A new hybrid Lagrangian numerical scheme utilizing phase space grid for XGC1 edge gyrokinetic code

S. Ku
Princeton Plasma Physics Laboratory, USA

In collaboration with
R. Hager, C.S. Chang

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Outline

• Tokamak edge plasmas and XGC1
• Total-f (full-f), conventional $\delta f$, and total-$\delta f$ PIC
• New hybrid Lagrangian scheme
  – Needed for edge simulation (reduces weight-growth from wall-loss, enables non-linear collision)
  – Use both particle and v-space-grid
  – Direct weight evolution
  – Used in XGC1/a for all physics
• Example in a simple ITG turbulence case
  – The $\alpha$-factor and numerical dissipation
  – Homogeneous marker distribution in v-space
Tokamak Edge Plasmas

- Non-Maxwellian
  - Steep H-mode gradient
  - In-contact with wall
  - Strong turbulence level
    \( \frac{\delta n}{\langle n \rangle} \sim 10\% \)

- Sources and Sinks
  - Wall loss
  - Neutral atoms
  - Radiative cooling
XGC1: X-point included Gyrokinetic Code

• Uses experimental EFIT data
  – Magnetic fields
  – Divertor and limiter

• Fully nonlinear Fokker-Plank – Landau collision on v-space grid

• Logical sheath to handle wall boundary

• Built-in neutral Monte-Carlo routine and atomic cross sections

• GPU+CPU hybrid capability

• Good weak and strong scaling to maximal capability of the leadership HPCs (titan, mira, and edison).
PIC simulation of Tokamak plamsas: Total-\( f \) vs conventional \( \delta f \)

- **Total-\( f \) (Full-\( f \)):** Solve \( f \) directly without manipulation
  - \( \frac{Df}{Dt} = C(f) + \text{Source} - \text{Sink} \)
  - Original XGC1
- **Conventional \( \delta f \) in Tokamak plasmas**
  - \( f = f_0(\text{fixed analytically}) + \delta f \)
  - \[
  \frac{D\delta f}{Dt} \equiv -\frac{D^* f_0}{D^* t} + C = -v_E \cdot \nabla f_0 + C
  \]
  - No neoclassical (grad-B drift) free energy on RHS
  - Scale separation between mean (\( f_0 \)) and perturbed \( \delta f \) is assumed
  - Main plasmas in most of core \( \delta f \) codes
Total-$\delta f$ particle methods

- Total-$\delta f$
  - $f = f_0 + \delta f$
  - $\frac{D\delta f}{Dt} = -\frac{Df_0}{Dt} + C + \text{Source} - \text{Sink}$
  - $D/Dt$ contains all physics
  - Mathematically identical to total-$f$
  - Mean and perturbed physics are solved together
  - Includes sources and sinks
  - $\delta f$ can can become large due to strong neo-collisional drive, wall loss, sources, or long time evolution.
    - Growing weight and noise problem
  - Difficult to handle wall loss and non-linear collision
Comparison between total-\(f\) and total-\(\delta f\)

[Ku et al., Nuclear Fusion 2009]
- Non-flux driven solutions decay
- Transient behavior is different, caused by the different Monte-Carlo noise level, but time integrated heat flux is the same
- Meaningful steady state solutions agree.

\[
\text{Total } \delta f \sim 0.5 \text{m}^2/\text{s}
\]
New hybrid Lagrangian scheme

- Solve total-$\delta f$ eq.
- $f = f_0 + f_P = f_a + f_g + f_P$, enables edge simulation
- $f_0$ contains slowly varying physics in time.
- $f_a$ is a fixed analytic distribution function (e.g. Maxwellian).
- $f_g$ is deviation from $f_a$ on 5D grid.
- $f_P$ represents $\delta f$ particles, driven by the free energy in $f_a$ and $f_g$.
- All physics information on continuum grid, with $f_P$ moved to v-grid.

$$f = f_0 + f_P = f_a + f_g + f_P$$
New hybrid Lagrangian scheme

- Time evolution:
  - Step 1: Solve particle motion and weight evolution as in the total-$\delta f$ scheme + S operation in $v$-grid
    \[
    \frac{Df_P}{Dt} = -\frac{D(f_a + f_g)}{Dt} + S(v\text{-grid})
    \]
  - Step 2: Redefine $f_P$ and $f_g$ with the following operation ($\alpha << 1$)
    \[
    f_P \leftarrow [1 - \alpha(X,V)]f_P, \quad f_g \leftarrow f_g + \alpha(X,V)f_P
    \]

