

Multiscale, multiphysics modeling of turbulent transport and heating in collisionless, magnetized plasmas

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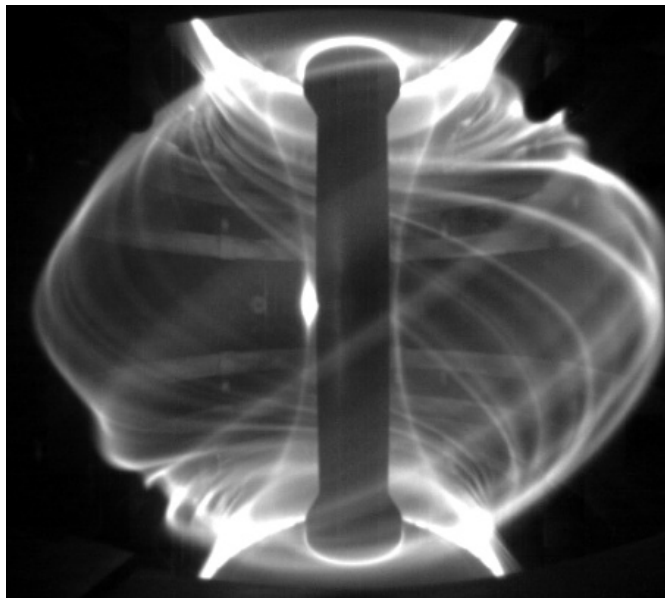
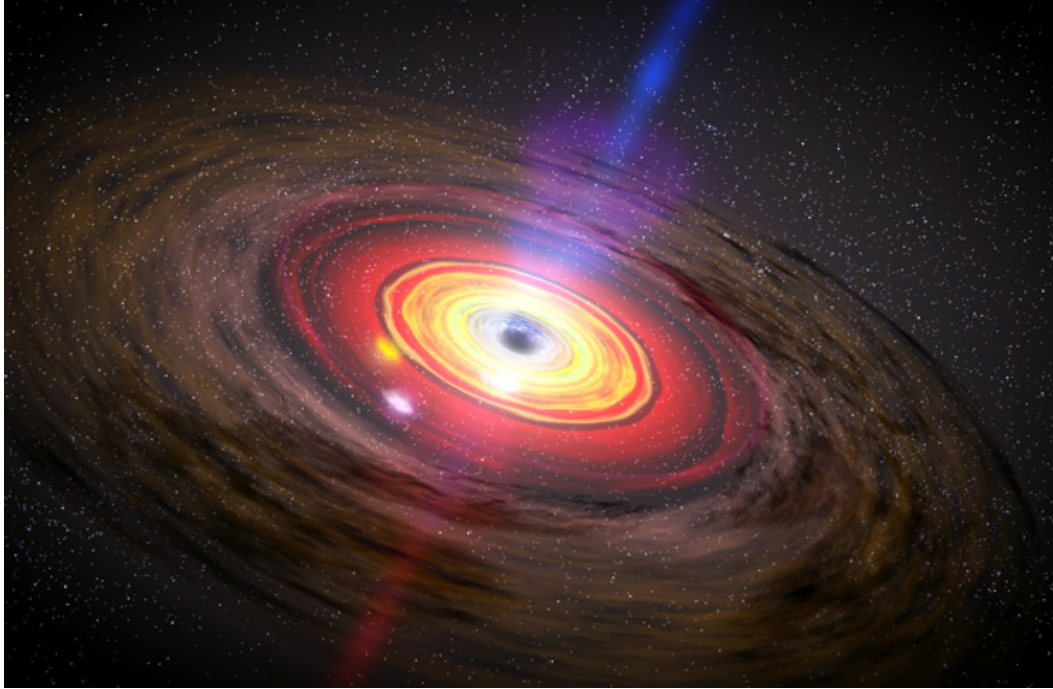
Collaborators: W. Dorland (Maryland), F. I. Parra (MIT), G. W. Hammett (PPPL),
I. G. Abel, A. A. Schekochihin (Oxford), S. C. Cowley (Culham),
T. Gorler (IPP-Garching), F. Jenko (IPP-Garching), ...



Overview

- Collisionless plasma dynamics are hard
- Let's make life simpler: a mean field approach for turbulence and transport/heating in tokamak plasmas
- Numerical modeling approach: multiscale, hybrid kinetic/fluid code Trinity
- Issues and opportunities

Hot, magnetized plasmas



What do we want?

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{\Gamma} = \dots$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{P} = \dots$$

...

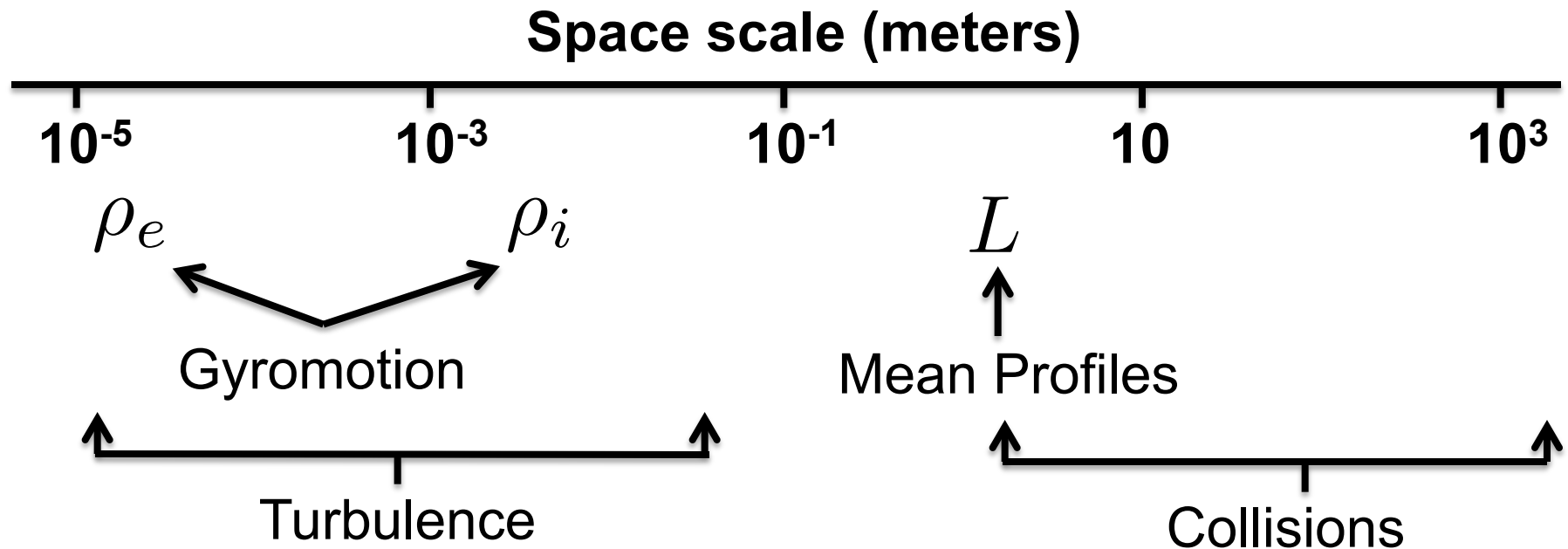
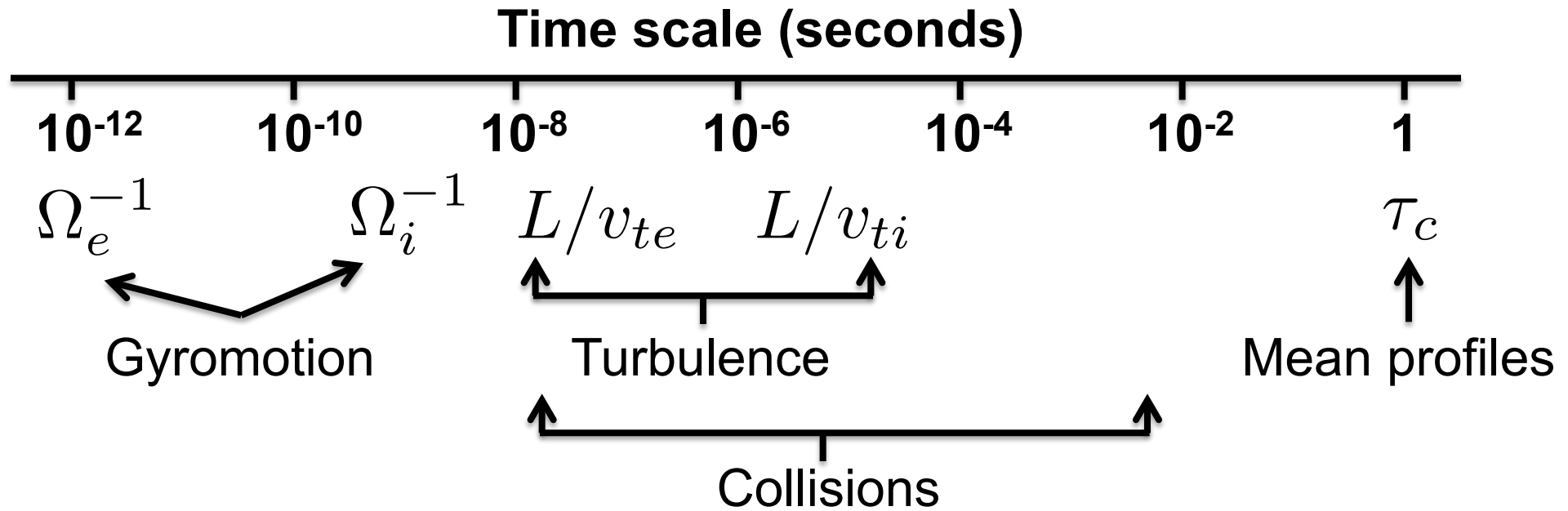
$$\frac{df}{dt} = C[f]$$

