Fall 2010
Applied Physics E4990
Kinetic Theory and Simulation of Plasmas

Tuesday 4:10 - 6:40 pm; Room 327, Mudd

Instructor: Wei-li Lee [wwl2113@columbia.edu; 609-243-2647]

Prerequisite: Introduction to Plasma Physics

1. Basics of Kinetic Theory
2. Kinetic Plasma Simulation
3. Simulation Models and Properties
4. Perturbative Particle Simulation
5. Gyrokinetic Theory and Simulation
6. Microinstabilities: linear and nonlinear properties
7. Shear-Alfven Waves: finite-β effects on microturbulence
8. Gyrokinetic MHD
9. High Frequency Gyrokinetics
10. Integrated Simulation
11. Applications to (Magnetic and Beam) Fusion and Space Physics

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Unique features of kinetic plasma physics

- Governing equations are based on Hamiltonian dynamics
  - -- 6 dimensional phase space (configuration & velocity)
  - -- Known conservation properties
- Collisionless Landau Damping at all wavelengths
  - -- velocity space effects
- Debye shielding effects in configuration space
  - -- neutral plasmas
- Resolutions in configuration and velocity space
  - -- determined by physics of interest
- Highly nonlinear global phenomena
  - -- multiscale simulation in time and space

Fully Electromagnetic Vlasov-Maxwell System

$$\frac{dF}{dt} \equiv \frac{\partial F}{\partial t} + \mathbf{v}\cdot\frac{\partial F}{\partial \mathbf{x}} + \frac{q}{m}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\frac{\partial F}{\partial \mathbf{v}} = 0$$ Vlasov equation

$$\nabla\cdot\mathbf{E} = 4\pi\rho \qquad \rho = e\int (F_i - F_e)d\mathbf{v}$$ Coulomb's law

$$\nabla\times\mathbf{B} = \frac{4\pi}{c}\mathbf{J} + \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t} \qquad \mathbf{J} = e\int \mathbf{v}(F_i - F_e)d\mathbf{v}$$ Ampere's law

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$$ Faraday's law

$$\nabla\cdot\mathbf{B} = 0$$ No magnetic monopole

Let $\mathbf{Q} = \mathbf{Q}^L + \mathbf{Q}^T$ such that $\nabla\cdot\mathbf{Q}^T = 0$ and $\nabla\times\mathbf{Q}^L = 0$

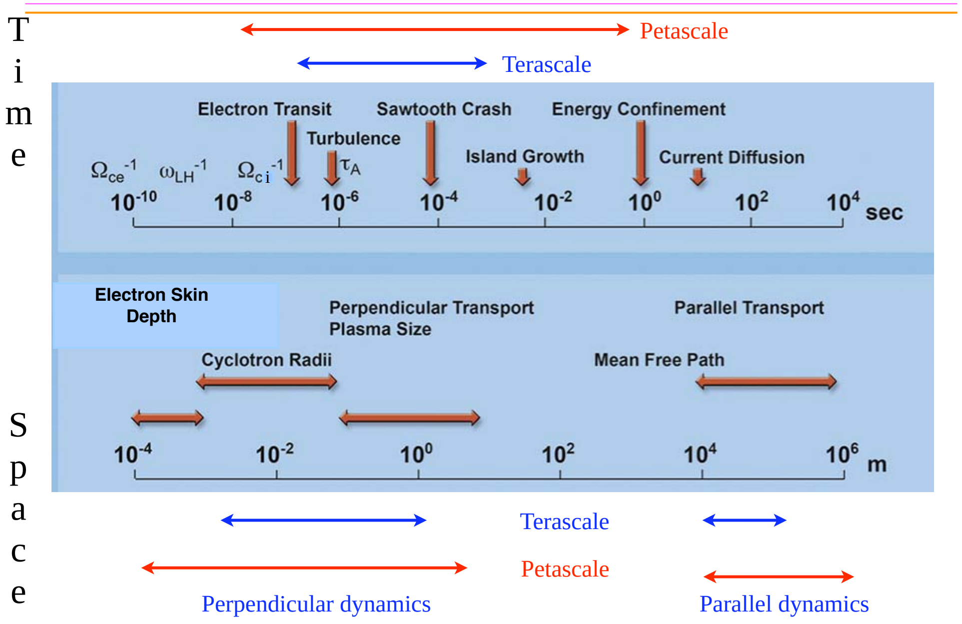
$$\nabla\cdot\mathbf{E}^L = 4\pi\rho$$

$$\nabla\times\mathbf{B}^T = \frac{4\pi}{c}\mathbf{J}^T + \frac{1}{c}\frac{\partial\mathbf{E}^T}{\partial t} \qquad 0 = \frac{4\pi}{c}\mathbf{J}^L + \frac{1}{c}\frac{\partial\mathbf{E}^L}{\partial t}$$ ---- can also be obtained from Vlasov + Poisson

