OASCR Multiscale Mathematics Research and Education Project
Multiscale Gyrokinetics for Fusion Plasmas*

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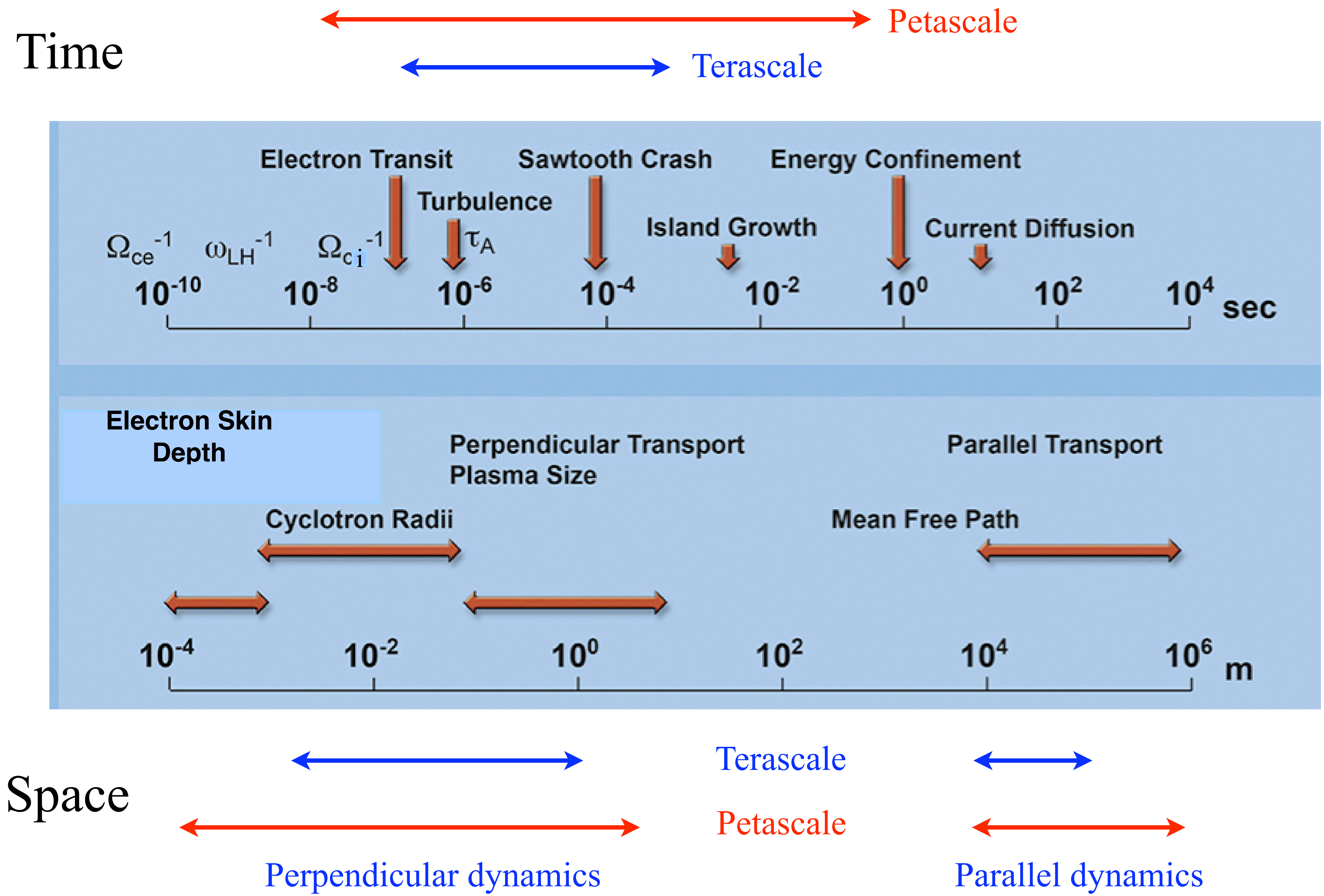
Presented at
PSACI PAC Meeting
June 2008

*This is also a pending project on Multiscale Mathematics for Complex Systems

Multiscale Fusion Plasmas on MPP Platforms

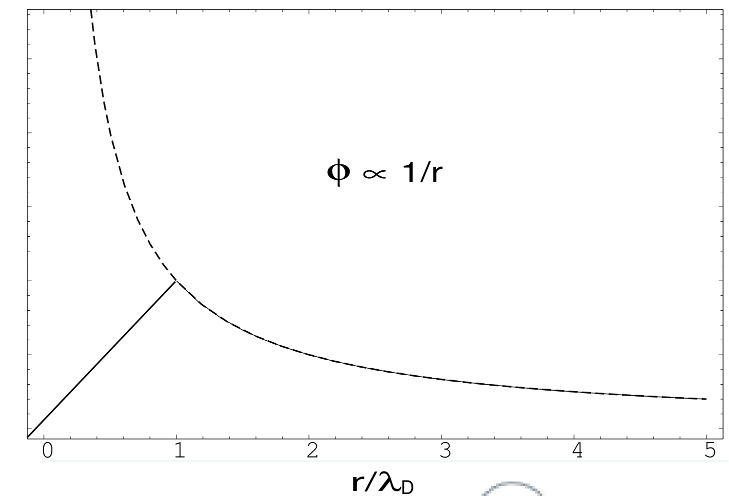


Scale separation is due to field line following coordinates

Multiscale Mathematics for Fusion Plasmas

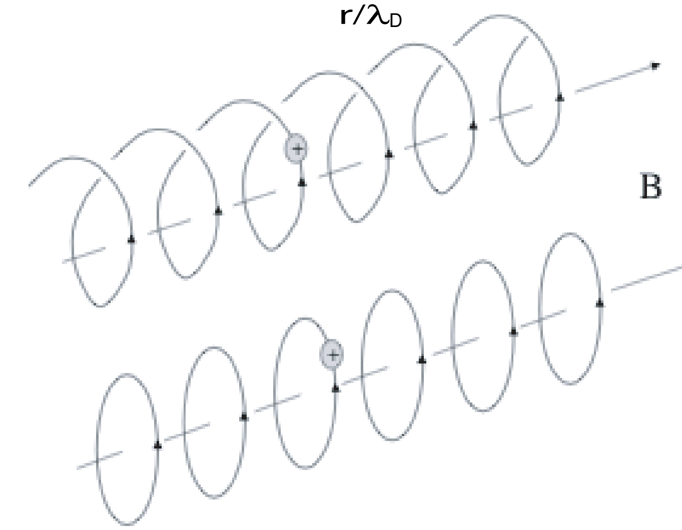
• Fusion physics a fertile ground for multiscale mathematics -- span more than eight orders of magnitude in spatial and temporal scales for tokamaks.

• Simulation algorithms based on finite-size particles are the first examples of mulitiscale mathematics based on the Debye shielding concept
⇒ relaxing the original requirement for the numbers of particles in the Debye sphere, i.e., $n\lambda_D^3 \gg 1$, in the mean time, by making collisions as subgrid phenomena.

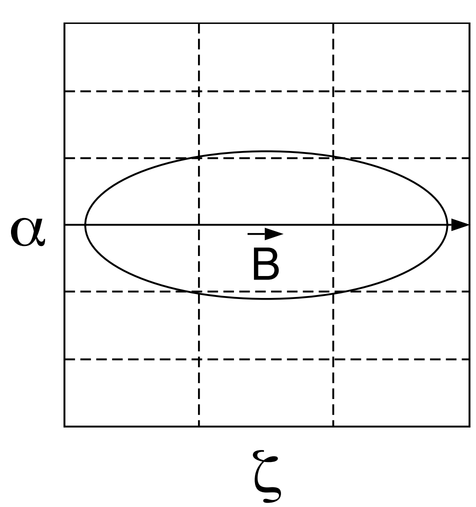


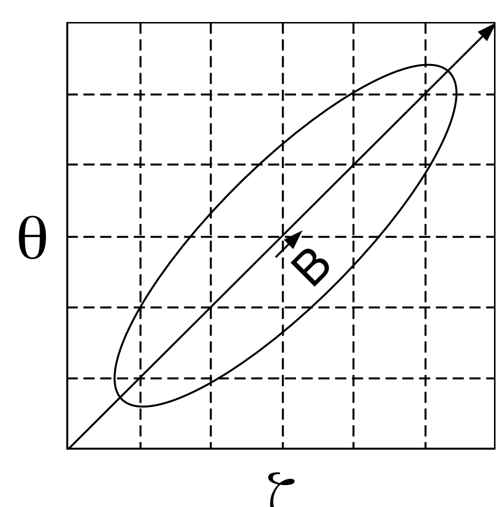
• Gyrokinetic formalism is another example of multiscale mathematics based on the use of gyrokinetic ordering
⇒ orders of magnitude improvement in computational requirements

