SciDAC ISEP
Integrated Simulation of Energetic Particles

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SciDAC ISEP Center:
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SPECIAL TOPIC:
Gyrokinetic Particle Simulation: A Symposium in Honor of Wei-li Lee

Gyrokinetic particle simulations of the effects of compressional magnetic perturbations on drift-Alvenic instabilities in tokamaks
by G. Dong, J. Bao, A. Bhattacharjee, A. Brizard, Z. Lin, and P. Porazik
Outlines

- SciDAC ISEP
- ISEP V&V
- Integrated EP simulation
- TAE saturation via zonal fields
- Excitation of BAAE
Confinement of Energetic Particle in Burning Plasmas

• The confinement of energetic particles (EP) is a critical issue for burning plasma experiments since the ignition in ITER relies on the self-heating by energetic fusion products (α-particles)

• Plasma confinement properties in the new ignition regime of self-heating by α-particles is one of the most uncertain issues when extrapolating from existing fusion devices to ITER

• Energetic particles turbulence and transport: EP excite meso-scale instabilities and drive large EP transport, which can degrade overall plasma confinement and threaten the machine integrity

• Interaction between energetic particles and thermal plasmas: since EP constitute a significant fraction of plasma energy density in ITER, EP will strongly influence microturbulence responsible for turbulent transport and macroscopic magnetohydrodynamic (MHD) instabilities potentially leading to disruptions
SciDAC ISEP: Integrated Simulation of Energetic Particles in Burning Plasmas

• SciDAC GSEP (2008-2017): established the new paradigm of nonlinear kinetic simulations of energetic particle turbulence by treating relevant physical processes from micro to macro scales on the same footing

• In 2017, GSEP & CSEP (2011-2017) jointly established ISEP, one of 9 SciDAC-4 centers funded by OFES & ASCR with the goal of validated whole device modeling (WDM)

• SciDAC ISEP (2017-2022) goals
  ▶ To improve physics understanding of EP confinement and EP interactions with burning thermal plasmas through exascale simulations
  ▶ To develop a multiscale and multiphysics ISEP framework with predictive capability as an EP module in future WDM project
ISEP Objectives

• Study EP physics needed for predictive capability
  – EP transport by mesoscale EP turbulence
  – EP coupling with microturbulence and macroscopic MHD modes
  – First-principles simulations: GTC, GYRO, FAR3D, M3D-K

• Develop integrated simulation capability for EP physics
  – ISEP framework based on GTC

• Develop EP module with predictive capability for WDM
  – Reduced EP transport models (CGM, RBQ)
  – First-principles ISEP framework

• EP module verification and validation (V&V via kick model)

• Computational partnership
  – Workflow/data management
  – Solvers
  – Optimization & portability
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• RSAEs near \( \rho \sim 0.4 \)
• TAEs > \( \rho \sim 0.7 \)
• ECEI Dual Array
  – 2 \( \rho \): 0.4–0.56, match RSAE location
  – 1 \( \rho \): 0.72–0.94, match TAE location

• RSAE, RSAE, microturbulence co-exist
• What is saturation & transport mechanisms?
• Linear & nonlinear V&V of 8 GK & MHD simulation of RSAE/TAE
• V&V of 3 reduced EP transport models
• Linear benchmark nearly done. Nonlinear simulation in progress
DIII-D shot 158243 at 805ms for ISEP V & V of AE Saturation & EP Transport
n=4 RSAE in DIII-D shot 158243 at 805ms
Validation via Synthetic Diagnostics

Comparison of GTC simulation with experimental ECE data using Synthetic Diagnostic Platform [Shi, 2017].