$$\nabla\times\mathbf{E}^T = -\frac{1}{c}\frac{\partial\mathbf{B}^T}{\partial t}$$

$$\nabla\cdot\mathbf{B}^T = 0$$

Plasma Physics is Multiscale in Time and Space



Scale separation is due to magnetic coordinates

Multiscale Properties for Vlasov-Maxwell Equations

- Debye Shielding ⇒ Finite Size Particles and Particle-In-Cell Simulations
- Low Frequency Gyrokinetics ⇒ Polarization Shielding & Charged Rings
- Low Frequency Darwin Gyrokinetics ⇒ Electron Skin Depth Shielding
- High Frequency Gyrokinetics ⇒ Kruskal Rings
- Perturbative Particle Simulation ⇒ Noise Reduction
- Gyrokinetic Poisson & Ampere Solvers ⇒ PETSc
- Magnetic Coordinates ⇒ separation of parallel and perpendicular dynamics with straight field line coordinates :

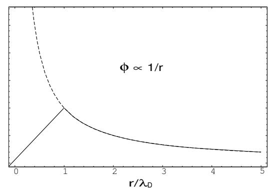
$$\mathbf{B} = I\,\nabla\Phi + \nabla\Psi \times \nabla\Phi$$

Multiscale Properties for Vlasov-Maxwell Equations (cont.)

- Fluctuation-Dissipation Theorem
  -- Intrinsic particle noise
- Stochastic Differential Equations
  -- Intrinsic particle noise
  -- Collisions
  -- Numerical coarse graining
- Singular Perturbation
  -- Shear Alfven waves and magnetic tearing
- Projective Integration
  -- Bridging the gaps between first principles simulations

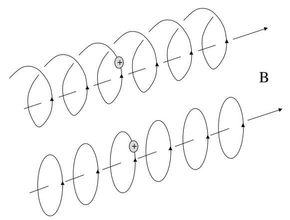
Multiscale Models for Fusion Plasmas

- Debye Shielding ⇒ Particle-In-Cell (PIC) Simulation [Dawson et al. 1968; Birdsall et al., 1968]



-- Coulomb interactions modified
-- No need for $n\lambda_D^3 \gg 1$
-- Collisions become sub-grid phenomena
-- N log N calculations on a grid
-- No need for N^2 calculations

- Low Frequency Gyrokinetics [Lee, 1983] -- charged rings and polarization shielding



-- Fast gyromotion approximated by rotating charged rings, which, in turn, give rise to large time steps

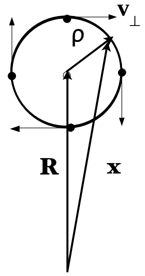
-- Debye shielding is replaced by Polarization shielding, which, in turn, gives rise to large grid spacing

- Gyrokinetic PIC Simulation [Lee, 1987]

-- numerical algorithm to transform the calculation of Bessel function of

$$J_0(k_\perp \rho)$$

from Fourier space + velocity space to configuration space.



Governing Low-Frequency Gyrokinetic Vlasov-Maxwell Equations

$$\boxed{\frac{dF_\alpha}{dt} \equiv \frac{\partial F_\alpha}{\partial t} + \frac{d\mathbf{R}}{dt}\cdot\frac{\partial F_\alpha}{\partial \mathbf{R}} + \frac{dv_\parallel}{dt}\frac{\partial F_\alpha}{\partial v_\parallel} = 0}$$