due to the presence of polarization shielding and rotating charged rings

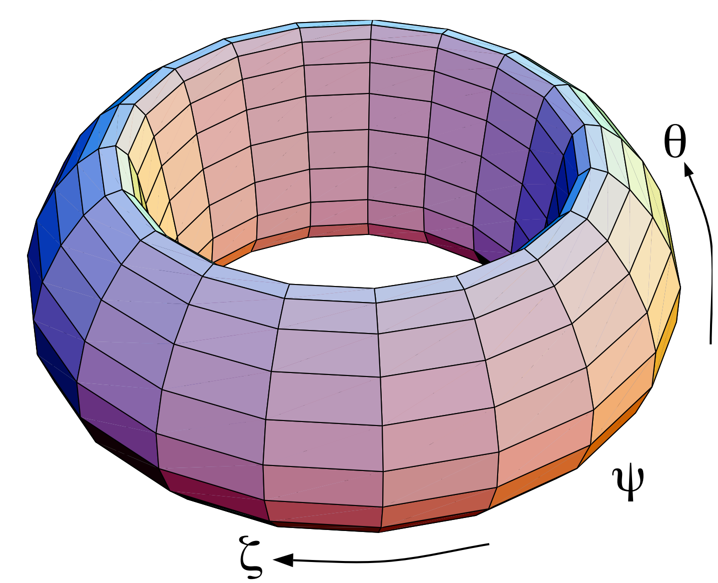


• Magnetic coordinates (ψ, θ, ζ) and field line following mesh (ψ, α, ζ) also greatly improve the computational requirements for fusion plasmas and are another example of multiscale mathematics





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



Governing Equations for Gyrokinetic Particle Simulation

- Gyrokinetic Vlasov Equation is solved using Particle-In-Cell (PIC) methods

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

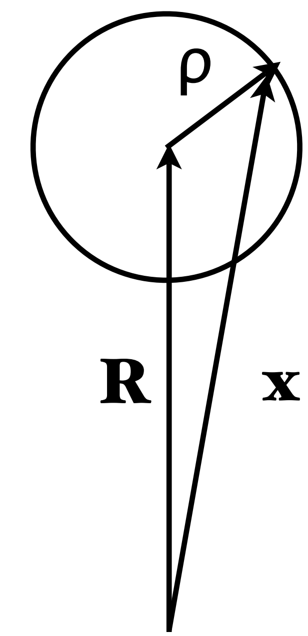
$$\frac{d\mathbf{R}}{dt} = v_\parallel \mathbf{b}^* + \frac{v_\perp^2}{2\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times \nabla lnB_0 - \frac{c}{B_0}\nabla\bar{\phi}\times\hat{\mathbf{b}}_0$$

$$\frac{dv_\parallel}{dt} = -\frac{v_\perp^2}{2}\mathbf{b}^*\cdot\nabla lnB_0 - \frac{q_\alpha}{m_\alpha}\left(\mathbf{b}^*\cdot\nabla\bar{\phi} + \frac{1}{c}\frac{\partial \bar{A}_\parallel}{\partial t}\right)$$

-- Velocity Nonlinearity

$$\mu_B \equiv \frac{v_\perp^2}{2B_0}\left(1 - \frac{mc}{e}\frac{v_\parallel}{B_0}\hat{\mathbf{b}}_0\cdot\nabla\times\hat{\mathbf{b}}_0\right) \approx cons.$$

$$\mathbf{b}^* \equiv \mathbf{b} + \frac{v_\parallel}{\Omega_{\alpha 0}}\hat{\mathbf{b}}_0 \times (\hat{\mathbf{b}}_0\cdot\nabla)\hat{\mathbf{b}}_0, \quad \mathbf{b} = \hat{\mathbf{b}}_0 + \frac{\nabla\times\bar{\mathbf{A}}}{B_0}$$



- Gyrokinetic Poisson's Equation is solved using PETSc (SciDAC TOPS)

$$\nabla^2\phi + \frac{\tau}{\lambda_D^2}[\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})] = -4\pi\rho_{gc}(\mathbf{x})$$

$\lambda_D \ll \rho_s$ →

$$\frac{\rho_s^2}{\lambda_D^2}\nabla_\perp^2\phi(\mathbf{x}) = -4\pi\rho_{gc}(\mathbf{x})$$

$k_\perp^2\rho_s^2 \ll 1$

- Gyrokinetic Ampere's Law

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

$\omega^2/k^2 v_A^2 \ll 1$

PPPL
PRINCETON PLASMA PHYSICS LABORATORY

Multiscale Maxwell's Equations

- $\nabla^2\phi = -4\pi q\delta(\mathbf{r})$ $\longrightarrow$ $\phi = \frac{q}{r}$ Bare charged particles

  $\nabla^2\phi - \frac{\phi}{\lambda_D^2} = -4\pi q\delta(\mathbf{r})$ $\longrightarrow$ $\phi = \frac{q}{r}e^{-r/\lambda_D}$ Debye-shielded particles $r \gg \lambda_D$

- $(\frac{\rho_s}{\lambda_D})^2\nabla_\perp^2\phi = -4\pi q\delta(\mathbf{r})$ $\longrightarrow$ $\phi = \frac{q}{r}\frac{\rho_s}{\lambda_D}$ Bare gyrokinetic particles

  $(\frac{\rho_s}{\lambda_D})^2\left[\nabla_\perp^2\phi - \frac{\phi}{\rho_s^2}\right] = -4\pi e\delta(\mathbf{r})$ $\longrightarrow$ $\phi = \frac{q}{r}\frac{\rho_s}{\lambda_D}e^{-r/\rho_s}$ Polarization-shielded particles $r \gg \rho_s$

- $(\frac{\rho_s}{\lambda_D})^2\left[\nabla^2\psi - \frac{\psi}{\delta_e^2}\right] = -4\pi qv\delta(\mathbf{r})$ $\longrightarrow$ $\psi = \frac{q}{r}\frac{\rho_s}{\lambda_D}e^{-r/\delta_e}$ Electron-skin-depth-shielded particles $r \gg \delta_e$

- $\nabla_\perp^2\phi - [\phi - \langle\phi\rangle] = \delta n_i$

  or $\nabla_\perp^2[\langle\phi\rangle + \delta\phi] - \delta\phi = \delta n_i$

  $\longrightarrow$ < > --- flux surfaced averaged quantity

  Combined zonal flow and perturbative potentials

  $|\langle\phi\rangle(k_r)| \gg |\delta\phi(\mathbf{k})|$

  $|\mathbf{k}| \gg |k_r|$

ACCOMPLISHMENTS

• Development of Mathematical and Numerical Algorithms

-- High-frequency-short-wavelength gyrokinetics

-- Low-frequency-mesoscale gyrokinetics

-- Low-frequency-long-wavelength gyrokinetics

-- Symplectic Integrator

• Preparations for Fusion Simulation Project (FSP)

-- Gyrokinetic Tokamak Simulation (GTS) code

• Developed and taught a graduate level course, “Kinetic Theory and Modeling of Plasmas” (APAM 4990), at the Department of Applied Physics and Applied Mathematics, Columbia University in Spring Semester 2008

• Publications

-- 4 published papers and 2 manuscripts in preparation

• Invited Talks

-- 2 talks at 20th International Conference on Numerical Simulation of of Plasmas