(a) Radial structure of $\delta T_e$. (b) The $n = 4$ mode's phase with respect to $R = 195.0$ cm
Nonlinear Interaction of RSAE, TAE, ITG

- Using EP profile from kick model, GTC finds $n=6$ TAE weakly unstable in the outer edge, good agreement with DIII-D
- GTC finds strong ITG instability in the outer edge, nonlinearly spreading to core
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Kinetic-MHD via Gyrokinetic Simulation

- Nonlinear gyrokinetic equation, Poisson equation, Ampere’s law

\[
\frac{\partial F}{\partial t} + (v_{\parallel} b + v_d) \cdot \frac{\partial F}{\partial R} + v_{\parallel} \frac{\partial F}{\partial v_{\parallel}} = 0
\]

\[
\phi - \tilde{\phi} = -\sum_s 4\pi e Z_s \bar{n}_s
\]

\[
\nabla^2 A_{\parallel} = -\sum_s \frac{4\pi e}{c} Z_s \bar{n}_s u_s
\]

- In fluid limit, gyrokinetic system recover linear MHD modes including Alfven wave, interchange mode, kink mode, KBM

\[
\frac{\omega(\omega - \omega_P)}{v_A^2} \nabla^2_{\perp} \delta \phi - iB_0 \cdot \nabla \left\{ \frac{b_0 \cdot \nabla \times [\nabla \times (k_{\parallel} \delta \phi b_0)]}{B_0} \right\}
\]

\[
-\frac{\dot{\omega}}{c} \delta B \cdot \nabla \left( \frac{b_0 \cdot \nabla \times B_0}{B_0} \right)
\]

\[
-\frac{i\omega}{c} \frac{4\pi}{c} \left[ \nabla \times b_0 \cdot \nabla \left( \frac{\delta P_{\parallel}}{B_0} \right) + b_0 \times \nabla B_0 \cdot \nabla \left( \frac{\delta P_{\perp}}{B_0^2} \right) + \frac{\nabla \times b_0 \cdot \nabla B_0}{B_0^2} \delta P_{\perp} \right]
\]

\[= 0\]

Difficult in Gyrokinetic Simulation of MHD Modes: $E_{||}$

- Parallel electric field $E_{||} = -\nabla_{||}\phi - \frac{\partial A_{||}}{\partial t}$ [Lin, SciDAC PMP meeting, GA, 2001]

- Need to calculate accurately scalar $\phi$ and vector potentials $A_{||}$
  
  $\phi - \tilde{\phi} = -\sum s 4\pi e Z_s n_s$

- Ideal MHD $E_{||} \sim 0$. $|E_{||}|/|\nabla_{||}\phi| \sim |E_{||}|/|\frac{\partial A_{||}}{\partial t}| \sim (k_{\perp}\rho_s)^2 \ll 1$

- Physics: cancellation between electrostatic and inductive $E_{||}$


- Canonical momentum used as independent velocity variable
  
  $\left(\nabla_{\perp}^2 - \frac{\omega_{pe}^2}{c^2} - \frac{\omega_{pi}^2}{c^2}\right)\Delta A_{||} = \frac{4\pi}{c} \left( e n_{e0} \delta u_{||e} - Z_i n_{i0} \delta u_{||i} \right)$.

- LHS: $|1^{\text{st term}}|/|2^{\text{nd term}}| \sim (k_{\perp} d_e)^2 \ll 1$. Small numerical error of RHS leads to large error of $A_{||}$

- Infamous “cancellation problem”: calculate $2^{\text{nd}}$-order $O(k_{\perp}^2\rho_s d_e)^2$ term from $0^{\text{th}}$–order $O(1)$ equation!
Solution: $E_\parallel$ from Electron Parallel Force Balance

- For $\omega/k_\parallel << v_e$, electron response mostly adiabatic (isothermal)
  Adiabatic $E_\parallel = -\nabla_\parallel (\phi + \phi_{ind})$ from massless electron \cite{Holod, PoP2009}

$$\frac{e\phi_{ind}}{T_e} = -\frac{e\phi}{T_e} + \frac{\delta n_e}{n_0} - \frac{\delta\psi^A}{n_0} \frac{\partial n_0}{\partial \psi}$$