GK Vlasov Equation

$$\left[\begin{array}{l} \dfrac{d\mathbf{R}}{dt} = v_\parallel \mathbf{b}^* + \dfrac{v_\perp^2}{2\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times \nabla lnB_0 - \dfrac{c}{B_0}\nabla\bar{\phi}\times\hat{\mathbf{b}}_0 \\ \dfrac{dv_\parallel}{dt} = -\dfrac{v_\perp^2}{2}\mathbf{b}^*\cdot\nabla lnB_0 - \dfrac{q_\alpha}{m_\alpha}\underline{\left(\mathbf{b}^*\cdot\nabla\bar{\phi} + \dfrac{1}{c}\dfrac{\partial \bar{A}_\parallel}{\partial t}\right)} \\ \mu_B = \dfrac{v_\perp^2}{2B_0}\left(1 - \dfrac{mc}{e}\dfrac{v_\parallel}{B_0}\hat{\mathbf{b}}_0\cdot\nabla\times\hat{\mathbf{b}}_0\right) \approx const. \end{array}\right]$$

Coordinates Transformation
and Gyrophase Averaging

$$\mathbf{b}^* \equiv \mathbf{b} + \frac{v_\parallel}{\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0\cdot\nabla)\hat{\mathbf{b}}_0 \qquad \mathbf{b} = \hat{\mathbf{b}}_0 + \frac{\nabla\times\bar{\mathbf{A}}}{B_0} \qquad \begin{pmatrix}\bar{\phi}\\ \bar{\mathbf{A}}\end{pmatrix}(\mathbf{R}_{\alpha j}) = \langle\begin{pmatrix}\phi\\ \mathbf{A}\end{pmatrix}(\mathbf{x}_{\alpha j})\rangle_\varphi$$

$$\boxed{\frac{\rho_s^2}{\lambda_D^2}\nabla_\perp^2\phi(\mathbf{x}) = -4\pi(1-\rho_i^2\nabla_\perp^2)\rho(\mathbf{x})} \qquad \rho(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N}\langle\delta(\mathbf{x}-\mathbf{x}_{\alpha j})\rangle_\varphi$$

GK Poisson's Equation
with Pede Approximation

$$\boxed{\nabla^2\mathbf{A}(\mathbf{x}) - \frac{1}{v_A^2}\frac{\partial^2\mathbf{A}_\perp(\mathbf{x})}{\partial t^2} = -\frac{4\pi}{c}\mathbf{J}(\mathbf{x})}$$

GK Ampere's Law

$$\mathbf{J}(\mathbf{x}) = \sum_\alpha q_\alpha \sum_{j=1}^{N}\left[(\mathbf{v}_{\parallel\alpha j} + \mathbf{v}_{d\alpha j})\langle\delta(\mathbf{x}-\mathbf{x}_{\alpha j})\rangle_\varphi + \langle\mathbf{v}_{\perp\alpha j}\delta(\mathbf{x}-\mathbf{x}_{\alpha j})\rangle_\varphi\right]$$

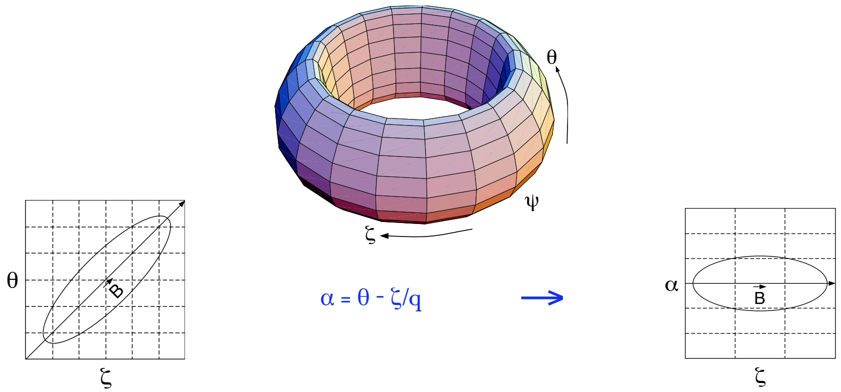
$$\mathbf{v}_d \equiv v_\parallel^2\hat{\mathbf{b}}_0\times(\hat{\mathbf{b}}_0\cdot\nabla)\hat{\mathbf{b}}_0 + \frac{v_\perp^2}{2}\hat{\mathbf{b}}_0\times\nabla lnB_0$$

[Lee, Dubin et al., Hahm, Brizard, Qin et al, PPPL]

Multiscale Models for Fusion Plasmas (cont.)

