Gyrokinetic simulations for tokamaks and stellarators

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Interest in global (full-volume) gyrokinetic particle-in-cell simulations for stellarators.

Two main areas of activity:
- Microinstabilities and turbulence
- MHD modes and their interaction with fast particles

Even linear electrostatic simulations for stellarators can become difficult due to high necessary resolution.

For electromagnetic perturbations already linear simulations in a tokamak can become very difficult (especially in the MHD limit, small $k_\perp \rho$)

⇒ necessity of algorithm development

MHD modes provide an excellent testing ground for codes since a very high quality of numerics is required.
Overview

1 Theory
- Electromagnetic gyrokinetic equations
- MHD hybrid model
- Electron fluid hybrid model

2 Results
- MHD hybrid model
- Electron fluid model
- Fully electromagnetic gyrokinetics
- Electrostatic ITG in stellarators
Fully gyrokinetic simulations are very time-consuming and difficult. Develop simplified models: Sacrifice physics for gain in speed.

⇒ EUTERPE, FLU-EUTERPE, CKA-EUTERPE
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All equations are derived from a Lagrangian via a variational principle in \( \{ \vec{R}, p_\parallel, \mu, \alpha \} \) coordinates (consistency and conserved quantities)

\[
L = \sum_{\text{species}} \int \left\{ f \left[ (q\vec{A} + p_\parallel \vec{b}) \cdot \dot{\vec{R}} + \frac{m}{q} \mu \dot{\alpha} - \frac{p_\parallel^2}{2m} - \mu B + q\left\langle \frac{p_\parallel}{m} A_\parallel - \Phi \right\rangle \right] + f_0 \left[ -\frac{q^2}{2m} \left\langle A_\parallel \right\rangle^2 + \frac{m}{2B^2} (\nabla \perp \Phi)^2 \right] \right\} \, dV \, dW - \frac{1}{2\mu_0} \int (\nabla \perp A_\parallel)^2 \, dV
\]

- \( \delta B_\parallel \) neglected
- \( \langle \cdot \rangle \): gyro-averaging operator
- \( dW = B_\parallel^* \, dp_\parallel \, d\mu \, d\alpha, \, dV = \sqrt{g} \, ds \, d\vartheta \, d\varphi, \, B_\parallel^* = B + \frac{1}{q} p_\parallel \vec{b} \cdot \nabla \times \vec{b} \)

adiabatic electron model: \( \frac{m}{2B^2} (\nabla \perp \Phi)^2 \implies \frac{e^2}{2k_B T_{e0}} (\Phi - \bar{\Phi})^2 \)

neglect \( q\langle \Phi \rangle \) for electrons
Cancellation problem

Electromagnetic simulations are hampered by the cancellation problem.

- Moment of $p \parallel$ does not give a physical current.
- Ampère’s law in $p \parallel$ formulation ($d_c$: collisionless skin depth)

\[-\frac{1}{\beta} \nabla^2 A \parallel + \frac{1}{d_c^2} A \parallel = j \parallel_i + j \parallel_e\]

- $\frac{1}{d_c^2} A \parallel \gg \frac{1}{\beta} \nabla^2 A \parallel$ (especially for MHD modes, since $k \perp \rho_i \approx 0$)
- $j \parallel_e$ contains adiabatic part $j \parallel_{e,ad} = \int e v \parallel \left[ \frac{e}{T} f_0 v \parallel A \parallel \right] \, d^3v$
- Numerical cancellation of the two large terms $\frac{1}{d_c^2} A \parallel$ and $j \parallel_{e,ad}$
- Different numerical representations: matrix $\iff$ particles

Cancellation problem mitigated by adjustable control variate method.

[Hatzky et al. 2007]

- Iterative method for determining a control variate
- Allows strong reduction in the number of necessary markers

Nevertheless, simulations require a very long time (small time step) or are still not feasible for certain parameters.
Equations of motion in $v_\parallel$ formulation (slab version for simplicity)

$$
\begin{align*}
\dot{R} &= v_\parallel \vec{b} + \frac{1}{B} \vec{b} \times \nabla \left[ \phi - v_\parallel A_\parallel \right] \\
\dot{v}_\parallel &= -\frac{q}{m} \left[ \nabla_\parallel \phi + \frac{\partial A_\parallel}{\partial t} \right]
\end{align*}
$$

