned}$$

on the line. This is self-similar under the natural parabolic scaling, indeed fixing $L > 1$, evolving for time $t = L^2$ and then rescaling both u and x by L yields a renormalization map

$$u_2 = R_L u_1 \equiv Lu(x/L, L^2).$$

Since the rescaled function also satisfies the heat equation in $y=x/L$ and $\tau = t/L^2$, we can naturally iterate the procedure obtaining

$$u_{k+1} = R_{L^{2k}} u_k$$

where through the Fourier Transform we easily see

$$\Im\left(R_L f\right)(k) = e^{-k^2(1-L^2)} \Im\left(f\right)\left(\frac{k}{L}\right).$$

The semigroup of the parabolic heat equation is naturally contractive, and the rescaling modifies this into a filter which extracts the Gaussian fixed point u_* with Fourier transform

$$\Im(u_*) = A_0 e^{-k^2}.$$

Undoing the rescaling shows that the long-time asymptotics of the heat equation are governed by the similarity structure of its Green's function, if the initial data converges sufficiently rapidly at spatial infinity. However, the similarity structure is somewhat special, and the framework can be made more general, and the underlying mechanisms more transparent, if one changes to similarity variables

$$\begin{aligned} \tau &= \ln(t), \\ \varsigma &= x/\sqrt{t} \end{aligned}$$

so that the heat equation becomes

$$\begin{aligned} u_\tau &= \frac{1}{2}\varsigma u_\varsigma + u_{\varsigma\varsigma}. \\ u(\varsigma,0) &= u_1(\varsigma) \end{aligned}$$

In the original variables the linear spectrum was a continuous line that touched the origin, working in an algebraically weighted norm in the similarity variables the spatial weight pushes the continuous spectrum into the left-half plane, leaving behind point spectrum located at the negative half integers

$$\left\{-\frac{1}{2}, -1, -\frac{3}{2}, \cdots\right\}.$$

The role of the rescaling is to discretize the spectra of the linear semigroup, with the salient asymptotics reducing to a spectral projection onto the eigenmodes of least decay. The

TRG approach subsumes the self-similar structure into a broader framework of identifying coherent structures whose linearization has eigenmodes compatible with its own tangent plane.

General outline of the TRG method

Given a manifold of quasi-steady equilibria, described parametrically as the graph above a reduced dimensional space, the full PDE is reduced to an adiabatic flow on the tangent plane of the manifold. Consider a manifold

$$M = \{\Phi(x;\vec{p}) \mid \vec{p} \in K\}$$

where K is a space of parameters and x represents the independent variables, and a governing equation written abstractly as

$$U_t = F(U).$$

In a neighborhood of the manifold M we decompose solutions U as

$$U(x,t) = \Phi(x,\vec{p}(t)) + W(x,t).$$

where the remainder W is small in an appropriate sense. The residual,

$$R(\vec{p}) = F(\Phi(\vec{p})),$$

engenders a drift along the tangent plane of the manifold. One key to the reduction is an analytic foliation of the phase space in a neighborhood of the manifold. The reduction is based upon the structure of the linearization of F about M. Substituting the decomposition into the flow we have the expression

$$W_t + \nabla_{\vec{p}}\Phi \cdot \vec{p}_t = F(\Phi) + L_{\vec{p}}W + N(W),$$

where $L_{\vec{p}}$ is the linearization of F about $\Phi = \Phi(\vec{p})$ and N represents terms that are quadratic or higher in W. A key assumption is that the eigenspace $Y_{\vec{p}}$ associated to the eigenvalues of $L_{\vec{p}}$ which are small or of positive real part, is approximately in agreement with the tangent plane of the manifold, spanned by the elements of

$$\nabla_{\vec{p}}\Phi.$$

Under this assumption, we define the $L_{\vec{p}}$ spectral projection $\pi_{\vec{p}}$ onto $Y_{\vec{p}}$, and have a foliation of the state space in a neighborhood of the manifold, that is each U_0 may be uniquely decomposed into a base point $\vec{p}_0$ and a spectrally orthogonal remainder W_0 satisfying

$$\pi_{\vec{p}_0} W_0 = \pi_{\vec{p}_0}\left(U_0 - \Phi\left(\vec{p}_0\right)\right) = 0$$

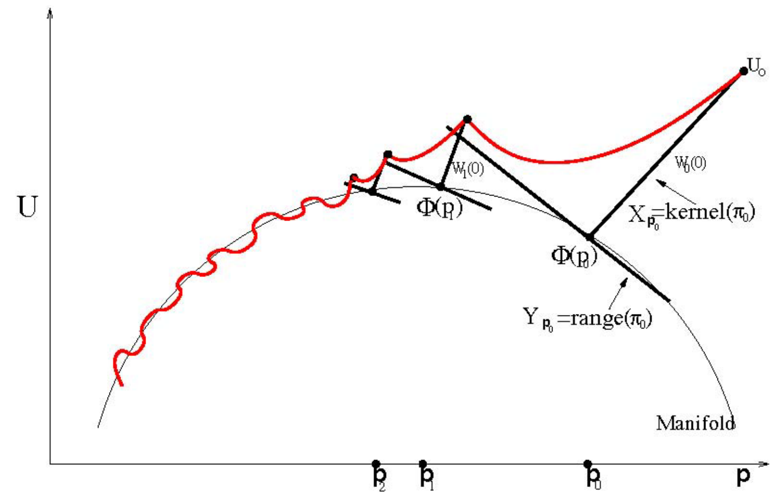

Figure 2. The adiabatic manifold *M* and the associated flow. Initial data that is sufficiently close to the manifold can be uniquely decomposed into a bare manifold coordinate and a remainder *W* that lies in the decaying space associated to the local linearization. After the manifold parameters have evolved away from the bare coordinate, the solution is renormalized, generating a new bare coordinate and associated decomposition.

Thus, given an initial data U_0 we define the bare quantity, $\vec{p}_0$, the manifold coordinate, and the associated spectral subspace $X_{\vec{p}_0}$ which is the compliment to $Y_{\vec{p}_0}$. This bare coordinate system is frozen in time and the renormalized quantities $\vec{p}(t)$ and $W(t)$ are updated so as the keep the remainder $W \in X_{\vec{p}_0}$ from diverging. We also freeze the linearized operator $L_{\vec{p}}$ at $L_{\vec{p}_0}$ and renormalize it to $\tilde{L}_{\vec{p}_0}$ in such a way that

$$S_{\vec{p}_0}(t)(I - \pi_{\vec{p}_0}(L_{\vec{p}_0} - \tilde{L}_{\vec{p}_0}))$$

is small, where $S_{\vec{p}_0}(t)$ is the linear semi-group associated to $L_{\vec{p}_0}$. This is a central step in the renormalization, exploiting the contractivity of the semigroup on certain subspaces to simplify the linearization and reduce the complexity of the projected dynamics. The evolution becomes

$$W_t + \nabla_{\vec{p}}\Phi \bullet \vec{p}_t = F(\Phi) + \tilde{L}_{\vec{p}_0}W + \left[(L_{\vec{p}} - \tilde{L}_{\vec{p}_0})W + N(W)\right]$$

and since

$$\pi_{\vec{p}_0}\tilde{L}_{\vec{p}_0}W = 0,$$

projecting the evolution onto $X_{\vec{p}_0}$ and $Y_{\vec{p}_0}$ yields an adiabatic flow on the manifold which uncouples from W at leading order,

$$\vec{p}_t = \left[\pi_{\vec{p}_0}\nabla_{\vec{p}}\Phi\right]^{-1}\pi_{\vec{p}_0}F(\Phi) + \pi_{\vec{p}_0}\left[(L_{\vec{p}} - \tilde{L}_{\vec{p}_0})W + N(W)\right],$$

and the evolution of the remainder

$$W_t = L_{\vec{p}_0}W + (I - \pi_{\vec{p}_0})\left[F(\Phi) - \nabla_{\vec{p}}\Phi \bullet \vec{p}_t + (L_{\vec{p}} - \tilde{L}_{\vec{p}_0})W + N(W)\right].$$

The secular terms, $(L_{\vec{p}} - \tilde{L}_{\vec{p}_0})$ grow slowly, and after a time Δt, dependent upon the evolution, it must be renormalized away through a reprojection. At leading order, however, the terms

$$(L_{\vec{p}} - \tilde{L}_{\vec{p}_0})W + N(W)$$

can be neglected on the right-hand side of the adiabatic evolution, which reduces to the closed form

$$\vec{p}_t = \mathbb{F}(\vec{p}) \equiv \left[\pi_{\vec{p}_0} \nabla_{\vec{p}} \Phi\right]^{-1} \pi_{\vec{p}_0} F(\Phi).$$

The evolution of the remainder can also be simplified by dropping the secular and nonlinear terms,

$$W_t = L_{\vec{p}_0} W + (I - \pi_{\vec{p}_0})\left[F(\Phi) - \nabla_{\vec{p}} \Phi \bullet \vec{p}_t\right].$$

The evolution of this equation only requires the evaluation of the full nonlinearity F on the manifold M which is typically significantly simpler than on the full system.

On the space $X_{\vec{p}_0}$, where the remainder equation lives, the linearization is asymptotically contractive, with a limiting exponential rate $\upsilon > 0$. However there can be transient growth associated with the linear evolution,

$$\left\| S_{\vec{p}_0} W_0 \right\| \le M e^{-\upsilon(t-t_0)} \left\| W_0 \right\|,$$

where M>1. A key step to prevent dynamic resonance of the temporal evolution of the adiabatic equation with the remainder equation is that

$$M e^{-\upsilon \Delta t} < 1.$$

If the adiabatic evolution is too fast, the secular transients in the remainder evolution may not die down before the renormalization point, which updates the linearized operator. In this case the putative exponential decay of the linear equation may not be achieved due to the temporal resonance. The temporal RG formulation identifies two testable criteria that insure the validity of the reduction to the adiabatic flow: the compatibility condition between the small eigenvalue eigenspace and the tangent plane of the manifold, and the dynamic resonance condition.

The temporal renormalization is enacted after the time Δt, which depends upon the rate of the evolution of the adiabatic equation, and the strength of the secular terms. The solution at time $t_1 = t_0 + \Delta t$ is reprojected, determining the renormalized bare quantity $\vec{p}_1$ and associated remainder W_1 which satisfy the nonlinear projection equation

$$W_1 \equiv \Phi(\vec{p}(t_1) + W(t_1)) - \Phi(\vec{p}_1) \in X_{\vec{p}_1}.$$

This gives a new decomposition, based upon $\pi_{\vec{p}_1}$, the associated spectral spaces $X_{\vec{p}_1}$ and $Y_{\vec{p}_1}$ and the reduced linearization $\tilde{L}_{\vec{p}_1}$. The procedure is then iterated.

Applications to Reaction Diffusion and Mixed Hyperbolic-Parabolic systems

The temporal RG procedure has been applied rigorously to systems of singularly perturbed reaction diffusion equations in the semi-strong regime, in which spatially localized pulses in a weakly diffusive component interact strongly through the nonlocalized, strongly diffusive components [Doelman, T. Kaper, K. Promislow, Nonlinear asymptotic stability of the semi-strong pulse dynamics in a regularized Gierer-Meinhardt model, *SIAM Math. Analysis* **38** (6) 1760-1787 (2007)], [P.A.C. Chang and K. Promislow, Nonlinear stability of oscillatory pulses in the parametric nonlinear Schrodinger equation, *Nonlinearity* **20** 743-763 (2007)], [R. Moore and K. Promislow, Renormalization group reduction of pulse dynamics in thermally loaded optical parametric oscillators, *Physica D* **206** 62-81 (2005), R. Moore and K. Promislow, The semi-strong limit of multipulse interaction in a thermally driven optical system, *J. Diff. Eqs*. accepted (2008)]. The resultant adiabatic flow is a family of N ordinary differential equations for the positions of the localized pulses, which change shape and speed at leading order as they evolve. Moreover the stability of the pulse configurations change as the pulses interact, leading to eigenvalues crossing into the right-half plane, violating the compatibility condition and signaling the need to augment the adiabatic manifold. These results have been extended to the case in which the essential spectrum approaches the origin, the nose of this essential spectrum is included in the space $Y_{\vec{p}}$, along with an associated extension of the adiabatic manifold, to include a dissipative tail added to the non-localized pulses. In this case the independent variables in the adiabatic flow become the localized pulse positions and a truncated description of the dissipative tail, [Doelman et al, *ibid*.].

<u>*Applications of TRG to Collisional Flows*</u>

A principal goal is the application of the temporal RG to the development of a multiscale simulation method for collisional flows of Maxwellian particles and coulomb collisions of ionized gases, combining particle and continuum approaches, adapting and extending the method developed earlier for the Flicker problem [RE. Caflisch, J. Devita, X. Yu, A. Christlieb and J. Luginsland. "WKB Solution for the Cathode Flicker Problem" UCLA CAM Report.]. In particular, we will develop criterion for the validity of reduced fluid models, giving rigorous quantization of thermalization/dethermalization rates, and extend equilibrium models to multi-Maxwellian regimes for Coulomb collisions for which thermalization rates are not uniform.