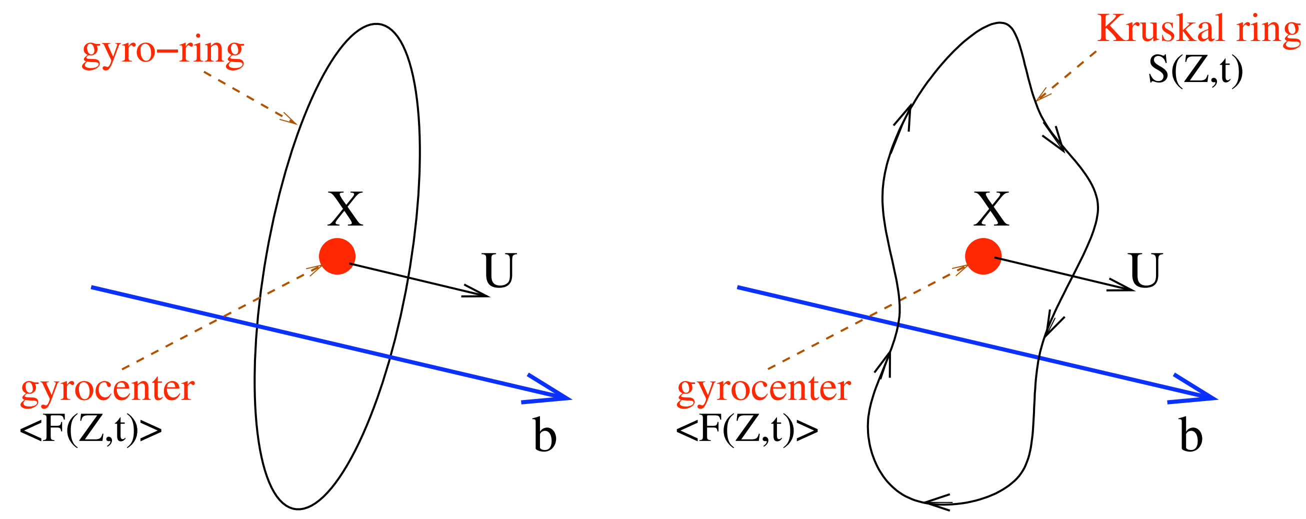
High Frequency Gyrokinetics

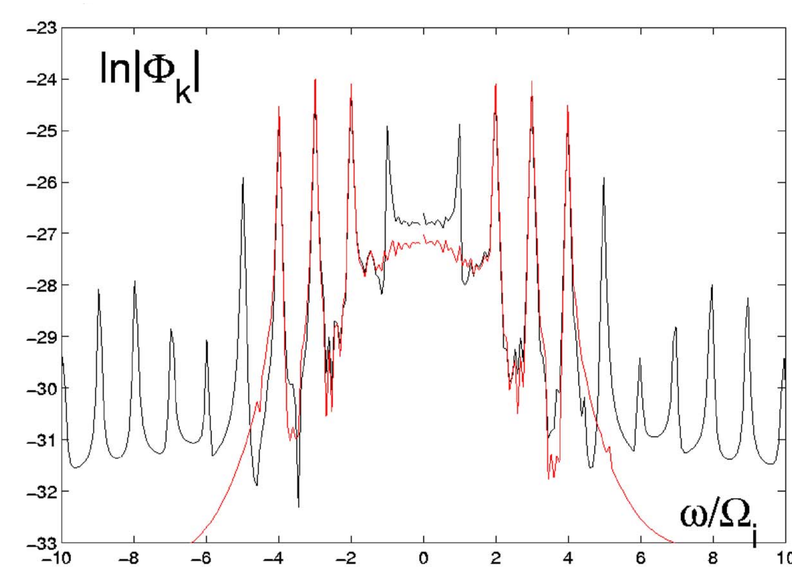
"High Frequency Gyrokinetic Particle Simulation"
R. A. Kolesnikov, W. W. Lee, H. Qin, and E. Startsev, Phys. Plasmas 14, 072506 (2007).

- A new gyrokinetic approach for arbitrary frequency dynamics in magnetized plasmas including ion cyclotron waves by viewing each particle as a quickly changing nearly periodic Kruskal ring rather than a rigid charged ring.

- This approach allows the separation of gyrocenter and gyrophase responses and thus allows for, in many situations, larger time steps for the gyrocenter push than for the gyrophase push.

- The gyrophase response which determines the shape of Kruskal rings can be described by the Fourier series in gyrophase, allowing control over the cyclotron harmonics at which the plasma responds and, thus, reducing the dimensionality.



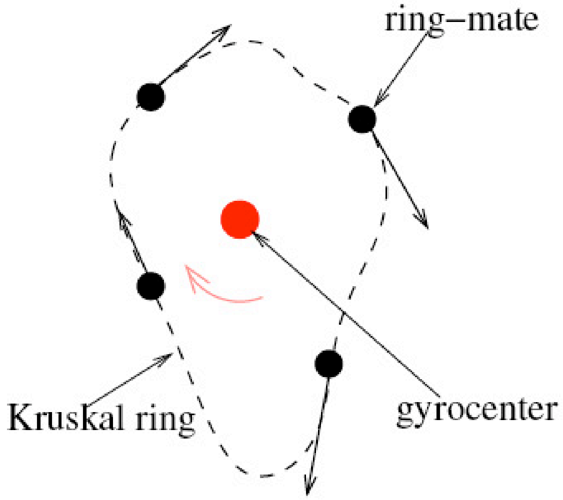


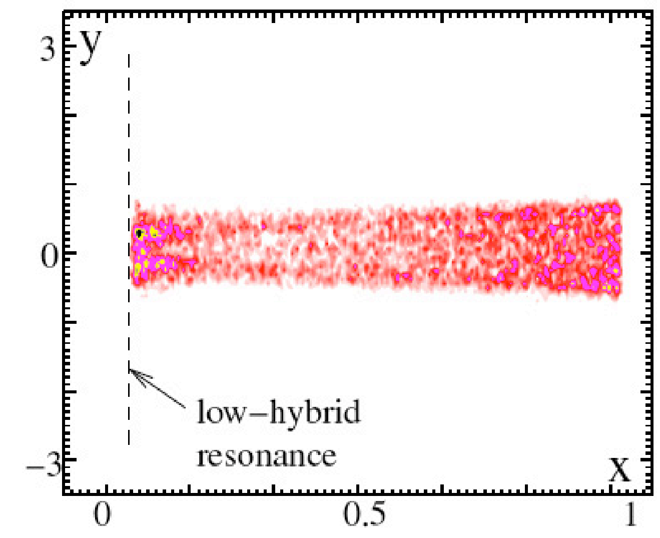
The frequency spectra for the ion Bernstein waves from the 6D (black) and 5D (red) the high frequency gyrokinetic code

High Frequency Gyrokinetics (cont.)

"Electromagnetic High Frequency Gyrokinetic Particle Simulation,"
R. A. Kolesnikov, W. W. Lee and H. Qin, Comm. in Comp. Phys. **4**, 575 (2008)

- A new electromagnetic version of the high frequency gyrokinetic numerical algorithm for particle-in-cell simulation is developed. The new algorithm offers an efficient way to simulate the dynamics of plasma heating and current drive with radio frequency waves.
- Moreover, the gyrokinetic formalism allows separation of the cold response from kinetic effects in the current, which allows one to use much smaller number of particles than what is required by a direct Lorentz-force simulation.
- Also, the new algorithm offers the possibility to have particle refinement together with mesh refinement, when necessary.
- Simulations of electromagnetic low-hybrid waves propagating in inhomogeneous magnetic field are shown here.





Simulations of lower-hybrid heating using Kruskal rings

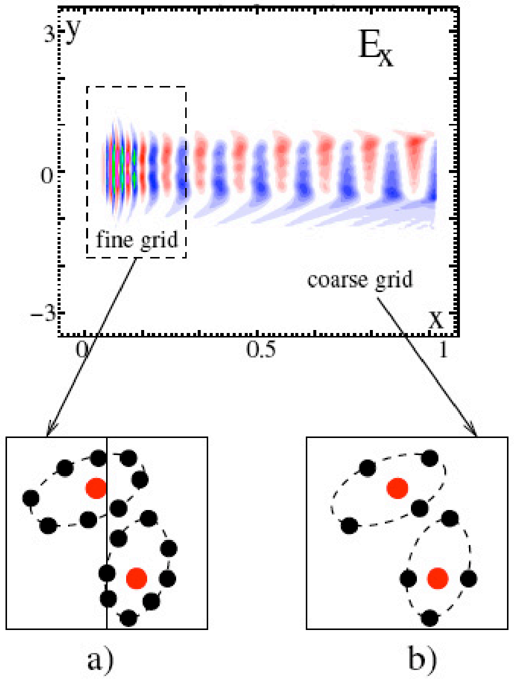
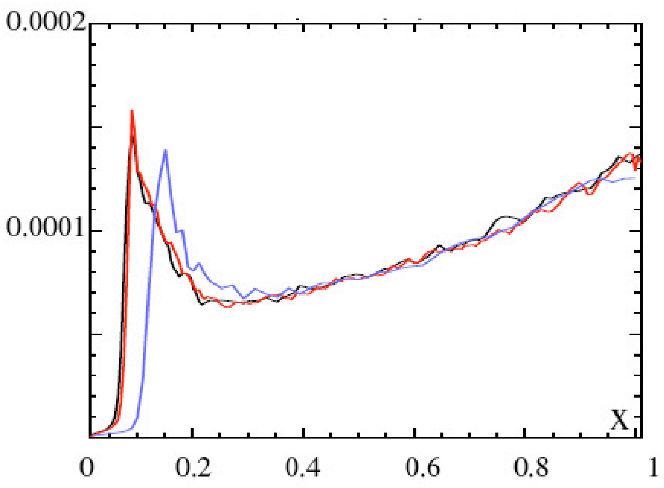