Use splitting $A_\parallel = A_\parallel^s + A_\parallel^h$, introduce $u_\parallel = v_\parallel + \frac{q}{m} A_\parallel^h$ and simplify equations by using the resulting freedom to postulate

$$
\frac{\partial A_\parallel^s}{\partial t} + \nabla_\parallel \phi = 0
$$

Field equations

$$
\begin{align*}
\frac{\partial A_\parallel^s}{\partial t} + \nabla_\parallel \phi &= 0 \\
- \frac{1}{\beta} \nabla_\perp^2 (A_\parallel^h + A_\parallel^s) + SA_\parallel^h &= j
\end{align*}
$$
Pullback scheme II

Kinetic equation:
\[ \frac{\partial \delta f}{\partial t} = -\dot{R} \cdot \nabla f_0 - \frac{q}{m} u || \nabla || A^h || \frac{\partial f_0}{\partial u ||} \]

second term can be reduced by keeping \( A^h || \) small \( \Rightarrow \) idea of restarting

1. Start with \( A^h || = 0 \), i.e. \( u || = v || \)

Scheme allows for much larger time steps and enables simulations in parameter regimes not accessible before.
Kinetic equation:
\[
\frac{\partial \delta f}{\partial t} = -\dot{R} \cdot \nabla f_0 - \frac{q}{m} u_\parallel \nabla_\parallel A^h_\parallel \frac{\partial f_0}{\partial u_\parallel}
\]

second term can be reduced by keeping \( A^h_\parallel \) small ⇒ idea of restarting

1. Start with \( A^h_\parallel = 0 \), i.e. \( u_\parallel = v_\parallel \)
2. Integrate system in \( u_\parallel \)-space: \( A^h_\parallel \) develops, leading to \( u_\parallel \neq v_\parallel \)

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2. Integrate system in \(u_\parallel\)-space: \(A^h_\parallel\) develops, leading to \(u_\parallel \neq v_\parallel\)
3. Transform from \(u_\parallel\)-space to \(v_\parallel\)-space (use pullback)

\[
\delta f(v_\parallel) = \delta f(u_\parallel) + \frac{q}{m} A^h_\parallel \frac{\partial f_0}{\partial u_\parallel}, \quad v_\parallel = u_\parallel - \frac{q}{m} A^h_\parallel
\]

Scheme allows for much larger time steps and enables simulations in parameter regimes not accessible before.
Kinetic equation:
\[
\frac{\partial \delta f}{\partial t} = -\hat{R} \cdot \nabla f_0 - \frac{q}{m} u\| \nabla A_h^h \frac{\partial f_0}{\partial u}\|
\]
second term can be reduced by keeping $A_h^h$ small $\Rightarrow$ idea of restarting

1. Start with $A_h^h = 0$, i.e. $u\| = v\|

2. Integrate system in $u\|$-space: $A_h^h$ develops, leading to $u\| \neq v\|

3. Transform from $u\|$-space to $v\|$-space (use pullback)

\[
\delta f(v\|) = \delta f(u\|) + \frac{q}{m} A_h^h \frac{\partial f_0}{\partial u\|}, \quad v\| = u\| - \frac{q}{m} A_h^h
\]

4. Keep the full solution by setting $A_s^s$ to $A_s^s + A_h^h$ and restart

Scheme allows for much larger time steps and enables simulations in parameter regimes not accessible before.
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   • Electromagnetic gyrokinetic equations
   • MHD hybrid model
   • Electron fluid hybrid model

2 Results
   • MHD hybrid model
   • Electron fluid model
   • Fully electromagnetic gyrokinetics
   • Electrostatic ITG in stellarators
- Use simplified way of describing the interaction of Alfvén modes with fast particles.
- CKA code (A. Könies) solves the linearised reduced MHD eigenvalue problem.
- Resulting mode structure and frequency used as a fixed input for a particle simulation ⇒ linear
- Allow trajectories to react ⇒ nonlinear
- Perturbative scheme

\( \Phi, A'' \ \frac{\omega}{\omega} \rightarrow \text{EUTERPE} \)

CKA

MHD equation eigenvalue problem

EUTERPE

particle motion gyrokinetic equation
MHD hybrid model II

- Time derivative of quasineutrality equation

\[
\frac{\partial}{\partial t} \nabla \cdot \left[ \frac{M_n}{B^2} \nabla \phi \right] = -\nabla \cdot \left[ -\vec{b} \frac{1}{\mu_0} \nabla^2 A_{||} + j^{(0)}_{||} \left( \frac{\vec{b} \times \vec{k}}{B} A_{||} - \frac{\vec{b} \times \nabla A_{||}}{B} \right) \right. \\
\left. + p_{\text{bulk}}^{(1)} \left( \frac{\vec{b} \times \vec{k}}{B} + \frac{\vec{b} \times \nabla B}{B^2} \right) + p_{||,\text{fast}}^{(1)} \frac{\vec{b} \times \vec{k}}{B} + p_{\perp,\text{fast}}^{(1)} \frac{\vec{b} \times \nabla B}{B^2} \right]
\]

