Steady State Gyrokinetic Transport Project Status: A SAP with FACETS

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Plasma Science Advanced Computing Institute (PSACI)

Program Advisory Committee (PAC) Meeting

Princeton, NJ

5–6 June 2008

TGYRO Goals

Integrate gyrokinetic simulations into transport calculations

- We summarize recent progress in the **Steady-State Gyrokinetic Transport (SSGKT) project**
  - → A *Scientific Discovery through Advanced Computing* (SciDAC) initiative funded the US Office of Advanced Computing Computing Research (OASCR).
  - → A Scientific Application Parternship with FACETS.
- Goal is to develop an algorithmic strategy to employ local and global gyrokinetic turbulence simulations in **steady-state transport calculations**.
- The prototype will be used to **predict steady-state temperature and density profiles in ITER** given fixed pedestal boundary conditions.

Project Status

Team Funding Review

- Mark Fahey, Oak Ridge National Laboratory, PI
  - → Funding arrived in December 2006
  - → Focus has been on TGYRO parallelization and integration into FACETS
- Jeff Candy, General Atomics
  - → Funding arrived in April 2007
  - → Focus has been on steady-state algorithmic approach and implementation
- Thomas Fouquet, General Atomics, postdoc
  - → Started work September 2007

We are just over a year into the project for the General Atomics team members.

Project Status

TGYRO Prototype

TGYRO has evolved significantly in the last 6 months. It has two basic operational modes, local and global.

Local Method

- For small $\rho_* = \rho_s/a$, global simulations are unnecessary (in fact, they are inefficient), as **gyroBohm scaling** and the **locality** of turbulence is largely assured.
- We've created a traditional transport code (prototype TGYRO) to compute steady-state profiles given fluxes using a novel iteration scheme.
- Local method in TGYRO can run separate instances of GYRO, or simpler transport models (IFS-PPPL or TGLF) at selected radii on any number of processors.
- We presently combine GYRO fluxes in the outer core with TGLF fluxes in the inner core for a single TGYRO simulation.

Global Method

- For large-ρ_* plasmas (DIII-D, NSTX), we also provide a **global feedback scheme** pioneered by R. Waltz. This solver is currently being used by **Holland, Budny, Waltz, Angioni** for experimental studies.

Project Status

Addressing charge questions

Progress toward achieving scientific targets with respect to clear deliverables during the second year of project.

- The **CS focus** of our SAP was to couple multiple instances of GYRO to a transport driver, which we have completed in the prototype. Currently integrating GYRO into FACETS, to be followed by TGYRO.
- The **physics focus** is to develop a steady-state transport iteration scheme that works for intermittent, time-dependent gyrokinetic data. We are still working on the physics credibility of this prototype.

Signficant interactions with respect to collaborations with the Computer Science and Math communities.

- This SAP is an active partnership between a computational fusion scientist (Jeff Candy, GA) and a computer scientist (Mark Fahey, ORNL).

Project Status

Addressing charge questions

How leadership-class computing resources have enabled the achievement of the target scientific goals as well as demonstrated the scalability of the science.

- The leadership-class resources (INCITE project of same name) allow us to run the TGYRO prototype in an efficient way. The GYRO instances are very expensive, thus we can run at different radii with many processors with the computational goal of minimizing the run time while approaching steady-state.
- The problems **scale up perfectly** as more radial gridpoints are added.
- Also, a user can perform a GYRO scan (without iteration) across, say, 10 points along the minor radius. In the past, this would require 10 separate runs AND a lot of bookkeeping/management. Now it is all automated, and we can directly compare GYRO results to TGLF results.
  - → Jeff is doing this sort of analysis now based on so-called ASTRA profiles for ITER. So, TGYRO is already doing exploratory ITER transport work.

Standard Transport Code Formulation

Historical approaches to transport simulations and modeling

In order of complexity:

1. **Fixed gradient:** fix (z_i, z_e, T_i, T_e) and compute (Q_i, Q_e).
   - This is the approach used by modern GK codes.
2. **Fixed flux:** fix (Q_i^T, Q_e^T) and compute (z_i, z_e, T_i, T_e).
   - Relevant to **experimental modeling**: what profiles are required to match experimental power output?
3. **Self-consistent transport:** compute (z_i, z_e, T_i, T_e) given pedestal values (T_i^*, T_e^*).
   - Relevant to **profile prediction**: what profiles and fusion power do I get in a given configuration?