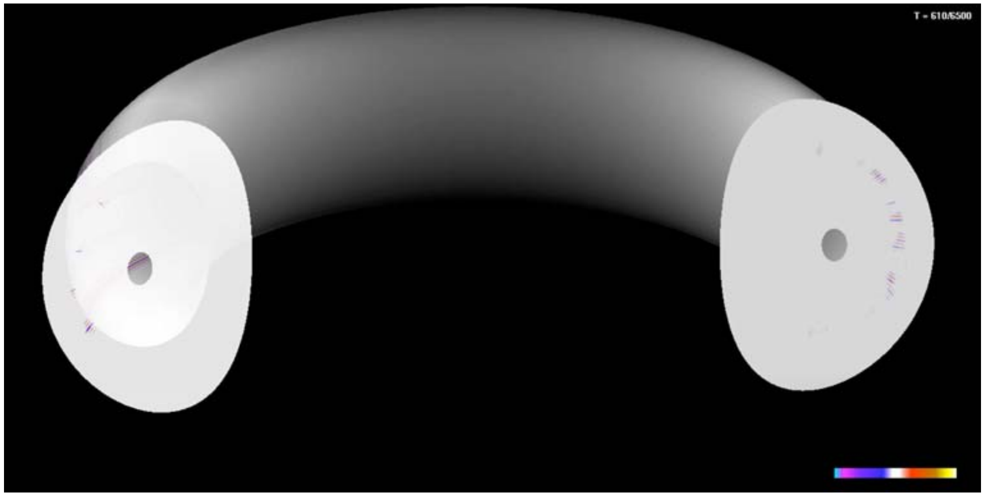
- Magnetic coordinates (ψ, θ, ζ) and field line following mesh (ψ, α, ζ) also greatly improve the computational requirements for fusion plasmas:

-- Coarse grid along the field-line-aligned coordinates
-- Large time steps for zeroth order orbit calculations
-- The Courant condition for particle motion along the field-lines is for accuracy not for stability for PIC codes.



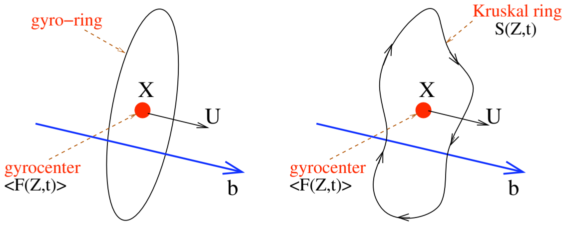
$\alpha = \theta - \zeta/q \quad \longrightarrow$

Gyrokinetic Particle Simulation of Magnetic Fusion Plasmas

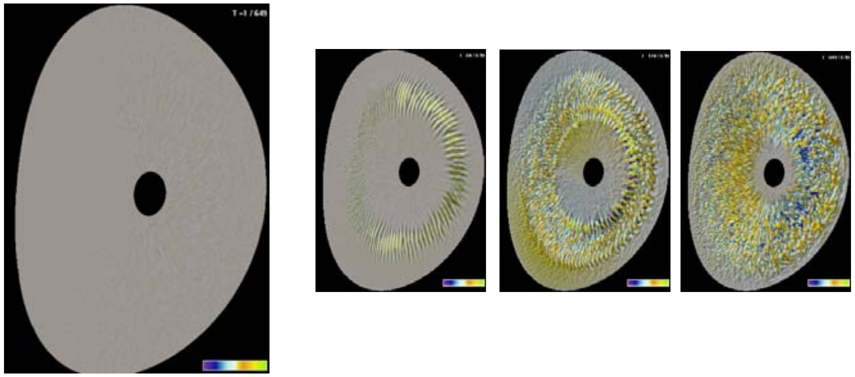


- Global PIC simulation
- Magnetic coordinates
- Grokinetic Vlasov-Maxwell Equations

High Frequency Gyrokinetics [Kolesnikov et al., 2008]: heating



Low Frequency Gyrokinetics [Wang et al., 2006]: turbulence



Theory Seminar

Gyrokinetic Particle-In-Cell Simulation:
Recent Controversy and Progress

W. W. Lee
PPPL

August 2010

Collaborators:
TechX: T. G. Jenkins
LANL: R. Kolesnikov
PPPL: S. Ethier, E. A. Startsev