CKA part, EUTERPE part

- Simple closure for bulk pressure (neglect compressibility and anisotropy)

\[
\frac{\partial p_{\text{bulk}}^{(1)}}{\partial t} = -\frac{\vec{b} \times \nabla \phi}{B} \cdot \nabla p_{\text{bulk}}^{(0)}
\]

- MHD closure (vanishing $E_{||}$)

\[
\frac{\partial A_{||}}{\partial t} = -\vec{b} \cdot \nabla \phi
\]
Alfvén modes are stable eigenmodes with frequency $\omega_0$

\[
\phi(\vec{r}, t) = \phi_0(\vec{r}) e^{i\omega_0 t}
\]
\[
A_{\parallel}(\vec{r}, t) = A_{\parallel 0}(\vec{r}) e^{i\omega_0 t}
\]
\[
p^{(1)}(\vec{r}, t) = p_0(\vec{r}) e^{i\omega_0 t}
\]

Allow for complex time dependent amplitude

\[
\phi(\vec{r}, t) = \hat{\phi}(t) \phi_0(\vec{r}) e^{i\omega_0 t}
\]
\[
A_{\parallel}(\vec{r}, t) = \hat{A}_{\parallel}(t) A_{\parallel 0}(\vec{r}) e^{i\omega_0 t}
\]
\[
p^{(1)}(\vec{r}, t) = \hat{p}(t) p_0(\vec{r}) e^{i\omega_0 t}
\]
\[
\frac{\partial \hat{\phi}}{\partial t} = i\omega_0 (\hat{A}_\parallel - \hat{\phi}) + 2(\gamma - \gamma_d)\hat{\phi} \\
\frac{\partial \hat{A}_\parallel}{\partial t} = -i\omega_0 (\hat{A}_\parallel - \hat{\phi})
\]

\[
\gamma = \frac{T}{2W}
\]

\gamma_d: ad-hoc damping

Wave-particle energy transfer:

\[
T = -\int dW dV f^{(1)}_{\text{fast}} \left[ \frac{1}{B} \vec{b} \times (m v^2_\parallel \vec{k} + \mu \nabla B) \cdot \nabla \phi^* \right]
\]

Wave energy:

\[
W = \int dV \frac{M n}{B^2} |\nabla_\perp \phi|^2
\]

Linear model: Growth rate of the mode given by \(\gamma\)

Nonlinear model: Use Re(\(\phi\)), Re(\(A_\parallel\)) for fast particle trajectories
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Electron fluid model [Cole et al. 2014]

- Linearised electron continuity equation ($v_\parallel$ formulation)

\[
\frac{\partial n_e}{\partial t} + n_0 \vec{B} \cdot \nabla \frac{u_e}{B} + B \vec{v}_{E \times B} \cdot \nabla \frac{n_0}{B} + (\nabla \times A_\parallel \vec{b}) \cdot \nabla \frac{n_0 u_e}{B} + n_0 (2\vec{v}_* - \vec{v}_{E \times B}) \cdot \nabla \frac{B}{B} + \frac{\nabla \times B}{B^2} \cdot \left( -\frac{1}{e} \nabla p_e + n_0 \nabla \phi \right) = 0
\]

with \( \vec{v}_* := \frac{\vec{b} \times \nabla p_e}{en_0 B} \)

- Ampère’s law and quasineutrality

\[
u_e = \frac{1}{en_0} \left( j_{i\parallel} + \frac{1}{\mu_0} \nabla^2 A_\parallel \right)
- \nabla \cdot \left( \frac{m_i n_0}{e B^2} \nabla \phi \right) = n_i - n_e
\]

- MHD ($E_\parallel = 0$) and pressure closure

\[
\frac{\partial A_\parallel}{\partial t} = -\vec{b} \cdot \nabla \phi \quad \quad \frac{\partial p_e}{\partial t} = -\vec{v}_{E \times B} \cdot \nabla p_e
\]

More physics can be included by improving the closures.
Global gyrokinetic code EUTERPE

