Steady State Gyrokinetic Transport Code (SSGKT): Multi-physics, multi-scale, integrated fusion simulation

M.R. FAHEY[a] AND J. CANDY[b]

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

[b]General Atomics, San Diego, CA

PROJECT OVERVIEW

The goal of this project is to develop a prototypical Steady State Gyrokinetic Transport Code (SSGKT) that integrates micro-scale gyrokinetic turbulence simulations into a framework for practical multi-scale simulation of the International Thermonuclear Experimental Reactor (ITER).

This code will have the capability to predict steady-state core temperature and density profiles given the H-mode pedestal boundary conditions.

The key numerical challenge is to determine the most efficient feedback algorithm, because code outputs are intermittent and extremely expensive.

SSGKT addresses a key problem of critical scientific importance; namely predicting the performance of ITER given an edge boundary condition.

The key scientific advance will be to show that gyrokinetic codes (simulating micro-scales) can be run practically within a transport code (simulating the macro-scale).

This is referred to as simulation of turbulence on transport timescales and is cited as one of the four leading Focused Integration Initiatives for a Fusion Simulation Project[5].

GYRO CODE HIGHLIGHTS

GYRO[2] solves the 5-D coupled gyrokinetic-Maxwell equations on distributed memory architectures.

Development of GYRO started in 1999, and by 2002 the fundamental design milestones were achieved.

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 [1].

For experimental studies, tools exist which can map TRANSP or ONETWO data into a form directly readable by GYRO.

Given an input equilibrium and profiles, 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[7]. This prevents numerical instability of pathological electron-scale waves.

Eulerian discretization makes GYRO suitable for very long (in time) simulations.

Ported to a variety of machines including Cray X1E and XT3, IBM Power4, Power5 and Blue Gene, SGI Altix, and various Opteron and Intel based clusters

THE OLD APPROACH

Presently, at the *macro-scale* end of the spectrum, predictive modeling of steady-state temperature and density profiles [6] is usually done with simplified local transport models like GLF23 [9].

At the *micro-scale* end the spectrum, the standard approach in the gyrokinetic simulation community is to compute the statistical steady-state of turbulence [4] which is generated by *fixed* plasma profiles.

GYRO is regularly used for fixed-profile simulations (i.e., without feedback) of global DIII-D, JET, C-MOD and NSTX experiments. Such simulations are far shorter than the global transport (energy confinement) time.

By separating the turbulence (internal, micro-scale physics) and transport (external, macro-scale physics) time scales, and introducing a feedback loop between them, one can arrive at the steady-state transport balance required for a true macro-scale steady-state solution.

PRIMITIVE EQUATIONS IN GYRO

GYRO solves the plasma kinetic equations (integro-differential) coupled to Maxwell's equations (time-independent) for electron and ion gyrocenter 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

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

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

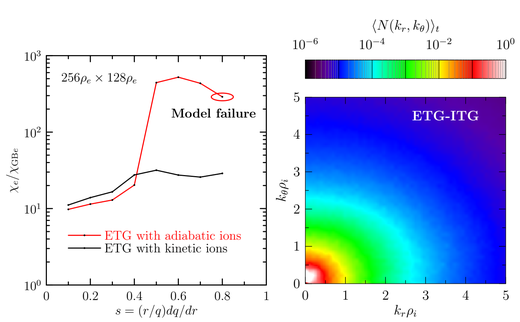
where $\mathcal{R}_s = \mathrm{V}[\mathcal{G}\mathcal{G}]$ is a velocity-space-integrated double gyroaverage.

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

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.

RECENT GYRO INCITE RESULTS



Recent INCITE results show that the adiabatic ion model of ETG is invalid for typical parameters (left). Also, huge, coupled ETG-ITG simulations show that the spectrum is really isotropic for $k_\perp\rho_i > 0.5$.

THE NEW APPROACH

Use a master transport code to coordinate and provide feedback to multiple separate GYRO [3] simulations.

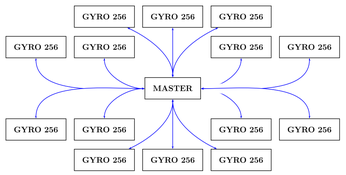
Each instance of GYRO will compute local radial fluxes that will be periodically communicated to the master. In comparison to the size of a local simulation distribution function, the amount of data to be communicated to the master will be minimal.

The master transport code, and in particular the feedback scheme (or schemes) it will employ, has not yet been developed.

The physical sources (beam ions, radio frequency heating, radiation, thermonuclear rates, etc.) which must be accounted for in the master are available as off-the-shelf technology.

The use of the transport power and plasma flow balance equation, rather than direct dynamical interactions, is potentially the key solution to connecting core turbulence to the edge pedestal.

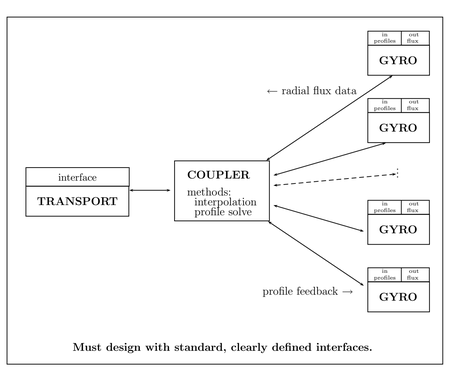
This new approach will allow highly efficient use of several thousand processors; the master code must only compute relatively simple feedback information based on transport power balance, and the independent instances of GYRO will scale very well because of the relatively low processor count per instance (32 to 256).



