Electromagnetic gyrokinetics and plasma turbulence: numerical methods and optimizations in GYRO

J. Candy,[a] R.E. Waltz,[a] and M.R. Fahey.[b]

[a]General Atomics, San Diego, CA

[b]Oak Ridge National Laboratory, Oak Ridge, TN

OVERVIEW

GYRO[1] is a large software project designed for solving the 5-D coupled gyrokinetic-Maxwell equations on distributed memory architectures.

GYRO can operate as a flux-tube (local) code, or as a global code, with electrostatic or electromagnetic fluctuations.

Full-physics simulations have reproduced within experimental errors the transport observed in DIII-D L-mode discharges[2].

Given an input equilibrium and profiles (local Maxwellian in velocity), GYRO computes the turbulent transport coefficients $\chi(r)$ and $D(r)$ for electrons and ions.

Time-integration is an implicit-explicit (IMEX) Runge-Kutta scheme[3]. This prevents numerical instability of pathological electron-scale waves.

GYRO has been ported to the Cray-X1 with excellent results, although linear simulations will run with ease on a modest laptop.

PRIMITIVE EQUATIONS

One must solve kinetic equations (integro-differential) coupled to field equations (time-independent) for electron and ion gyro-center distributions, which we decompose spectrally in the toroidal direction:

$$h(r,\theta,\varphi,\lambda,\epsilon;t) \to h_n(r,\theta,\lambda,\epsilon;t)$$

(λ,ϵ) are velocity-space variables, while (r,θ,φ) are toroidal coordinates.

Gyrokinetic Equation

$$\frac{\partial h_n}{\partial t} - \mathcal{C}[h_n - z_s\alpha_s v_{\parallel s}(\mathcal{G}A_\parallel)_n] = \mathrm{RHS}_n(r,\theta;\lambda,\epsilon)$$

$$\mathrm{RHS}_n = \left[-\frac{1}{R_0 q}\frac{v_{\parallel s}(r,\theta)}{g_\theta(r,\theta)}\frac{\partial}{\partial\theta} + \imath\omega_{ds}^{(1)} + \imath\omega_{ds}^{(r)}\frac{\partial}{\partial r}\right](h_n + z_s\alpha_s(\mathcal{G}u_s)_n) - \imath n_s\,\omega_{*s}\,(\mathcal{G}u_s)_n + \imath\hat{\rho}\,\{\mathcal{G}u_s, h\}_n \ ,$$

where $u_s \doteq \phi - v_{\parallel s}A_\parallel$,

$$v_{\parallel s}(r,\theta) \doteq \sigma\mu_s\sqrt{2\epsilon T_s(r)\left(1-\lambda\hat{B}(r,\theta)\right)} \ .$$

Field equations

$$\sum_{s=1}^{n_{\rm ion}}\alpha_s z_s^2(1-\mathcal{R}_s)\,\phi_n = \sum_{s=1}^{n_{\rm kinetic}} z_s \mathrm{V}[\mathcal{G}(h_n)_s] \ ,$$

$$-\frac{2\rho_s^2}{\beta_e}\nabla_\perp^2 A_{\parallel n} + \sum_{s=1}^{n_{\rm kinetic}}\alpha_s z_s^2\,\mathrm{V}[v_{\parallel s}^2 A_{\parallel n}] = \sum_{s=1}^{n_{\rm kinetic}} z_s \mathrm{V}[v_{\parallel s}\mathcal{G}(h_n)_s] \ ,$$

where $\mathcal{R}_s = \mathrm{V}[\mathcal{G}\mathcal{G}]$ is a velocity-space-integrated double gyroaverage.

$$\mathrm{V}[f_s] \doteq \sum_\sigma \frac{1}{2\sqrt{\pi}}\int_0^\infty d\epsilon\, e^{-\epsilon}\sqrt{\epsilon}\int_0^1 \frac{d(\lambda\hat{B})}{\sqrt{1-\lambda\hat{B}}}\, f_s(r,\theta,\zeta;\epsilon,\lambda,\sigma;t) \ ,$$

Definitions

- $\mathcal{C}$ is the collision operator (dominantly diffusion in λ).
- σ denotes the sign of velocity, z_s the species charge, β_e the plasma pressure, $\alpha = n/T$, and ρ_s is the local ion-sound gyroradius.
- $v_\parallel$ is the parallel velocity which passes through zero at bounce points, complicating the numerical treatment.
- $\mathcal{G}$ is the nonlocal gyroaveraging operator.
- ϕ is the electrostatic potential, and $A_\parallel$ is the magnetic potential for transverse fluctuations.