- δf particle-in-cell code
- Global simulation domain: full-volume
- 3D stellarator equilibria (from VMEC equilibrium code)
- Multiple kinetic species (ions, electrons, fast ions/impurities)
- Electrostatic/electromagnetic
- Linear/nonlinear
- Pitch-angle collision operator (⇒ neoclassics)

⇒ Code platform for implementation of different models
   (GYGLES: basically a reduced, linear, axisymmetric version of EUTERPE)
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W7-X equilibrium with \( \beta \approx 3\% \)

Flat bulk plasma profiles
\[ n_{\text{bulk}} = 10^{20} \text{ m}^{-3} \]

TAE mode found (CKA)
Destabilise TAE mode by fast particle interaction:
Maxwellian fast particles
\[ n_{\text{fast}} \] profile fixed with
\[ n_{\text{fast},0} = 10^{17} \text{ m}^{-3} \]

FLR effects important

Reaction on external radial electric field
\[ (\vec{E}_0 = E_s \nabla s, \ E_s = \text{const.}) \]

\[ M_E = \frac{1}{v_{th}} \langle |\vec{E}_0 \times \vec{B}| \rangle \]

[\text{Mishchenko et al. 2014}]
Fast ions from ICRH

Very simple model for ICRH: anisotropic Maxwellian power deposition localised in space

Less-pronounced finite orbit-width effects

Strong influence of anisotropy on growth rate (more/less parallel temperature)
Nonlinear CKA-EUTERPE: amplitude development

- ITPA benchmark case: circular $A = 10$ tokamak, $(m, n) = (10/11, -6)$ TAE
- Without artificial damping mode amplitude does not saturate.
- Feature robust with respect to time step and particle number: no numerical artefact
- Artificial damping necessary ($\gamma_d \approx 2.5 \cdot 10^3 \, \text{s}^{-1}$) in order to reach saturation (damping of same order also used by other codes).
For small growth-rates theory (Berk-Breizmann model) predicts relationship between saturation amplitude and growth rate: \( \delta B / B \sim \gamma_{\text{eff}}^2 \)

Scaling confirmed by other codes

Symmetric frequency chirping observed.
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- **Electron fluid model**
- Fully electromagnetic gyrokinetics
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Internal kink in a screw pinch. Scan over position of $q = 1$ surface.

ITPA benchmark: **EUTERPE, FLU-EUTERPE and CKA-EUTERPE**
Internal tokamak kink mode

- Finite $\nabla T$ used to destabilise the mode.
- In fluid limit (no gyrokinetic ions), direct comparison possible with MHD code CKA:
  $\gamma_{FLU} = 1.29 \times 10^6 \text{s}^{-1}$
  $\gamma_{CKA} = 1.27 \times 10^6 \text{s}^{-1}$
- Strong stabilisation with JET/ITER-like aspect ratio and elongation.
- Further stabilisation with inclusion of bulk ion gyrokinetic effects.

Resistive layer physics lost but tokamak simulations become practical.

[Cole et al. 2014]
Fast particle effects: Linear fishbone

- Maxwellian fast species (D), $T_{\text{fast}} = 300$ keV
- Initial stabilisation of the mode (perturbative effect) overcome by unstable branch.
- Frequency jump with onset of fast particle destabilisation.
- Non-perturbative mode structure for larger fast particle density.

![Graph showing growth rate and frequency vs. fast particle density](image-url)
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For ITPA case TAE had no continuum interaction.

- Use steeper $q$-profile $\Rightarrow$ continuum interaction.

- MHD mode structure strongly modified by interaction with KAW. [Cole et al. 2015]

- Change of mode structure not captured by CKA-EUTERPE.

- FLU-EUTERPE: follows change in mode structure but break-down of fluid closure?
Pull-back scheme: simulations for stellarator

Electromagnetic ITG for LHD-like configuration
\( (\beta_{eq} = 1.5\%, \beta_e = 0.85\%) \)

**Standard \( \delta f \) scheme:**
- Numerical instability quickly develops
- Wrong mode structure

**New scheme:**
- Simulation stays stable
- Clean mode structure

[Mishchenko et al. 2014]
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Simplified profiles for $L_T-L_n$-scans

For global simulations profiles are a critical issue: One gains a functional degree of freedom but loses flexibility to produce parameter sequences.

- **Simplified profiles:**
  - piece-wise linear
  - \( \frac{d \ln T_{i,e}}{ds} \) and \( \frac{d \ln n_{i,e}}{ds} \)
  - \( s = \frac{\Psi_{\text{tor}}(r)}{\Psi_{\text{tor}}(0)} \).