Alfven wave, IAW, drift wave

- Vector potential $A_\parallel$ calculated from $E_\parallel$
  \[ \frac{\partial A_\parallel}{\partial t} = \nabla_\parallel \phi_{ind} \]

- Perturbed current $\delta u_e$ from Ampere’s law
  \[ n_0 e \delta u_e = -\nabla_\perp^2 A_\parallel \]

- Perturbed density $\delta n_e$ from continuity equation
  \[ \frac{\partial \delta n_e}{\partial t} = -\nabla_\parallel n_0 \delta u_e \]

- Electrostatic potential $\phi$ from Poisson equation using perturbed density $\delta n_e$

- No cancellation problem or electron particle noise

  \textit{A Fluid-Kinetic Hybrid Electron Model for Electromagnetic Simulations,}
  \textit{Lin and Chen, Phys. Plasmas 8, 1447 (2001)}

- Mixed-variable gyrokinetics \cite{Mishchenko et al, PoP (2014)} separates $A_\parallel$ into
  “symplectic” and “Hamiltonian”; ideal MHD as “symplectic” $\phi_{ind} = -\phi$: Alfven wave.
  However, IAW, drift wave have cancellation problem and electron particle noise
Fluid-Kinetic Hybrid Electron Model [Lin & Chen, PoP2001]

- Total $E_\parallel$ corrected by non-adiabatic $E_\parallel$ from kinetic electron response using split-weigh scheme [Manuilskiy and Lee, PoP2000] to reduce noise

$$f_e = f_0 e^{(\phi + \phi_{\text{ind}})/T_e} + \delta g_e$$

- Collisionless tearing mode removed in this expansion based on small electron mass; Resistive tearing mode kept via Ohm’s law

- Electrostatic version [Lin et al, PPCF2007] removes numerical $\omega_h$ mode, enabling simulation of trapped electron mode

- Electron model extensively utilized by GSEP for simulating microturbulence, Alfvén eigenmodes, kink & resistive tearing modes

$$\left[ \frac{\partial}{\partial t} + (v_\parallel b + v_d + v_E) : \frac{\partial}{\partial x} - b^* \cdot \nabla (\mu B - e\phi) \frac{\partial}{m_e \partial v_\parallel} - C_e \right] \delta g_e^{(1)}$$

**A Conservative Scheme Solving Exact DKE**

- Calculate total $E_{||}$ as sum of adiabatic and non-adiabatic parts

$$A_{||} = A_{||}^A + A_{||}^{NA}$$

$$\frac{\partial A_{||}^A}{\partial t} = \nabla_{||} \phi_{ind}$$

$$\frac{e \phi_{ind}}{T_e} = -\frac{e \phi}{T_e} + \frac{\delta n_e}{n_0} - \frac{\delta \psi^A}{n_0} \frac{\partial n_0}{\partial \psi}$$

- Define electron adiabatic responses using adiabatic $E_{||}$

$$f_0 + \delta f_A = f_0 e^{(\phi + \phi_{ind})/T_e} + \delta \psi^A \frac{\partial f_0}{\partial \psi}$$

- Solve exact DKE by calculating kinetic electron non-adiabatic responses $\delta h_e$

$$f_e = f_0 + \delta f_A + \delta h_e$$

- Non-adiabatic part of $E_{||}$ calculated via electron parallel momentum equation (generalized Ohm’s law) using non-adiabatic response

A Conservative Scheme Solving Exact DKE

• Recover collisionless tearing mode with current sheet at $d_e$ scale
• Non-tearing current screened by $d_e$, no “cancellation problem”
• Recover nonlinear MHD dynamo term, “nonlinear polarization term”, “ponderomotive force”:
  $ \delta j_{pol} \times \delta B_\perp$

$$\left( \nabla_\perp^2 - \frac{1}{d_e^2} \right) \frac{\partial A_{\parallel NA}^A}{\partial t} = \frac{1}{d_e^2} \chi_\parallel - c \nabla_\perp^2 (\nabla_\parallel \delta \phi_{ind})$$

$$\chi_\parallel = \frac{c}{en_0} \mathbf{b}_0 \cdot \nabla \delta P_{\parallel}^{NA} - \frac{c}{en_0 B_0} \delta \mathbf{B}_{\parallel}^{NA} \cdot \nabla P_{\parallel}^{NA} - \frac{c}{en_0 B_0} \delta \mathbf{B} \cdot \nabla \delta P_{\parallel}^{NA} - \frac{c}{B_0} \delta \mathbf{B} \cdot \nabla \delta \phi_{ind}$$