Illustration of the idea of particle refinement technique

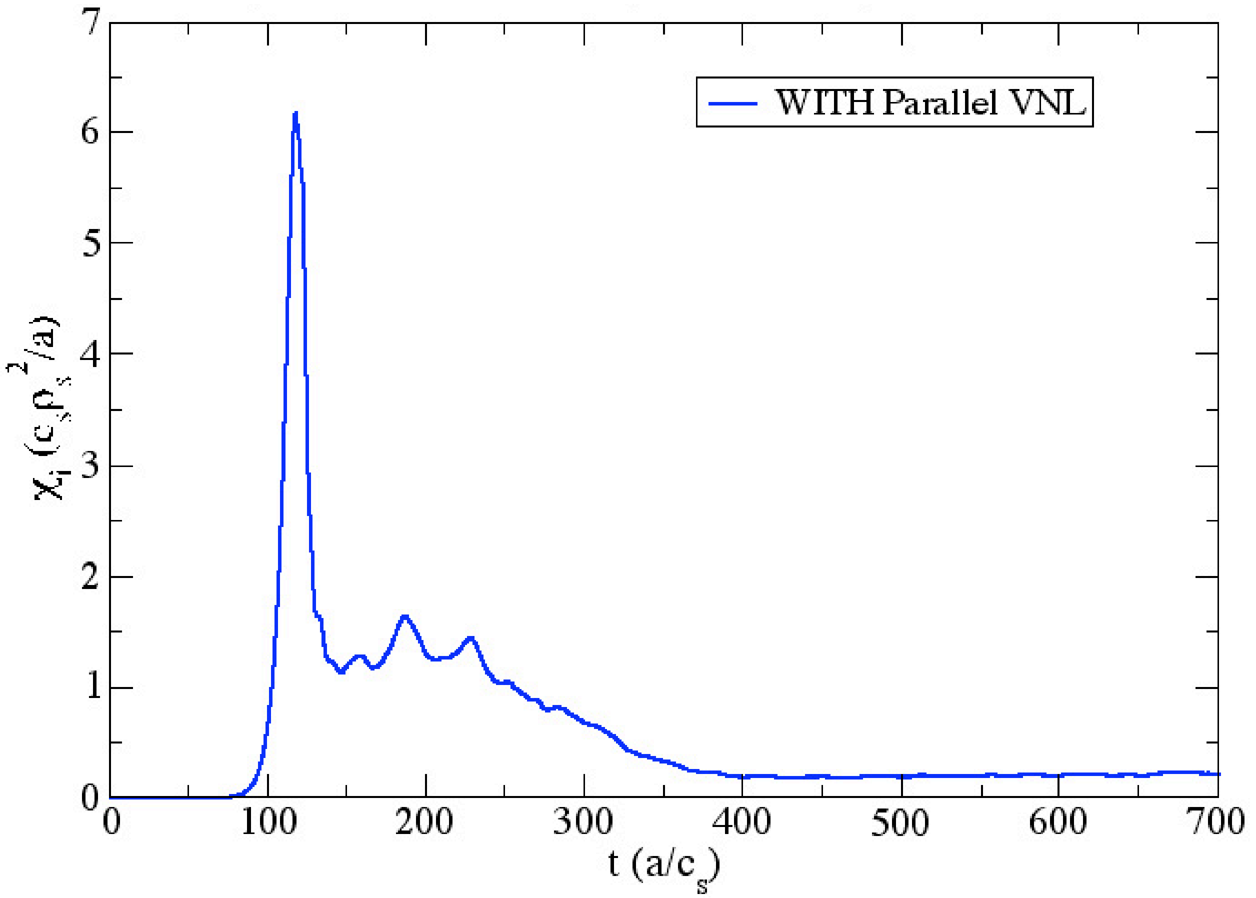


Stochastic heating of plasma ions for lower-hybrid waves for a different grid

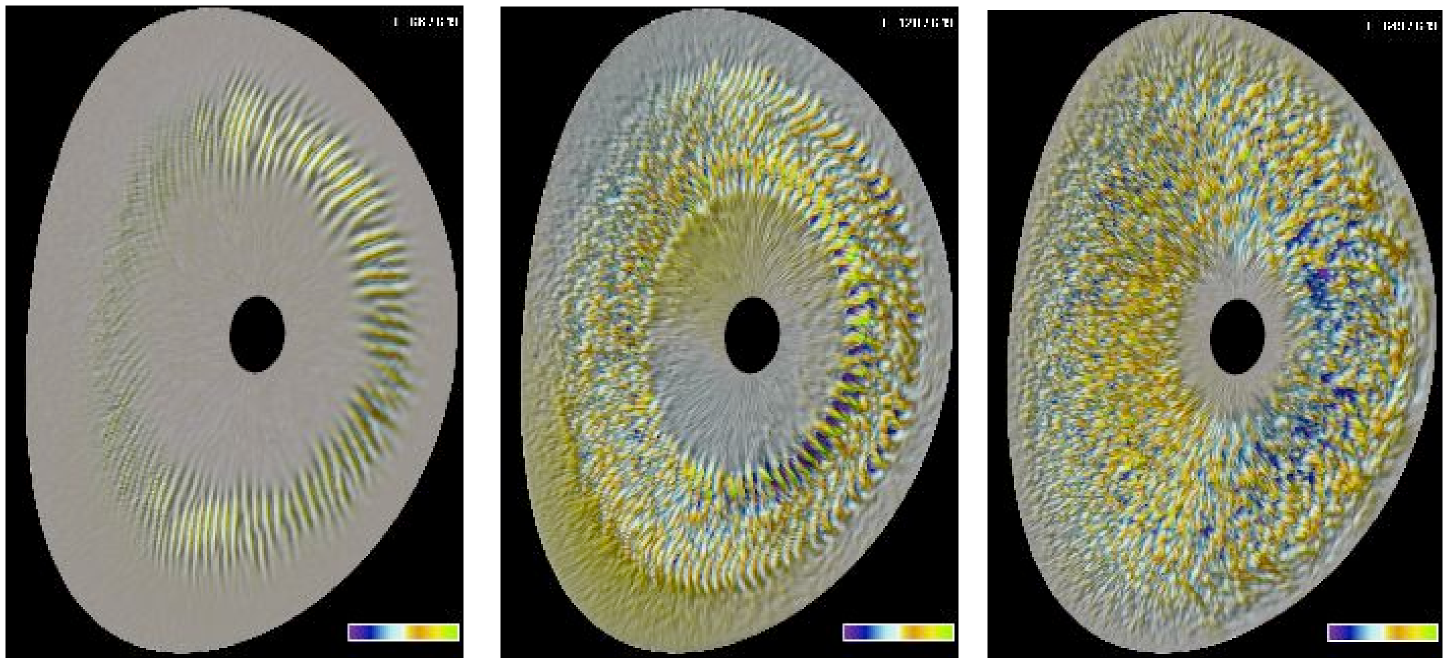
Global-scale and Meso-scale Gyrokinetics

"Steady State Turbulent Transport in Magnetic Fusion Plamsas,"
W. W. Lee, S. Ethier, R. Kolesnikov, W. X. Wang and W. M. Tang,
submitted to Computational Science and Discovery (2008)