Quasi-Equilibrium reductions of Maxwellian collisions

For rarified gas dynamics and other collisional models which are governed by a Maxwellian or hard-sphere collision kernel the rates of thermalization are relatively uniform in the velocity [E. Carlen and X. Lu, Fast and Slow Convergence to Equilibrium for Maxwellian Molecules via Wild Sums**,** *Journal of Statistical Physics,* **112**, Nos. 1/2, July 2003]. Moreover, since the collision kernel is independent of the relative velocity of the particles, depending only upon the angle of collision, one may exploit a Wild summation approach, which decomposes the semi-group associated to a Maxwellian collision operator based upon a binning of particles with common numbers of prior interactions [E. Carlen, M. Carvalho, and E. Gabetta, Central Limit Theorem for Maxwellian Molecules and Truncation of the Wild Expansion, *Comm. Pure and Applied Math*., **53**, 370-397 (2000)]. For a simple, purely collisional flow

$$U_t = M(U)$$

where M is a Maxwellian collision operator, the maxwellian velocity distributions

$$\Phi_M(\vec{v};\vec{u},T,n) = n(2\pi T)^{-\frac{3}{2}} e^{-|\vec{v}-\vec{u}|^2/2kT},$$

are well know equilibrium distributions parameterized by average velocity, temperature, and density. The linearization of the collision operator about a Maxwellian velocity distribution has a five dimensional kernel comprised exactly of elements of the tangent plane

$$\frac{\partial \Phi_M}{\partial p_i}$$

where

$$\vec{p}(x,t) = (p_1(x,t),\cdots,p_5(x,t)) = (\vec{u}(x,t),T(x,t),n(x,t)).$$

The inclusion of convection, or an external force, drives the collisional system away from the Maxwellian distribution. There are two questions of interest; the first is to quantify the scalings in which the adiabatic flow generated by projecting the perturbation onto the kernel of the Maxwellian remains a valid reduction. This requires a quantization of thermalization/ dethermalization rates. The second is to identify new equilibria, or quasi-steady equilibria, which may be generated in cases of prescribed external forces. We fix our attention on the Boltzmann equation

$$U_t + v \bullet \nabla U = \frac{1}{\varepsilon} M(U)$$

in a heavily collisional case $\varepsilon << 1$. The linearization, $L_{\vec{p}}$ of the collision operator about $\Phi_M(\bullet, \vec{p})$ has a 5 dimensional kernel. Working with a more than quadratically weighted velocity norm

$$\|U\|_\delta = \int_{\mathbb{R}^3} \left(1 + |\vec{v}|^{2+\delta}\right) U(\vec{v}) d\vec{v},$$

then the remainder of the spectrum is uniformly bounded in the left-half complex plane for an integrable Maxwellian collision kernel, [Carlen, 2003 *ibid*.]. Given a velocity distribution U which is sufficiently close to a Maxwellian, it can be uniquely decomposed into a Maxwellian and a non-thermalized component

$$U = \Phi_M(x, \vec{v}; \vec{p}) + W.$$

Under the adiabatic reduction the Maxwellian parameters evolve at leading order according to

$$\vec{p}_t = \left[\pi_{\vec{p}_0} \nabla_{\vec{p}} \Phi\right]^{-1} \pi_{\vec{p}_0} v \bullet \nabla_x \Phi_M,$$

which corresponds to the Navier-Stokes and energy equation. The non-thermalized particles, W evolve according to the exact equation

$$W_t = \frac{1}{\varepsilon} L_{\vec{p}_0} W + (I - \pi_{\vec{p}_0}) \left[-v \bullet \nabla_x \Phi_M - \nabla_{\vec{p}} \Phi \bullet \vec{p}_t + (L_{\vec{p}} - L_{\vec{p}_0}) W - v \bullet \nabla_x W + \frac{1}{\varepsilon} N(W) \right]$$

with the linearized term generating a strongly contractive semigroup which can be efficiently approximated by a few terms of a Wild expansion. The fundamental issue is to identify regimes in which the kinetic particles, W, may be neglected. At leading order the dethermalization rate is given by the influence of the convective and the adiabatic evolution of the Maxwellian parameters,

$$(I - \pi_{\vec{p}_0}) \left[v \bullet \nabla_x \Phi_M + \nabla_{\vec{p}} \Phi \bullet \vec{p}_t \right]$$

which appear on the right-hand side of the W evolution. When this term is small in the $\|\bullet\|_\delta$ norm, the uniform decay of the linear semigroup suggests controllability of the kinetic term, however one must also check the nonlinear-resonance condition which verifies if the time dependence of the linear operator impacts the observed decay rates. This is a significant extension of the nonlinearity into the linear semigroup theory and requires either we obtain decay rates which are uniform in the linear phase space, or obtain information about where in the linear phase space the kinetic terms reside. Without resolving the kinetic terms, under assumptions of ergodicity, the effective linear decay rates can be computed by Monte Carlo sampling. Without ergodicity, one must investigate the Fokker-Planck equations for the probability distribution of the kinetic terms to estimate the effective decay rate; we have begun this process for simple linear models, and plain to extend to the full system.

The extension to the full system will provide a rigorous analytic framework for splitting the distribution into Maxwellian and kinetic parts. This splitting will enable the development of a numerical framework that will greatly reduce the overhead associated with the collision integral, since the Maxwellian lies in the null space of the collision operator. As long as the smallness and resonance conditions are not violated, the system may be numerically evolved solving $\vec{p}_t$ and W_t equations to leading order. It is anticipated that a Wild expansion may be employed to efficiently handle the evolution of *W*, as long as the tail of the kinetic part is not to 'fat' [Carlen, 2003 *ibid*.]. The two analytic conditions, smallness and renounce, are essential to this rigorous approach. As discussed in the general TRG section, the temporal renounce condition is important because it identifies the time, $t_1 = t_0 + \Delta t$, that renormalization about new bare coordinates, $\vec{p}_1$, needs to take place. If the smallness condition is violated, the condition tells us that the system is far from Maxwellian that was initially linearized about and the chosen ansatz is no longer valid. At this point, the smallness condition is informing the algorithm that the whole system needs to be treated kinetically.

Coulomb collisions: Bump on Tail instability

For charged particles, which interact through a long-range potential, the collision kernel is substantially different. The relative velocity of interacting particles defines the time scale of the interaction, and thus a large relative velocity implies a weak collision. A Coulomb collision kernel scales like the inverse cube of the relative velocity. For the simple, purely collisional flow

$$U_t = C(U)$$

where *C* is the Coulomb collision operator, which also possesses equilibrium Maxwellian velocity distributions, however since the collision kernel depends strongly upon relative velocities, there is no natural Wild summation for the linear propagator. Consider a velocity distribution characterized by two Maxwellians,

$$\Phi = \Phi_{M,1}(\vec{v}) + \Phi_{M,2}(\vec{v}),$$

with parameters $\vec{u}_i, T_i$, and n_i for $i \in \{1,2\}$. If the Maxwellians are well separated

$$\varepsilon \equiv \frac{k\left(T_1 + T_2\right)}{\left|\vec{u}_1 - \vec{u}_2\right|^2} << 1,$$

then the collision rate within a Maxwellian, which scale like $T_i^{-\frac{3}{2}}$ can dominate those between the two Maxwellians, which scale with $\left|\vec{u}_1 - \vec{u}_2\right|^{-3}$.

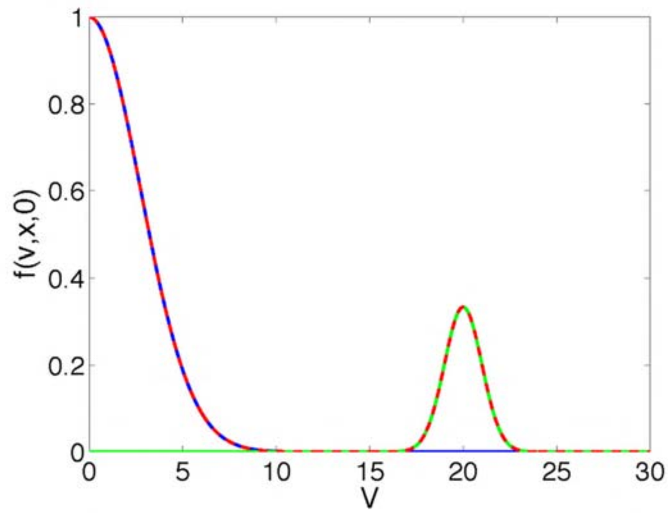

Figure 3. Velocity profile of a double Maxwellian with average velocities $\vec{u}_1 = 0$ and $\vec{u}_2 = 20$. The collisional interactions will be relatively weak and the distribution will evolve as two Maxwellians until the tails overlap substantially.

Because of the weak collisional interaction between the well-separated Maxwellians, to leading order they act as independent velocity distributions and the associated linearization of the collision operator about Φ has ten small eigenvalues, whose eigenfunctions are well approximated by, but not identical to, the 10 dimensional tangent space spanned by $\nabla_{\vec{p}}\Phi$. The two-humped Maxwellian is not invariant under the collisional flow and the inter-Maxwellian collisions will generate non-Maxwellian, or kinetic particles. The relaxation rate of the kinetic particles onto a Maxwellian distribution can be arbitrarily slow if the tail of the velocity distribution is fat, due to the inverse cubic dependence of the collision kernel on relative velocity. The linearization $L_{\vec{p}}$ of the Coulomb collision operator about the double-Maxwellian will have 10 Maxwellian eigenvalues within $O(\varepsilon)$ of the origin, continuous spectrum which approaches the origin corresponding to the fast tail of the particle distribution, $|\vec{v}| >> |\vec{u}_1| + |\vec{u}_2|$, and spectrum which is uniformly in the left-half complex plain, corresponding to kinetic particles whose velocity is comparable to that of the Maxwellian distribution. With this decomposition we associate spectral projections π_M, π_W, and π_K, associated to Maxwellian, non-thermalized, and extremely kinetic particles. Given a velocity distribution *U* which is sufficiently close to a well-separated double Maxwellian, it can be uniquely decomposed into a double-Maxwellian, non-thermalized, and kinetic parts

$$U(\vec{v}) = \Phi_M(\vec{p}) + W + K,$$

where $\vec{p}$ represents the 10 Maxwellian parameters, *K* lies in the range of $\pi_{K,\vec{p}}$ and *W* lies in the range of $\pi_{W,\vec{p}}$. The exact evolution under the collision operator becomes

$$\vec{p}_t = \left[\pi_{\vec{p}_0}\nabla_{\vec{p}}\Phi_M\right]^{-1}\pi_{\vec{p}_0}C(\Phi) + \pi_{\vec{p}_0}\left[(L_{\vec{p}} - L_{\vec{p}_0})(K+W) + N(K,W)\right],$$

where the last term on the right hand side indicates the impact of collisions among the kinetic and non-thermalized particles on the Maxwellian. The dominant impact on the adiabatic evolution of the Maxwellian parameters comes from the inter-Maxwellian terms, which reduce to

$$C(\Phi_M) = C(\Phi_{M,1}, \Phi_{M,2}) + C(\Phi_{M,2}, \Phi_{M,1}),$$

since the self-interactions are zero. These terms can be computed efficiently, particularly when the second Maxwellian has a low density. The Wild summable and Kinetic terms evolve according to

$$W_t = L_{\vec{p}_0} W + (\pi_{W,\vec{p}})\Big[C(\Phi_M) - \nabla_{\vec{p}}\Phi \bullet \vec{p}_t + (L_{\vec{p}} - L_{\vec{p}_0})W + N(W,K)\Big],$$

$$K_t = L_{\vec{p}_0} K + (\pi_{K,\vec{p}})\Big[C(\Phi_M) - \nabla_{\vec{p}}\Phi \bullet \vec{p}_t + (L_{\vec{p}} - L_{\vec{p}_0})K + N(W,K)\Big],$$

with the distinction that $L_{\vec{p}_0}$ generates a rapidly convergent semi-group on *W*, but not on *K*. The dethermalization of particles is represented by the terms

$$\pi_{W,\vec{p}} C(\Phi_M) \quad \text{and} \quad \pi_{K,\vec{p}} C(\Phi_M)$$

which appear on the right-hand side of the *W* and *K* evolutions. The thermalization of particles is accounted for naturally by the term

$$\pi_{\vec{p}_0} N(W+K)$$

as well as at the renormalization steps when the bare quantities which determine the coordinate system are updated. If the Maxwellians are sufficiently well separated, the non-thermalized particles *W* can be ignored. However as the Maxwellians evolve and become less well separated, the non-thermalized particles will become important, and their propagation, which is dominated by the linear operator $L_{\vec{p}}$, will be determined by Monte-Carlo methods. Eventually the two Maxwellians will no-longer be well separated, and the 10x10 matrix on the right-hand side of the adiabatic evolution will become singular, this is associated with the delocalization of the 10 Maxwellian eigenvalues from the origin, giving a criterion for detecting the failure of the ansatz. At this point one must renormalize the bare quantities down to a single Maxwellian. While thermalization/dethermalization is accounted for naturally during the evolution of the observables, $\vec{p}(t)$, this is also manifested through the re-projecting which occurs at the renormalization steps. In particular at the failure point of the double Maxwellian ansatz, the particles in the second Maxwellian will subsequently be treated completely kinetically until their thermalization with the bulk distribution.