Transport Code Formulation

Steady-state problem

Steady-state **transport equations** for electrons and ions

$$\frac{1}{V'(r)}\frac{\partial}{\partial r}\left[V'(r)Q_i(r)\right] = (1-\lambda)S_\alpha + S^{ei}_{\text{exch}} + S^{i}_{\text{aux}}$$

$$\frac{1}{V'(r)}\frac{\partial}{\partial r}\left[V'(r)Q_e(r)\right] = \lambda S_\alpha - S^{ei}_{\text{exch}} + S^{e}_{\text{aux}} - S_{\text{rad}}$$

Integrating leads to a coupled system

$$Q_i(z_i, z_e, T_i, T_e) - Q_i^T(T_i, T_e) = 0$$

$$Q_e(z_i, z_e, T_i, T_e) - Q_e^T(T_i, T_e) = 0$$

with $z_i \doteq -\frac{a}{T_i}\frac{\partial T_i}{\partial r}$ and $z_e \doteq -\frac{a}{T_e}\frac{\partial T_e}{\partial 4}$.

We enforce pedestal boundary conditions are $r = r_*$: $\quad T_\sigma(r_*) = T^*_\sigma$.

Discretizing and applying Newton's method we have this system

$$(\mathcal{J}_{\sigma\sigma',jj'} - \mathcal{J}^T_{\sigma\sigma',jj'})\delta z_{\sigma',j'} = -\left[\hat{Q}_{\sigma,j}(z^0) - \hat{Q}^T_{\sigma,j}(z^0)\right]$$