COMPUTER SCIENCE CHALLENGES

We intend that the software framework we form will lay a foundation for even more powerful and comprehensive simulations in the future. We will strive to develop prototypical standards (interfaces and components) and documented application programming interfaces for fusion application modules, which will allow incorporation of other modern fusion applications codes into the framework. We will be working with the Framework Application for Core-Edge Transport Simulations (FACETS) of which we are a Scientific Application Partnership (SAP).

Furthermore, we will need to resolve: (1) exactly what data needs to be communicated between the two codes, and (2) what is the most efficient way to communicate such data. Data exchanged among the models may reside on differing spatial meshes, requiring interpolation between the source and target components respective grids. The models may also differ in how they discretize time, requiring some scheme to either interpolate or average/accumulate data for translation between the source and target components' time meshes.



PHYSICS CHALLENGES

Must determine plasma temperature and density profiles which give rise to steady-state power and particle balance.

For a single ion species, such that $n \doteq n_e = n_i$, we can write master equations of the form

$$\Gamma_e(x,y,z,\tau) = \Gamma_e^{\mathrm{target}}(n,T_e,T_i) \ , \quad (1)$$

$$Q_e(x,y,z,\tau) = Q_e^{\mathrm{target}}(n,T_e,T_i) \ , \quad (2)$$

$$Q_i(x,y,z,\tau) = Q_i^{\mathrm{target}}(n,T_e,T_i) \ . \quad (3)$$

We want to solve this at radial points r_p for $p = 1,\ldots,N_p$, with $N_p \sim 16$. Here, Q is the *GYRO heat flux*, Γ is the *GYRO particle flux*, Q^{target} is the *target heat flux* and Γ^{target} is the *target particle flux*. Above, we have defined the following normalized quantities

$$x = -\frac{a}{n}\frac{\partial n}{\partial r} \ , \quad y = -\frac{a}{T_e}\frac{\partial T_e}{\partial r} \ , \quad z = -\frac{a}{T_i}\frac{\partial T_i}{\partial r} \quad \text{and} \quad \tau = T_i/T_e \ . \quad (4)$$

Given $\{x,y,z\}$, the profiles updated according to

$$n(r) = n(r_*)\exp\left(\frac{1}{a}\int_{r_1}^{r_*} x(r')dr'\right) \ , \quad (5)$$

$$T_e(r) = T_e(r_*)\exp\left(\frac{1}{a}\int_{r_1}^{r_*} y(r')dr'\right) \ , \quad (6)$$

$$T_i(r) = T_i(r_*)\exp\left(\frac{1}{a}\int_{r_1}^{r_*} z(r')dr'\right) \ . \quad (7)$$

Here, $r_* > r_{N_p}$ is the position of the boundary condition (which specifies the H-mode pedestal height).
We have two proposed schemes to solve the iteration problem: diagonal relaxation and semi-analytic solution.

Additional considerations

Each instance of GYRO operates on its own intrinsic time-scale, a/c_s, length scale, ρ_s, and therefore its own local (gyroBohm) diffusion scale $\rho_s^2 c_s/a$. We remark that at the small values of $\rho_* = \rho_s/a$ in ITER, gyroBohm scaling and the locality of turbulence is largely assured.

The cost of a local simulation is independent of ρ_*, whereas the cost of a global simulation increases dramatically as $\rho_* \to 0$.

At a fixed number of *macro-zones*, N_p, the method we propose has an asymptotic efficiency which ought to be at least $\mathcal{O}\left(\rho_*^{-2}\right)$ times better than a single global gyrokinetic simulation.

References

[1] J. Candy and R.E. Waltz. Anomalous transport in the diii-d tokamak matched by supercomputer simulation. *Phys. Rev. Lett.*, 91:045001–1, 2003.

[2] J. Candy and R.E. Waltz. An eulerian gyrokinetic-maxwell solver. *J. Comput. Phys.*, 186:545, 2003.

[3] J. Candy and R.E. Waltz. An Eulerian gyrokinetic-Maxwell solver. *J. Comput. Phys.*, 186:545, 2003.

[4] J. Candy and R.E. Waltz. Velocity-space resolution, entropy production and upwind dissipation in Eulerian gyrokinetic simulations. *Phys. Plasmas*, page to be published, 2006.

[5] Fusion Energy Sciences Advisory Committee (FESAC): Office of Advanced Computer Science Research/Office of Fusion Energy Sciences *Dahlburg Committee Report* (2002); see http://www.isofs.info.

[6] J.E. Kinsey, G. Bateman, T. Onjun, A.H. Kritz, A. Pankin, G.M. Staebler, and R.E. Waltz. Burning plasma projections using drift-wave transport models and scalings for the H-mode pedestal. *Nucl. Fusion*, 43:1845, 2003.

[7] L. Pareschi and G. Russo. High order asymptotically strong-stability-preserving methods for hyperbolic systems with relaxation. In *Hyperbolic problems: Theory, Numerics, Applications*. Springer, 2002.

[8] R.E. Waltz. Rho-star scaling and physically realistic gyrokinetic simulations of transport in DIII-D. *Fusion Sci. Technol.*, 48:1051, 2005.

[9] R.E. Waltz, G.M. Staebler, W. Dorland, G.W. Hammett, M. Kotschenreuther, and J.A Konings. A gyro-Landau fluid transport model. *Phys. Plasmas*, 4:2482, 1997.