We anticipate that the exact algorithm will have the following form:

- Given a double Maxwellian, compute the eigendistributions of the associated linearization, which can be preconditioned using the partial derivatives of the ansatz with respect to the parameters.
- Given an bump on tail distribution, solve the spectrally orthogonal decomposition, essentially the inversion of an explicit 10x10 matrix.
- Estimate the inter-Maxwellian terms, $C(\Phi_M)$, to bound the renormalization time Δt by controlling the secularity.
- Ignore the secular and nonlinear terms in the adiabatic evolution and estimate the leading terms in the *W* and *K* evolution to determine their growth, and self-check on the nonlinear term ignored during the adiabatic evolution.
- Renormalize and iterate the procedure until either the double-Maxwellian ansatz fails, or the kinetic terms become significant, in which case they can be handled explicitly by Monte-Carlo methods.
- In the case that kinetic terms dominate and the nonlinearity *N* cannot be ignored in the adiabatic equation, then a fully kinetic approach is needed.

Extension to Boltzmann-Poisson Systems

As in the Maxwellian collision kernel, the inclusion of convection and long-range coulomb forces will drive the Coulomb system away from the Maxwellian distribution. The principal question of interest is to quantify the scalings in which the adiabatic flow generated by a single Maxwellian remains a valid reduction. Writing the Vlasov-Poisson system in a heavily collisional scaling

$$U_t + v \bullet \nabla_x U + a \bullet \nabla_v U = \frac{1}{\varepsilon} C(U)$$

where the acceleration a is determined from the electric field and $\varepsilon << 1$, one can again decompose as

$$U = \Phi_M + W + K ,$$

where Φ_M is a single Maxwellian parameterized by position dependent Maxwellian parameters $\vec{p}(x)$. The goal is to understand the regimes for which the long-range Coulomb interaction can be held in check by the contractivity of the collision operator. Given the relatively weak impact of the collision operator on the kinetic particles, K, they will need to be handled explicitly through Monte-Carlo methods.

Task 4 – Implementation of RG-inspired advanced particle shape functions for PIC

This task builds on the developments of tasks 1 and 2 to implement dynamic RG-inspired charge/current weighting in particle codes. We will examine this both in the particle-in-cell context and the gridless treecode milieu. A variety of practical issues must be confronted to be an effective method. These include, but are not limited to charge/current conservation, symmetry between weighting from the grid to the particle and vice-versa, and development of boundary conditions that handle the extended stencil of these particles without loss of accuracy. These issues will be assessed in multiple dimensions by implementation in software, verification against test problems previously developed in this effort, and finally testing in comparison to standard weighting in PIC and gridless methods.

In developing this task, we should stress that we are focused on just the algorithms associated with the particle weighting. These modifications apply equally well, therefore, to both electrostatic and electromagnetic field solutions. Care will be taken to keep the fundamental numerical interaction in the field solutions essentially un-changed, thus allowing these methods to be rapidly applied to the range of kinetic problems of interest to the Air Force.

This task will serve to develop a general means to include dense plasmas in kinetic methods by using a RG description of particle weighting, or shape function to deal with the multiple scale issues associated with grid heating. This builds directly on the Debye shielding work presented earlier. The impact of grid heating is strongly tied to the fact that the presence of the grid introduces aliasing between wavenumbers in momentum space. The mathematics of this is quite similar to our RG treatment of the Debye length, except that in this case we simply use the functional form of the Debye shielding to rescale the charge on a macro-particle to reflect the shielding associated with the large number of physical particles in phase space that the macro-particle is representing. In this context, the particle charge simply becomes

$$e \rightarrow e \bullet \exp\left\{ {}^{-r}\!/\!{}_{\lambda_D} \right\}$$

where λ_d has the traditional meaning. Expanding this scaling leads to an infinite series

NGP Scaling

$$e \rightarrow e \bullet \exp\left\{ {}^{-r}\!/\!{}_{\lambda_D} \right\} = e\left\{ 1 - \frac{r}{\lambda_D} + \frac{1}{2}\left(\frac{r}{\lambda_D}\right)^2 + \ldots \right\}$$

PIC Scaling

where the renormalized macro-particle charge is now an explicit function both of space and of the Debye length. Inspection allows identification of traditional particle-in-cell weighting of the particle to the grid, where the first term is simply nearest grid point weighting [Birdsall and Langdon, *Plasma Physics via Computer Simulation*. CRC Press, New York, 2004], while retaining two terms in the expansion yields particle-in-cell weighting. Thus, RG offers an interpretation of grid heating where the quality of the expansion in terms of r/λ_d gives an immediate assessment of the fidelity of the shielding physics. Furthermore, this identification gives a functional form for extension to higher order particle methods simply by keeping more terms. Based on Phase I work, this RG-inspired particle weighting is shown to be competitive with 5th order standard PIC weighting. Finally, this offers a dynamic means to control the particle's characteristics as the plasma transitions from kinetic to continuum regimes as a function of density and temperature. Thus, it can be thought of as a "complex" particle in the sense of [D. Hewett. "Fragmentation, merging, and internal dynamics for PIC simulation with finite size particles" J. Comp. Phys. 189(2003) 390-426], where the additional physical information present in the particle enhances the fidelity of the numerical method. The Debye problem developed earlier provides a rigorous basis for the evolution of these complex particles in the dense plasma context, providing accuracy even when the discretization, either in terms of grids or particles, is insufficient to explicitly resolve all short length scale details of a given plasma.

Task 5 – Testing and evaluation of advanced multi-scale algorithms

The methods developed in tasks 3 and 4 will be evaluated for accuracy, speed, and effectiveness against more general test problems. These include, but are not limited to

- Debye and flicker
- Langmuir probe simulations
- bump-on-tail particle distributions
- Dense kinetic plasma effects in space-propulsion devices, and
- Dense anode plasma in HPM sources

RG plays a dual role in this task by virtue of providing enhanced analytic tools to find solutions to multi-scale test problems for verification and validation, in addition to its crucial role in the development of new numerical algorithms. The connections between the RG theory and the development of better particle methods for dense plasmas will be the central focal point of the work. This work will provide a systematic validation of both new theory and new algorithms. The approach is designed to provide new test problems as well as the necessary self-checks on the methodology. Three examples of our approach are summarized below:

Debye Shielding and the Impact of Statistical Fluctuations

We start with the following work plan in this task:

- Applying RG theory to reproduce known results (e.g. Debye Shielding),
- Use the RG theory to account for numerical defects (e.g. statistical fluctuations on the mesh as well as to take into account effect of finite mesh in a periodic domain)
- Having accounted for numerical defects, use RG to compute effective shielding distance with a given noise level in PIC.
- Verify the shielding RG results via numerical simulation.

Thus giving us a new test problem specifically designed to validate existing PIC codes. In addition, the validation via simulation provides a self-check that the theoretical results are correct. The application of Temporal RG to the cathode flicker problem will also lead to new test problems that traditional PIC codes can be validated against.

Further, the RG approach can be used to develop tools that can enhance existing legacy codes for dense plasma problems. An example of this is the planned use of RG to explain numerical heating and develop alternative weightings that avoid numerical heating, in short weightings that are ideal for dense plasma simulations with particle methods;

- Use path integral form of RG theory to investigate and rigorously explain phenomenon such as numerical heating in under resolved dense plasma particle codes.
- Based on the RG, develop new particle shape functions and new weighting consistent schemas for PIC. (PIC RG)
- Put new weighing into RG theory and show reduced heating in dense plasmas.
- Validate reduced heating via simulation.

This tight coupling between particle code theory and the particle methods of plasma simulations is what makes this approach novel and potentially very powerful.

Bump on Tail Instability and Temporal RG Decomposition

The RG approach will also lead to new algorithms and tight coupling with new validation is critical. An example of a new algorithm coming out of this work is the development of the Temporal RG for the Bump on Tail work:

- Apply TRG metrology, as described in the TRG section, to construct a rigorous numerical approach to the orthogonal splitting of the distribution and evolve the split system.
- Validate the TRG approach by comparing with traditional MCC methods for the Bump on Tail problem.

The TRG approach will be first applied to the cathode flicker problems and comparing with simulations will validate the theoretical results. This will provide the team with confidence in the theoretical framework out lined in the TRG section and will also provide a new test problem. Then the approach will be applied to the Maxwellian molecule collision operator and the methodology will be turned into a numerical method, which will be compared with DSMC results of gas dynamics problems. Finally, the approach will be applied to the Bump on Tail and external field problem.

This task supports all the technical goals of this project, and provides a capstone effort for the development of new plasma simulations techniques.

Task 6 – Documentation

The results of this Phase II STTR effort will be documented in a final report.

Project Management

Consistent with the level of effort specified in the budget, we offer the following work load breakdown: Tasks 1-2 shall be completed in the six months of the Phase II effort, with the effort spread roughly equally between the UCLA and NumerEx. We then, in tasks 3 and 4, transition from the application of RG methods to specific, but representative plasma physics problems to development of general protocols for understanding the multi-scale nature of the problem, development of criteria for choosing between various methods depending on these scale lengths, and finally, develop of algorithms that offer dynamic range in dealing with kinetic and fluid effects in a single code. In the spirit of risk reduction, we will study both the use of RG to dynamically control the plasma shielding length, and the implementation of new collision operators to include BGK-like kinetic effects in a continuum formulation. These tasks will consume roughly one year of effort, with task 3 work being carried by UCLA with strong assistance from Michigan State and task 4 effort being dominated by NumerEx. Tasks 5 and 6 will consume the rest of the effort, with roughly equal contribution from the team, consistent with budgetary level of effort.

The great strength of this team is the diverse set of skills and viewpoints we bring to this problem. The great challenge is that we are geographically distributed around the world. In light of this, we plan on continuing our practice from Phase I of holding bi-weekly tele-conferences. These telecons proved critical to achieve our current successes, and we look forward to the continued intellectual stimulation and interchange they provide. Additionally, these bi-weekly meetings will be supplemented with travel as warranted to central locations where the team can meet in person.

Related Work

NumerEx has been involved with a wide variety of pulsed power and RF source physics problems since it was founded in the late 1980s. NumerEx has been involved with the continuing development of ICEPIC, a three-dimensional particle-in-cell (PIC) code since 1997, and has made continuous use of ICEPIC for modeling various narrowband RF devices of interest to the Air Force Research Laboratory since that time. The most relevant work has been recent modeling efforts to understand the Michigan experimental demonstration of magnetic priming.

Figure 4 shows the NumerEx simulation of the U of Michigan low-noise microwave oven magnetron [Luginsland et. al., Appl. Phys. Lett. **84**, 5425, 2004]. These calculations used ICEPIC, and were performed on 4 nodes of a LINUX cluster. Each calculation took up to two days to complete, but included a detailed description of the fields resulting from the permanent magnets, high resolution of the strapping structure present in these devices, and careful modeling of the power output structure. Benchmarking these ICEPIC calculations against experiments performed at the University of Michigan showed excellent agreement in the output power as well as the reduction in starting current for pure mode operation. The accompanying figure 5 shows the geometric detail included in the calculation.

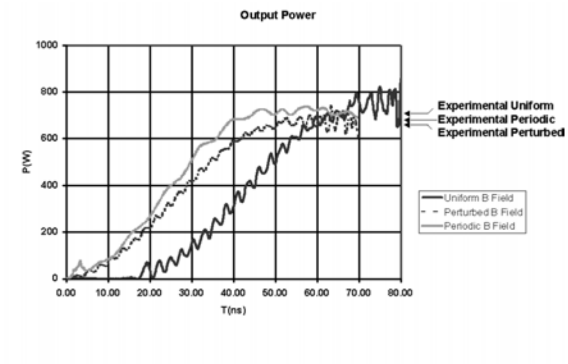

Figure 4. ICEPIC simulations for a variety of magnetic priming conditions. Compared to the uniform case, the magnetic priming results in lower noise, decreased time to full power operation, and enhanced mode control.

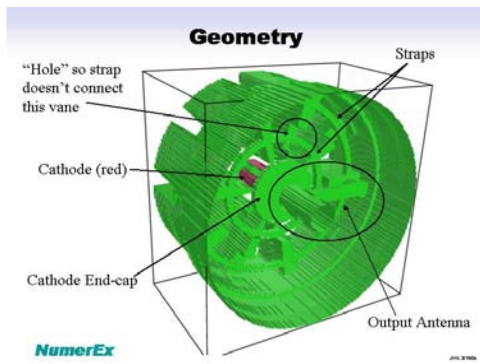

Figure 5. Conventional S-band magnetron demonstrating magnetic priming computationally.

NumerEx staff has extensive experience in the PIC simulation, analysis and design of space-charge limited diodes, a critical component in any vacuum electronics source. The customer was the Air Force Research Laboratory (POC Dr. Donald Shiffler, 505-853-3906 and Dr. Keith Cartwright, 505-846-9101). This work focused on multi-dimensional space-charge limited flow, plasma-filled diodes for impedance reduction, dense anode plasma formation, and bipolar flow from a variety of material. For example, recent work focused on plasma formation in the magnetically insulated line oscillator. Plasma production on the anode was sufficient to eliminate magnetic insulation, leading to poor microwave production. These simulations clarified the pulse-shortening mechanism for the first time. Finally, NumerEx has extensive experience with the development of novel emission algorithms to handle space charge limited flows in a variety of situations.