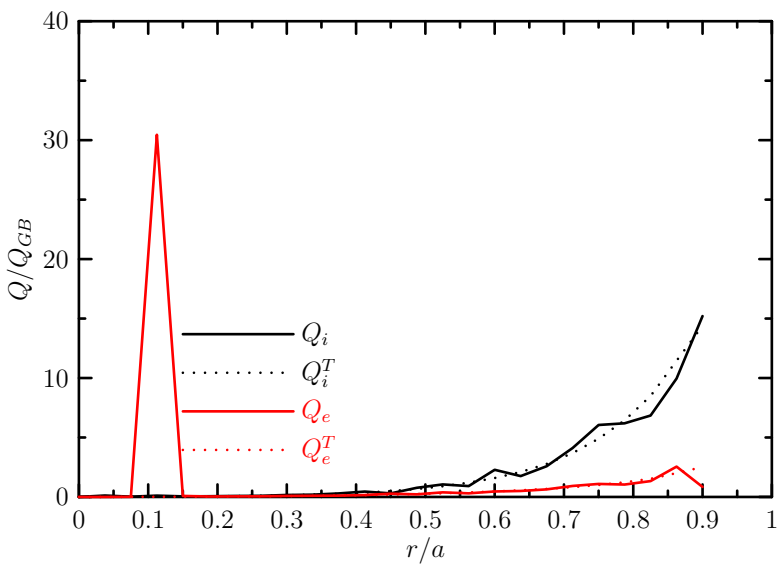
Test Case: ITER-like plasma

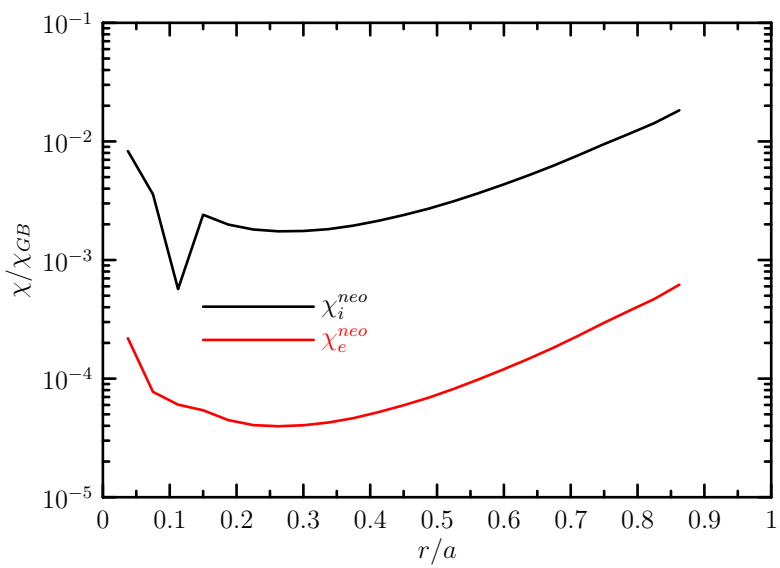
Flux and Diffusivities

12 hour simulation with 1284 processors

25 radial grid points:

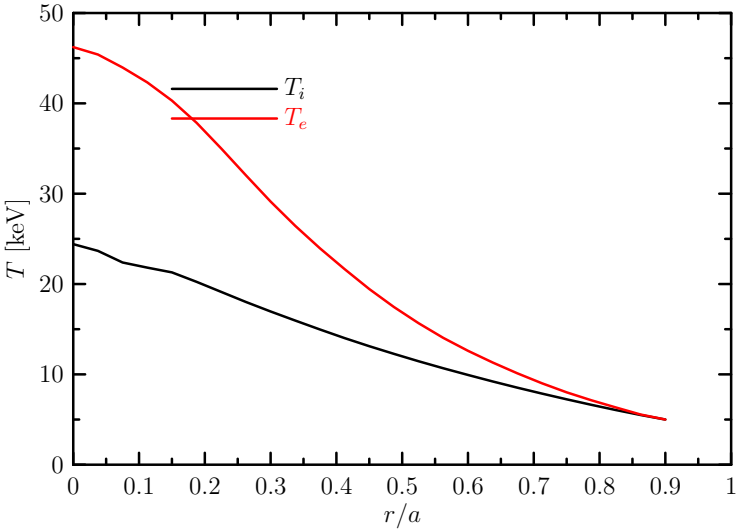
- 4 instances of TGLF from $r/a = 0.0375$ to 0.15 (1 processor each)
- 20 instances of GYRO from $r/a = 0.1875$ to 0.9 (64 processors each)