\{III\} \quad \{IV\} \quad \{V\} \quad \{VI\}

\begin{align*}
+ & \frac{c}{B_0} \delta \mathbf{B} \cdot \nabla \langle \phi \rangle - \frac{cm_e}{en_0} \nabla \cdot \left[ n_0 \delta u_{\parallel e} \left( 3 \mathbf{V}_c + \mathbf{V}_e \right) + n_0 u_{\parallel e} \mathbf{V}_e \right] - \frac{cm_e}{en_0} \nabla \cdot \left( n_0 \delta u_{\parallel e} \mathbf{V}_e \right) \\
\{VII\} \quad \{VIII\} \quad \{IX\}
\end{align*}

\begin{align*}
+ & \frac{c}{en_0} \frac{P_{\parallel 0} - P_{\perp 0}}{B_0^2} \delta \mathbf{B} \cdot \nabla B_0 + \frac{c}{en_0} \frac{\delta P_{\parallel NA}^{NA} - \delta P_{\perp NA}^{NA}}{B_0^2} B_0 \cdot \nabla B_0 \\
\{X\}
\end{align*}
Compressible Magnetic Perturbations via Perpendicular Force Balance for Slow Modes

\[ \delta B_\parallel B_0 \left\{ 1 + \beta_e + \beta_i \left[ I_0 \left( k_\perp^2 \rho_i^2 \right) - I_1 \left( k_\perp^2 \rho_i^2 \right) \right] \exp \left( -k_\perp^2 \rho_i^2 \right) \right\} \]

\[ \frac{8\pi}{16\pi T_i} \left\{ I_0 \left( k_\perp^2 \rho_i^2 \right) - I_1 \left( k_\perp^2 \rho_i^2 \right) \exp \left( -k_\perp^2 \rho_i^2 \right) - 1 \right\} \delta B_\parallel e \delta \phi \]

\[ = -\pi \Omega_e^2 \left( \int d\mu d\nu B_0 \int_0^{\rho_e} F_\text{gyro e} r dr - \pi \Omega_i \right) \]

\[ \times \left( \int d\mu d\nu B_0 \left\langle \int_0^{\rho_i} F_\text{gyro i} r dr \right\rangle \right). \quad (13) \]

When \( k_\perp \rho_i \ll 1 \), Eq. (13) reduces to

\[ \delta B_\parallel B_0 \left( 1 + \beta_e + \beta_i \right) \]

\[ \frac{4\pi}{4\pi} = -\delta P_{e\perp} - \delta P_{i\perp}, \quad (14) \]

Gyrokinetic particle simulations of the effects of compressional magnetic perturbations on drift-Alfvénic instabilities in tokamaks, Dong et al, Phys. Plasmas 24, 081205 (2017)

- Significant effects of \( \delta B_\parallel \) on KBM
- Effects of \( \delta B_\parallel \) on TAE linear dispersion very small
**Gyrokinetic Toroidal Code**

- First-principles, integrated simulation capability for nonlinear interactions of multiple kinetic-MHD processes

- Current capability in a single version
  - Global 3D toroidal geometry & experimental profiles
  - **Microturbulence**: 5D gyrokinetic ions & electrons, electromagnetic fluctuations (including compressional perturbations, tearing & non-tearing parity)
  - **MHD and energetic particle**: Alfven eigenmodes, kink, tearing modes
  - **Neoclassical transport**: Fokker-Planck operators
  - **Radio frequency waves**: 6D Vlasov ions

