The role of global gyrokinetic simulations in multi-scale transport modeling

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Multi-Scale Methods For Waves And Transport Processes In Fusion Plasmas:
The Legacy Of Grigory Pereverzev
Motivation

• To determine the fusion power of future machines it is necessary to accurately predict the time evolution of density, temperature and rotation profiles on an energy confinement time.

• Reduced 1D integrated transport modeling (ASTRA, TRANSP, JETTO) are used to determine the relation between profiles, sources/sinks and fluxes.

• Multiple local flux-tube simulations at different radial positions can be used to evolve the macroscopic profiles in time. But the boundary conditions and the treatment of sources & sinks can be a problem.

• Global full-f gyrokinetic simulations simultaneously evolve the fluctuations and the equilibrium in time while taking heat sources and sinks into account.----> self-consistent
Large scale separation in ITER plasmas

- Grid spacings $\sim$ 3D space x 3D velocity x time

--> Multi-scale methods that use physics guidance are required
Large scale separation in ITER plasmas

**Multiscale model for Collisions:** Relaxing the original requirement for the numbers of particles in the Debye sphere by making collisions a subgrid phenomena.
Large scale separation in ITER plasmas

Gyrokinetic formalism eliminates the gyroangle dependency reducing the problem size from 3D to 2D in velocity space.

\[
(r, v) \rightarrow (\vec{R}, v_\parallel, v_\perp)
\]
Large scale separation in ITER plasmas

Magnetic coordinates (ψ, θ, ζ) take advantage of a $k_{||} << k_{\perp}$ and greatly improve the computational requirements for fusion plasmas.
Large scale separation in ITER plasmas

\[
\left( \frac{L_\parallel}{\Delta_\parallel} \right) \times \left( \frac{L_\perp}{\Delta_\perp} \right)^2 \times \left( \frac{L_v}{\Delta_v} \right)^2 \times \left( \frac{L_t}{\Delta_t} \right)
\]
Critical issues for global simulations (I)

**Messo scale transport**

- Local gyrokinetic turbulence simulations have been found to agree well with experiments in the high temperature core region \((r/a<\sim 0.8)\) of both L-mode and H-mode regimes.
  - Energy fluxes
  - Density fluctuation levels
  - Correlation lengths

- Local gyrokinetic simulations generally under-predict energy transport in the L-mode for \(r/a>\sim 0.8\)

- Can the radial propagation of meso-scale non-linear structures explain the systematically under-prediction? ----> global simulations required
Critical issues for global simulations (II)

Turbulence interaction with large scale flows

• Velocity shearing of turbulent fluctuations by large scale flows generate transitions improved confinement regimes. But what is generating the velocity shear?

• $E_r$ radial dependence fairly well predicted by neoclassical theory. However, Reynolds stress from turbulence generate corrugations of $E_r$.
  – Critical for ExB flow shear of the turbulent fluctuations
  – Can transport momentum from the edge to the core

• Coupling of global codes to the edge is essential but extremely challenging: electromagnetic, ions & electrons, geometry, plasma-wall interaction, neutrals.
Critical issues for global simulations (III)

Turbulence and MHD modes

- Several global codes have been developed for electromagnetic turbulence to study the self-consistent interplay between magnetic islands and turbulence but are still numerically very challenging.

- The interplay between turbulence and sawtooth/ELM crashes is so far unexplored territory.
Numerical PIC approach: ELMFIRE
Gyrokinetic full-f code: ELMFIRE

ELMFIRE properties:

- Nonlinear gyrokinetic electrostatic 5D full-f particle code.
- Species: e,i, impurity.
- Binary collision model.
- Quasineutrality enforced through polarization drift and electron parallel non-linearity.
- Applicable for kinetic analysis of neo-classical physics and microturbulence.

Heikkinen et al. JCP '08 & '11, PoP'10

Instantaneous density fluctuation normalized to flux-surface averaged density, poloidal section.
\[
\frac{dR}{dt} = Ub' + \frac{\mu}{q} \hat{b} \times \nabla B + \hat{b} \times \nabla \Phi \\
\frac{dv}{dt} = \frac{b'}{m} (\mu \nabla B + e \nabla \Phi)
\]

\[
\frac{dR_I}{dt} = \frac{1}{B\Omega} \frac{dE}{dt} \\
\frac{dv_{\|,e}}{dt} = \frac{qE_{\|}}{2m}
\]

J.A. Heikkinen PoP 2010
Momentum or Energy conserving interpolation.