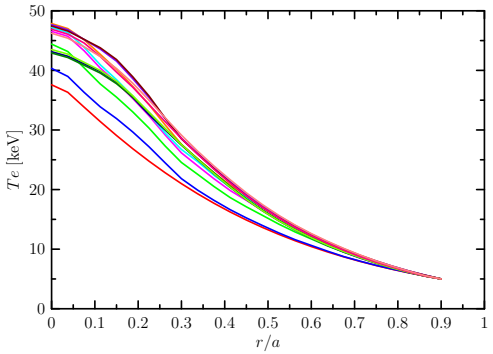


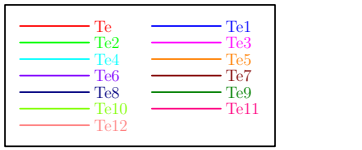


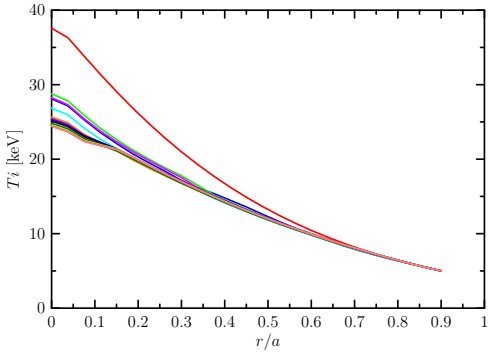
Test Case: ITER-like plasma

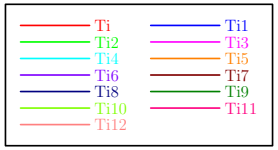
Electron and Ion profile convergence





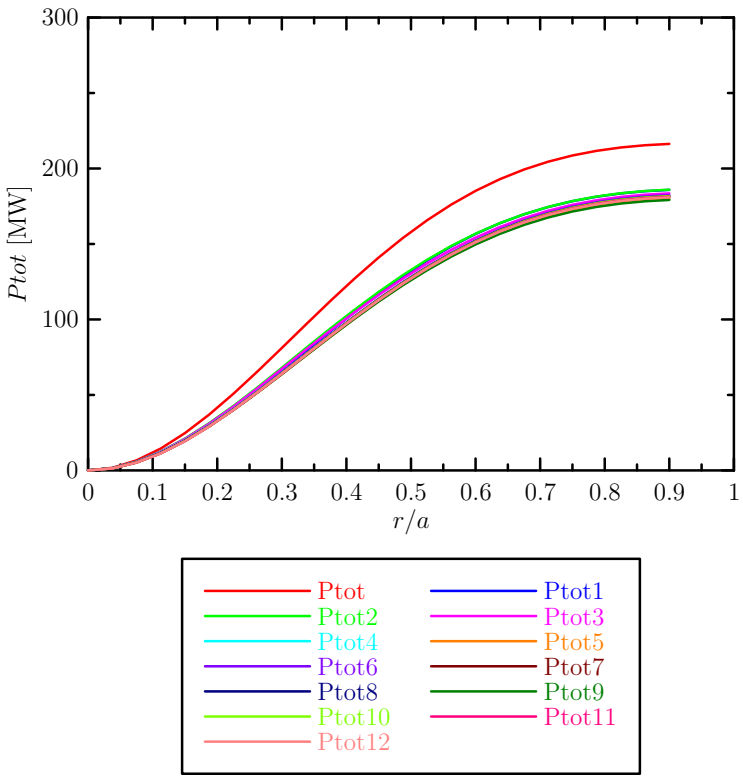


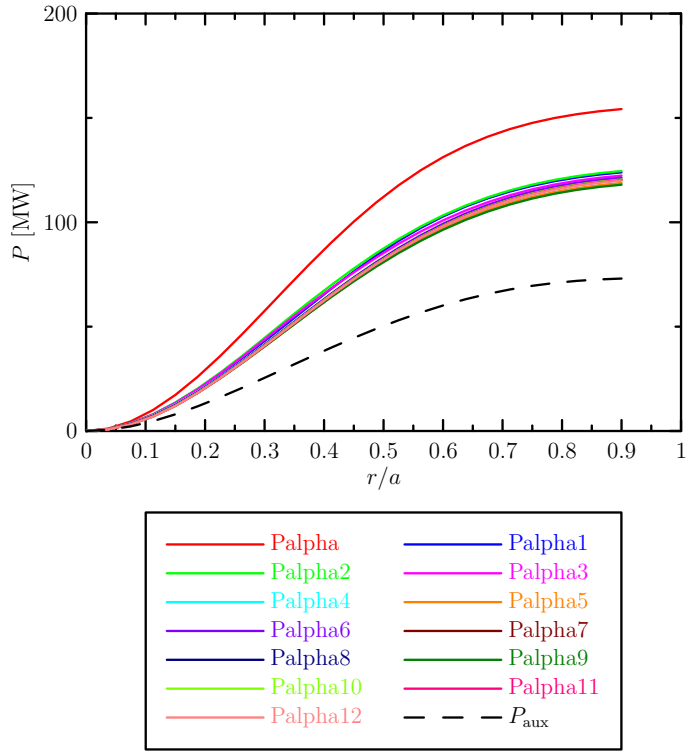




Test Case: ITER-like plasma

Total and alpha power





Conclusions

- Coupled IFS-PPPL/TGLF/GYRO simulations implemented in our TGYRO prototype.
- Actively working on getting GYRO into the FACETS framework.
- We are working on “steady-state convergence”. Initial results using direct iteration; we can get to a fairly crude steady-state in just a few iterations. We are investigating the Newton step-size as well as the GYRO time-averaging length to see just how good we can make the direct method. Code is improvely weekly.
- “TGYRO is shaping up to become a really unique, powerful tool, and for a fact I know that lots of groups around the world will soon want to get their hands on it.” Candy

Extra slides

Standard Transport Code Formulation

Restrict attention to the steady-state problem

Steady-state **transport equations** for electrons and ions

$$\frac{1}{V'(r)}\frac{\partial}{\partial r}\left[V'(r)Q_i(r)\right] = (1-\lambda)S_\alpha + S^{ei}_{\text{exch}} + S^{i}_{\text{aux}}$$

$$\frac{1}{V'(r)}\frac{\partial}{\partial r}\left[V'(r)Q_e(r)\right] = \lambda S_\alpha - S^{ei}_{\text{exch}} + S^{e}_{\text{aux}} - S_{\text{rad}}$$

