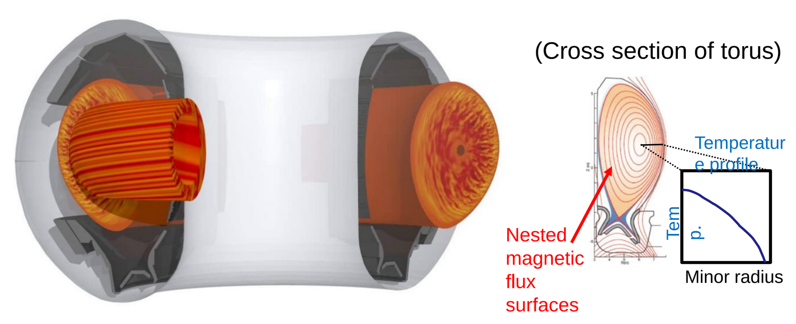
Bringing Global Gyrokinetic Turbulence Simulations to the Transport Timescale using a Multiscale Approach

Lawrence Livermore National Laboratory

Jeff Parker [parker68@llnl.gov], L. LoDestro, L. Ricketson, A. Campos, J. Hittinger (LLNL); D. Told (IPP); G. Merlo (UT Austin); F. Jenko (UT Austin/IPP)

Vision: Global gyrokinetic simulations coupled to transport solver, as key component of high-fidelity WDM



Turbulent fluxes in the core are small, resulting in long timescales for the evolution of macroscopic profiles, e.g., T(r)

Turbulence time ~ 10 μs
Energy confinement time ~ 1 s

Direct numerical integration capturing both turbulence and confinement time scales → computationally expensive!

Assuming a separation of timescales exists, how can we efficiently study the self-consistent evolution on the long timescale? How do we bridge the timescale gap?

Vision: Multiscale method to exploit the timescale gap.

- Couple a *transport solver* with gyrokinetic simulation for calculation of fluxes
- *Challenge*: Need efficient methods and algorithms for coupling directly with global turbulence simulation

Benefits: High-fidelity predictive turbulence + transport simulations. Can be a key component of a whole-device model

- Transport at the confinement timescale, using best available gyrokinetic simulations as a high-cost, high-benefit alternative to computationally cheaper quasilinear transport models
- Nonlocal effects – e.g., internal transport barriers (ITBs)
- Enabling a new form of discovery science

Theoretical Background:

Multiscale Gyrokinetics Ordering, applicable to core of a tokamak:

$$\frac{\omega}{\Omega} \sim \frac{\rho}{L} \sim \frac{k_\parallel}{k_\perp} \sim \frac{\delta f}{f} \sim \frac{|\delta \mathbf{B}|}{|\mathbf{B}|} \sim \frac{|\delta \mathbf{E}|}{|\mathbf{E}|} \sim \epsilon \qquad k_\perp \rho \sim O(1) \qquad \frac{1}{\omega\tau} \sim \epsilon^2$$

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f + \frac{q}{m}[\mathbf{E} + \mathbf{v}\times\mathbf{B}]\cdot\frac{\partial f}{\partial \mathbf{v}} = C[f]$$

Can derive:

Transport Equations (slow timescale, 1D)

$$\frac{\partial n}{\partial t} + \frac{1}{V'}\frac{\partial}{\partial \psi}\left[V'\langle \mathbf{\Gamma}\cdot\nabla\psi\rangle\right] = S_n$$

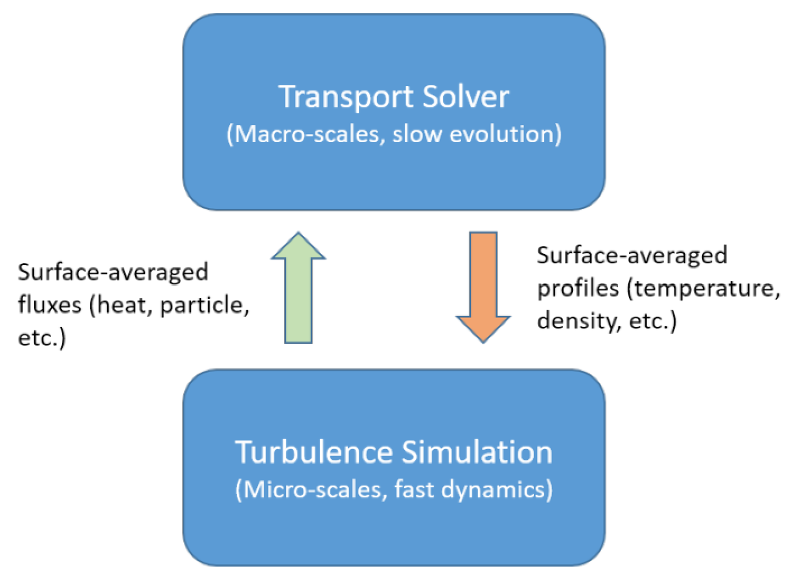
$$\frac{3}{2}\frac{\partial p}{\partial t} + \frac{1}{V'}\frac{\partial}{\partial \psi}\left[V'\langle \mathbf{Q}\cdot\nabla\psi\rangle\right] = S_E$$