In PIC/CIC scheme one may interpolate in two ways:

1) \( E(x) = -\text{grad} \Phi = -\sum \Phi_k \text{grad} S_k (x) \)

2) \( E(x) = \sum E_k S_k (x) \)

Scheme 1) conserves energy and is numerically stable against divergent ExB flow (J.A. Byers et al., 1994) but has a self force.

Scheme 2) conserves momentum, but is prone to numerical instability by divergent ExB flow
Momentum conserving interpolation scheme drives instabilities by divergent E×B flow.

SOLUTION: Ensure zero ExB divergence by modifying the expression for $E_r$.

\[
\left( \nabla \times \vec{E} \right)_\phi = 0 \quad \rightarrow \quad \frac{\partial (r E_\theta)}{\partial r} = \frac{\partial E_r}{\partial \theta}
\]

\[
E_r(r, \theta, \phi) = \int_0^\theta \frac{\partial}{\partial r} (r E_\theta) \, d\theta + E_r(r, 0, \phi)
\]
Energetic consistency

• Where is the energy lost?
  → Electron parallel motion.

• 1\textsuperscript{st} order Implicit Euler tends to cool electrons, only 2-point method stable

• Improvement by using 2\textsuperscript{nd} order velocity verlet integration.
Validation of the ELMFIRE code for ohmic FT-2 tokamak discharges
FT-2 tokamak @ the Ioffe Institute, St. Petersburg

- Large aspect ration: $R_0 = 55$ cm, $a = 8$ cm
  
  \[ B_t < 2.7 \text{ T}, \quad I_p < 50 \text{ kA} \]

  \[ N_e < 7 \cdot 10^{19} \text{ m}^{-3}, \quad T_e < 1 \text{ keV}, \quad T_i < 0.4 \text{ keV} \]

- Operational since 1981

- Used for the development of new diagnostics & turbulence and GAM studies

- CX analyser & visible light spectrometry
- Multi-pulse Thomson scattering
- Doppler reflectometry: Cutoff layer, $k_\theta \rho_s \sim 0.1$, rad. res. ~0.5 cm
- Enhanced scattering: Upper hybrid resonance layer, $k_\theta \rho_s \sim 2-5$, rad. res. ~0.1 cm
Confinement time simulation within 5 days with 2048 processors

- Confinement time $\tau_E \sim 1$ ms / 30ns time step \(\sim 30\,000\) time steps
- low beta --> electrostatic assumption valid
- large aspect ratio --> analytical magnetic field background

1 time step takes 1 min with 1 000 000 particles per proc.

- High collisionality $v^* \sim 10$-25 & steep gradients ($\delta n/n \sim 1$-8 %)
  \(\rightarrow\) 3000 ppc needed to overcome the noise level
- $1/p^* = a/p_s = 50$-350, grid is set to 120r/150p/t8

430 000 000 particles in total
Steady state profiles obtained 30 μs after start up

\[ B=2.2\text{T}, \; I=18.9\; \text{kA}, \]
\[ \text{Hydrogen plasma,} \]
\[ Z_{\text{eff}} \sim 3.1, \text{Impurity } O^{+6} \]

Sources & Sinks
- Ohmic heating model by loop voltage
- radiation & CX losses
- “Poloidal limiter model”
- recycling
From noise to turbulence spectrum

- Wave number spectrum from different time instants demonstrates how one moves from white noise to physical spectrum in modes.
Noise fluctuation level

Noise level

Turbulence fluctuation level

Graphs showing the fluctuation levels of noise and turbulence with varying parameters.
The Neoclassical equilibrium $E_r$

The neoclassical equilibrium is obtained by removing the modes with toroidal mode number $n \neq 0$ => NC filtering

$$E_{r,HH} = \frac{T_i n_i'}{q_i n_i} + C \frac{T_i'}{q_i} + B_p U_i$$

$$C = 1 - \frac{\left(1.17 - 0.35 \sqrt{\nu}\right) - 2.1 \nu^2 \epsilon^3}{1 + 0.7 \sqrt{\nu} + \nu^2 \epsilon^3}$$

The poloidal variation of the impurity density in the presence of steep gradients has an influence on the poloidal flow. Main ions in Plateau regime & Impurities in PS regime

Landreman, PoP 2011
The synthetic diagnostic is constructed using the complex instrumental DR weighting function.
Mean poloidal flow is well reproduced by ELMFIRE

\[ v_\theta = 2\pi f_D/k_\theta = v_{\text{ExB}} + v_{\text{ph}} \]
$E_r$ bursts measured with the ES and reproduced by ELMFIRE

The experimental signal is low-pass filtered with a Nyquist frequency of $F_N = 156.25$ kHz.
Effect of the impurities on the GAM frequencies