Fluxes are the sum of **neoclassical transport** (Hinton-Hazeltine analytic theory, NEO) and **turbulent transport** (TGLF, GYRO)

$$Q_i = Q_i^{\text{Neo}} + Q_i^{\text{Turb}}$$

$$Q_e = Q_e^{\text{Neo}} + Q_e^{\text{Turb}}$$

Standard Transport Code Formulation

Account for Sources, Radiation and Exchange

$S_\alpha \longrightarrow$ Thermonuclear source

$S^{ei}_{\mathrm{exch}} \longrightarrow$ Electron-ion energy exchange

$S^{i}_{\mathrm{aux}} \longrightarrow$ Ion Auxilliary heating

$S^{e}_{\mathrm{aux}} \longrightarrow$ Electron Auxilliary heating

$S_{\mathrm{rad}} \longrightarrow$ Electron radiation

$\lambda \longrightarrow$ Fraction of heating to electrons

Standard Transport Code Formulation

Solve volume-integrated form of the equation

Define **target fluxes** via integration:

$$Q_i^T(r) \doteq \frac{1}{V'(r)} \int_0^r dx\, V'(x) \left[(1-\lambda)S_\alpha + S_{\text{exch}}^{ei} + S_{\text{aux}}^{i}\right]$$

$$Q_e^T(r) \doteq \frac{1}{V'(r)} \int_0^r dx\, V'(x) \left[\lambda S_\alpha - S_{\text{exch}}^{ei} + S_{\text{aux}}^{e} - S_{\text{rad}}\right]$$

The result is a curious system which depends on both the temperatures and the temperature gradients:

$$Q_i(z_i, z_e, T_i, T_e) - Q_i^T(T_i, T_e) = 0$$

$$Q_e(z_i, z_e, T_i, T_e) - Q_e^T(T_i, T_e) = 0$$

$$z_i \doteq -\frac{a}{T_i}\frac{\partial T_i}{\partial r} \quad \text{and} \quad z_e \doteq -\frac{a}{T_e}\frac{\partial T_e}{\partial r}$$

Standard Transport Code Formulation

Connection between profiles and gradients

Enforce **pedestal boundary conditions** at $r = r_*$:

$$T_\sigma(r_*) = T_\sigma^*$$

In this case, the gradient z_σ uniquely determine T_σ:

$$T_\sigma(r) = T_\sigma^* \exp\left(\int_r^{r_*} dx\, z_\sigma(x)\right)$$

On a discrete grid, this is just

$$T_\sigma(r_{i-1}) = T_\sigma(r_i) \exp\left\{\left[\frac{z_\sigma(r_i) + z_\sigma(r_{i-1})}{2}\right][r_i - r_{i-1}]\right\}$$

Standard Transport Code Formulation

Reduction to nonlinear algebraic system

Let's bring the problem into canonical form. First, put problem in discrete form:

- $z_{\sigma,j} = z_\sigma(r_j)$
- $Q_{\sigma,j} = Q_\sigma(r_j)$
- $Q^T_{\sigma,j} = Q^T_\sigma(r_j)$

Then the equations to be solved are

$$\hat{Q}_{\sigma,j} = \hat{Q}^T_{\sigma,j}$$

where the hat denotes gyroBohm normalization.

Standard Transport Code Formulation

Numerical Method

We then apply Newton's method while making the assumption that the transport fluxes depend only locally on the gradients so that the Jacobian associated with $Q_{\sigma,j}$ is block diagonal. This then leads to the system

$$(\mathcal{J}_{\sigma\sigma',jj'} - \mathcal{J}^T_{\sigma\sigma',jj'})\delta z_{\sigma',j'} = -\left[\hat{Q}_{\sigma,j}(z^0) - \hat{Q}^T_{\sigma,j}(z^0)\right]$$