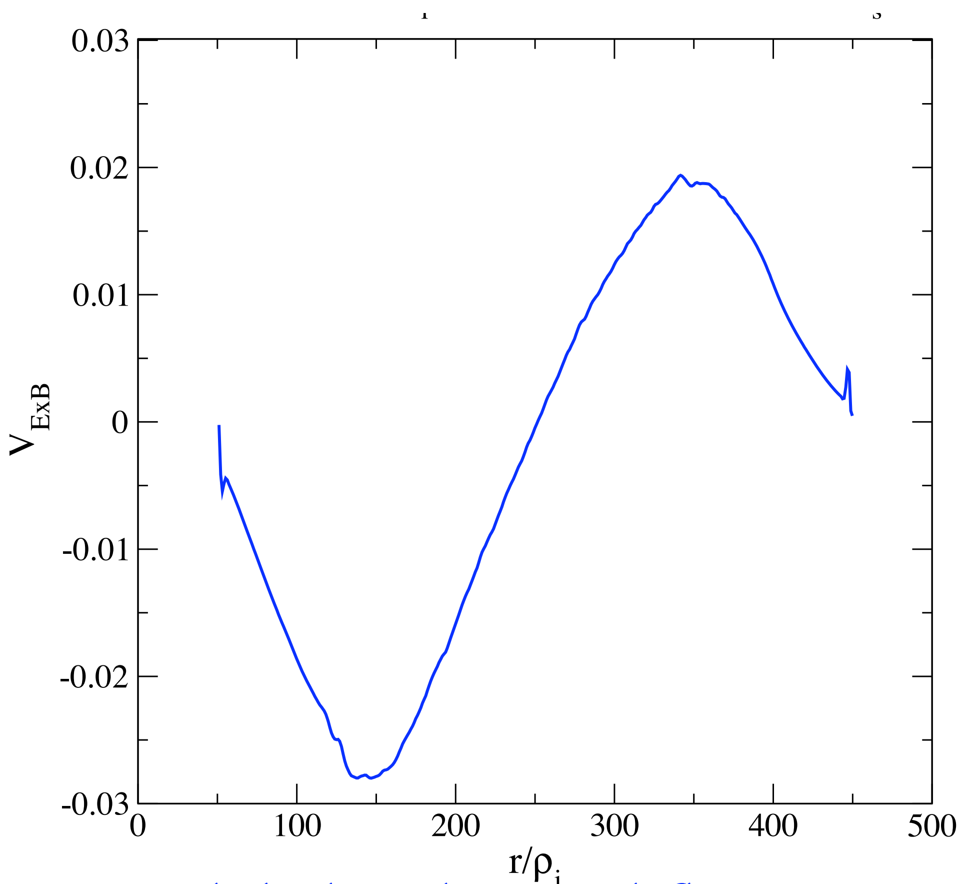
"Effects of Profile Relaxation on Ion Temperature Gradient Drift Instabilities,"
R. Ganesh, W. W. Lee, R. Kolesnikov, S. Ethier, and J. Manickam, manuscript in preparation.



Time evolution of ion thermal diffusivity



Global simulations of mesoscale ITG fluctuations



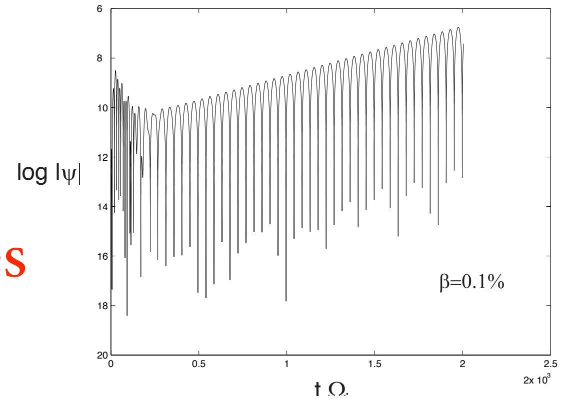
Large global scale zonal flow structure

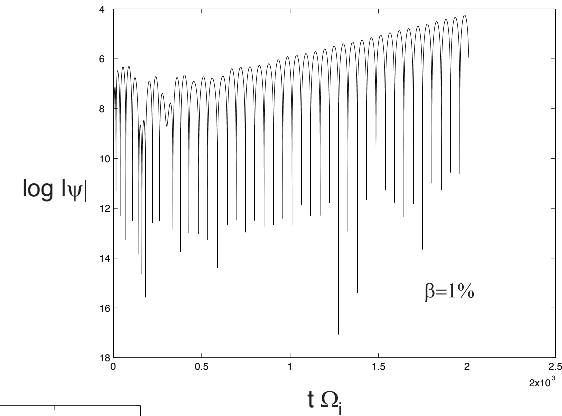
Low-Frequency Finite-Beta Gyrokinetics

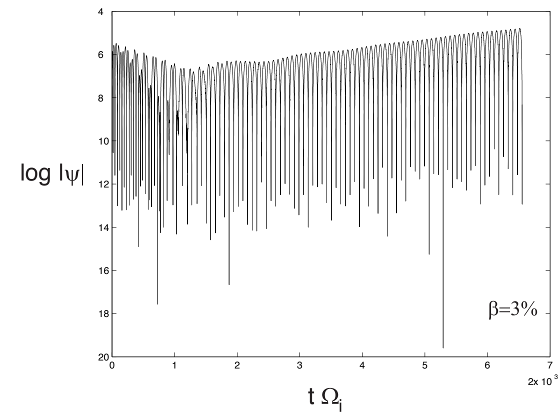
"Simulation of Finite-beta Effects in Gyrokinetic Plasmas,"

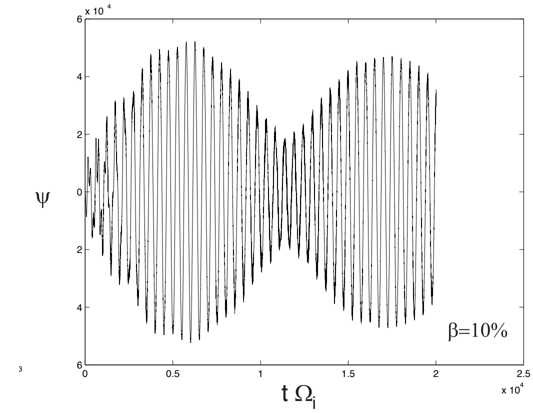
E. A. Startsev, W. W. Lee and W. X. Wang, manuscript in preparation.

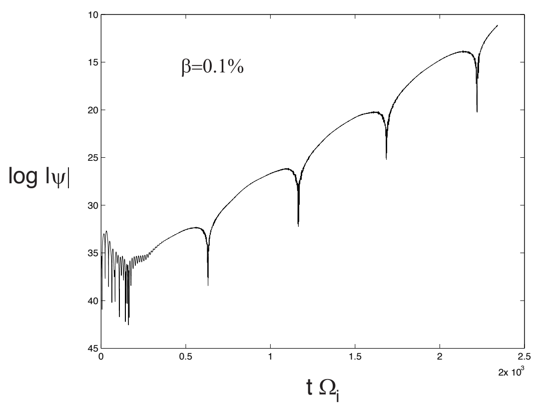
- Finite-beta stabilization of drift waves

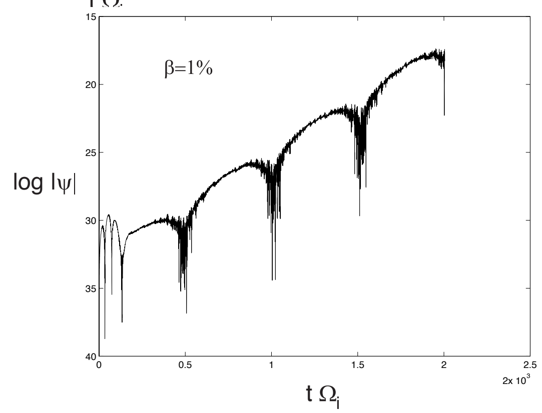


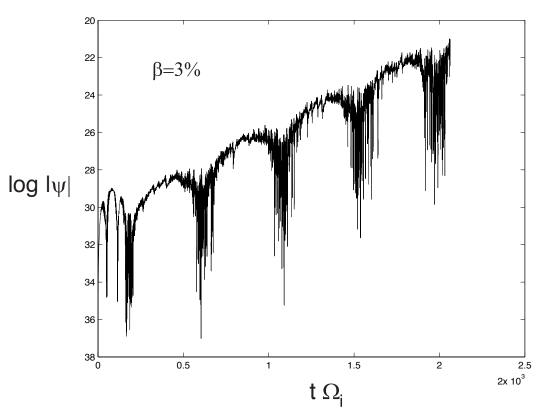


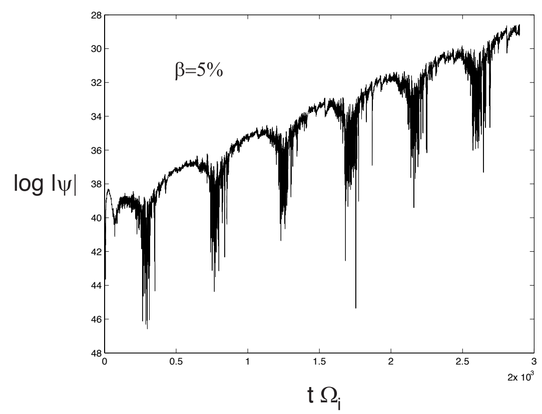




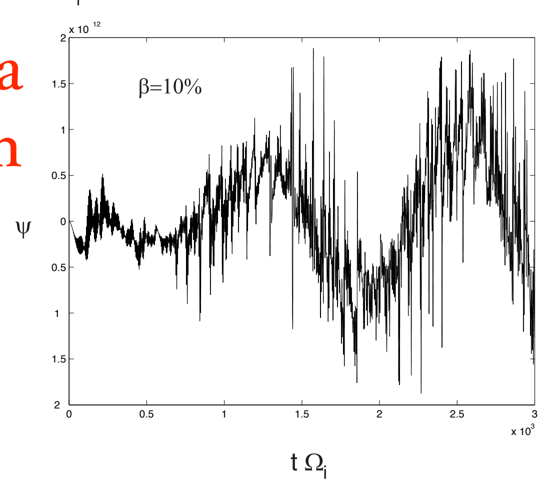








- Finite-beta stabilization of ITG modes



- A new double-split scheme is used

$$F = (1+\psi)F_0 + \int dx_{||}\kappa \cdot (\nabla A_{||} \times \hat{\mathbf{b}}_0) + \delta g$$