Under the ICEPIC development effort, NumerEx personnel have created and implemented a new space-charge-limited emission algorithm as noted above and made significant contributions to the range of capabilities of ICEPIC (applied magnetic field model, planewave generator, dielectric materials, permeable materials, lossy conductors, two-dimension version, initial cylindrical coordinates version, various antenna models and transmission-line-mode launchers). NumerEx personnel have also made extensive comparisons between ICEPIC calculations and various experimental efforts. These efforts were all funded by AFRL (point of contact: Dr. Keith Cartwright, AFRL/DEHE, (505)846-9101).

Recently, NumerEx is involved in the simulation, analysis, and design of gas-puff radiation sources (Figure 6). In this case, gas sprayed from a nozzle is ionized and pinched by the application of electrical energy. The customer is DTRA and the Naval Research Laboratory (POC Dr. Jack Davis 202-767-3278). The MACH software is being used to investigate the details of nozzle design and the relationship between nozzle design and radiative performance.

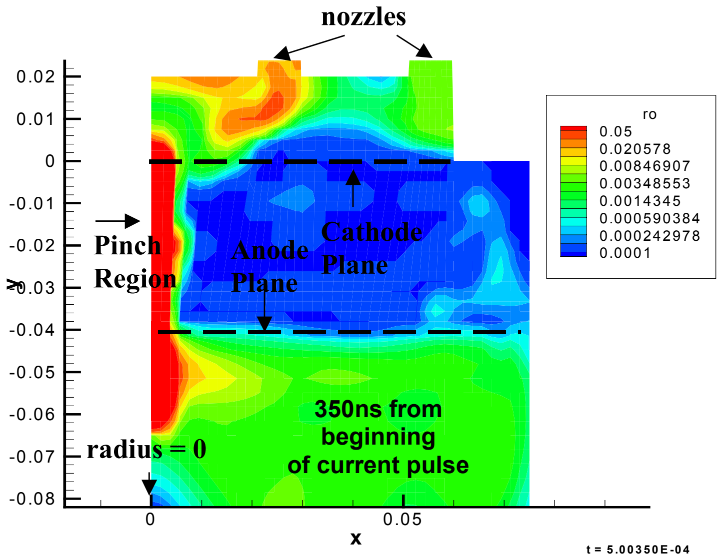

Figure 6. Gas-puff Z-pinch.

Finally, we have recently begun investigating various aspect of plasma combustion for Eglin AFB under a Phase II SBIR, including the various roles played in detonation by electrically exploding wires, including hypervelocity impact, ohmic heating, and deflagration-to-detonation transition [POC: Lt. Mark Wuertz 850-882-7990]. Critical to this effort was the development of a two-stage induction/reaction model to serve as a bridge between fast chemical kinetics reaction rates and rather slower hydrodynamic shocks. This work has been extended to study the impact of transient plasma ignition on hydrocarbon chemistry for pulse detonation and internal combustion engines [POC: Dr. G. Roy, 703-696-5588].

Caflisch and his collaborators at UCLA have worked on multiscale mathematics and numerical methods in several application areas. In collaboration with Lorenzo Pareschi, Caflisch has developed a hybrid method for rarefied gas dynamics that represents the velocity distribution function as a combination of a continuum Maxwellian equilibrium and a collection of particles. This method combines a fluid solver for the Maxwellian component with a DSMC method for the particles and the interaction between the particles and the Maxwellian. Figures 7 shows results of this method applied to a shock wave at Mach 1.4 and for flow past a leading edge, respectively.

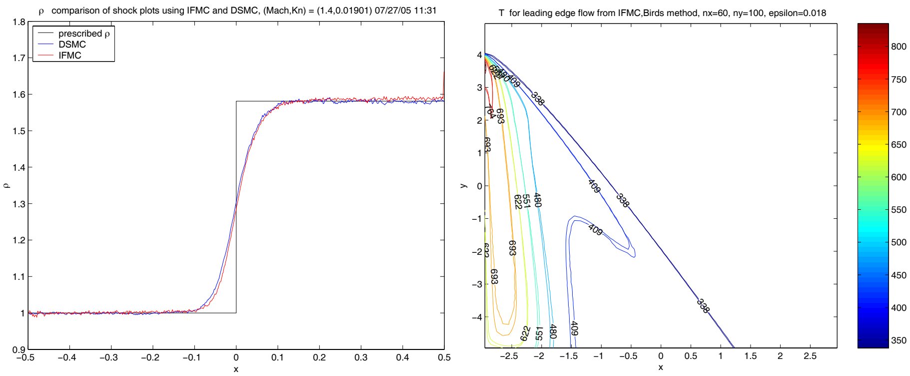

Figure 7. Comparison of hybrid method and DSMC results for density in a shock wave at Mach 1.4 (left) and temperature in flow past a leading edge (right).

In recent work with Richard Wang at UCLA and Andris Dimits and Bruce Cohen at LLNL, Caflisch has started to extend this hybrid method to Coulomb collisions in a plasma. Figure 8 shows a comparison of the hybrid method and a direct Monte Carlo method for relaxation of an initially anisotropic distribution of electrons in a plasma.

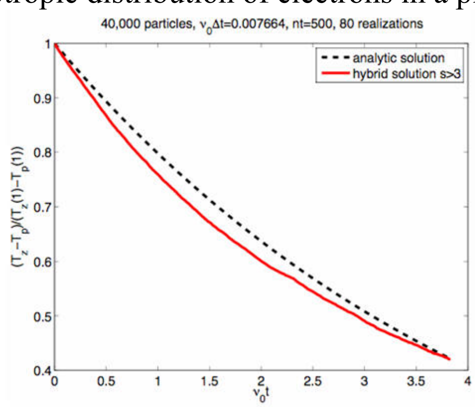

Figure 8. Comparison of analytic solution (dashed line) and results from hybrid method (solid line) for decay of anisotropy in electron distribution function.

Caflisch and Dimitri Vvedensky have developed a number of multiscale numerical methods for simulation of epitaxial growth. In collaboration with researchers at HRL Labs and UCLA, they developed an island dynamics model and a level set simulation method that applies coarse graining to the lateral features of an epitaxial surface, but retains atomistic scale detail in the height of the crystal layers. Figure 9 shows a typical result from this method. The different colors are the epitaxial surface at different numbers of crystal layers; i.e., across each interface the surface height changes by a single crystal layer.

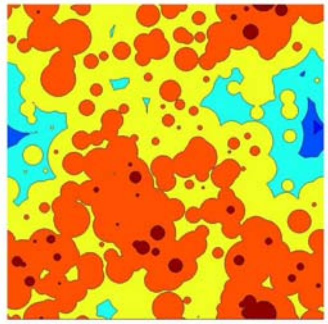

Figure 9. Surface height of epitaxial thin film simulated using the island dynamics/level set method.

Relationship to Future Research or Research and Development

RG-based computational methods for plasma physics fits naturally into our team's research and development plans. For our renormalization experts, this works extends their talents into the plasma regime, providing new vistas in range of problems to solve. Similarly, for the plasma physics specialists, the RG-methods offer an opportunity to develop new equations, new algorithms, and new test problems for verification and validation of multiple scale plasmas, especially those associated with kinetic plasmas, with density bordering on the typical fluid limits. From plasma thrusters to directed energy sources to space-weather, this quasi-kinetic dense plasma phenomena is in the direct design path for advanced technology of interest to the Department of Defense. As such, this effort natural fits the progression of topics necessary to perform our research. The strong advantage of pursuing these topics under the Phase II STTR auspices, however, is the assembling of this team of high diversity in scientific understanding. The current Phase I effort has demonstrated that our team is well positioned to rapidly advance the state-of-the-art in multi-scale plasma computation.

Future research and development efforts look to build on our newly found capability to handle multiple scale physics from both analytic and computational perspectives, with a strong emphasis on dynamically assessing the quality of approximations, numerical methods, and fidelity of algorithms. From here, the team has discussed looking at the transition from quantum mechanical field emission to fully space-charge limited flows consistent with our flicker formulation for application in tera-hertz sources of coherent radiation, studying the transition from kinetic through two-fluid to single fluid (MHD) physics in plasma opening switches, magnetic reconnection in space-plasma systems, and finally advanced diagnostics based on improved understanding of Langmuir probes and sheaths consistent with our Debye shield work in Phase I. All of these advances are enabled by our growing capability in RG-based techniques. In short, this Phase II effort is providing a critical building block for the advances in multiple scale techniques needed by the computational plasma physic community at large.

Commercialization Strategy

NumerEx has two arenas of potential commercialization. The first is in the military context. The Air Force and the Department of Defense in general is committed to both transformation in weapon systems and the rapid prototyping of advanced technology. The Department of Defense is targeting $10 to $30 billion per year into modernization efforts, out of a nearly $500 billion budget. Clearly, this market dwarfs the commercial market for application of advanced scientific modeling of plasmas and electromagnetics in the near term. As such, NumerEx is committed to developing advanced simulations tools for the government and its contractors. NumerEx also plans to exploit existing relationships with high technology system integrators, such as Science Applications International Corporation and ATK-Mission Research, in conjunction with consultation with our government partners, to push this simulation technology from research and development to deployment in researcher's hand for computer-aided engineering. Furthermore, industrial companies often develop parametric tools to aid the design of technology. The application of RG for model reduction offers tremendous potential to tie first-principles, physics-based software to these more approximate formulations. Given the increasing focus within the Air Force on Simulation-based Acquisition, NumerEx can exploit this effort not only in the design of advanced capability technological devices, but also provide expertise to the test/evaluation community and the war gaming community for exploitation of plasma technology through deployment to the warfighter. NumerEx is committed to developing state-of-the-art techniques on the wider question of acquisition streamlining and cost control of new technology systems [see https://www.dmso.mil/public/ and http://www.msiac.dmso.mil/sba/].

Specifically, NumerEx will approach our government partners to investigate the potential for matching funds for phase III applications of plasma modeling technology based on the Renormalization Group techniques proposed herein. Given the important role that optimization is currently playing in high technology development, especially in the area of reduced order modeling for parametric searching, the time may be ripe for controlled application of higher/lower fidelity models, especially in the context where multiple scales present a particular challenge to parametric and reduced order models obtained from proper orthogonal decomposition. Furthermore, there are a variety of opportunities to work with members of the fusion and space-weather communities where our RG approach to assessing correctness may be synergistically applied to other computational techniques. Our team looks forward to investigating these prospects where phase III matching funds can bring value to both the Air Force and other branches of government

A longer-term exploitation of this STTR Phase II research in the commercial sector involves enhanced efficiency internal combustion, pulse detonation engines, transient plasma ignition, and ramjet hypersonic engines through our existing relationship with General Electric and Nissan. One potential method to enhance diesel engines is "vortex" or turbulent mixing of the fuel and oxidizer to ensure full consumption (burning) of the fuel as well as pulsed power based plasma ignition technology. All of these features introduce multiple time-scales to the problem at hand. With the deployment of such technology, the diesel engine becomes both more efficient and cleaner in terms of byproducts. Diesel engines are a major technology available to increase the fuel efficiency of transportation vehicles, one of the major sources of greenhouse gases and pollution. Detailed understanding of the roles of hydrodynamics, source geometry, chemistry, and the resulting ignition energy is important to this new community. Additionally, novel ignition methods, such as transient plasma ignition have been shown to reduce NO_x and soot emissions in internal combustion gasoline engines. The physics associated with this transient plasma covers the range of kinetic plasmas associated with plasma streamers through reactive fluid limits due to the modified chemistry associated with the application of pulsed power. Better understanding of these issues offers potential for the both more efficient engines as well as more flexibility in the precise fuel condition leading to combustion. As noted in President Bush's State of the Union speech on January 28, 2003, the federal government has earmarked 1.2 billion dollars for the development of clean burning hydrogen fuel cells. However, the expected deployment of such technology is still 15 years away. Recent studies have suggested that stopgap technology, such as improved internal combustion engines based on plasma combustion techniques, may have significant merit in this arena. NumerEx will approach General Electric and Nissan to investigate appropriate alliances that will lead to Phase III matching funds.

Without adding in the potential gains associated with Phase III cost sharing, RG-based plasma simulation technology offers true value to a number of stakeholders. Given these avenues for growth, NumerEx expects potential gains in revenue from the licensing of modeling software, and increased engineering services revenue. These potential gains are summarized in Table 1, and will be reported in our Company Commercialization Report Update. These gains suggest that NumerEx will grow by roughly 15% in sustained business due to the Phase II award.

Table 1. Expected revenue stream to NumerEx from RG-based simulation technology due to engineering services and licensing/royalties of modeling tools.