Slowly varying in time
Fast varying in time
Direct weight evolution

- Gyrokinetic Vlasov-Boltzmann eq.
  \[
  \frac{Df_p}{Dt} = -\frac{Df_0}{Dt} + S(f)
  \]

- Differential form of weight evolution (2 weights, Hu and Kromess)
  \[
  \frac{dw_1}{dt} = \frac{(1-w_2)}{f_0} \left[ \frac{Df_0}{Dt} + S \right] \\
  \frac{dw_2}{dt} = \frac{(1-w_2)}{f_0} \frac{Df_0}{Dt}
  \]

- Direct weight evolution (new)
  \[
  \frac{(1-w_2)}{f_0} = \text{constant} \\
  \Delta w_1 = \Delta w_2 + S \frac{(1-w_2)}{f_0} \Delta t
  \]
  - Maker particles conserve phase space density
    - Unlike conventional \( \delta f \): Due to inaccuracy in \( D^*/D^*t \) operation
    - Avoid \( w_2 \) errors from time integrator and \( D/Dt \) error from gradient
Weight evolution of wall loss

• Marker particle is reflected at wall
  – Elastic reflection
  – Conserve phase space volume
  – \( w_2 \) remains the same
  – cf. reflection by sheath potential

• \( f = 0 \) with wall loss
  – Reflected marker particle cancels \( f_0 \)

\[
\begin{align*}
  w_1 &= -1 + w_2 \\
  f &= f_0 + w_1 g = 0 \\
  (1 - w_2) g &= f_0
\end{align*}
\]
Advantage in continuum grid

- Weight reduction using v-space $f_g$
- Continuum space physics operation with $f_p$ moved to continuum grid
  - Nonlinear collision
  - Neutral ionization and C-X
  - Radiation
ITG turbulence in cyclone geometry

- Collisionless
  - Collision capability presented by R. Hager
- 0.3M real space grid
- 32 by 31 v-space grid
  - Slow physics on v-grid
- 400M particles
  - 1500 ptls/real space grid
  - 1.5 ptls/v-space grid
  - Fast physics in the particles
α factor and numerical dissipation

\[ f_p \leftarrow (1 - \alpha) f_p \]
\[ f_g \leftarrow f_g + \alpha f_p \]

- Non-flux driven, total-deltaf
- Particle \(\rightarrow\) v-space operation gives numerical dissipation from interpolation (damping of Landau resonance).
- Too large \(\alpha\) reduces turbulence and time integrated heat flux
- Optimal \(\alpha \sim C(\Delta v) \Delta t/[\text{turbulence corelation time scale}]\)
V-space grid resolution also matters

- Fine grid: v-space grid from 32 x 31 to 62 x 61
- Reduced numerical dissipation in v-space $\rightarrow$ restore original heat flux even at $\alpha = 0.004$

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Homogeneous probabilistic marker initialization in v-space for better statistics at higher energy

Number of particles in v-space cells

Maxwellian distribution

Homogeneous distribution
Homogeneous Marker distribution in v-space and greater # of particles can allow bigger $\alpha$

- Homogeneous marker distribution gives better statistics
- Maxwellian distribution resembles less # ptls results
Particle Noise Reduction

- Variance of $w_1g$ in $v$-space cell ($g$: Marker distribution)
- $\alpha = 0.001 \rightarrow$ reduce particle noise variance by 4 in 1500 time steps.
- Particle noise reduction
Flux driven simulation

- Heat and cooling is applied to near axis and edge
- Close to steady state
- \( \alpha = 0 \) and \( \alpha = 0.001 \) converges to similar gradient.
- Time integrated heat flux is different for \( \alpha = 0.01 \) from \( \alpha = 0 \).
Summary

• A new hybrid Lagrangian scheme for gyrokinetic simulation of tokamak edge plasma is implemented in XGC1.
  – Combination of particle and continuum
  – Lagrangian particle push
  – Difficult physics operation and noise reduction in continuum space
  – Direct weight evolution and homogeneous marker distribution help simulation accuracy

• The new scheme is equivalent to ‘total-f’ with
  – Sources and Sinks
  – Non-maxwellian distribution

• \( f_{\text{particle}} \) is slowly converted to \( f_{v\text{-grid}} \).
  – Slow time varying function \( \rightarrow v\text{-space grid} \)
  – Fast time varying function remains in particles
  – Magnitude of \( \alpha \) depends upon \( \Delta v \) and particle number.
  – The new scheme relaxes growing weight problem.