After a Newton iteration, we measure the residual

$$R^1_{\sigma,j} = \frac{\left[\hat{Q}_{\sigma,j}(z^1) - \hat{Q}^T_{\sigma,j}(z^1)\right]^2}{\left[\hat{Q}_{\sigma,j}(z^1)\right]^2 + \left[\hat{Q}^T_{\sigma,j}(z^1)\right]^2}$$

TGYRO memory model

TGYRO

```
use tgyro_globals
use gyro_globals
use transport_globals
```

TRANSPORT

```
use transport_globals
```

GYRO

```
use gyro_globals
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GYRO

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use gyro_globals
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use gyro_globals
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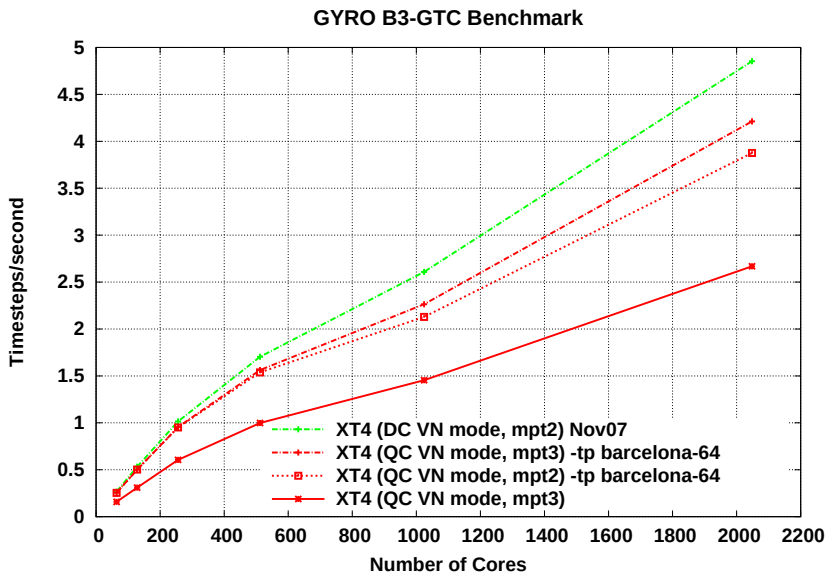
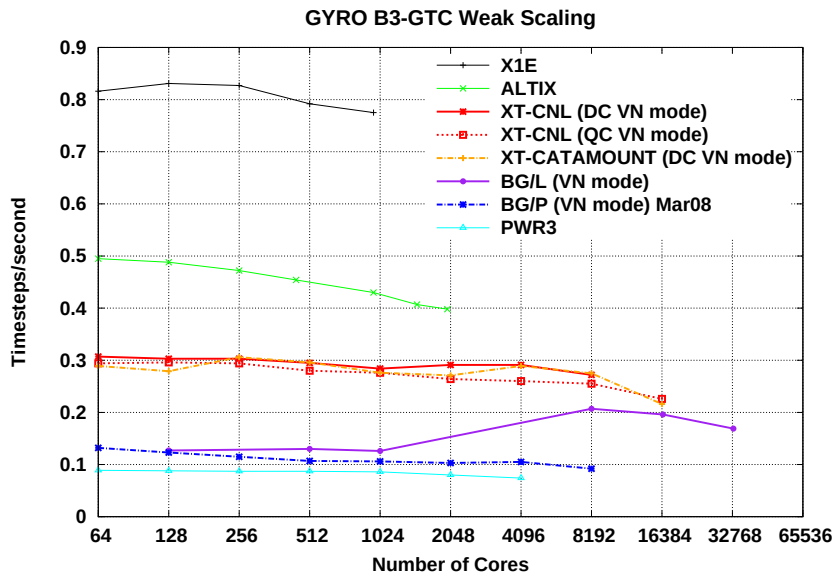
GYRO scaling





Implications for Gyrokinetic Transport Calculations

Working in the near-threshold regime

New issues related to reactor modeling

- Power-balance indicates that codes will operate in the **sub χ_{GB} (near-threshold) regime**.
- In this regime, simulations are characterized by a **long transient phase**.
- Long simulation times are required to acquire good turbulence statistics.
- Significant new **GK simulation logic** will be required to run in ITER near-threshold regime .
- Possible implication is that simulating well into the **ETG range** will be required to get the correct ratio of electron to ion energy flux.