- **Further simplification:**
  - keep equilibrium configuration fixed and change parameters \( (L_T, L_n) \) only in the simulations.
Quasi-realistic profiles for $L_T - L_n$-scans

Quasi-realistic: simplified but derived from equilibrium
(assuming finite residual pressure $\delta p_0$)

\[
\frac{p}{p_0} = 1 - 2s + s^2 + \frac{\delta p_0}{p_0}
\]

\[
\frac{T_{i,e}}{T_0} = \left( \frac{1}{2} \frac{p}{p_0} \right)^{1-\chi}, \quad (T_e = T_i)
\]

\[
\frac{n_{i,e}}{n_0} = \left( \frac{1}{2} \frac{p}{p_0} \right)^\chi, \quad (n_e = n_i)
\]

\[
\eta_i = 1 - \chi \div \chi = \text{const.}
\]

$\Rightarrow \eta_i$-scan implies $L_{T,n}$-scan

Advantage: not necessary to recalculate equilibrium for new parameter settings
Clear onset of linear ITG instability for $\eta_i \geq 1$ observed.

Similar growth rates for W7-X and LHD.
W7-X: ITG mode pattern

W7-X ($\beta = 2\%, \ T_\ast = 1 \text{ keV}$)

Electrostatic potential (absolute values) normalized to maximum $s = 0.5$

$a/L_T = 1.41, \ a/L_n = 0.0, \ (m_0, n_0) = (210, -190)$

- ITG mode resides in region of unfavourable curvature.
- High-shear region or 'helical edge' avoided.
LHD (β = 1.5%, \(T_\ast = 1\) keV, \(R_0 = 3.75\) m)

electrostatic potential (absolute values) normalized to maximum at \(s = \text{const.}\).

\[ \eta_i = 2, \ s = 0.61, \ \gamma = 0.12 \frac{v_T}{a} \]
\[ \eta_i = 1, \ s = 0.75, \ \gamma = 0.02 \frac{v_T}{a} \]

- Helical edge less pronounced than in W7-X
\( L_T - L_n \)-scan for simplified profiles

\[ \text{LHD} \ (\beta = 1.5\%, \ T_* = 1 \text{keV}) \]
Quasi-realistic profile scan yields 'configuration characteristic'.

Consistent profiles are a unique challenge of global simulations.

Reasonable assumptions about residual pressure are crucial.
Radial electric field effects

W7-X ($\beta = 2\%, \ T_* = 1\ keV$)

Two different radial electric field models used (variation of $\alpha$):

- **Physical**: $E_s = \alpha \frac{p_i'}{q_i n_i} \Rightarrow$ model A
- **Simple**: $E_s = -\alpha \Rightarrow$ model B
- Asymmetric damping effect
Conclusions

EUTERPE: global (full-volume) gyrokinetic particle-in-cell code for stellarators.

Hierarchy of models implemented:
MHD hybrid, electron fluid, fully gyrokinetic.

New numerical schemes allow faster and more robust electromagnetic simulations.

Examples:
- Fast particle interaction with TAE and internal kink mode.
- Electrostatic ITG with (quasi-)realistic profiles for stellarators.

Progress, especially for electromagnetic simulations, has been made but further testing is necessary.
International benchmark case for Alfvén wave fast-particle interaction.

- Circular tokamak \( A = 10, R = 10 \text{ m}, B = 3 \text{ T}, \) bulk ions: D

- \( n_e = 2 \cdot 10^{19} \text{ m}^{-3}, \)
  \( T_i = T_e = 1 \text{ keV} \)

- \( q = 1.71 + 0.16s \)

- \( T_{\text{fast}} = 400 \text{ keV (Maxwellian)} \)

- \( n_{\text{fast}} = n_0 \exp \left( -\frac{\Delta n}{L_n} \tanh \frac{s - s_0}{\Delta n} \right) \)
  with \( n_0 = 0.75 \cdot 10^{17} \text{ m}^{-3}, \)
  \( \Delta n = 0.2, L_n = 0.3, s_0 = 0.5 \)
- $\beta_e$-effect on growth rate relatively weak.

- In contrast to tokamak no AITG/KBM branch found in $\beta_e$ scan.

- Pullback scheme allows much faster (one day) simulations than adaptive control variate scheme.

$\Rightarrow$ More careful tests necessary to validate schemes.