A tempting thought

“Think? Why think?! We have computers to do that for us.”

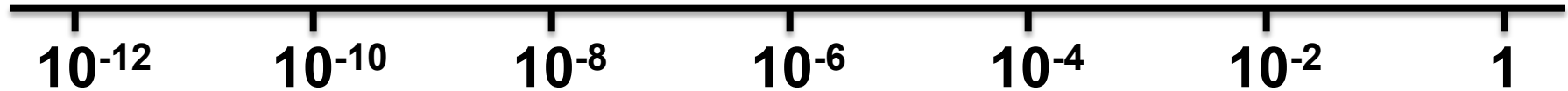
-- Jean Rostand

Range of scales



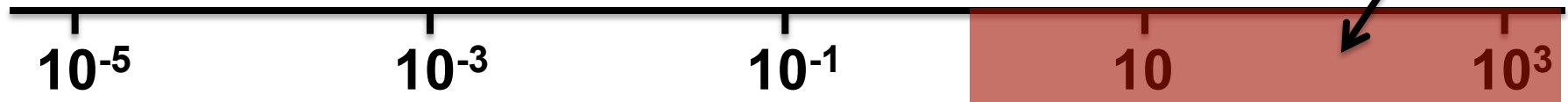
Expense (brute force)

Time scale (seconds)



Temporal grid: $\sim 10^{13}$ time steps

Space scale (meters)

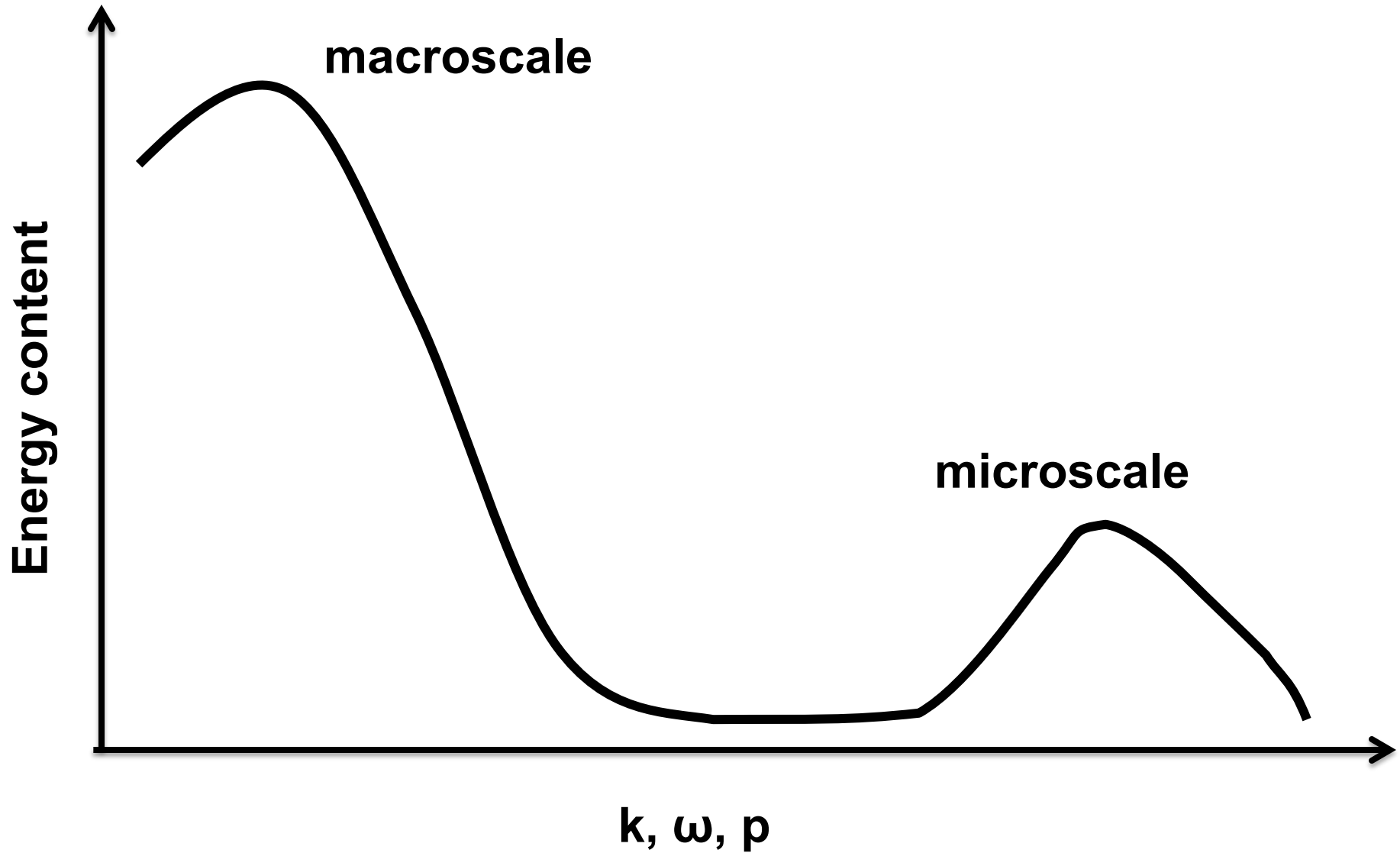


Spatial grid: $\sim 10^6$ grid points x 3-D = 10^{18} grid points

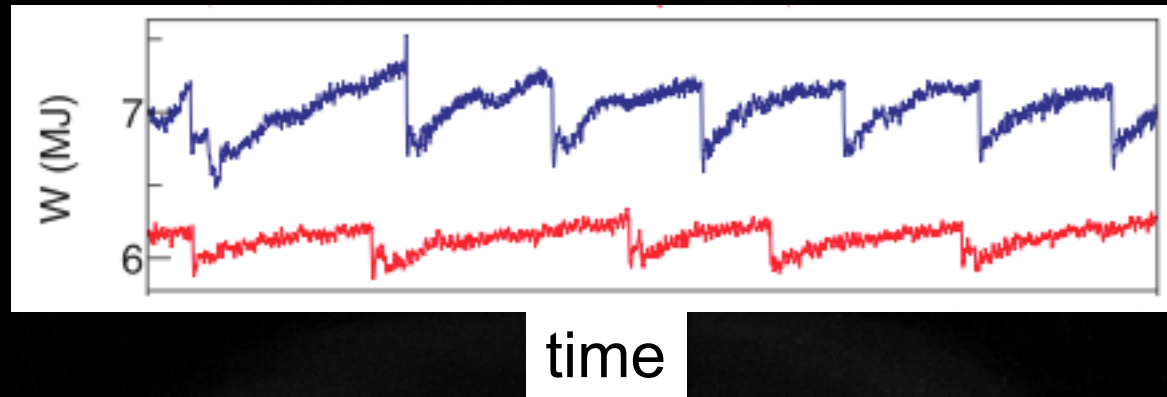
Velocity grid: ~ 10 grid points x 3-D = 10^3 grid points