GAM frequency:

\[ \omega_{GAM} = \frac{v_{t,i}}{R} \sqrt{\frac{7}{4} \frac{T_e}{T_i}} \]

GAM frequency including impurity contribution:

\[ \omega_{IMP} = \frac{7/4(n_i+n_Z)+A}{n_i m_i+n_Z m_Z} + \frac{23/8(n_i/m_i+n_Z/m_Z+B)}{7/4(n_i+n_Z)+A} q^2 \]

Guo et al. PoP 17 2010
Correlation measurements with ES Diagnostic

Two signals at probing frequencies with difference $|f_2 - f_1| < 4$ GHz, corresponding to spatial separation $|\Delta L| < 2$ cm in plasma, are measured simultaneously.
GAM propagating radially outwards with 1.1 km/s

ES: two $f_D$-signals

ELMFIRE: $E_{r1}$ & $E_{r2}$

$k_r \sim 2.8 \text{ cm}^{-1}
\lambda_r \sim 2.2 \text{ cm}
V_r \sim 1.1 \text{ km/s}
Profiles and transport results (ctd)

\[ \chi_e = \frac{P_{OH} - P_{rad} - \frac{3}{2} \frac{d}{dt} \int n_e T_e dV}{4\pi^2 R r n_e \Delta T_e} \]

\[ \chi_i = \frac{P_{ei} - P_{CX} - \frac{3}{2} \frac{d}{dt} \int n_i T_i dV}{4\pi^2 R r n_i \Delta T_i} \]

\[ Q = \frac{\sum S(x_p \Delta r)(m_p / 2(v_p - u)^2 - q_p(\Phi_p - \Phi_{FS}))}{4\pi^2 R r} \]

What is wrong/missing?
- Definitions of \( \chi \)? Grid resolution?
- Boundary treatment? Physics?
Conclusions

• Good correspondence between experiments and simulation have been obtained for:
  – Mean $E \times B$ flows.
  – DR spectra.
  – Oscillations in zonal flows.
  – GAM spatial correlation properties.

• Clear influence of the impurity species on the poloidal flow is observed.

• The transport coefficient agree in size but the trend is opposite......Why?
Radial electric field

Radial profile

Top pedestal

Half way pedestal
Ion heat conductivity

Radial profile

Top pedestal

Half way pedestal
Ion particle flux

Radial profile

Top pedestal

Half way pedestal
Sosenko's PIC model

- P. Sosenko's model uses an alternative definition of gyrocenter.
  
  \[ \mathbf{P. P. Sosenko et al., Physica Scripta 64 (2001) 264} \]

- Polarization drift is included in the Eqs of motion.
- This introduces changes on Poisson's equation.

\[
\mathbf{x} = \mathbf{R} - \mathbf{\dot{\rho}} \left\{ \begin{array}{l}
\mathbf{\ddot{\rho}} = \frac{\mathbf{b} \times \mathbf{\dot{v}}}{\Omega} \quad \text{Lee} \\
\mathbf{\dot{\rho}} = \frac{\mathbf{b} \times (\mathbf{v} - \mathbf{\dot{v}})}{\Omega} \quad \text{Sosenko}
\end{array} \right. 
\]
Sosenko's PIC model

Extra term in the equations of Motion:

\[
\frac{dR}{dt} = U\hat{b}_* + \frac{\mu}{e} \frac{\hat{b} \times \nabla B}{B} + \frac{\hat{b} \times \nabla \Phi}{B} + \frac{1}{\Omega} \frac{d}{dt} - \nabla \Phi
\]

\[
\frac{d\mathbf{v}}{dt} = \frac{\hat{b}_*}{m} (\mu \nabla B + e \nabla \Phi)
\]

And extra term in the Poisson equation
(for fluid model there is also a Jacobian term in the poisson eq.):

\[
\nabla^2 \Phi + \frac{q^2}{m_0 B e} \int f' \left( (\Phi - \langle \Phi \rangle) \frac{\delta f}{\delta \mu} + \frac{m}{q} \langle f \rangle \nabla^2_{\perp} \langle \Phi \rangle \right) \left| d\mathbf{v} \right| = \frac{1}{\varepsilon_0} (e n_e(\mathbf{r}) - q n_i(\mathbf{r}))
\]

For \( k_{\perp} \rho_i \to 0 \), \( \int \left| (\Phi - \langle \Phi \rangle) \frac{\delta f}{\delta \mu} + \frac{m}{q} \langle f \rangle \nabla^2_{\perp} \langle \Phi \rangle \right| d\mathbf{v} \to 0 \)}