$$\frac{d\delta g_e}{dt} = -F_0 \left[\frac{\partial \psi}{\partial t} + \nabla\psi \times \hat{\mathbf{b}}_0 \cdot \kappa \right]$$

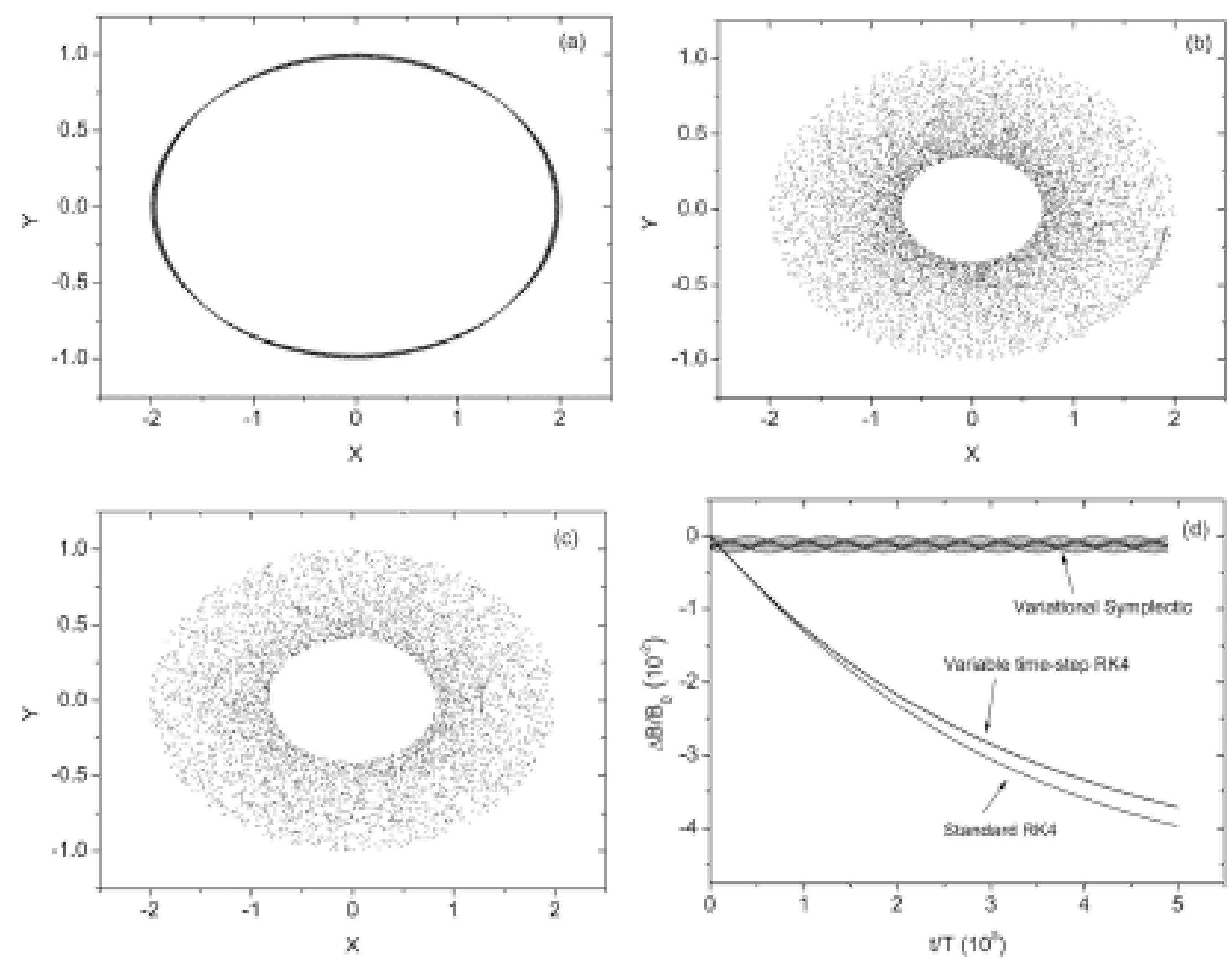
$$\psi = \phi + \int (\partial A_{||}/\partial t) dx_{||}/c$$

- It is found that GK PIC simulations for the finite beta stabilization of ITG modes in the presence of FLR effects needs also to resolve the electron skin depth.
- This need coming from the multiscale Poisson's equation, even in the absence of collisionless tearing, can be understood from the point of view singular perturbation methods.

Phase pace preservation integrator for long time simulations

"Variational Symplectic Integrator for Long Time Simulations of the Guiding Center Motion of Charged Particles in General Magnetic Fields,"
Hong Qin and Xiaoyin Guan, Phys. Rev. Lett. **100**, 035006 (2008)

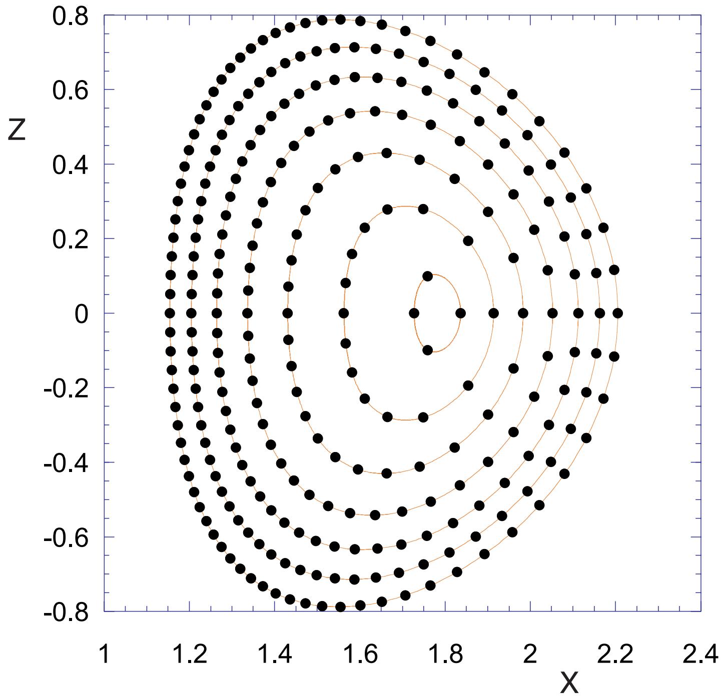
The guiding-center dynamics in general magnetic field does not possess a (global) canonical symplectic structure, and the conventional symplectic integrator does not apply. Marsden and West [2001] recently developed the method of variational symplectic integrator for dynamic systems with a well-defined Lagrangian, and the variational symplectic integrator conserves exactly a non-canonical symplectic structure. Here, we develop the variational symplectic integrator for the guiding-center dynamics from the guiding-center Lagrangian and demonstrate its superior numerical properties compared with the standard fourth order Runge-Kutta methods.