DISCRETIZATION SCHEMES

Orbit-time Grid

Highest accurcy for treatment of trapped and pinch orbits is obtained via an orbit-time for discretization:

$$\frac{v_\parallel(\theta)}{qR}\frac{\partial}{\partial\theta} \longrightarrow \omega_b(\lambda)\frac{\partial}{\partial\tau}$$

Expand ϕ and $A_\parallel$ in series of blending functions (finite elements) to avoid a poloidal grid:

$$\phi\left[\theta(\lambda,\tau_j)\right] = \sum_{m=1}^{n_b} c_m F_m\left[\theta(\lambda,\tau_j)\right]$$

$$F_m(\theta) = N(\theta - m\Delta\theta) + e^{-2\pi i n q}N(\theta-(m+n_b)\Delta\theta).$$

Entropy-conserving Nonlinearity

Nonlinear advance uses a difference-spectral analogue of the Arakawa symmetrization method:

$$\{F,G\} = \frac{1}{3}\left[\partial_\alpha(F\,\partial_r G - G\,\partial_r F) + \partial_r(G\,\partial_\alpha F - F\,\partial_\alpha G) + (\partial_\alpha F)(\partial_r G) - (\partial_\alpha G)(\partial_r F)\right]$$

- $\partial_r \to$ 6th-order centred difference.
- $\partial_\alpha \to$ pseudo-spectral.
- Difference-spectral scheme conserves integrals of

$$\int_V d\alpha\, dr\,\{F,G\}, \quad \int_V d\alpha\, dr\, F\{F,G\} \quad \text{and} \quad \int_V d\alpha\, dr\, G\{F,G\}$$

Banded-pseudospectral Gyroaverages

$$\mathcal{G}_n^{ii'} = \begin{cases} \dfrac{1}{2J}\displaystyle\sum_{p=-J}^{J-1} z_p^{i-i'}J_0\left(k_p^i\rho_\perp\right) & \text{if } |i-i'|\le i_g \\ 0 & \text{if } |i-i'| > i_g \end{cases}$$

$$\mathcal{R}_n^{ii'} = \begin{cases} \dfrac{1}{2J}\displaystyle\sum_{p=-J}^{J-1} z_p^{i-i'}e^{-b_p^i}I_0\left(b_p^i\right) & \text{if } |i-i'|\le i_g \\ 0 & \text{if } |i-i'| > i_g \end{cases}$$

Velocity-Space Integration

Since $\mathrm{V}[1] = 1$, it follows automatically that $\mathcal{F}\mathrm{V}[1] = 1$, where $\mathcal{F}$ is a flux-surface average. Equivalently,

$$\frac{1}{2\sqrt{\pi}}\int_0^\infty d\epsilon\, e^{-\epsilon}\sqrt{\epsilon}\int_0^{\lambda^*} d\lambda\,\bar{\tau}(\lambda)\oint d\tau = \mathcal{J}_0 \ ,$$

with $\lambda^* = 1/\hat{B}(r,0)$ the maximum possible value of λ. Above, we have used the integral identity

$$\sum_\sigma\int_{-\pi}^{\pi} d\theta\, g_\theta(r,\theta)\int_0^{1/\hat{B}(r,\theta)}\frac{d\lambda}{\sqrt{1-\lambda\hat{B}(r,\theta)}} = \int_0^{\lambda^*} d\lambda\,\bar{\tau}(\lambda)\oint d\tau \ .$$

Since the numerical evaluation of integrals of this type will involve separate integration weights in each of the variables ϵ, λ and τ, it is useful to make the decomposition $\mathcal{F}\mathrm{V} = \mathrm{V}_\epsilon\times\mathrm{V}_\lambda\times\mathrm{V}_\tau$, where

$$\mathrm{V}_\epsilon[h] \doteq \frac{2}{\sqrt{\pi}}\int_0^\infty d\epsilon\, e^{-\epsilon}\sqrt{\epsilon}\,h \ ,$$