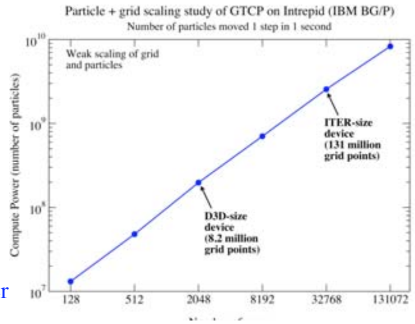
• Old Controversy: Particle Noise

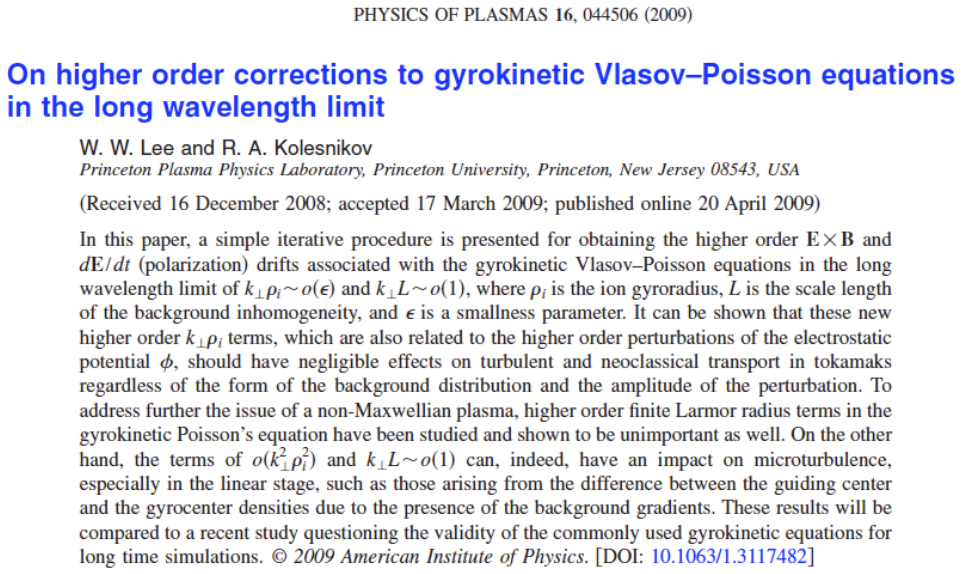
- "Discrete particle noise in particle-in-cell simulations of plasma microturbulence" [W. M. Nevins, G. W. Hammett, et al., Phys. Plasmas, 2005]: for system in equilibrium
- "Fluctuations and Discrete Particle Noise in Gyrokinetic Simulation of Drift Waves" [T. G. Jenkins and W. W. Lee, Phys. Plasmas, 2007]: for nonlinearly saturated system

• Recent Controversy & Progress:

1) validity of gyrokinetic Poisson's equation for global modes
   - "Limitation of gyrokinetics on transport times scales" [Parra and Catto, PPCF 2008]
   - "On higher order corrections to gyrokinetic Vlasov–Poisson equations in the long wavelength limit," [Lee and Kolesnikov, PoP 2009]: Comment by Parra&Catto, Response by Lee&Kolesnikov
2) δf to full-F simulations:
   - "A Generalized Weight-Based PIC Simulation Scheme," Lee, Jenkins and Ethier, CPC (to appear).
3) finite-β effects:
   - "Finite-β Stabilization of Microinstabilities," Startsev and Lee (in preparation).

- Global Gyrokinetic PIC codes for tokamaks in the US:
  - GTC [Lin, Hahm et al., Science, 1998]
  - GTS [Wang, Lin et al., Phys. Plasmas, 2006]
  - XGC [Ku, Chang et al., Nucl. Fus., 2009]
- Most suitable for modern massively parallel computers
  - GTCP on BlueGene [Ethier]
  - A top breakthrough in computational science [Tang]
  - Involved in 3 proposals for Exascale Co-Design Center




PHYSICS OF PLASMAS 16, 044506 (2009)

On higher order corrections to gyrokinetic Vlasov–Poisson equations in the long wavelength limit