	Software License/Royalty	Engineering Services	Total Revenue
PII Start + 1 year	$40,000.00	$50,000.00	$60,000.00
PII Start + 2 years	$50,000.00	$75,000.00	$120,000.00
Post Phase II	$50,000.00/year	$125,000.00/year	$175,000.00/year

Key Personnel

John W. Luginsland (Co-Principal Investigator)

Dr. Luginsland is a staff member at NumerEx where he performs advanced research in the application of computational kinetic and magneto-hydrodynamic plasma physics to the development of electromagnetic systems. He is currently the lead investigator of a Phase II SBIR effort to enhance and focus the pressure associated with plasma ignition of fuel-air mixtures. Additionally, he is principle investigator on efforts to enhance the state-of-the-art in meso-band RF sources, based on non-linear transmission line technology with the Air Force Research Laboratory, multi-scale physics (kinetic to fluid limits) issues associated with pulse detonation engine using transient plasma ignition for the Office of Naval Research, and efforts to apply renormalization group mathematics to computational plasma physics problems for the Air Force Office of Scientific Research. He has extensive experience with parallel particle-in-cell simulation, including the analysis of both conventional vacuum electronics and high power microwave systems, such as magnetrons. A particular focus is vacuum and plasma diode physics, dealing with such issues as quantum mechanical cold cathode field emission, multi-dimensional space charge limited flow, plasma filled diodes, bipolar flow, and anode plasma formation.

He has over 15 years experience in research and development of electromagnetic high technology products, and a history of close interactions with experimental teams. He has worked with both the DOE and DOD, primarily in the areas of computational science and engineering. Dr. Luginsland's experience includes development of high current particle accelerators for medical and industrial applications, and high power microwave systems for military and industrial uses. Prior to joining NumerEx, he worked for Science Applications International Corporation, developing first principles simulation codes and parametric tools for the modeling and design of advanced armor and survivability systems. In addition to his research duties, he was a program manager at SAIC for an effort to integrate advanced armor systems into next generation military platforms and was acting test planner for a live-fire experimental facility dedicated to advanced armor concepts based at the Aberdeen Proving Grounds. Previously, Dr. Luginsland worked at the Air Force Research Laboratory for 5 years where he was responsible for both HPM source and computational modeling software development, leading to the weaponization of directed energy systems for non-lethal electronic attack. He was the lead for computational physics in the Narrowband High Power Microwave Technology Area, charged with facilitating applied research for modeling in support of experimental HPM source development. During this tenure, he was a member of a three-person team winning the Department of the Air Force's Science and Engineering Award for Exploratory and Advanced Technology Development. In 2006, Dr. Luginsland was honored with the IEEE Nuclear and Plasma Science Society's Early Achievement Award. He continues to serve as a technical resource to the Air Force in supporting the development of compact HPM and vacuum electronics sources as well as various types of computational analysis, including high performance computing algorithms. His wider interests include the design, integration, and assessment of military utility for directed energy devices, high power microwave systems, millimeter-wave and THz vacuum electronics systems, battle-damage assessment technology, and advanced fuel/air munitions. Dr. Luginsland has supported various US government agencies in the assessment of foreign technology.

B.S.E, Nuclear Engineering, University of Michigan, 1992
M.S.E, Nuclear Engineering, University of Michigan, 1994
Ph.D., Nuclear Engineering, University of Michigan, 1996

Dr. Luginsland's publication list follows:

REFEREED PUBLICATIONS

• Pengvanich, Chernin, Lau, Luginsland, and Gilgenbach. "Effect of Random Circuit Fabrication Errors on Small-Signal Gain and Phase In Traveling-Wave Tubes." IEEE Trans. Electron Devices, **55**, 916, 2008.
• Lau, Luginsland, Cartwright, and Haworth. "Role of Ions in Crossed-field Diodes." Phys. Rev. Lett., **98**, 015002, 2007.
• Kowalczyk et. al. "AC space charge effects on beam loading of a cavity." IEEE Trans. Elect. Dev., **52**, 2087, 2005.
• Jones et. al. "Simulations of magnetic priming in a relativistic magnetron." IEEE Trans. Elect. Dev., **52**, 858, 2005.
• Neculaes et. al. "Rapid kinematic bunching and parametric instability in a crossed-field gap with periodic magnetic field." 33, 654, 2005.
• Neculaes et. al. "Magnetic priming effects on noise, startup, and mode competition in magnetrons". IEEE Trans. Plasma Sci., **33**, 94, 2005.

• Umstattd, Carr, Frenzen, Luginsland, and Lau. "A simple physical derivation of Child-Langmuir space-charge-limited emission using vacuum capacitance." Am. J. of Physics, **73**, 160, 2005.
• Greenwood, Cartwright, Luginsland, and Baca. "On the elimination of numerical Cerenkov radiation in PIC simulations." J. Comp. Phys., 201, **665**, 2004.
• Luginsland et. al. "Three-dimensional particle-in-cell simulations of rapid start-up in strapped oven magnetrons due to variation in the insulating magnetic field." Appl. Phys. Lett., **84**, 5425, 2004
• Lopez et. al. "Relativistic magnetron driven by a microsecond E-beam accelerator with a ceramic insulator." IEEE Trans. Plasma Sci., **32**, 1171, 2004.
• Shiffler et. al. "Emission uniformity and shot-to-shot variation in cold field emission cathodes." IEEE Trans. Plasma Sci., **32**, 1262, 2004.
• Lopez et. al. "Limiting current in a relativistic diode under the condition of magnetic insulation." Phys. Plasmas, **10**, 4489, 2003.
• Lopez et. al. "Cathode effects on a relativistic magnetron driven by a microsecond e-beam accelerator." IEEE Trans. Plasma Sci., **30**, 947, 2002.
• Wilsen et. al. "A simulation study of beam loading on a cavity." IEEE Trans. Plasma Sci., **30**, 1160, 2002.
• Shiffler et. al. "Effect of anode materials on the performance of explosive field emission diodes." IEEE Trans. Plasma Sci., 30, 1232, 2002.
• Luginsland, Lau, Umstattd, and Watrous. "Beyond the Child-Langmuir law: A review of recent results on multidimensional space-charge-limited flow." Phys. Plasmas, **9**, 2371, 2002.
• Peterkin and Luginsland. "A virtual prototyping environment for directed-energy concepts." Computing in Science and Engineering, **4**, #2, 42, March/April 2002.
• Umstattd, and Luginsland. "Two-dimensional space-charge-limited emission: Beam-edge characteristics and applications." Phys. Rev. Lett., **8714**, 5002, 2001 (Article number 145002).
• Watrous, Luginsland, and Frese. "Current and current density of a finite-width, space-charge-limited electron beam in two-dimensional, parallel-plate geometry." Phys. Plasmas, **8**, 4202, 2001.
• Shiffler et. al. "Emission uniformity and emission area of explosive field emission cathodes." Appl. Phys. Lett., **79**, 2871, 2001.
• Haworth, Luginsland, and Lemke. "Improved cathode design for long-pulse MILO operation." IEEE Trans. Plasma Sci., **29**, 388, 2001.
• Luginsland et. al. "Computational Techniques." – in Schamiloglu, and Barker, Eds. High-Power Microwave Sources and Technologies. Wiley/IEEE Press, 2001.
• Hendricks et. al. "Gigawatt Class Sources." – in Schamiloglu, and Barker, Eds. High-Power Microwave Sources and Technologies. Wiley/IEEE Press, 2001.
• Watrous, Luginsland, and Sasser. "An Improved Space-charge-limited Emission Algorithm for use in Particle-in-cell Codes." Phys. Plasmas, **8**, 289, 2001.
• Blahovec et. al. "3-D ICEPIC Simulations of the Relativistic Klystron Oscillator." IEEE Trans. Plasma Sci., **28**, 821, 2000.
• Haworth, Luginsland, and Lemke. "Evidence of a New Pulse-shortening Mechanism in a load-limited MILO." IEEE Trans. Plasma Sci., **28**, 511, 2000.
• Haworth et. al. "Comprehensive Diagnostic Suite for a Magnetically Insulated Transmission Line Oscillator." Rev. Sci. Inst., **71**, 1539, 2000.
• Luginsland, McGee, and Lau. "Virtual Cathode Formation Due to Electromagnetic Transients." IEEE Trans. Plasma Sci., **26**, 901, 1998.
• Spencer, Hendricks, Luginsland, and Stump. "Dynamics of the Space-Charge Limiting Current in Gyro-type Devices." IEEE Trans. Plasma Sci., **26**, 854, 1998.
• Luginsland, Arman, and Lau. "High-Power Transit-Time Oscillator: Onset of Oscillation and Saturation." Phys. Plasma, **4**, 4404, 1997.
• Luginsland, Lau, and Gilgenbach. "2-Dimensional Child-Langmuir Law." Phys. Rev. Lett., **77**, 4668, 1996.
• Luginsland, Valfells, and Lau. "Effects of a Series Resistor on Electron-Emission from a Field Emitter." Applied Phys. Lett., **69**, 2770, 1996
• Luginsland, Lau, Hendricks, and Coleman. "A Model of an Injection-Locked Relativistic Klystron Oscillator." IEEE Trans. Plasma Sci., **24**, 935, 1996.
• Walter et. al. "Effects of Tapering on Gyrotron Backward-wave Oscillators." IEEE Trans. Plasma Sci., **24**, 636, 1996.
• Lau, and Luginsland. "Beam Breakup Instability in an Annular Beam." J. Appl. Phys., **74**, 5877, 1993.

Russel Caflisch (Co-Principal Investigator)

Russel E. Caflisch
Resume

Birth: April 29, 1954, Charleston, WV

Address:
Mathematics Department
University of California
Los Angeles, CA 90024-1555

Tel: 310-206-0200
Fax: 310-206-6673
E-mail: caflisch@math.ucla.edu
URL: http://www.math.ucla.edu/~caflisch/

Research Interests: Materials science, mathematical finance, Monte Carlo methods, kinetic theory, plasma dynamics, fluid dynamics, PDEs.

Education

Ph.D. Mathematics, Courant Institute of Math Sciences, NYU, June 1978
M.S. Mathematics, Courant Institute of Math Sciences, NYU, February 1977
B.S. Mathematics, Michigan State University, June 1975

Awards & Honors

Invited Lecturer, International Congress of Mathematicians, Madrid 2006
Alfred P. Sloan Research Fellow, 1984-1989
Hertz Foundation Graduate Fellow, 1975-1978

Professional Experience

1989-present Professor, Mathematics Department, UCLA
2001-present Founding Member, California NanoSystems Institute (CNSI), UCLA
2002-present Professor, Materials Science & Engineering Department, UCLA
1988-1989 Professor, Courant Institute of Mathematical Sciences, NYU
1984-1988 Associate Professor, Courant Institute of Mathematical Sciences, NYU
1984-1984 Assistant Professor, Courant Institute of Mathematical Sciences, NYU
1979-1982 Assistant Professor, Department of Mathematics, Stanford University
1978-1979 Visiting Member, Courant Institute of Mathematical Sciences, NYU

Editorial Board Member:

Editor-in-Chief, Multiscale Modeling and Simulation, 2008-present
Continuum Mechanics and Thermodynamics
Applied Mathematical Finance
Multiscale Modeling and Simulation 2002-2008
Mathematical Analysis and Applications
European Journal of Applied Mathematics
Mathematical Research Letters
Transport Theory and Statistical Physics
SIAM Journal on Applied Mathematics 1989-1995
Mathematical Modeling and Numerical Analysis 1988-1995

Professional Activities:

Information Technology Planning Board, UCLA (2004-present)
Board of Trustees, Institute for Pure and Applied Mathematics (IPAM) (2003-2006)
Scientific Board, American Institute of Mathematics (AIM) Research Conference Center (2002-2006)
Chair, IT Infrastructure Committee, California NanoSystems Institute (CNSI) (2000-2005)

Chair, IT Infrastructure Committee, California NanoSystems Institute (CNSI) (2000-2005)
Chair, Org. Comm., IPAM Prog. on Math. for Nanoscale Science and Eng. (2003)
Prog. Comm., IPAM Workshop on Material Interfaces and Geometrically Based Motion(2000)
PI, Virtual Integrated Prototyping for Epitaxial Growth, UCLA/Hughes Research Labs (1997-2000)
Chair, Research Computing Committee, Div. Phys. Science, UCLA (1994-present)
Policy & Standards Committee, UCLA Connectivity Project (1995)
Director of Applied Mathematics, UCLA Mathematics Department (1994-1995)
Chair, Review committee for DOE grants in continuum mechanics (1993)
NATO Workshop on Singularities in Fluids, Plasmas and Optics, co-Director (1992)
SIAM Publications Committee (1990-1995)
DiPrima Prize Committee, SIAM (1992)
Future Carrier Technology Study, Naval Studies Board, National Academy of Sciences (1990)
University Scientists Program, Institute for Defense Analyses (1989-present)
PI, URI Center for Analysis of Heterogeneous and Nonlinear Media, NYU (1986-1989)
NSF Postdoctoral Fellowship Selection Committee (1987-1989)
Defense Science Study Group, Institute for Defense Analyses (1985-1988)
Organizer for Workshop on Mathematical Aspects of Vortex Dynamics, Leesburg, VA (1988)
Program Committee for National SIAM Meeting, Boston (1986)

Relevant and Selected Publications (over 130 total publications)