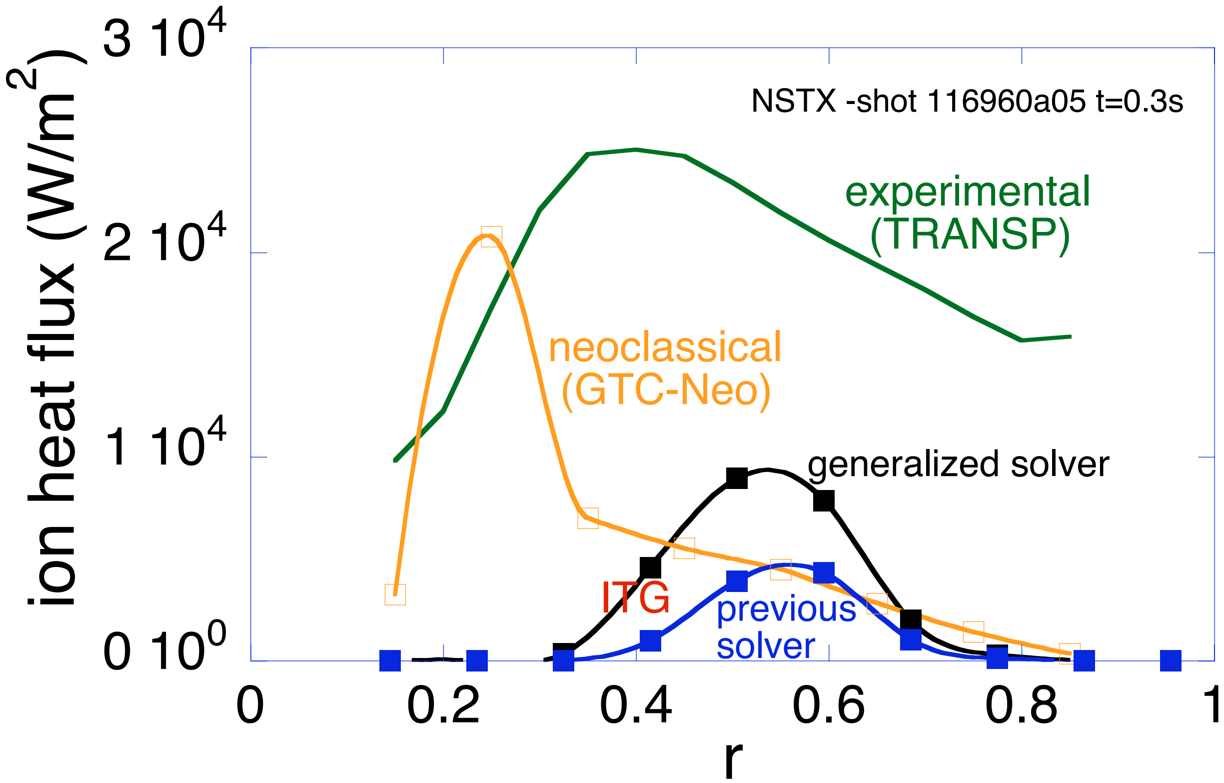


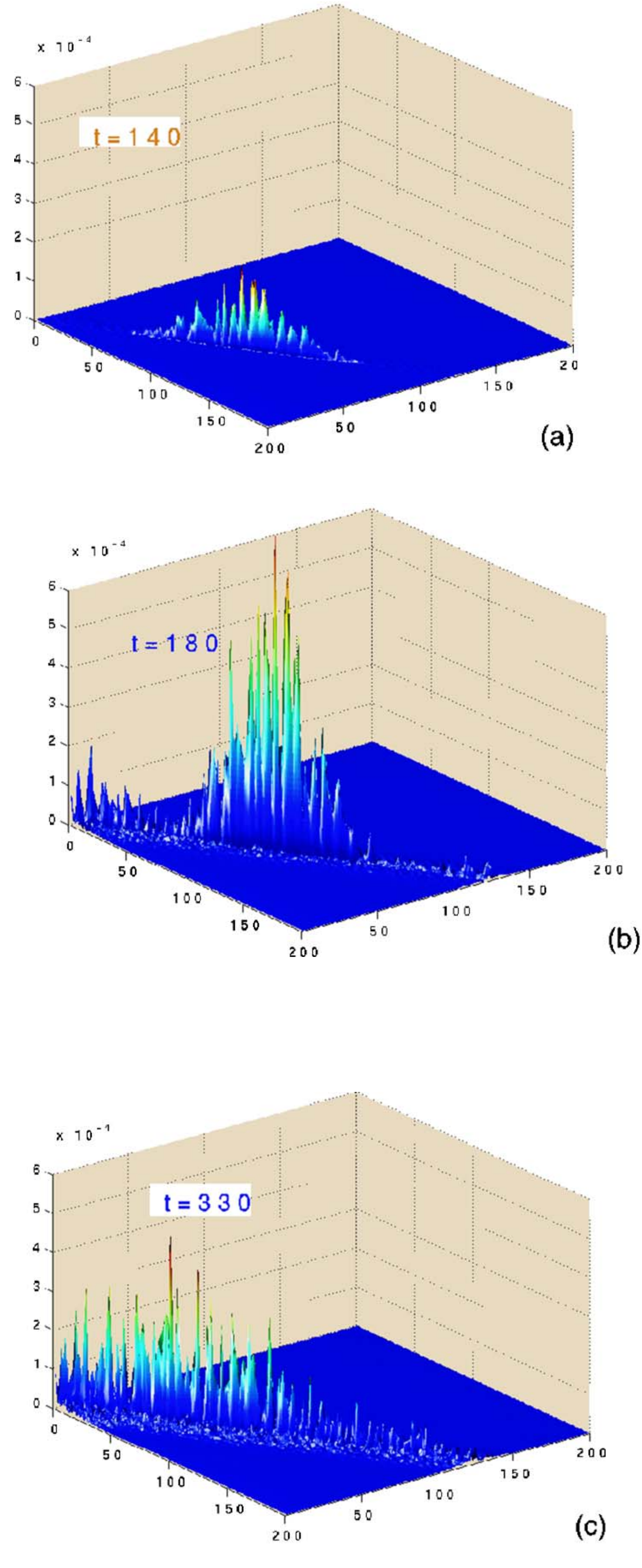
Gyrokinetic Tokamak Simulation (GTS) Code

[Wang et al., 2006 and 2007]

- General geometry interfaced with TRANSP and JSOLVER: capable for validation exercises and synthetic diagnostics based on experimental data from NSTX and DIIID