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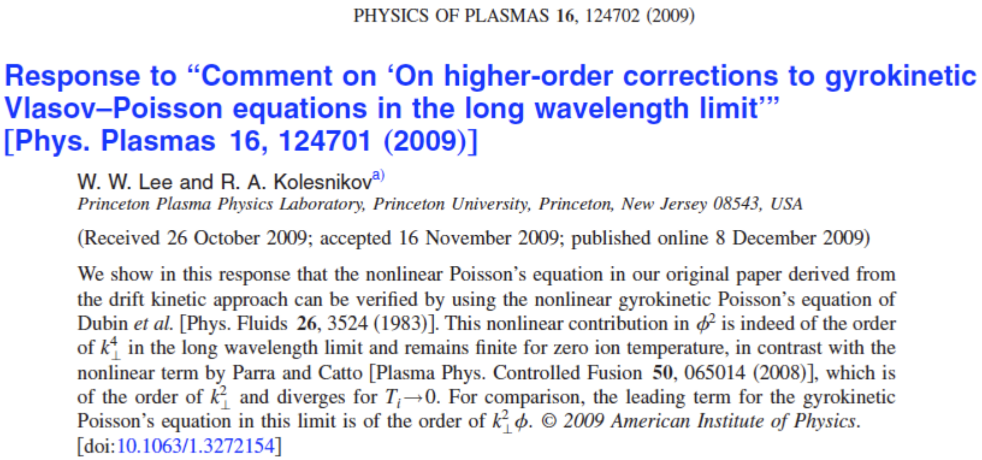
(Received 16 December 2008; accepted 17 March 2009; published online 20 April 2009)

In this paper, a simple iterative procedure is presented for obtaining the higher order $\mathbf{E}\times\mathbf{B}$ and $d\mathbf{E}/dt$ (polarization) drifts associated with the gyrokinetic Vlasov–Poisson equations in the long wavelength limit of $k_\perp\rho_i\sim o(\epsilon)$ and $k_\perp L\sim o(1)$, where ρ_i is the ion gyroradius, L is the scale length of the background inhomogeneity, and ϵ is a smallness parameter. It can be shown that these new higher order $k_\perp\rho_i$ terms, which are also related to the higher order perturbations of the electrostatic potential ϕ, should have negligible effects on turbulent and neoclassical transport in tokamaks regardless of the form of the background distribution and the amplitude of the perturbation. To address further the issue of a non-Maxwellian plasma, higher order finite Larmor radius terms in the gyrokinetic Poisson's equation have been studied and shown to be unimportant as well. On the other hand, the terms of $o(k_\perp^2\rho_i^2)$ and $k_\perp L\sim o(1)$ can, indeed, have an impact on microturbulence, especially in the linear stage, such as those arising from the difference between the guiding center and the gyrocenter densities due to the presence of the background gradients. These results will be compared to a recent study questioning the validity of the commonly used gyrokinetic equations for long time simulations. © *2009 American Institute of Physics*. [DOI: 10.1063/1.3117482]


PHYSICS OF PLASMAS 16, 124702 (2009)

Response to "Comment on 'On higher-order corrections to gyrokinetic Vlasov–Poisson equations in the long wavelength limit'" [Phys. Plasmas 16, 124701 (2009)]

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We show in this response that the nonlinear Poisson's equation in our original paper derived from the drift kinetic approach can be verified by using the nonlinear gyrokinetic Poisson's equation of Dubin *et al.* [Phys. Fluids **26**, 3524 (1983)]. This nonlinear contribution in ϕ^2 is indeed of the order of $k_\perp^4$ in the long wavelength limit and remains finite for zero ion temperature, in contrast with the nonlinear term by Parra and Catto [Plasma Phys. Controlled Fusion **50**, 065014 (2008)], which is of the order of $k_\perp^2$ and diverges for $T_i\rightarrow 0$. For comparison, the leading term for the gyrokinetic Poisson's equation in this limit is of the order of $k_\perp^2\phi$. © *2009 American Institute of Physics*. [doi:10.1063/1.3272154]

A Generalized Weight-Based Particle-In-Cell Simulation Scheme

W. W. Lee, T. G. Jenkins¶ and S. Ethier

(to appear in Computational Physics Communications)

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Abstract

A generalized weight-based particle simulation scheme suitable for simulating magnetized plasmas, where the zeroth-order inhomogeneity is important, is presented. The scheme is an extension of the perturbative simulation schemes developed earlier for particle-in-cell (PIC) simulations. The new scheme is designed to simulate both the perturbed distribution (f) and the full distribution (full-F) within the same code. The development is based on the concept of multiscale expansion, which separates the scale lengths of the background inhomogeneity from those associated with the perturbed distributions. The potential advantage for such an arrangement is to minimize the particle noise by using f in the linear stage of the simulation, while retaining the flexibility of a full-F capability in the fully nonlinear stage of the development when signals associated with plasma turbulenceare at a much higher level than those from the intrinsic particle noise.