1. R.E. Caflisch, "The Fluid Dynamic Limit of the Nonlinear Boltzmann Equation," *Comm. Pure Appl. Math.*, 33 (1980), pp. 651-666.
2. "Shock Profile Solutions of the Boltzmann Equation" (with B. Nicolaenko), Comm. Math. Phys., 89 (1982), pp. 161-194.
3. "Global Existence for a Nonlinear Theory of Bubbly Liquids," Comm. Pure Appl. Math., 38 (1985) 157-166.
4. "Variance in the Sedimentation Speed of a Suspension" (with J. Luke), Phys. Fluids, 28 (1985) 759-760.
5. "Singularity Formation and Ill-Posedness for Vortex Sheets" (with O. Orellana) SIAM J. Math. Anal. 20 (1989) 293-307.
6. "Singularity Formation for Complex Solutions of the 3D Incompressible Euler Equations" Physica D, 67 (1993) 1-18.
7. "Valuation of Mortgage Backed Securities Using Brownian bridges to reduce effective dimension" (with W. Morkoff and A. Owen) J. Computational Finance, 1 (1997) 27-46.
8. R.E. Caflisch, "Monte Carlo and Quasi-Monte Carlo Methods" *Acta Numerica* (1998) 1-49.
9. S. Chen, M. Kang, B. Merriman, R.E. Caflisch, C. Ratsch, R. Fedkiw, M.F. Gyure, and S. Osher, "Level Set Method for Thin Film Epitaxial Growth", *J. Comp. Phys.* 167 (2001) 475-500.
10. L. Pareschi, R.E. Caflisch *An Implicit Monte Carlo Method for Rarefied Gas Dynamics I. The Space Homogeneous Case* J. Comp. Phys. 154 (1999) 90-116.
11. C. Wang, T. Lin, R.E. Caflisch, B. Cohen and A. Dimits, "Particle simulation of Coulomb collisions: Comparing the methods of Takizuka & Abe and Nanbu" J. Comp. Phys. to appear.
12. R.E. Caflisch and Dionisios Margetis. Anisotropic step stiffness from a kinetic model of epitaxial growth" Multiscale Modeling & Sim. to appear (2008).
13. R.E. Caflisch, C. Wang, Giacomo Dimarco, B. Cohen and A. Dimits, "A Hybrid Method for Accelerated Simulation of Coulomb Collisions in a Plasma" MMS, submitted

Facilities/Equipment

All of NumerEx's work will be performed at our offices at 2309 Renard Place SE, Suite 220, Albuquerque, NM 87106 and 401 E. State St., Suite 304, Ithaca, NY 14850. The Phase I work is mainly computational in nature. NumerEx possesses a number of LINUX-based Beowulf-class clusters for running the high performance computing plasma software, such as ICEPIC and MACH software. The NumerEx facilities meet federal, state (NM and NY), and local laws for airborne emission, waterborne effluents, external radiation levels, outdoor noise, solid and bulk waste disposal, and handling and storage of toxic and hazardous materials.

Subcontractors/Consultants

NumerEx and UCLA will work with Prof. Dimitri Vvedensky, Prof Keith Promislow, and Assistant Professor Andrew Christlieb, noted experts in renormalization group methods and plasma physics. Their resumes follow:

Dimitri Dimitrievich Vvedensky

Current Appointment

Professor of Physics, The Blackett Laboratory, Imperial College, London SW7 2AZ, United Kingdom
Tel: +44–20–7594–7605; Internet: d.vvedensky@imperial.ac.uk

Citizenship: USA

Education

Ph.D	(Materials Science)	Massachusetts Institute of Technology	1979
S.M.	(Materials Science)	Massachusetts Institute of Technology	1976
B.S.	(Mathematics)	University of Maryland	1974

Employment History

Head of Condensed Matter Theory	Imperial College	1998–2005
Professor of Theoretical Solid State Physics	Imperial College	1992–
Reader in Theoretical Solid State Physics	Imperial College	1989–1992
Lecturer in Theoretical Solid State Physics	Imperial College	1985–1989
British Petroleum Venture Research Fellow	Imperial College	1982–1985
NATO Postdoctoral Fellow	University College London	1981–1982
Research Fellow	Massachusetts Institute of Technology	1979–1981

Concurrent and Visiting Appointments (1997–)

Guest Professor	Institut de Recherche sur les Phénomènes Hors Équilibre, Université de Provence	2008
Guest Professor	Institut de Recherche sur les Phénomènes Hors Équilibre, Université de Provence	2007
Senior Fellow	Institute for Pure and Applied Mathematics, University of California, Los Angeles	2005
Wilhelm Röntgen Professor	Fakultät für Physik und Astronomie, Universität Würzburg	1999
Guest Professor	Laboratorium für Festkörperphysik, Eidgenössische Technische Hochschule Zürich	1998
Visiting Professor	Department of Mathematics, University of California, Los Angeles	1997–2003

Professional and Administrative Duties (1997–)

Scientific committee, *5th International Congress of Material Sciences and Engineering*	2008
Scientific committee, *Material Informatics and Density Functional Theory*	2008
International committee, *Cargèse Summer School on NanoSteps: Self-Organized Nanostructures on Crystal Surfaces*	2008
Organizing committee, *3rd International Workshop on DFT Applied to Metals and Alloys*	2007
Organizing committee, *International Workshop on Physics and Technology of Thin Films*	2006
Co-organizer, IPAM Workshop on *Multiscale Modeling in Condensed Matter and Materials Sciences*	2005
Co-organizer, ICCG14 Topical Session on *Self-Assembled Nanostructures for Quantum Dots*	2004
Organizer, EPS Condensed Matter Division Colloquium on *Quantum Dots for Quantum Computing*	2004
Review Panel, Research Council for Natural Sciences and Engineering, Academy of Finland	2003
Director, NATO ARW on *Quantum Dots: Fundamentals, Applications, Frontiers*	2003
Co-organizer, MPI–PKS Seminar on *Models of Epitaxial Crystal Growth*	2002
Co-organizer, NATO ARW on *Atomistic Aspects of Epitaxial Growth*	2001
Board of Directors, Society for Engineering Science	1999–2000

Doctoral Thesis Supervision (1997–)

Makoto Itoh (April 1997–September 1999)
Atomic-Scale Homoepitaxial Growth Simulations of Reconstructed III–V Surfaces

Raffaele Vardavas (October 1998–March 2002)
Fluctuations and Scaling in One-Dimensional Irreversible Film Growth Models

Alessio Farhadi (October 2000–April 2004)
Statistical Properties of Light Transmission through Clouds

Alvin Chua (April 2002–July 2004)
Coarse-Grained Kinetics of Nonequilibrium Systems

Christoph Haselwandter (October 2003–2006)
Multiscale Theory of Fluctuating Interfaces

Bahman Farnudi (October 1997–April 2008)
Scaling and Universality in Deposition Models of Growth

Alberto Cozzini (October 2006–)

Masters Thesis Supervision (1997–)

Chiara Baggio (2000–2001)
Equations of Motion for Discrete Models of Epitaxial Growth

Sabrina Rabello (2002–2003)
The Edwards-Wilkinson Model of Epitaxial Growth

Georg Schusteritsch (2005–2006)
Theoretical Descriptions of Epitaxially Grown Low-Dimensional Semiconductor Nanostructures

Honors and Awards

Fellow, American Physical Society	2007
Fellow, Institute of Physics	2005
Imperial College Award for Teaching Excellence	2004
Wilhelm Röntgen Professorship, Institüt für Theoretische Physik, Universität Würzburg	1999
Imperial College Award for Teaching Excellence	1996
NATO Postdoctoral Fellowship	1981
American Society for Testing and Materials Student Award	1974
Tau Beta Pi (American National Engineering Honor Society)	1973
University Scholarship	1970–1974

Press Citations

UK welcomes help from Japan
D. Swinbanks and P. Aldhous, *Nature*, January 25, 1990, p. 300.

Japan chips in to the UK
S. Croft, *Physics World*, March 1990, pp. 8–9.

Japanese in 6£m research deal with UK universities
P. Large, *The Guardian*, March 17, 1990, p. 9.

Atomic arrangements brings Japanese to UK universities
Metals and Materials, April 1990, p. 280.

Anglo–Japanese project
Chemistry in Britain, May 1990.

Rising funds
J. Schofield, *The Guardian*, July 19, 1990, p. 29.

Links that mean good business
I. Katz and S. Surkes, *The Sunday Correspondent*, July 22, 1990.

Mystery of quantum dots to be revealed
S. Bush, *Electronics Weekly*, January 27, 2003

Keith PROMISLOW

Professional Preparation

North Carolina State University	Mathematics	B.S.	1986
North Carolina State University	Physics	B.S.	1986
Indiana University	Applied Math	Ph.D.	1991
Pennsylvania State University	Applied Math		1991-95
Université de Paris XI, Orsay	Applied Math		1992-93

Positions Held

2006-Current	Executive Committee/Co-Founder	MCIAM†
2007-Current	Professor	Michigan State University
2003-06	Associate Professor	Michigan State University
2000-03	Associate Professor	Simon Fraser University
2001-02	Visiting Professor	Brown University
1995-00	Assistant Professor	Simon Fraser University
1991-95	NSF Postdoctoral Fellow	Pennsylvania State University
1992-93	NATO Postdoctoral Fellow	Université de Paris XI, Orsay

Publications related to proposal (45 total)

[1] R. Moore and K. Promislow, The semi-strong limit of multipulse interaction in a thermally driven optical system, *J. Diff. Eqs.* accepted March 2008.

[2] Mohar Guha and K. Promislow, Front propagation in a noisy, nonsmooth excitable media, *Discrete and Cont. Dyn. Systems, Ser. A* submitted Aug 2007.

[3] P. A. C. Chang and K. Promislow, Nonlinear stability of oscillatory pulses in the parametric nonlinear Schrödinger equation, *Nonlinearity* **20** 743-763 (2007).

[4] A. Doelman, T. Kaper, K. Promislow, Nonlinear asymptotic stability of the semi-strong pulse dynamics in a regularized Gierer-Meinhardt model, *SIMA* **38** (6) (2007) 1760-1787.

[5] R. Moore and K. Promislow, Renormalization group reduction of pulse dynamics in thermally loaded optical parametric oscillators, *Physica D* **206** (2005) 62-81.

[6] Keith Promislow, A renormalization method for modulational stability of quasi-steady patterns in dispersive systems, *SIMA* **33** No. 6 (2002), 1455-1482.

Other significant publications

[7] Z. Zhang, A. Marble, B. MacMillian, K. Promislow, J. Martin, H. Wang, B. Balcom, Spatial and Temporal Mapping of Water Content across Nafion Membranes under Wetting and Drying Conditions, *J. Magnetic Resonance* submitted Jan. 2008.

[8] K. Promislow, P. Chang, H. Haas, and B. Wetton, A Two Phase Unit Cell Model for Slow Transients in Polymer Electrolyte Membrane Fuel Cells, *J. Electrochem. Soc.* submitted Oct. 2007.

[9] I. Nazarov and K. Promislow, The impact of membrane constraint on PEM fuel cell water management, *J. Electrochem. Soc.* **154** (7) (2007).

[10] A. Shah, G.-S. Kim, and K. Promislow, Mathematical modelling of the catalyst layer of a polymer electrolyte fuel cell, *IMA J. Applied Math.* **72** (2007), 1-29.

[11] P. A. C. Chang, G.-S. Kim, K. Promislow, B. Wetton, Reduced dimensional computational models of polymer electrolyte membrane fuel cell stacks, *J. Comp. Physics* **223** 797-821 (2007).

[12] J. St-Pierre, B. Wetton, G.S.-Kim, K. Promislow, Limiting current operation of proton exchange membrane fuel cells, *J. Electrochem. Soc.* **154** (2) (2007) B186-B193.

Synergistic Activities

[1] Developed the Fuel Cell working group at Michigan State University with Greg Swain (Chemistry) and Greg Baker (Chemistry), which meets monthly to direct common research projects. Developed contacts with the Fuel Cell modeling group at Ford Motors, this resulted in submission of a 2006 Univerisity Research Project (URP) proposal to Ford Motors.

[2] Scientific leader of the interdisciplinary Computational Fuel Cell Dynamics group at SFU/UBC: 7 year industrial partnership with Ballard Power Systems, world leader in PEM fuel cells for automotive applications. Preparation of Development of computational software for fuel cell design. Has supported 5 postdoctoral fellows, and funded 8 graduate students. Recognized with PIMS Industrial Outreach award 2000, Science Council of BC Young Innovator 2002.

[3] Co-editor, with PI S.J. Paddison, of Springer book *Device and Materials Modeling of PEM Fuel Cells*, to appear in 2006, approximately 400 pages, 16 chapters from different authors, including the PIs.

[4] Organization of international conferences on PEM fuel cell modeling: Banff Internationl Research Station: Computational Fuel Cell Dynamics III, March 19-24, 2005, Computational Fuel Cell Dynamics II, April 19-24, 2003, and the Pacific Institute of Mathematical Sciences workshop, Computational Fuel Cell Dynamics June 4-8, 2001.