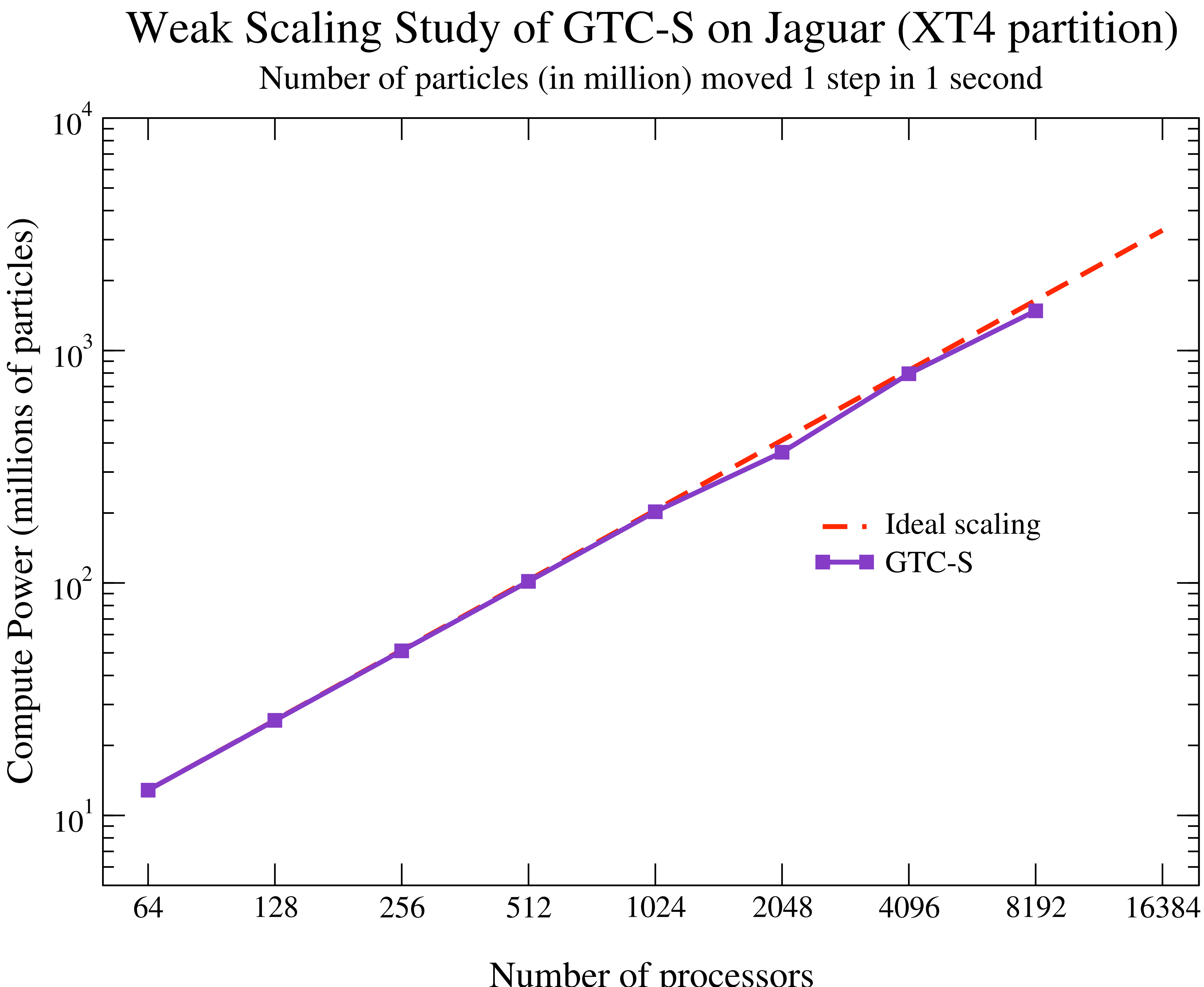


- Generalized Poisson solver involving two iteration loops using PETSc

$$\left(1+\frac{T_i}{T_e}\right)\frac{e\Phi}{T_i}-\frac{e\widetilde{\Phi}}{T_i}=\frac{\delta\bar{n}_i}{n_0}-\frac{\delta n_e^{(1)}}{n_0}+\frac{e\langle\Phi\rangle}{T_e}$$

- Multiscale phenomena have been observed

Performance of our gyrokinetic PIC code on MPP Platforms



S. Ethier, PPPL, Aug. 2007

Marching toward Fusion Simulation Project (FSP)

• Developing multiscale algorithms in toroidal geometry and testing them on GTS

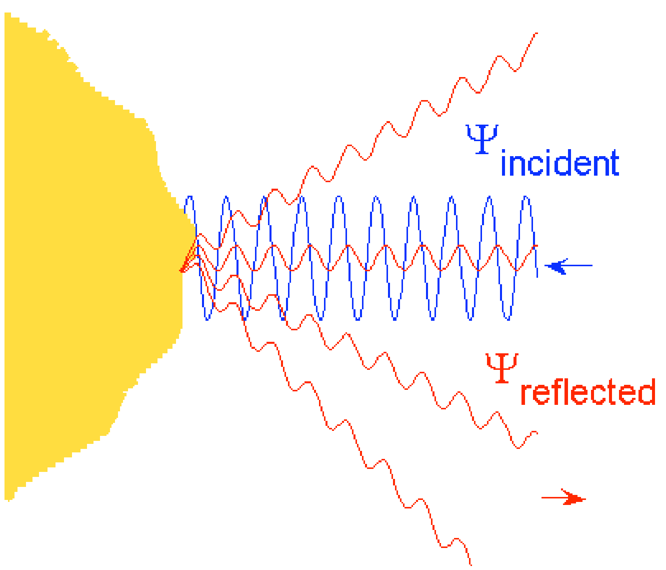
• Using inverse problems based on synthetic diagnostics for studying fluctuations and developing predictive capabilities

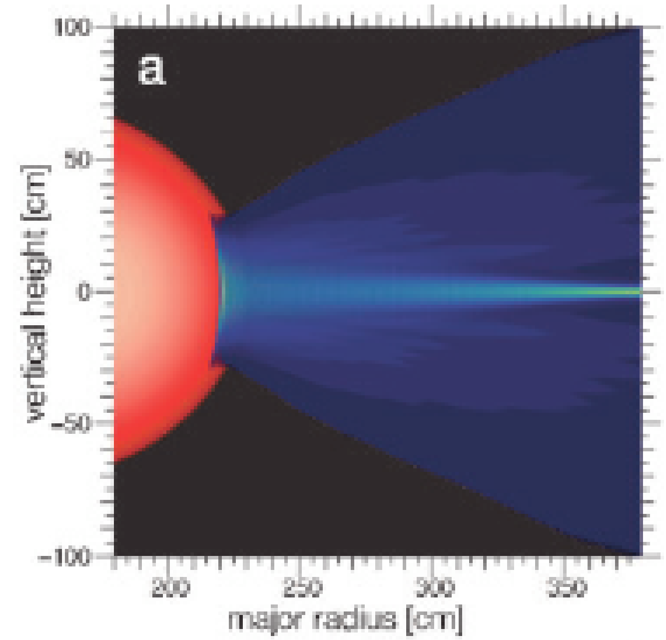
• Using projective integration in time to achieve integrated simulations by connecting separate first principles gyrokinetic PIC simulations for heating, transport and MHD

• Using Lattice-Boltzmann-like methods to simplify electron dynamics for gyrokinetic MHD simulations

• Developing an implicit wave equation solver for GTS

Diagnostics (Real/Synthetic) as an Inverse Problem





- Measurement: $\Psi_{reflected} = L\Psi_{incident}$
- $L = L(\delta n_e)$
- Inverse problem: Determine δn_e from L. Ill posed problem!
- Instead recover statistical properties of δn_e, e.g. $\langle \delta n_e \rangle$, σ, correlation-length,...
- Statistical inversion: Find $\pi(\sigma|L) \propto \pi_{prior}(\sigma)\pi(L|\sigma)$

THEORY AND MODELING OF KINETIC PLASMAS

APAM 4990, Spring 2008
W. W. Lee, Adjunct Professor
Department of Applied Physics and Applied Mathematics, Columbia University
(assisted by M. Adams)

1. Basics of kinetic plasma theory and simulation
   - Vlasov-Poisson Equations
   - Landau Damping and collisions
   - Particle codes
     - Klimontovich-Dupree representation
   - Vlasov codes
     - Semi-Lagrangian method and others
   - PIC simulation
     - NGP & SUDS, form factors
   - Computing Considerations
   - Remarks

2. Theoretical and numerical properties of plasmas
   - Linear Properties
   - Fluctuation-Dissipation Theorem
   - Numerical Noise
   - Time Step Restrictions
   - Grid Spacing Restrictions
   - Initial loading: Quiet Start - Fobanacci numbers
   - Implicit Schemes and Collisonal Models

3. Perturbative Particle Simulation and Other Schemes
   - Linearized trajectory method
   - Delta-f methods
     - Weight evolution method
     - Perturbed moments method
   - Split-weight method
     - Quasineutral model
   - Other innovative schemes
     - Adiabatic pusher, subcycling and orbit averaging
     - Drift Kinetic Model

THEORY AND MODELING OF KINETIC PLASMAS (cont.)

4. Gyrokinetic Theory and Simulation

- Drift Kinetic Vlasov-Poisson equations
  - Guiding center motion
  - ExB drift and Polarization Drift
  - Lowest order gyrokinetic-Poisson equations
- Gyrokinetic Vlasov-Poisson equations
  - Gyrokinetic ordering
  - Gyrocenter coordinates
  - Gyrophase averaging
- Gyrokinetic particle pushing
  - Coordinates transformation
- Gyrokinetic field solver
  - Integral equation
  - Pede approximation

5. Drift Wave Instabilities and Ion Temperature Gradient Modes

- Linear properties
- Numerical Schemes
- Nonlinear Saturation
- Hasegawa-Mima Equation
- Entropy conservation

6. Electromagnetic Models for Plasmas

- Fully Electromagnetic Maxwell Equations in Coulomb Gauge
- Darwin Model
- MHD model
- Electrostatic model

7. Alfven Waves in Gyrokinetic Plasmas

- Shear-Alfven waves
- Compressional-Alfven waves
- Comparisons with reduced MHD equations
- Finite-beta stabilization of microinstabilities

17 students taking for credit
3 students auditing (2 from PPPL)
6 home work assignments
1 take home final

Summary and Conclusions

• It has been an exciting three years of multiscale research and education under the present OASCR project.

• We hope that we will have the opportunity for three more years.

• Hopefully, we have also helped laying the foundations for integrated simulation of fusion plasmas and are looking forward to participate in the fusion simulation project (FSP) using the gyrokinetic PIC approach for heating, turbulence, MHD and transport physics.

• For the immediate future, in conjunction with SciDAC activities, we plan to participate in the simulations of ITER plasmas using GTS on the NCCS petaflop leadership system as a Science-at-Scale Pionnering Application.