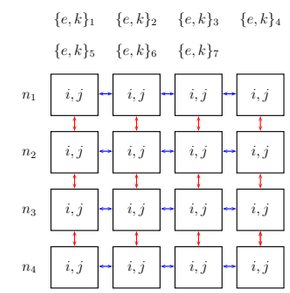
$$\mathrm{V}_\lambda[h] \doteq \frac{1}{2\,\mathcal{J}_0}\int_0^{\lambda^*} d\lambda\,\bar{\tau}(\lambda)\,h \ ,$$

$$\mathrm{V}_\tau[h] \doteq \frac{1}{2}\oint d\tau\, h \ .$$

COMMUNICATION ALGORITHM

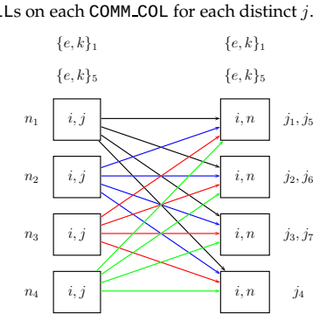
TSUB Library: Base distribution

Split `MPI_COMM_WORLD` into (say) 4 instances of `COMM_ROW` and `COMM_COL`



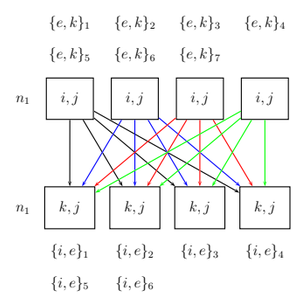
TSUB Library: Column transpose

`MPI_ALLTOALL`s on each `COMM_COL` for each distinct j.



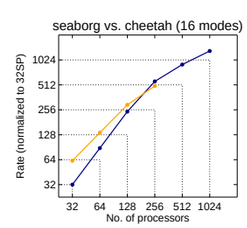
TSUB Library: Row transpose

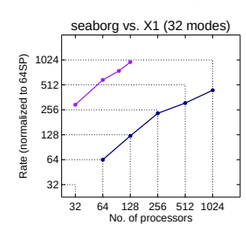
Complicated series of `MPI_ALLTOALL`s on each `COMM_ROW`.



Performance on IBM and Cray

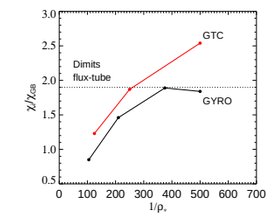
- cheetah suffers from poor Colony interconnect.
- 32 MSPs on the X1 can match 512 processors on seaborg.

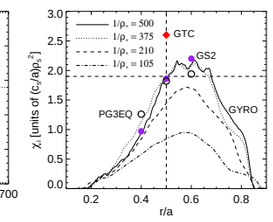




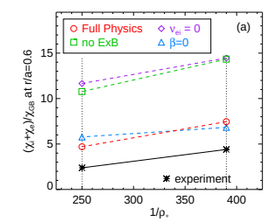
NUMERICAL RESULTS

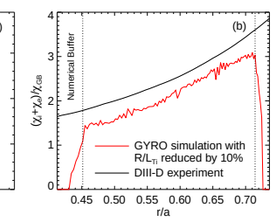
Local-limit Benchmarks





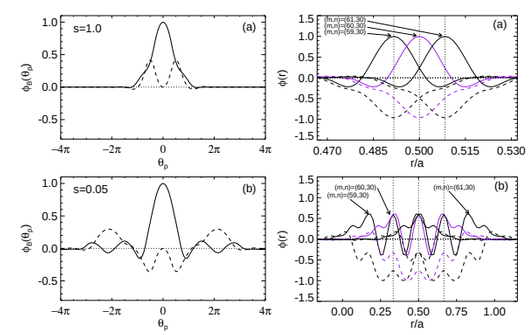
DIII-D Simulations



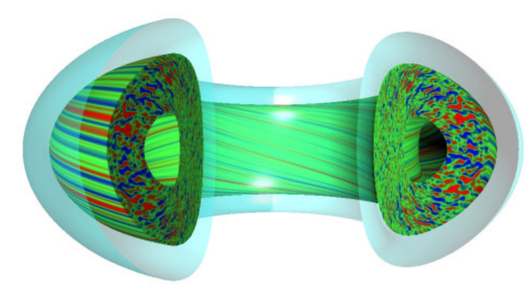


Weak Shear Eigenmodes

Compare moderate ($s = 1.0$) and low-shear ($s = 0.05$) modes in ballooning (left) and real space (right).



Shaped Plasma Visualization



References

[1] J. Candy and R.E. Waltz. *J. Comput. Phys.* **186**, 545 (2003).

[2] J. Candy and R.E. Waltz. *Phys. Rev. Lett.* **91**, 045001–1 (2003).

[3] L. Pareschi and G. Russo. in *Hyperbolic problems: Theory, Numerics, Applications*. Springer, (2002).