Total: $\sim 10^{34}$ total grid points

Scale separation



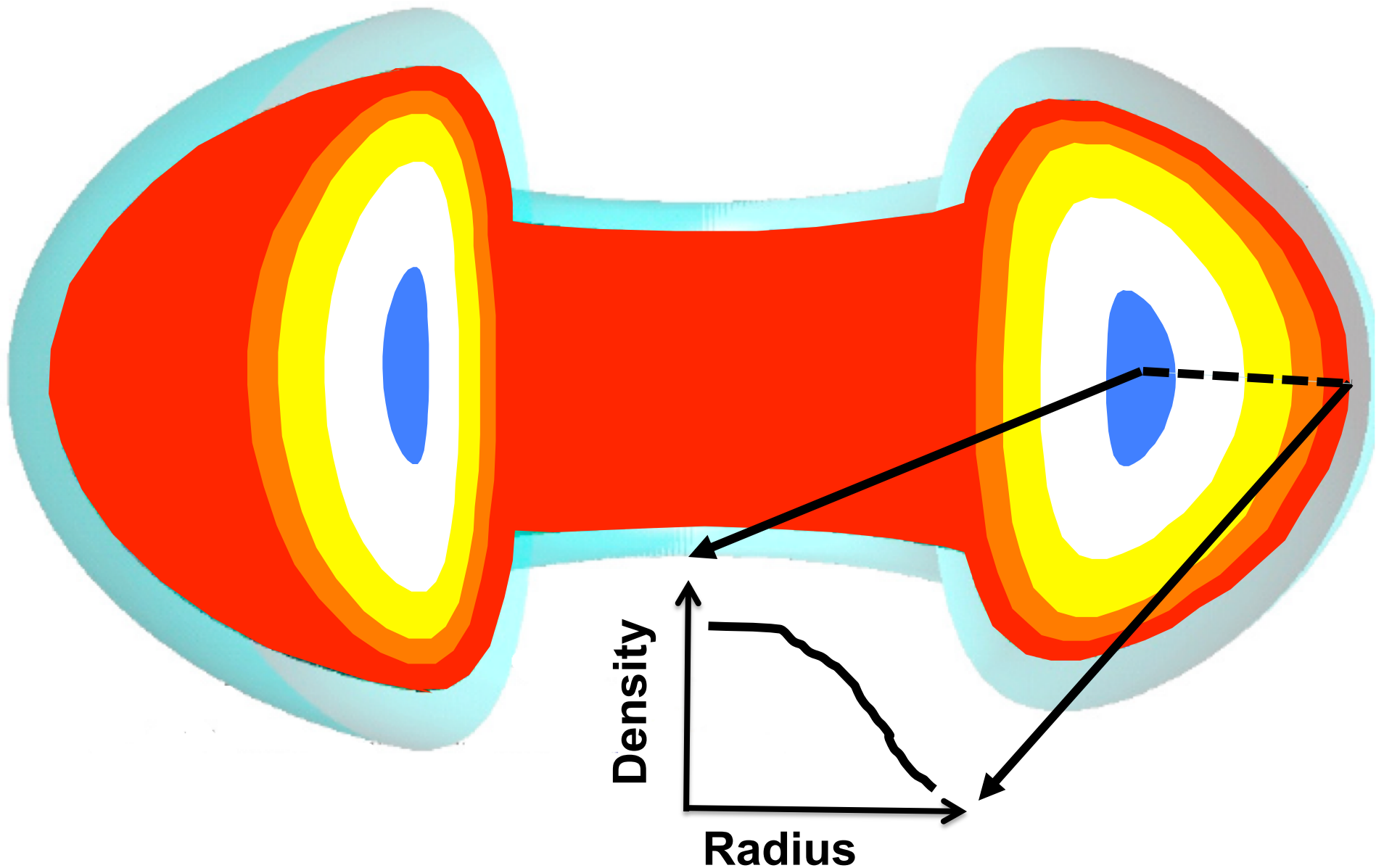
Multiscale, multiphysics



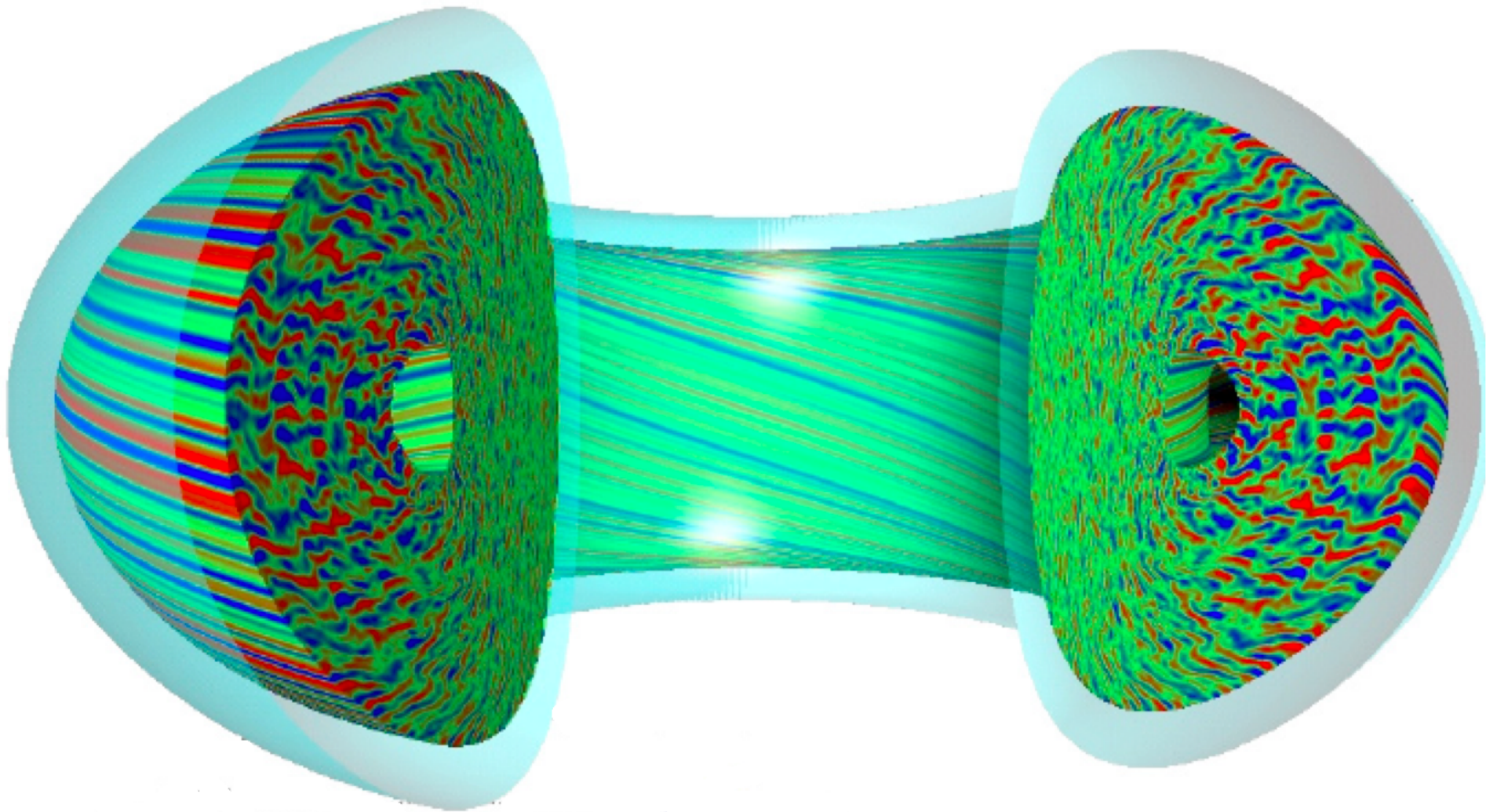
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Fast camera image of MAST plasma