Gyrokinetic Equations (fast timescale, 5D)

$$\frac{\partial h}{\partial t} + \left(v_\parallel \hat{\mathbf{b}} + \mathbf{V}_D + \langle \mathbf{V}_\chi\rangle_{\mathbf{R}}\right)\cdot\frac{\partial h}{\partial \mathbf{R}} = \langle C_L[h]\rangle_{\mathbf{R}} + \frac{ZeF_0}{T}\frac{\partial\langle\chi\rangle_{\mathbf{R}}}{\partial t} - \frac{\partial F_0}{\partial\psi}\langle\mathbf{V}_\chi\rangle_{\mathbf{R}}\cdot\nabla\psi$$

(Some terms suppressed, for simplicity)

Schematic Diagram of Numerical Solver



Method for numerical coupling

Paradigm transport equation

- Assume turbulent flux $\Gamma[n]$ is computed from a simulation

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial \psi}\Gamma[n] = S$$

Solve using an *implicit timestep* (so we are not constrained to tiny Δt)

- Stiff nonlinear problem – $\Gamma[n]$ depends strongly on the profile n
- What method for converging to self-consistent solution within a timestep?

Key Elements of our method (More detail in [1,2])

Let $n_{m,l}$ be the lth iterate of the mth timestep.

- Represent turbulent flux as diffusive (+ possibly convective), with numerically computed, evolving transport coefficients

$$\Gamma_{m,l} \to -D_{m,l-1}(\partial_x n_{m,l}) + c_{m,l-1}n_{m,l}$$

- Variant of Picard iteration (no Newton steps) – No Jacobian-vector products or any finite-difference estimation of derivatives

$$D_{m,l-1} \equiv -\theta\frac{\Gamma[n_{m,l-1}]}{\partial_x n_{m,l-1}}$$

$$c_{m,l-1} \equiv (1-\theta)\frac{\Gamma[n_{m,l-1}]}{n_{m,l-1}}$$

- Computationally advantageous

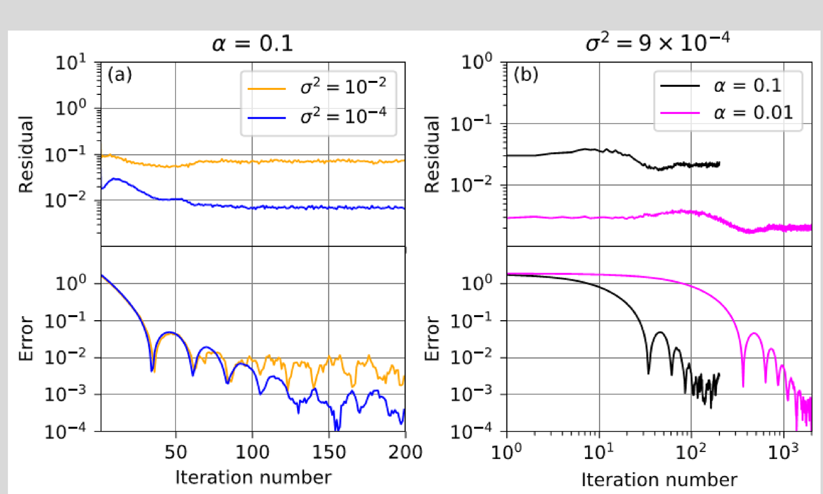
This gives a tractable, linear equation to solve for each iterate $n_{m,l}$:

$$\frac{n_{m,l} - n_{m-1}}{\Delta t} + \partial_x\left[-D_{m,l-1}\partial_x n_{m,l} + c_{m,l-1}n_{m,l}\right] = S_m$$

If it converges, it doesn't matter how you represented the turbulent flux: it's the right answer

Method is robust to turbulent fluctuations:
Fluctuations in the turbulent flux always occur in simulations. This method is robust.

Example: *analytic model* for $\Gamma[n]$ with added random noise. Solution still converges to the correct solution. **Shown:** Error decreases to an acceptably small level.



Contrast this method with a Newton-type of iteration, which would Taylor expand the turbulent flux:

$$\Gamma_{m,l} = \Gamma[n_{m,l}] \approx \Gamma[n_{m,l-1}] + \left.\frac{\delta\Gamma}{\delta n}\right|_{n_{m,l-1}}\cdot(n_{m,l} - n_{m,l-1})$$

This procedure requires calculation of Jacobian terms $\delta\Gamma/\delta n$. Two problems:

- **Computationally expensive** to calculate Jacobians or Jacobian-vector products. This problem is exacerbated for *global* turbulence simulations, where turbulence can depend in principle on the profiles everywhere (i.e., dense Jacobians)
- Fluxes are intrinsically noisy due to statistical fluctuations of turbulence simulations. **Errors are amplified** in a finite-difference calculation of Jacobian