[5] Co-founder, with Gang Bao (MSU), of the Michigan Center for Industrial Mathematics (2005) which seeks collaborations with industrial groups for longterm partnerships. Current industries include Ford Motors, Pfizer, KLA Tenkor, and Honeywell. The center has a strong educational component, overseeing the industrial internship program and the professional MSc in industrial mathematics, which as graduated 40+ MSc students over the past 5 years.

Thesis Advisor (3 PhD) and PostDoctoral Fellow Sponsor (9 PDF)

Hang Zhang	PDF	Current	Albert Cohen	PDF	Current
Greg Hayrepetyan	PhD	Current	Igor Nazarov	PDF	Lyman Briggs Col.
Mohar Guha	PhD	U. of Michigan	Paul Chang	PhD	UBC
Richard Moore	PDF	NJIT	Peter Berg	PDF	UOIT
Arian Novrusi	PDF	U. of Ottawa	Ricardo Carretero	PDF	San Diego State
Radu Bradean	PDF	Ballard Power	John Stockie	PDF	Simon Fraser Univ.

Biographical Sketch
Andrew J. Christlieb

1. **Professional Preparation**

Institution	Major/Area	Degree/Training
Univ. of Michigan-Dearborn	Mathematics	BS (1991 - 1996)
Univ. of Michigan-Dearborn	Electrical Engin.	BS (1991 - 1996)
Univ. of Michigan-Dearborn	Engin. Math	BS (1991 - 1996)
Univ. of Wisconsin-Madison	Applied Math	MS (1996 - 1998)
Univ. of Wisconsin-Madison	Mathematics	Ph.D. (1998 - 2001)
Univ. of Michigan-Ann Arbor	Aerospace Engin.	PostDoc (2001 - 2002)

2. **Appointments**

Date Start/End	Title	Institution
5/06 - Present	Assis. Prof.	Department of Mathematics Michigan State University
9/02 - 5/06	Term Assis. Prof.	Department of Mathematics University of Michigan-Ann Arbor
7/01 - 9/02	Research Fellow	Department of Aerospace Engin. University of Michigan-Ann Arbor

3. **Relevant Publications**

   (a) Journal

   i. A.J. Christlieb, R. Krasny and J.P. Verboncoeur, "Efficient Particle Simulation of a Virtual Cathode using a Grid-Free Treecode Poisson Solver", *IEEE Trans. Plasma Sci.*, 32 (2): 384-389 Part 1 APR 2004

   ii. A.J. Christlieb, R. Krasny and J.P. Verboncoeur, "A Treecode Algorithm for Simulating Electron Dynamics in a Penning-Malmberg Trap", *Comp. Phys. Comm.*, 164: 306-310, 2004

   iii. A.J. Christlieb, R. Krasny, J.P. Verboncoeur, J. Emhoff and I.D. Boyd , "Grid-Free Plasma Simulation Techniques", *IEEE Trans. Plasma Sci.*, 34(2): 149-165 Part 1 APR 2006

   iv. A. VanderWyst, A. Christlieb, M. Sussman, and I.D. Boyd, "Simulation of Liquid Metal Droplets from Field Emission", *Comm. in Comp. Phys.* 2(4): 640-661, 2007.

   v. A.J. Christlieb and S. Olson , "Grid-Free Direct Simulation Monte Carlo", Submitted

   (b) Thesis

   i. 'Computational Methods for Long Mean Free Path Problems', Christlieb A.J, Ph. D. thesis, University of Wisconsin-Madison, 2001.

4. **Synergistic Activities**

   (a) **Conferences:** I have presented on grid-free methods at several conferences, where I have received positive feed back. These include: IEEE International Conference on Plasma Science (2003,2004,*invited 2005*), APS Divstion of Plasma Physics (2004,2005,2007), and SIAM Computational Science and Engineering (2005,2007).

   (b) **Mentoring:** I have been a Co-Advisor to Jerry Emhoff (Aerospace, PhD 2005), Spencer Olsion (Physics, PhD 2006) and Anton VanderWyst (Aerospace, PhD 2006) for at least half of the work related to there thesis. I have mentored two undergraduates; Stephen Marin and Benjamin Sonday. Stephen was a summer REU student in 2005 and his work was on simulating the dynamics of point vortices. Benjamin was supported as research assistant as part of my AFOSR grant. Benjamin's work concerned the extension of point insertion methods to phase space problems.

   (c) **Teaching:** In addition to calculus 1, 2 and linear algebra, I have taught undergraduate numerical analysis and and graduate numerical analysis of ODE's and PDE's, undergraduate and graduate dynamical systems, as well as undergraduate PDE's. As part of the Current CSUMS proposal from MSU, I plans to develop a new course at the undergraduate level focusing on Numeral PDE's.

5. **Grants**

   - (2007–2010) Air Force Office of Scientific Research – **Young Investigator Award** – Computational Mathematics, *Grid-Free Electromagnetic Plasma Simulations*, PI: A.J. Christlieb, ($300, 156 total direct cost)
   - (2007–2009) Air Force Research Lab – IPA – Kirtland Air Force Base, Extended Particlein-Cell, PI: A.J. Christlieb, ($64, 000 total direct cost)

6. **Collaborators & Other Affiliations**

Recent Collaborators:

Name	Title	Institution	Department
Russel E. Caflisch	Prof.	Univ. of California-LA	Mathematics
Jean-Luc Cambier	Senior Sci.	AFRL Edward's	Advanced
	Tech. Staff	Edward's	Propulsion
Robert Krasny	Prof.	Univ. of Michigan	Mathematics
Mark Sussman	Asso. Prof.	Florida State Univ.	Mathematics
John P. Verboncoeur	Prof.	University of California Berkeley	ECE

Advisors:

Iain D. Boyd	Prof.	Univ. of Michigan	Postdoctoral
W. Nicolas G. Hitchon	Prof.	Univ. of Wisconsin	Graduate

Prior, Current, Pending Support of Similar Proposals or Awards

In addition to the Phase I STTR from AFOSR that the current Phase II effort is based upon, NumerEx currently is under contract to the Air Force Research Laboratory through the DETAR contract to provide support for the development of both ICEPIC and MACH as well as application of these software packages to support development of directed energy technology. As part of this work, NumerEx develops heuristic models of high power microwave devices and studies the multiple scale physics associated with the transition from quantum mechanical field emission to classical space-charge limited flows, but not in the formal framework of renormalization groups. Thus, this work does not touch on this proposed effort. Additionally, NumerEx is investigating both fluid and kinetic physics associated with transient plasma ignition for the Office of Naval Research, but fluid/kinetic coupling is not performed.

UCLA's current contracts for Prof. Caflisch are listed below. Note that only two combine plasma physics with multiple scale computation. The first contract, with the Department of Energy, while dealing with multi-scale plasma issues, does not deal just with renormalization group methods. The second contract with multi-scale plasma physics is the Phase I STTR from AFOSR that the current Phase II effort is based upon. As such, these do not conflict with the current effort to develop the renormalization group method in the plasma physics context. This proposal is the only support pending at this time.

CURRENT SUPPORT FOR RUSSEL E. CAFLISCH

MARCO (Wang, K.) 9/1/03 – 8/31/09 1 month summer
Microelectronics Advanced Research Corp. $409,762
"Functional Engineered Nano Architectonics"

NSF DMS-0402276 (Caflisch, R.) 7/1/04-6/30/08 as needed
NSF $338,080
"Kinetic Pathways to Formation and Self-Organization of Quantum Dots"

NSF DMS-0354488 (Caflisch, R.) 7/1/04-6/30/08
NSF $337,700
"FRG: Singularity Formation for the Three-Dimensional Euler Equations and Related Problems"

DOE DE-FG02-05ER25710 (Caflisch, R.) 9/1/05-8/31/08 1 month summer
DOE $630,901
"Multiscale Mathematics for Plasma Kinetics Spanning Multiple Collisionality Regimes"

NSF DMS-0707557 (Caflisch, R.) 7/01/07-06/30/10 1 month summer
NSF $236,020
"Collaborative /research: Numerics and Analysis of Singularities for the Euler Equations"

NUMEREX Award (Caflisch, R.) 9/15/07-06/14/08
DOD $50,006
"Development of a Renormalization Group Approach to Multi-Scale Plasma Physics Computation"

NumerEx
2309 Renard Place SE, Suite 220
Albuquerque, New Mexico 87106-4259

NumerEx Contact:

Michael H. Frese, 505-842-0074/FAX 505-842-5699

Date: 3/20/08
Quote for: AFOSR
Solicitation No.: FA9550-07-C-0131
Phase II -- F2-4459
Title: Development of a Renormalization Group Approach to Multi-Scale Plasma Physics Computation

Cost Estimate--Loaded Rates

Category	FY09 10/1/08 - 9/30/09			FY 10 10/1/09 - 9/30/10			Total	
	Hours	Loaded Rate*	Amount	Hours	Loaded Rate*	Amount	Hours	Amount
NumerEx-Site								
Sr Scntst/Engr	65	177.86	11,561	76	186.35	14,163	141	25,724
Sr Scntst/Engr	57	148.77	8,480	64	155.86	9,975	121	8,480
Scntst/Engr	413	154.33	63,739	451	161.69	72,923	864	136,662
Clerical/Admn	61	68.02	4,149	59	71.25	4,204	120	8,353
Total Labor	596		87,929	650		101,265	1246	189,194
Research Institution**			150,001			149,999		300,000
Subcontractor***			75,015			75,015		150,030
Consultant			20,000			20,000		40,000
Other Direct Costs			848			1,747		2,595
Total Hours/Costs	596		333,793	650		348,025	1246	681,818
Fee		10.0%	33,379		10.0%	34,803		68,182
Subtotal			367,172			382,828		750,000
NMGRT			0			0		0
Total Price			367,172			382,828		750,000

*Loaded rates are approximate, calculated from hours and amounts.
**See UCLA quote.
***See MSU quote.

Other Direct Costs:
Ithaca, NY to Los Angeles, CA--three trips
One person; 2.5 days/2 nights (one night traveling)
(118/64)

Air	445	Car	110
M&IE	160	Parking	15
Hotel	118		848

Includes 3% inflator per year

ORGANIZATION: The Regents of the University of California

PI: Caflisch Proposal to NUMEREX for STTR

	CALC 1	CALC 2	CALC	2008-09	2009-10	TOTAL
A. Senior Personnel	SAL YR 1	SAL YR 2				
1 Russel Caflisch	$191,600	$201,180	1 mo.	$21,289	$22,353	$43,642
2		$0		$0	$0	$0
Total Senior Personnel				$21,289	$22,353	$43,642
B. Other Personnel						
1. Postdoc (includes .5%)	$56,785	$57,921	0	$0	$0	$0
2. Graduate Student	$20,740	$21,155	1	$20,740	$21,155	$41,895
Total Salaries				$42,029	$43,508	$85,537
C. Fringe Benefits						
Faculty- Summer	12.7%	12.7%		$2,704	$2,839	$5,543
Postdoc	17.0%	17.0%		$0	$0	$0
Student	2.1%	2.1%		$436	$444	$880
Non Resident Tuition NRT)	$14,694	$15,429	1	$11,021	$11,572	$22,592
Fee Remission	$8,656	$9,089	1	$8,656	$9,089	$17,745
Fringe Benefits				$22,816	$23,944	$46,760
Total Salaries, Benefits				$64,845	$67,452	$132,297
D. Equipment				$0	$0	$0
Items under $5K subject to overhead.						
E. Travel				$4,000	$3,000	$7,000
F. Participant Costs						
Stipend				$0	$0	$0
Subsistence						$0
Total Participant Costs				$0	$0	$0
				YEAR 1	YEAR 2	TOTAL
G. Other Direct Costs						
1. Materials & Supplies				$2,000	$850	$2,850
2. Publication Costs				$260	$147	$407
3. Equipment items less than $5K				$0	$0	$0
4. Subcontract - Imperial College & Vvedensky				$40,900	$40,900	$81,800
Total Other Costs				$43,160	$41,897	$85,057
H. Total Direct Costs				$112,005	$112,349	$224,354
I. Indirect Costs	54.00%			$27,771	$27,426	$55,197
Subcontract in London	25.00%			$10,225	$10,225	
J. Total Costs				$150,001	$149,999	$300,000

Michigan State University (MSU)

1st yr			2nd year		
Cohen	1/4 salary AY	11,250	Cohen	1/4 salary AY	11,250
	fringes	2,813		fringes	2,813
		14,063			14,063
Promislow	.5 su	5,889	Promislow	.5 su	5,889
	fringes	451		fringes	451
		6,339			6,339
Promislow	1 crse buyout	17,000	Promislow	1 crse buyout	17,000
	fringes	5,950		fringes	5,950
		22,950			22,950
Supplies and short term visitors		3,500	Supplies and short term visitors		3,500
Travel		2,500	Travel		2,500
Total Direct		49,352	Total Direct		49,352
Overhead		25,663	Overhead		25,663
Total		75,015	Total		75,015

Small Business Technology Transfer (STTR) Program
Cost Proposal

Firm:	NumerEx
Address:	2309 Renard Place SE Suite 220 Albuquerque, NM 87106-4259
Location Where Work Will Be Performed:	NumerEx's Ithaca Office, UCLA, and MSU