Equilibrium macroscale spatial profile



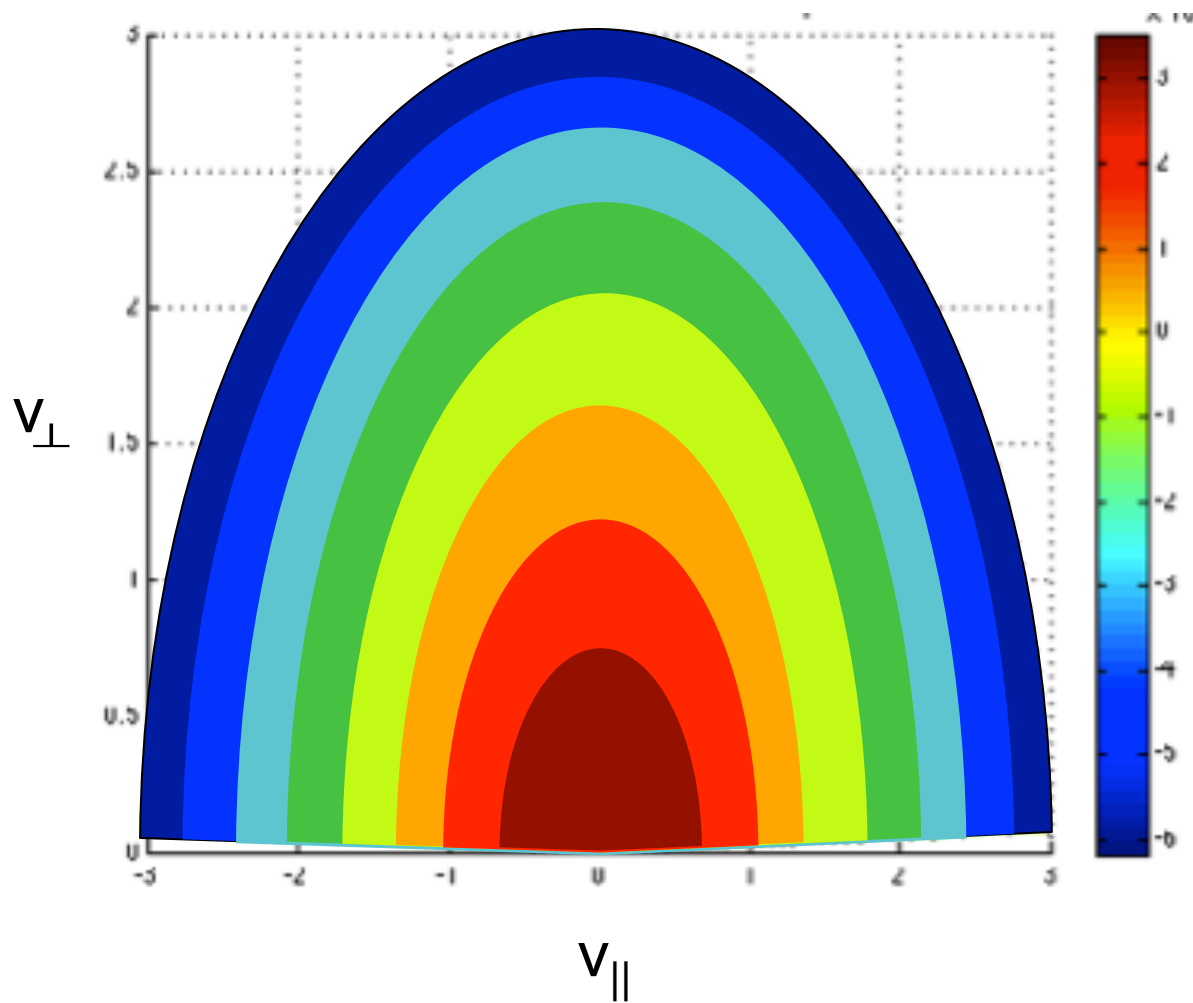
Microscale fluctuations



GYRO simulation
J. Candy and R. Waltz

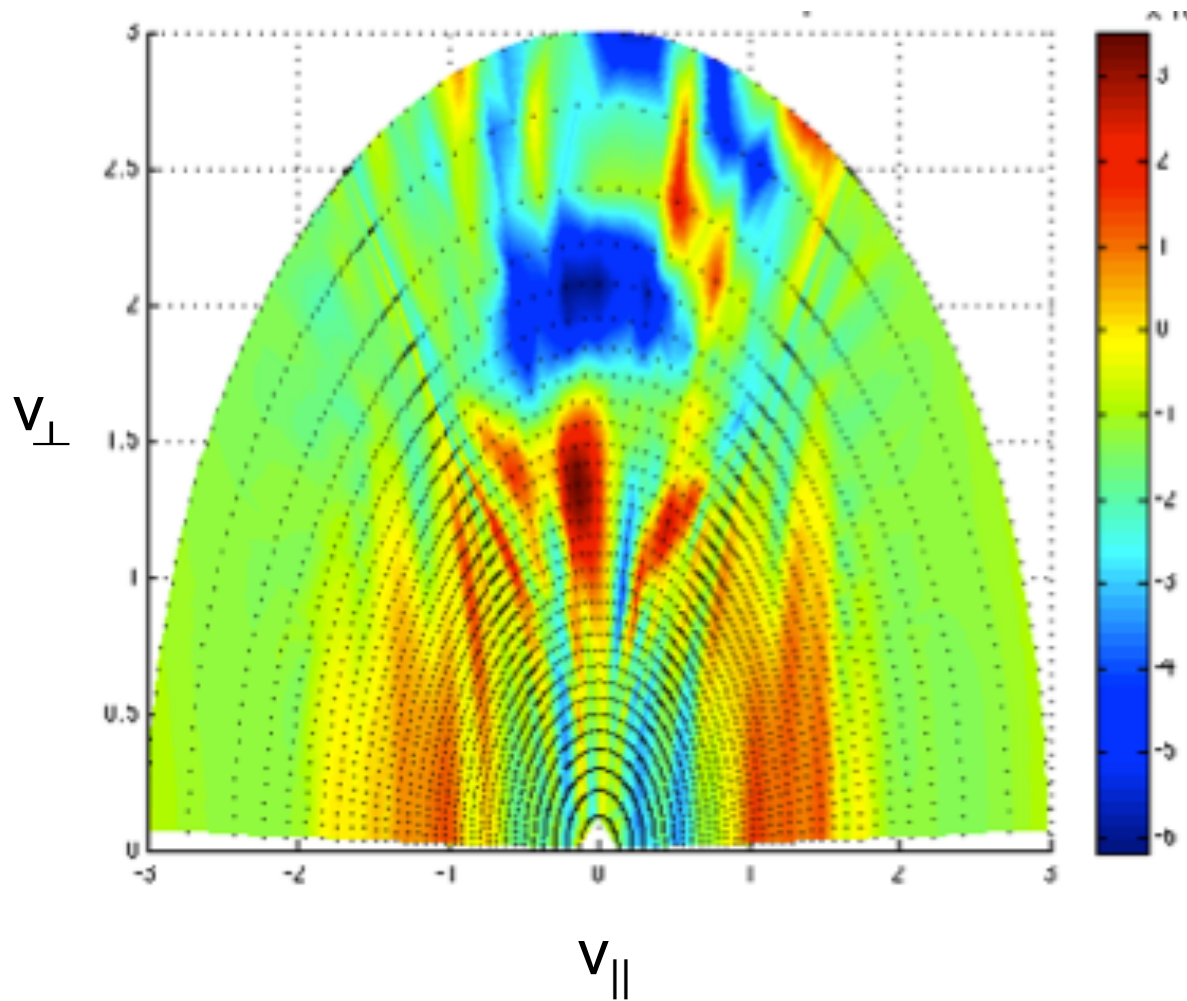
Equilibrium macroscale speed distribution