Finite-β Effects in Magnetized Plasmas (DRAFT)

E. A. Startsev and W. W. Lee

Princeton Plasma Physics Laboratory, Princeton University, Princeton, NJ 08543

(Dated: August 25, 2010)

Abstract

A new split-weight perturbative particle simulation scheme for finite-β plasmas is presented. The scheme is an improvement over the original split-weight scheme [W. W. Lee *et. al*, Phys. Plasmas **8**, 4435 (2001)], which splits the perturbed particle response into adiabatic and non-adaibatic parts. In the new scheme, by further separating out the non-adaibatic response of the particles associated with the quasi-static bending of the magnetic field lines in the presence of background inhomogeneities of the plasma, we are able to demonstrate the finite-β stabilization of drift waves and ion temperature gradient modes using a simple gyrokinetic particle code based on realistic fusion plasma parameters. However, for $\beta m_i/m_e \gg 1$, it becomes necessary to use the electron skin depth as the grid size of the simulation to achieve accuracy in solving the resulting singular perturbation equations. The proposed scheme is most suitable for studying shear-Alfvén physics in general geometry using straight field line coordinates for microturbulence and magnetic reconnection problems.

Gyrokinetic Particle Simulation Center

[SciDAC Proposal, May, 2010]

Scott Parker, Univ. of Colorado; Boulder, Peter Catto, MIT;
Wendell Horton, Univ. of Texas, Austin; Scott Klasky, ORNL;
Wei-li Lee, PPPL; Zhihong Lin, Univ. of California, Irvine

This project involves the two high-fidelity GTC and GEM particle codes and a supporting research program in verification and validation (V&V), theoretical formulation, algorithms and parallel performance. Gyrokinetic particle simulation is well suited for high phase space resolution and has demonstrated excellent parallel scalability and efficient utilization of hundreds of thousands of processors. The significant benefit of the excellent parallel performance is two-fold. First, it provides the capability to simulate large plasma volumes with few approximations using fully global calculations. Second, it allows investigating convergence with respect to phase space resolution useful for verification of simulation results. These codes are now fairly comprehensive in terms of physics, including, kinetic electrons, electromagnetic perturbations, collisionality, realistic magnetic equilibria, non-perturbative (full-f) capability, multiple ion species and interfacing with interpretive transport codes. The scientific goal of the Gyrokinetic Particle Simulation (GPS) Center will be, stated quite broadly, the basic understanding of turbulent transport in tokamak plasmas using gyrokinetic particle simulations efficiently optimized to run on hundreds of thousands of processors. More specifically, the project will target research needed for predictive modeling in preparation for the Fusion Simulation Project. The GPS Center will focus on studies of closed flux surface regions, but will include investigations of steep gradient edge pedestal turbulence. While the gyrokinetic simulations are quite widely applicable to a variety of fusion plasma research problems, there will be four primary foci of the Gyrokinetic Particle Simulation Center: First, there will be a strong verification and validation effort involving GTC and GEM and experimental data from the NSTX, DIII-D, and Alcator C-Mod tokamaks as well as the CLM and LAPD basic plasma experiments. Second, a theoretical and computational effort will be initiated to develop a computational framework for determining the global axisymmetric radial electric field and toroidal plasma rotation in burning plasma conditions. Third, research on modeling transport barriers and edge pedestal turbulence will be performed using global calculations that take into account steep variation in density and temperature profiles, equilibrium Er profile and the q profile. The project will emphasize global calculations where fewer assumptions are made. Fourth, we will examine the role of density fueling and impurity transport in tokamak plasmas using gyrokinetic particle simulation. These investigations will include all relevant ion species (D, T, He, impurities), and kinetic electrons. Additionally, algorithm development and computational research will include performance optimization of the two particle codes on peta-scale computers and preparation work for future exascale computers. Advanced data management tools will be utilized for the particle codes, as will fast parallel I/O, with the goals of both improving performance and facilitating the sharing of data and efficient collaboration amongst the research team. The proposed work is also expected to benefit all the codes in the fusion community that are based on Particle-In-Cell methodology.