[Lin et al, Science1998]
Phoenix.ps.uci.edu/GTC
Optimizing GTC for Exascale Computing

- GTC being developed as energetic particle module in fusion WDM by SciDAC ISEP collaborations: UCI, GA, PPPL, ORNL, LBNL, LLNL
- GTC speeds up 20X from CPU to GPU on SUMMIT (world’s fastest computer) by CAAR (Center for Accelerated Application Readiness) project: UCI, PU, ORNL, NVIDIA, IBM
- GTC recently selected by NVIDIA as one of Top 15 App Worldwide

*Wall-clock time for one trillion particle pushes in GTC weak scaling test on Summit*
GTC Simulation of Current Driven Instabilities: Kink, Resistive & Collisionless Tearing Modes

• GTC finds ion kinetic effects and toroidicity reduce growth rate of kink [McClenaghan, PoP2014] and resistive tearing mode [Liu, PoP2014]
• GTC simulations of collisionless tearing mode [Bao, 2017]
  ✓ GTC kinetic $\gamma=0.0031C_s/R_0$, [Drake & Lee, PF1977] kinetic theory $\gamma=0.0027$
  ✓ GTC fluid $\gamma=0.0014C_s/R_0$, [Liu & Chen, PPCF1977] fluid theory $\gamma=0.0015$

![GTC simulation of resistive tearing mode in cylinder [Liu, PoP2014]](image1)

![GTC simulation of collisionless tearing mode in cylinder [Bao, PoP2017]](image2)
KBM Saturation via Zonal Fields (ZF)

- ZF generated ($2y^{lin}$) via KBM 3-wave coupling, in contrast to ITG modulational instability
- Localized current sheet generated ($3y^{lin}$) by ponderomotive force

![Graph showing ITG and KBM effects](image-url)
KBM Mode Structure Broken by Zonal Fields

Nonlinear Saturation of Kinetic Ballooning Modes by Zonal Fields in Toroidal Plasmas, G. Dong, J. Bao, A. Bhattacharjee, and Z. Lin, submitted to PRL, 2018
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Measurement Shows Fast Radial Drift of TAE in DIII-D

- TAE moves rapidly while thermal plasma profiles barely change
- Cannot be explained by perturbative theory: thermal plasma profiles set MHD mode structure, EP only drives growth rate
GTC Simulations Find TAE Radial Localization

- Simulations scan EP profiles within experimental uncertainty
- Unstable TAE radial structures move with EP density gradient
- In contrast, stable TAE excited by antenna has larger radial width
- EP non-perturbative contribution induces TAE radial localization

TAE in DIII-D shot # 142111 at 525ms
Comparison of TAE Mode Structures between Simulation & Experiment

- EP non-perturbative contribution breaks radial symmetry of TAE eigenmode

**TAE in DIII-D shot # 142111 at 525ms**

[Z. X. Wang et al, PRL2013]
Comparison of TAE Frequency between Simulation & Experiment

- EP non-perturbative contribution and trapped electron effects induce TAE frequency dependence on toroidal mode number n

**TAE in DIII-D shot # 142111 at 525ms**
TAE Saturation via Zonal Fields

- Conventional model: Perturbative theory and reduction from 3D to 1D, i.e., single toroidal mode, radially local
- Non-perturbative simulation: Nonlinear physics beyond 1D model
  - Zonal fields (flow & current)
  - Fast chirping induced by radial variations of amplitude & guiding center dynamics
    
    [Zhang et al, PRL2012]

- TAE saturates by zonal flow
- Zonal current has little effects on TAE saturation
**TAE Saturation via Zonal Fields**

- ZF generated via 3-wave coupling, \( \gamma_{ZF} = 2\gamma_{lin} \)
- Generation of localized current sheet \( \gamma_{CS} = 3\gamma_{lin} \)
Radial profiles of zonal flows and zonal currents, thermal ion particle diffusivity and heat conductivity.
TAE Saturation via Zonal Fields