$$f = f(\mathbf{r}, \mathbf{v}, t)$$



Microscale fluctuations

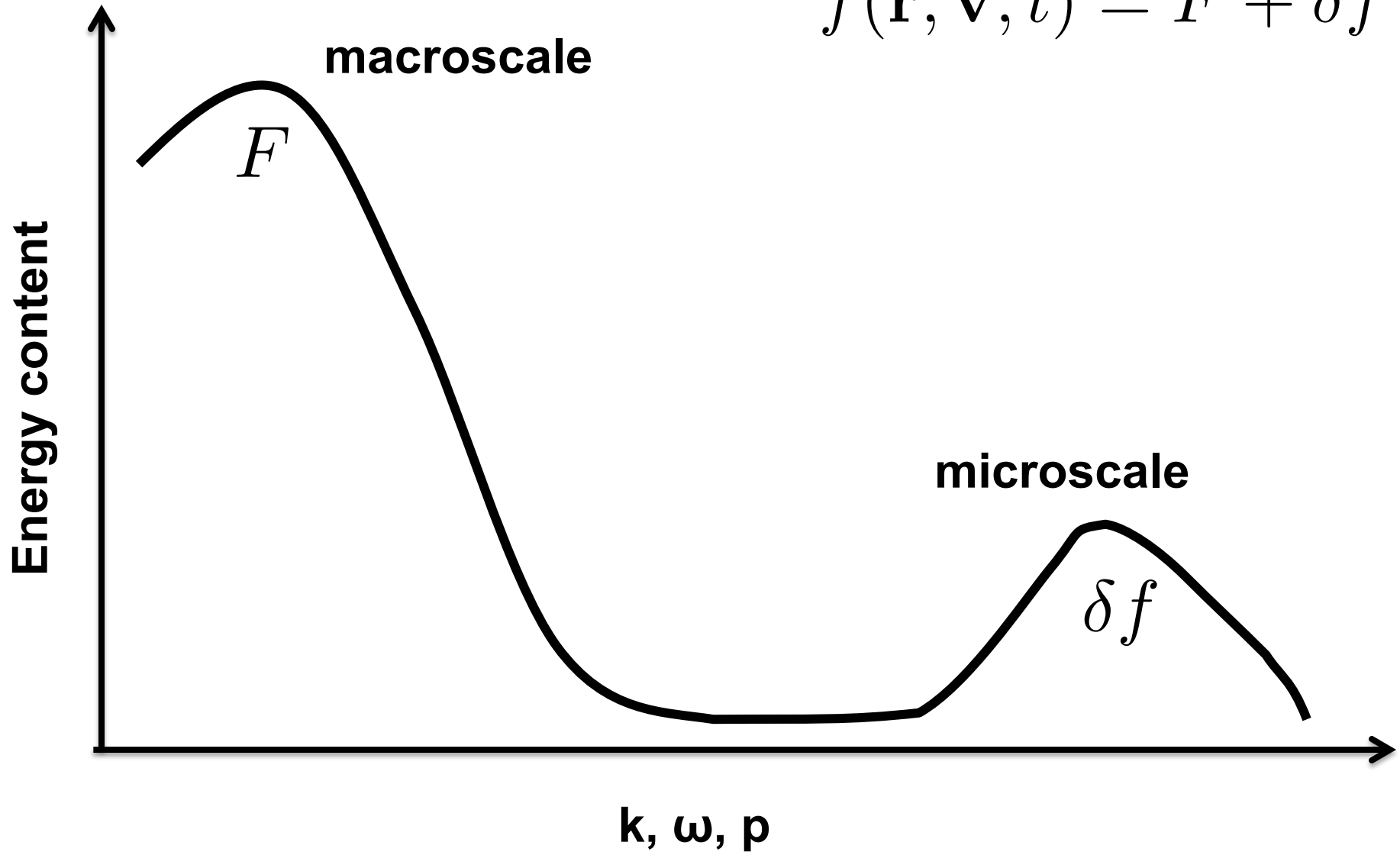
δf



GS2 simulation

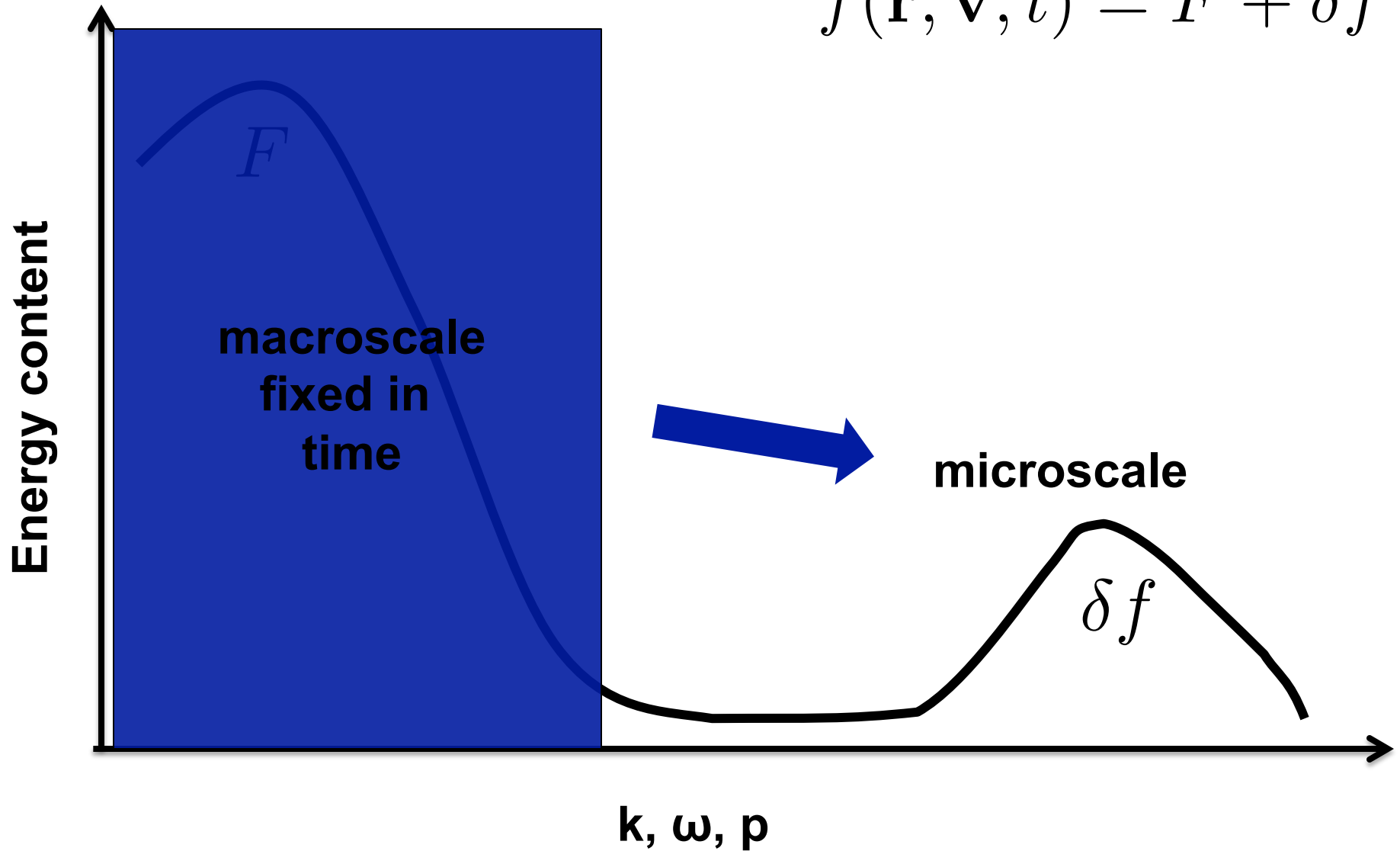
Scale separation

$$f(\mathbf{r}, \mathbf{v}, t) = F + \delta f$$



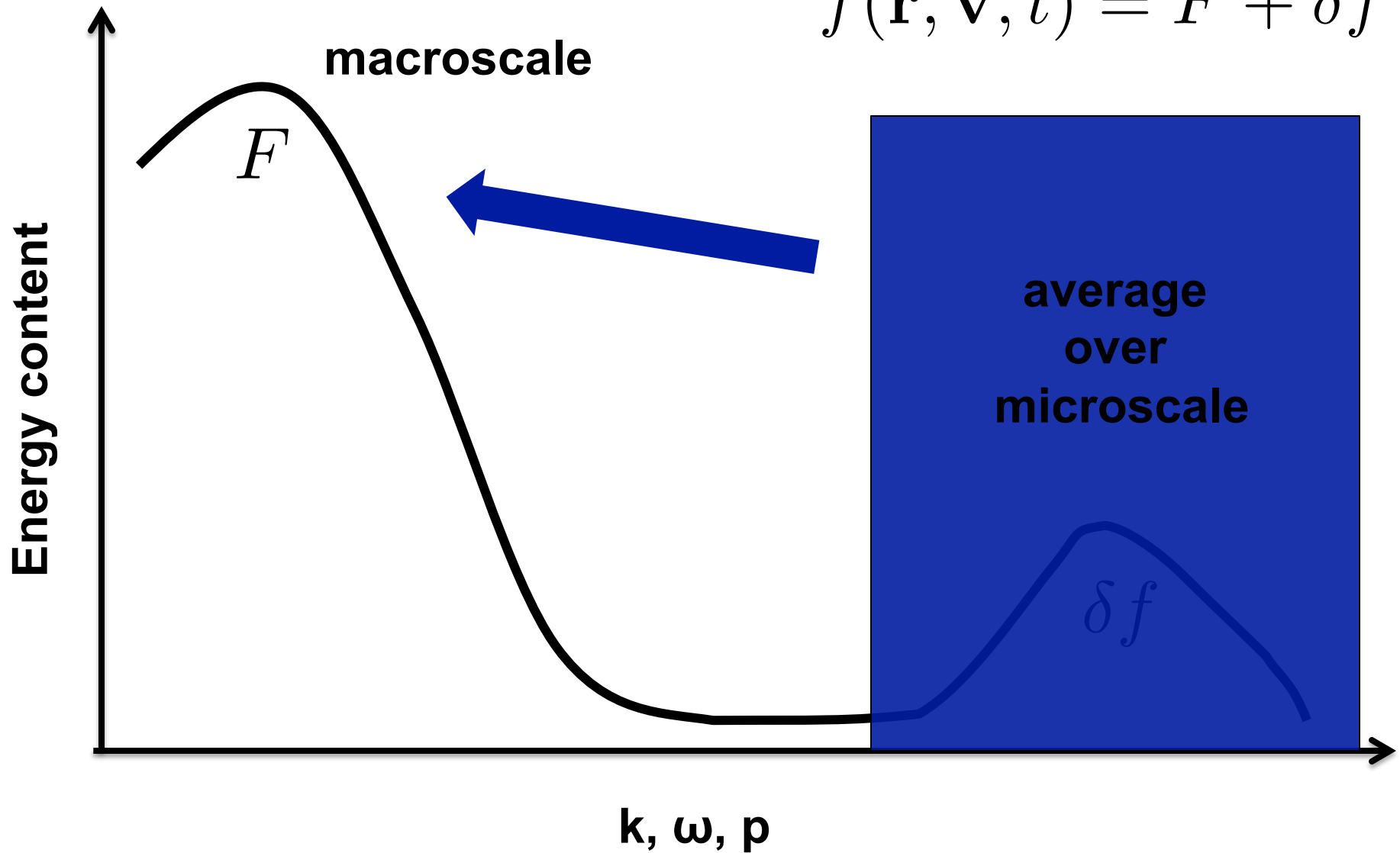