Princeton Plasma Physics Laboratory

Co-Design Center for Exascale Simulations of Fusion Plasmas

[Co-Design Proposal, July, 2010]

W. W. Lee (PI), PPPL, Princeton, NJ 08543 (609-243-2647; wwlee@pppl.gov)
Z. Lin (UC Irvine); G. Chiu (IBM); B. F. Smith (ANL); E. Strohmaier (LBNL); C. Kamath (LLNL);
D. Spong (ORNL); R. Lucas (USC); K. L. Ma (UC Davis); V. Decyk (UCLA); A. Sanderson (U. Utah)

The capability of simulating realistic fusion plasmas is an important step in the design and operation of experimental thermonuclear devices, such as ITER, presently under construction in France, with the United States as a major partner. For the success of ITER tokamak experiments, it is critical that we understand, predict, and control turbulent transport in fusion plasmas, so that the high-pressure plasmas remain confined and are self-sustained by the heating from the fusion reaction.

An important tool for understanding plasma turbulence in magnetic fusion research is the gyrokinetic Particle-In-Cell (PIC) simulation, which started in the 1980s at PPPL. PIC codes solve the equations of motion for the particles, and the associated field equations, in three-dimensions (instead of the usual phase space in 5~6 dimensions). As these equations are essentially linear, they are amenable to the complicated three-dimensional toroidal geometry of the tokamak, and the resulting physics is nearly two-dimensional. This allows us to naturally express the parallelism and locality in the problem, making these codes adaptable to modern-day, multi-core, massively parallel computers. When combined with the advances in gyrokinetic theory and algorithms, and the computational power of the proposed exascale systems, PIC codes make it a real possibility that we can realistically simulate an ITER burning plasma in one code with comprehensive physics using a single computing platform.

However, there are several challenges in moving PIC codes to the exascale systems. The systems proposed for 2015 and 2018 are likely to have many lightweight cores, increasing the node-level parallelism. At the same time, the amount of memory per floating point operation will drop significantly, the cost of moving data on and off chip will dominate the performance and energy budgets, and I/O bandwidth will not keep up with the needs of check-pointing, analysis, and visualization. This paradigm shift in the system architecture will require a re-design of PIC codes to move them to the exascale.

Co-Design Center for Exascale Simulations of Fusion Plasmas (cont.)

We propose to establish an exascale co-design center consisting of an integrated team of scientific researchers, applied mathematicians, computer scientists, and computer architects, to develop the capability of simulating realistic fusion plasmas using PIC codes. The centerpiece of the proposal is the state-of-the-art GTC code, which is the key code in two fusion SciDAC centers. It is scalable on petascale systems with 10^5 cores and currently is the only PIC code with all the physics capabilities to simulate burning plasmas.

We will address the challenges in scaling GTC in several ways, namely, by i) incorporating data compression in the gather-scatter operation used in particle computation; ii) developing efficient fine-grain parallelism in the Poisson solver and reorganizing the algorithm to reduce communication; and iii) moving the data analysis and visualization *in-situ*, along with new Alfven physics capabilities. This work will be done in close collaboration with the vendor (IBM), who will help in addressing architecture-driven questions, and a programming models, parallelization, and optimization team, who will help the physics, analysis, and visualization teams to extract the most from the hardware. In addition, a code team composed of key developers from each component will meet quarterly with the vendor and programming models team to ensure that scientific problem requirements influence the architecture design, and system constraints help to formulate the design of the algorithms and software.

We will also exploit the opportunities offered by the exascale system to improve GTC. Specifically, we will enhance verification and validation using the *in-situ* data analysis, and exploit the additional compute power to incorporate uncertainty quantification into the redesigned code and add new physics. In addition to enabling the co-design of exascale simulation of fusion plasmas and contributing to the simulation of a realistic ITER plasma, this work will also form an important component in the future for the Fusion Simulation Project (FSP), now in the planning stage under the auspices of US DoE.