Proposal #: F2-4459 — Title of Proposed Effort: Development of a Renormalization Group Approach to Multi-Scale Plasma Physics Computation

Firm's Taxpayer ID: 76-0811150 — CAGE Code: 0XLG7 — DUNS: 612410605

Topic Number: AF07-T022

TOTAL DOLLAR AMOUNT FOR THIS PROPOSAL: **$750,000.00**

DIRECT LABOR:	Phase II:			Option:		
Category and/or Individual:	Rate/Hour	Est.Hours	Cost	Rate/Hour	Est.Hours	Cost
Sr Scientist1	76.61	65	4,979.65	80.26	76	6,099.76
Sr Scientist2	64.08	57	3,652.56	67.14	64	4,296.96
Scientist	66.48	413	27,456.24	69.65	451	31,412.15
Administrative	29.30	61	1,787.30	30.70	59	1,811.30
Subtotal Direct Labor (DL):			37,875.75			43,620.17
Fringe Benefits, if not included in Overhead, (rate 0.0000 %) x DL =			0.00			0.00
Labor Overhead (rate 132.1500 %) x (DL + Fringe) =			50,052.80			57,644.05
Total Direct Labor (TDL):			87,928.55			101,264.22

DIRECT MATERIAL COSTS:	Phase II:	Option:
Subtotal Direct Materials Costs (DM):	0.00	0.00
Material Overhead (rate 0.0000 %) x DM:	0.00	0.00
Total Direct Materials Costs (TDM):	0.00	0.00

OTHER DIRECT COSTS:	Phase II:	Option:
Research Institution (UCLA)	150,001.00	149,999.00
Subcontractor (MSU)	75,015.00	75,015.00
Consultant (Christlieb)	20,000.00	20,000.00
Travel	848.15	1,747.26
Subtotal Other Direct Costs (ODC):	245,864.15	246,761.26
Direct Cost Overhead (rate 0.0000 %) x ODC	0.00	0.00
Total Other Direct Costs (TODC):	245,864.15	246,761.26

G&A (rate 0.0000 %) x (base: TDL)	0.00	0.00
Total Cost:	333,792.70	348,025.48
Fee or Profit (rate 10.0000 %)	33,379.27	34,802.55
TOTAL ESTIMATED COST:	**367,171.97**	**382,828.03**

Explanatory material relating to the cost proposal:

Travel: Ithaca, NY to Los Angeles, CA--three trips. Air-$445, M&IE-$160, Hotel-$118, Car-$110, Parking-$15. Second year includes a 3% inflator. UCLA budget includes time for Dr. Caflisch, one postdoc and one graduate student. MSU includes tiem for Cohen and Promislow. The Consultant's rate is $115/hour plus travel expenses.

>>Has any executive agency of the United States Government performed any review of your accounts or records in connection with any other government prime contract or subcontract within the past twelve months? Yes

If Yes, please provide the following:

Reviewing Office: DCAA

Individual: — Phone: 505-248-5000

Address: 505 Marquette Avenue NW
Suite 1100

Albuquerque, NM 87102

>>Will you require the use of any government property in the performance of this proposal? No

>>Specify the type of payment desired: Partial payments

Company Commercialization Report
Summary Page

Firm Name:	**NumerEx**	**Point of Contact:**	**Michael H. Frese**
Mail Address:	**2309 Renard Place SE**	**Phone Number:**	**(505) 842-0074**
	Suite 220	**Fax Number:**	**(505) 842-5699**
	Albuquerque, NM 87106-4259	**E-Mail:**	**Michael.Frese@numerex.com**
Phone:	**(505) 842-0074**		

<u>Commercialization Achievement Index</u>: N/A

This Index is a measure of how commercialization resulting from the proposer's prior phase II SBIR/STTR awards (from 2005 and before) compares with the commercialization resulting from groups of DoD SBIR/STTR projects selected at random from comparable time periods. (Commercialization includes both military and private sector markets.) The index score is a percentile ranking which ranges from 100 (highest) to 0 (lowest). Its statistical meaning is described in detail at http://www.DoDSBIR.net/Submission/CompanyCommercialization/Instructions/DefCAI.asp.

An Index score is only calculated for proposers that have received at least 4 phase II awards in years up to and including 2005.

(END OF SUMMARY)

Company Commercialization Report
Full Report and Company Certification

Commercialization Achievement Index:	**N/A**	
Phase I Awards:	**10**	Number of Employees in **1995**: **4**
Phase II Awards:	**3**	Current Number of Employees: **14**
Number of Patents resulting from SBIR/STTR:	**0**	
FIRM's total revenue:	**$1,000,000-$4,999,999**	Year Founded: **1988**
SBIR/STTR Funding as % of revenue:	**11**%	IPO resulting from SBIR/STTR: **No**

PHASE II PROJECTS:

Agency: NASA Year of Award: 1995 Topic #: 09.06 Contract #: NAS7-1380

Project Title: Innovative Design for Stationary Plasma Thrusters

Sales to:	(a)DoD/Primes: $0	(b)Other Federal Agencies: $0	(c)Export: $0
	(d)Private Sector: $0	(e)Others: $0	(f)3rd Party: $0
Additional Investment from:	(a)DoD: $0	(b)Other Federal Agencies: $0	(c)Private Sector: $0
	(d)Others: $0		

Used in Federal system or acquisition program?: No

Is the technology developed under this project related to manufacturing? No

Has the technololgy developed under this project achieved a cost saving or cost avoidance for the government or end user? NO

Agency: AF Year of Award: 1997 Topic #: DNA 93-015 Contract #: F40600-97-C-0018

Project Title: An Improved Plasma Opending Swtich for DECADE

Sales to:	(a)DoD/Primes: $0	(b)Other Federal Agencies: $0	(c)Export: $0
	(d)Private Sector: $0	(e)Others: $0	(f)3rd Party: $0
Additional Investment from:	(a)DoD: $0	(b)Other Federal Agencies: $0	(c)Private Sector: $0

(d)Others: $0

Used in Federal system or acquisition program?: No
Is the technology developed under this project related to manufacturing? No
Has the technololgy developed under this project achieved a cost saving or cost avoidance for the government or end user? NO

Agency: AF Year of Award: 2006 Topic #: AF05-163 Contract #: FA8651-06-C-0140

Project Title: Towards Weaponizing Next-Generation Volumetric Explosives--Computational Research and Development of Robust, Flexible, and Compact Munitions Based on Advanced Fuel-Air and Energetic Material Mixtures

Sales to:	(a)DoD/Primes: $0	(b)Other Federal Agencies: $0	(c)Export: $0
	(d)Private Sector: $0	(e)Others: $0	(f)3rd Party: $0
Additional Investment from:	(a)DoD: $0	(b)Other Federal Agencies: $0	(c)Private Sector: $0
	(d)Others: $0		

Used in Federal system or acquisition program?: No
Is the technology developed under this project related to manufacturing? No
Has the technololgy developed under this project achieved a cost saving or cost avoidance for the government or end user? NO

Firm Information Last Updated on: 3/20/2008 3:22:48 PM

Company Commercialization Information Last Updated on: 9/18/2007 12:08:36 PM

VERIFICATION AND VALIDATION OF RENORMALIZATION GROUP INSPIRE PARTICLE WEIGHTS FOR PIC CODES*

J.W. Luginsland
NumerEx, LLC
Ithaca, NY 14850, USA

A. Christlieb
Michigan State University, East Lansing, MI, USA

R. Caflisch
UCLA, Los Angeles, CA, USA

Simulations of dense kinetic plasmas are an area of active research. A variety of devices from high power microwave devices to Hall thrusters involve situations with dense fluidlike plasmas coexisting with important kinetic non-Maxwellian particle distributions. These plasmas exhibit a range of length and time scales, making accurate simulation a challenging and computationally intensive task. Currently, we are applying renormalization group methods to provide a systematic means to investigate multi-scale plasma behavior from the kinetic to the MHD regime. One development has been the discovery of a relationship between traditional particle-in-cell weights and the renormalized charge associated with Debye shielding. The development of algorithms to handle these multi-scale circumstances is facilitated by high-fidelity test problems suitable for verification and validation studies. Specifically, we report on the development of ordinary differential equations appropriate for studying kinetic plasmas with short Debye lengths relative to the system size. Via analytic and numerical solutions, we study the impact of collective shielding on Langmuir waves. Both our analytic and PIC simulations indicate the existence of harmonic mixing driven by nonlinear excitation of Langmuir waves in highly shielded (dense) plasmas.

* Work supported by Air Force Office of Scientific Research

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ELECTRON HOP FUNNEL MEASUREMENT AND SIMULATION FOR VARIOUS GEOMETRIES AND MATERIALS*

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J. Luginsland
NumerEx, Ithaca, NY 14850, USA

Vacuum electron hop funnel devices can be used to collect and spatially average electron emission current[1] from field emission arrays (FEAs). At the proper operating voltage the funnels provide unity gain of the injected emission current. The resulting beams can be more uniform than from typical FEAs, and the funnel technique might be used to generate very uniform electron sheet beams. In the work described here, hop funnels have been fabricated from Low Temperature Co-fired Ceramic (LTCC). Other materials will also be tested including SiO_2 and Macor in order to measure and simulate the effect that different secondary emission yield curves has on the insulating surface charge distribution and I-V characteristics. For each insulating material, hop funnel structures with varying wall slopes will be constructed to measure the relationship of the slope of the hop funnel wall with the "knee" of the I-V curve. In addition, the electron energy distribution of the hop funnel electron beam, as well as the beam spread, will be measured for each material and wall slope to create a matrix of data which will be used to determine an optimal hop funnel structure for a minimal average transverse electron energy component of the exit beam. The data will be compared against the predictions of the particle trajectory computer simulation Lorentz[2] and will be used to refine the statistical parameters in the numerical simulation. Based on the results, a novel slit design will be constructed of LTCC to be used with the FEAs to generate an electron sheet beam.

1. B H W Hendriks, G G P van Gorkom, N Lambert, and S T de Zwart, J. Phys. D: Appl. Phys. **30** pp. 1252–1264 (1997).
2. www.integratedsoft.com

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* This research is supported by the Air Force Office of Scientific Research (AFOSR) under the DEPSCOR Grant # FA9550-08-1-0396 and by the Electrical and Computer Engineering Department at Boise State University. FEAs are supplied by Stellar Micro Devices of Austin, TX.

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ROLE OF IONS IN A CROSSED-FIELD DIODE II: MONTE CARLO COLLISIONS

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J.W. Luginsland
NumerEx, Ithaca, NY 14850, USA

The effect of ions in a magnetically insulated crossed-field gap is studied using a particle-in-cell simulation with Monte Carlo collisions (MCC). (Code available through the PTSG at UC Berkeley.) These results are compared with the predictions from single particle orbit, shear flow models and previous particle-in-cell simulations in which the ions were modeled as a sheet of charge fixed at different positions within the gap[1]. The results of this experiment indicate that the diode loses insulation much more rapidly than shown in the immobile ion sheet model. The reasons for this increased rate of electron migration toward the anode are that the ions in this simulation are mobile and that the effects of MCC are being taken into account. Thus, ambipolar transport plays a role in the migration as does the fact that ions are being created throughout the gap by collisions. The implications of these findings, as suggested in previous work, are that of pulse shortening in relativistic magnetrons and bipolar flows in pulsed power systems.

1. Y.Y. Lau, J.W. Luginsland, K.L. Cartwright, and M.D. Haworth, "Role of ions in a crossed-field diode", Phys. Rev. Lett. 98 (2007).

A Renormalization Group Approach to Particle-in-Cell Weighting for Dense Plasmas

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Russel Caflisch
UCLA., Los Angeles, CA USA

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Imperial College, London, UK

The Particle-in-Cell (PIC) method offer a robust means to tackle a wide diversity of kinetic plasma physics problems in a variety of application areas. One challenging class of problems for PIC, however, deals with the simulation of dense plasmas. The dense plasma introduces both short time scale (via the plasma frequency) and short wavelength (via the Debye length) features that must be resolved for stability and accuracy. At sufficient density, it becomes natural to simulate these dense plasmas with either implicit kinetic methods or fluid methods (either two-fluid, or magneto-hydrodynamic). In many cases, however, the dense plasma is restricted to a relatively small volume of the calculation, while the rest the problem remains essentially kinetic. For example, high power microwave devices can develop dense plasma phenomena just near the region of the anode. The rest of the problem, however, requires fully explicit, kinetic methods to study the beam/wave interaction in tenuous electron plasma. We report on the development of a heuristic[1] renormalization method that rescales the bare electron charge assuming the existence of a screening cloud of dense plasma in a manner identical to the formation of the Debye sheath. We use this renormalization to provide an interpretation of the standard PIC weighting of particle information to the grid. This provides a natural scheme to interpret grid heating, and offers a means to systematically increase the accuracy of the particle weighting based on local information, such as plasma density and co-located grid resolution, to achieve desired fidelity. The new technique offers the potential of progressively higher order particle methods at reasonable computational costs.

1. W.D. McComb, *Renormalization methods*, Oxford University Press, Oxford, 2004.

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* Work supported by AFOSR