Macro drives micro

$$f(\mathbf{r}, \mathbf{v}, t) = F + \delta f$$

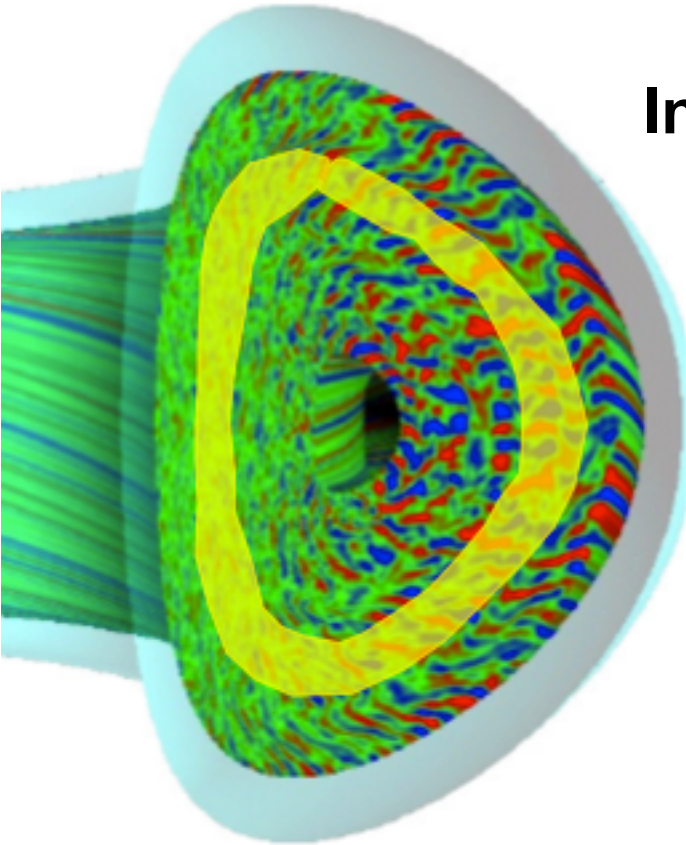


Micro feeds back into macro

$$f(\mathbf{r}, \mathbf{v}, t) = F + \delta f$$

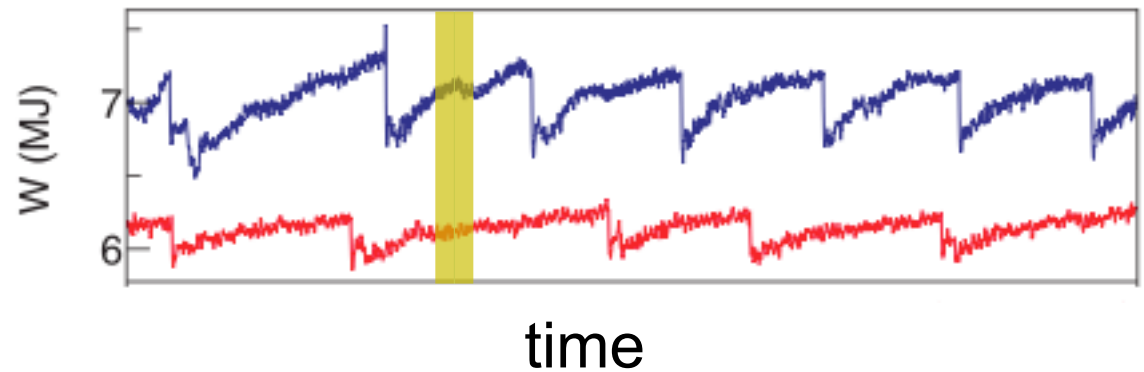


Coarse-grain average



In space...