- TAE linear mode structure broken by ZF
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Low Frequency Modes Induced Fast Ion Loss in DIII-D

- Both high frequency Alfvén eigenmodes (AE) and low frequency modes (LF)
- Up to 45% neutron deficit observed; Half induced by AE; The other half caused by LF modes
- LF: Beta-induced Alfvén eigenmode (BAE)? beta-induced Alfvén-acoustic eigenmode (BAAE)?
Low Frequency Alfven Eigenmodes

• Motivation
  – Loss of energetic particles due to low frequency BAAE & BAE
  – Strong coupling of BAAE & BAE with thermal plasmas: impact on confinement of thermal plasmas, transfer of energy from energetic to thermal ions?

• Existence & excitation of BAAE
  – Discrete BAAE has not been predicted by MHD or kinetic analytic theory
  – Does BAAE exist despite heavy damping by thermal ions?
  – Can BAAE be excited by realistic fast ion density gradient?

• Nonlinear interaction between BAAE & BAE
  – Can BAAE be nonlinearly generated?
  – What is nonlinear dynamics of BAAE?
Transition from BAE to BAAE for Larger Device $T_i = 0.5T_e$

Polarization of Unstable BAAE and BAE Alfvénic

- All poloidal harmonics of unstable BAAE and BAE are Alfvénic
- Gradually decrease the drive → damped modes.

\[ \frac{E_{\parallel}}{E_{\parallel \text{ES (BAAE)}}} \ll 1, \ m=6 \ \text{Alfvénic} \]

\[ \sim 1, \ m = 5,7 \ \text{Acoustic} \]

\[ \frac{E_{\parallel}}{E_{\parallel \text{ES (BAE)}}} \ll 1, \ m=5,6,7 \ \text{Alfvénic} \]

- Perturbative, radially local theory not valid for BAAE
Linear Wave-Particle Energy Exchanges

- BAAE & BAE excited by transferring from fast ion perpendicular energy
- BAAE damped by transferring to thermal ion parallel & perpendicular energy
- BAE damped by transferring to thermal ion perpendicular energy
- BAAE: $\omega_{r}=0.50v_{i}/R_{0}, \gamma=0.04, \gamma_{EP}=0.08, \gamma_{D\_unstable}=-0.04, \gamma_{D\_stable}=-0.22$
- BAE: $\omega_{r}=2.5v_{i}/R_{0}, \gamma=0.28, \gamma_{EP}=0.44, \gamma_{D\_unstable}=-0.16, \gamma_{D\_stable}=-0.05$
- BAAE excited even $\gamma_{EP} \ll \gamma_{D\_stable}$: perturbative theory not valid for BAAE

Nonlinear Generation of BAAE by BAE

- Linearly stable BAAE NL driven by BAE with $n_f = 9.5\%n_e$

- $\gamma_{BAAE} \sim const$ when BAE saturates

- NL generation of BAAE by BAE in DIII-D?

- Threshold $n_f = 9\%n_e$
The University of California, Irvine (UCI) invites applications for two Postdoctoral Researcher positions in integrated fusion simulation beginning in September 2018. The fusion simulation group at UCI is led by Professor Zhihong Lin, who directs the Center for Integrated Simulation of Energetic Particles (ISEP), part of US Department of Energy (DOE) Scientific Discovery through Advanced Computing (SciDAC) initiative. The successful candidates will develop advanced simulations on the world’s fastest supercomputers to study energetic particle confinement and turbulent transport in fusion experiments including tokamak, stellarator, and field reversed configuration. See http://phoenix.ps.uci.edu/zlin/ for additional information.

The successful applicants will have a Ph.D. degree in plasma physics or fusion energy science; salary will be commensurate with experience and qualifications. Applicants should submit a curriculum vitae, statement of research interests, a list of publications, and three names for letters of recommendation to Professor Zhihong Lin by email zhihongl@uci.edu.