Code implementing this approach: Tango

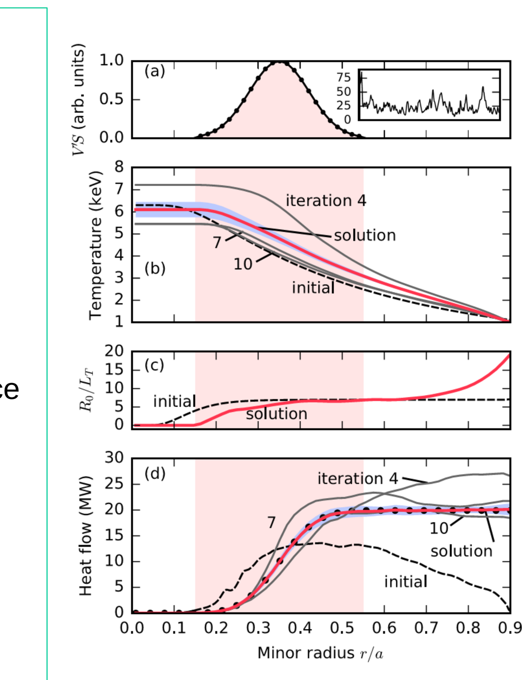
Tango is:

- 1D transport solver implementing this numerical method
- Coupled with global GENE
- Written in Python and open source, available at github.com/LLNL/tango

Results

Tango-global GENE run: Successfully found steady state temperature profile for a specified input heating power

- GENE parameters:
  - Domain: $\frac{r}{a} \in [0.1, 0.9]$
  - a=1.0 m, R_0=3.0 m
  - Bref=2.5 T, mref=2
  - **ρ_*= 1/292**
  - Circular geometry, adiabatic electrons, CBC-like
- Tango parameters:
  - Domain: $\frac{r}{a} \in [0, 0.9]$
  - Looking for a steady-state solution with an applied heat source
  - Relaxation EWMA parameter $\alpha = 0.3$ (fairly large)
  - 50 iterations
  - 50 GENE time units (Lref/cref = R/v_{ti}) per iteration
  - Evolving ion pressure only; density profile is prescribed and held fixed
  - Boundary conditions:
    - r=0: Neumann
    - r/a = 0.9: Dirichlet, fixed pressure/temperature
  - **Applied heat source 20 MW localized in 0.15 < r/a < 0.55**

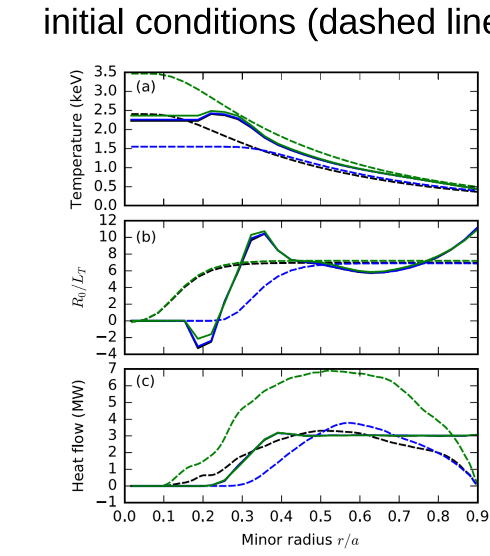


Required computational time
This example: 30-50 iterations required to attain converged steady-state solution: total GENE simulation time of 1500 – 2500 R/v_{ti}. (~35,000 cpu hours for this example)

Estimate of time in physical units:

- Confinement time estimate: $\tau_E \sim \frac{W_i}{P_{in}} \sim$ 55 ms
- Simulation time ~ 15 – 23 ms

Achieved same steady-state solution, starting from different initial conditions (dashed lines)



Goals and Moving Forward

- Ratchet up to increasing physics fidelity – requires generalizations of the coupling method, handling multi-channel turbulent transport, etc.
  - Synergies with AToM possible?
- Simulate frontier physics, such as ITBs
- Demonstrate real-world value by enabling quantitative predictions for experiments

References

[1] A. Shestakov, R. Cohen, J. Crotinger, L. LoDestro, A. Tarditi, X. Xu, "Self-consistent modeling of turbulence and transport," *J. Comp. Phys.* (2003)
[2] J. Parker, L. LoDestro, D. Told, G. Merlo, L. Ricketson, A. Campos, F. Jenko, J. Hittinger, "Bringing global gyrokinetic simulations to the transport timescale using a multiscale approach," *Nucl. Fusion* (2018)
[3] J. Parker, L. LoDestro, A. Campos, "Investigation of a multiple-timescale turbulence-transport coupling method in the presence of random fluctuations," *plasma* (2018)

Acknowledgments

Work supported by the SciDAC Partnership for Multiscale Gyrokinetic Turbulence. Work also supported by the Exascale Copmuting Project (17-SC-20-SC). This work was performed under the auspices of the US DOE by LLNL under Contract DE-DE-AC52-07NA27344.