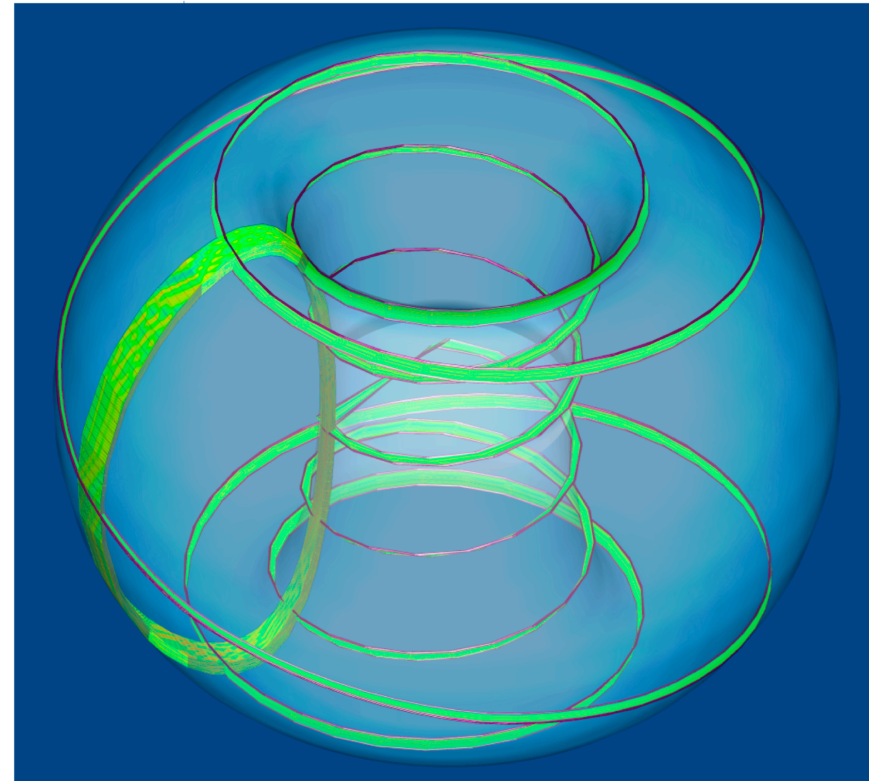
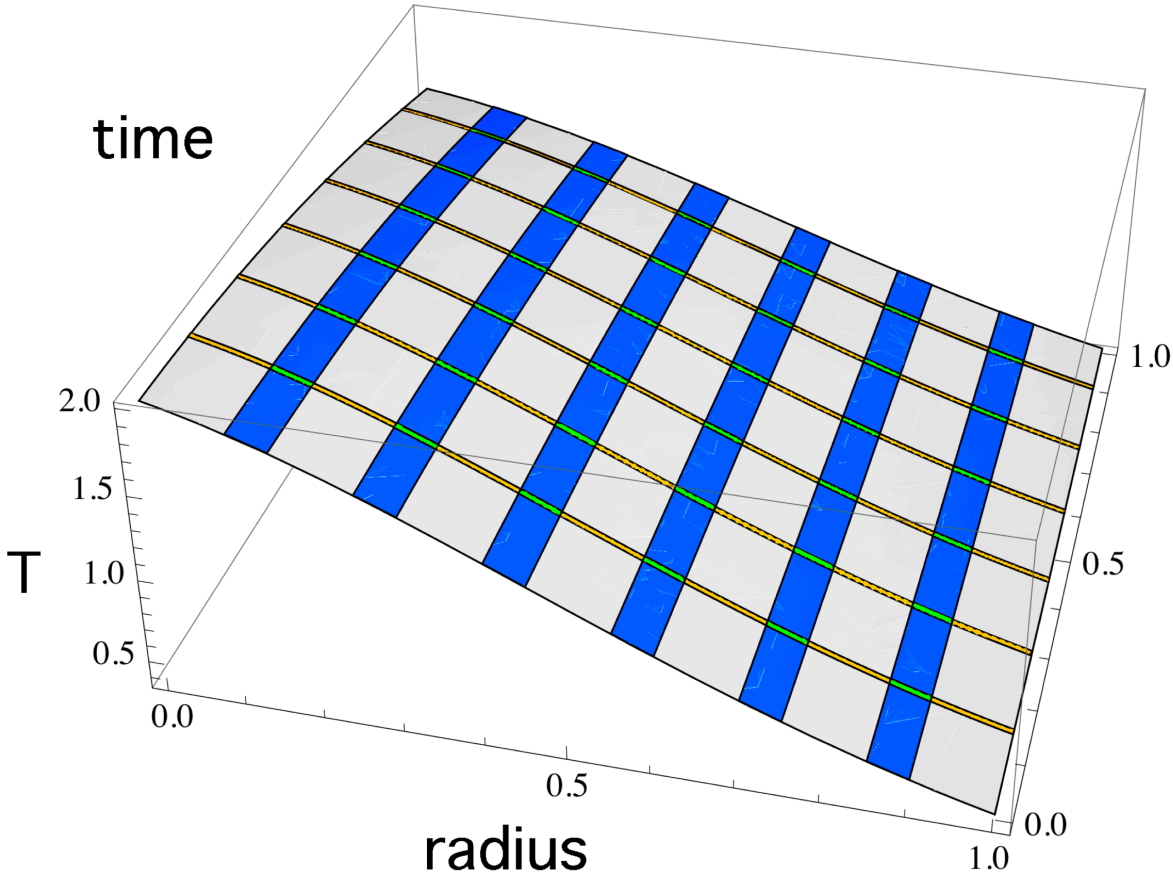
...and in time...



**...and moment approach in
velocities**

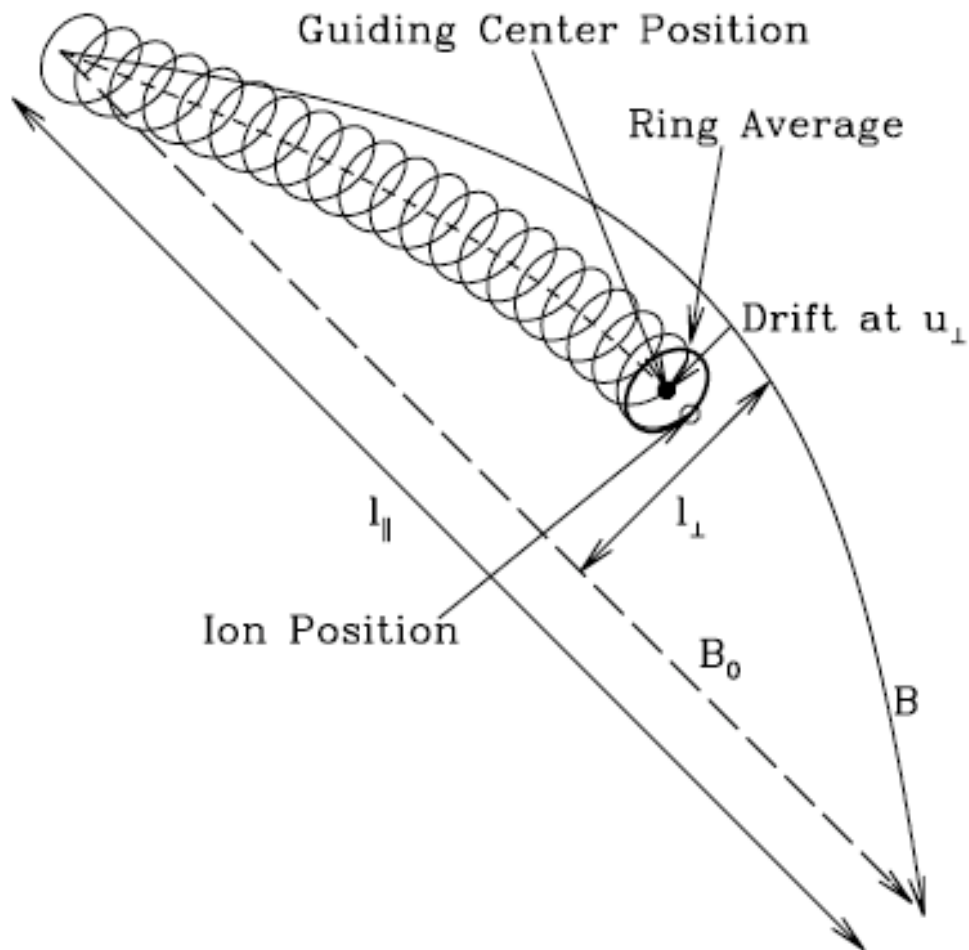
Multiscale model

Turbulent fluctuations calculated in small regions of fine space-time grid embedded in coarse grid for mean quantities (implemented in TRINITY code)



Gyrokinetic description of dynamics

$$\frac{\partial f_s}{\partial t} + \frac{d\mathbf{r}}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{r}} + \frac{d\mathbf{v}}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{v}} = C[f_s]$$



- Average over fast gyromotion and follow 'guiding center' position
- Eliminates fast time scale and gyro-angle variable (6-D \rightarrow 5-D)

Multiscale gyrokinetics

Decompose f into mean and fluctuating components:

$$f = F + \delta f$$

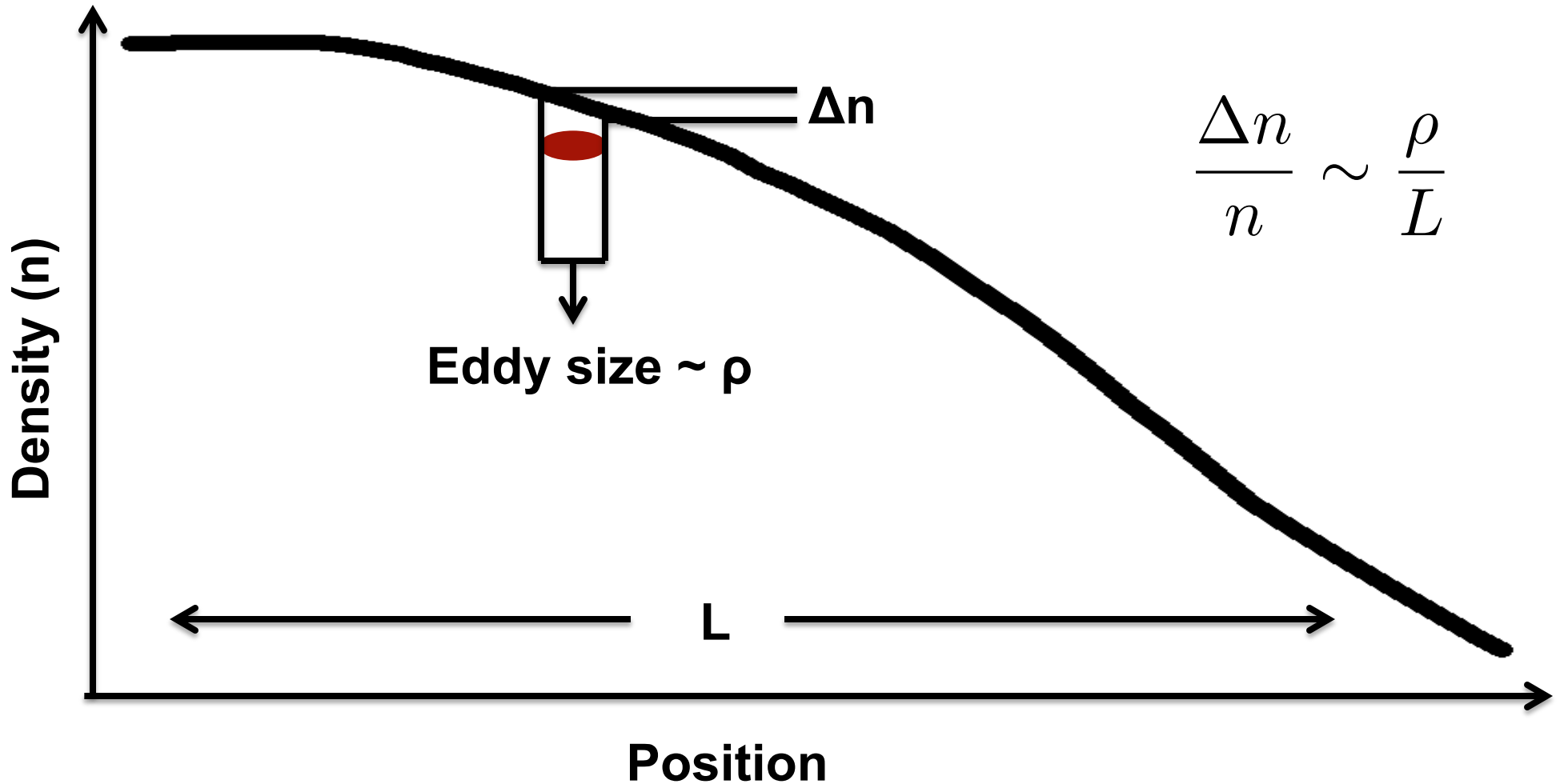
Mean varies perpendicular to mean field on system size while fluctuations vary on scale of gyro-radius:

$$\nabla_{\perp} \ln F \sim L^{-1} \quad \nabla_{\perp} \ln \delta f \sim \rho^{-1}$$

Fluctuations are anisotropic with respect to the mean field:

$$\nabla_{\parallel} \ln \delta f \sim L^{-1}$$

Mixing length estimates



Mixing length $\sim (\text{step size}) \times (\# \text{ steps})^{1/2}$

Macro time scale $\sim (\text{step time}) \times (\# \text{ steps to mix over length } L)$
 $\sim (L/\rho)^2 \times (\text{step time})$

Multiscale gyrokinetics

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$$f = F + \delta f$$

Mean varies perpendicular to mean field on system size while fluctuations vary on scale of gyro-radius:

$$\nabla_{\perp} \ln F \sim L^{-1} \quad \nabla_{\perp} \ln \delta f \sim \rho^{-1}$$

Fluctuations are anisotropic with respect to the mean field:

$$\nabla_{\parallel} \ln \delta f \sim L^{-1}$$

=> Turbulent fluctuations are low amplitude: $\delta f \sim \epsilon f$

=> Mean profile evolution slow compared to turbulence:

$$\frac{\partial \ln F}{\partial t} \sim \epsilon^2 \omega \sim \epsilon^3 \Omega$$

$$\epsilon \equiv \frac{\rho}{L} \ll 1$$

Multiscale gyrokinetics

Gyrokinetic equation for fluctuation dynamics:

$$\frac{\partial \langle \delta f \rangle}{\partial t} + \left\langle \frac{d\mathbf{R}}{dt} \right\rangle \cdot \frac{\partial}{\partial \mathbf{R}} \left(\langle \delta f \rangle - q \langle \delta \Phi \rangle \frac{\partial F}{\partial \varepsilon} \right) + \left(\left\langle \frac{d\mathbf{R}}{dt} \right\rangle - \overline{\left\langle \frac{d\mathbf{R}}{dt} \right\rangle} \right) \cdot \frac{\partial F}{\partial \mathbf{R}} = \langle C[\delta f] \rangle$$

Fluid conservation equations for mean dynamics:

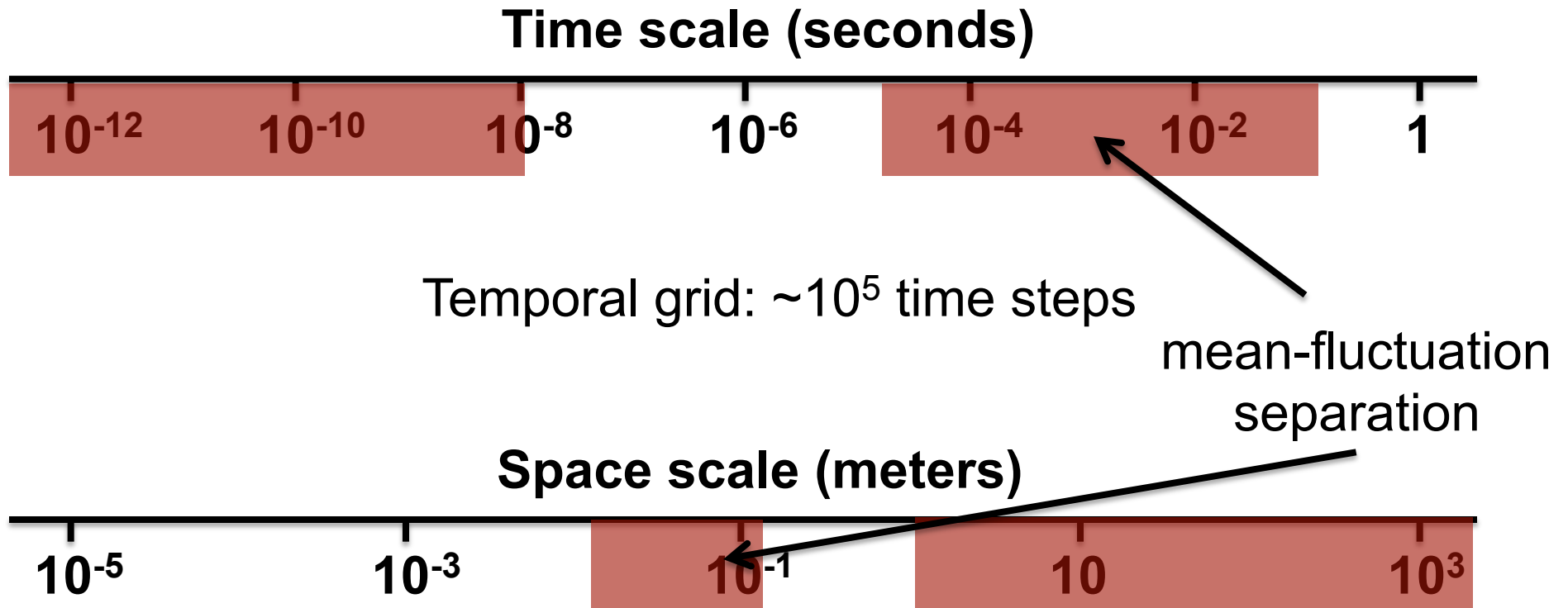
$$\frac{\partial \bar{n}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} (V' \bar{\Gamma}) = \bar{S}_n$$

$$\frac{\partial \bar{L}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} (V' \bar{\Pi}) = \bar{S}_L$$

$$\frac{3}{2} \frac{\partial \bar{p}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} (V' \bar{Q}) = \bar{S}_p$$

Fluxes are functions of fluctuating quantities

Expense (multiscale gyrokinetics)



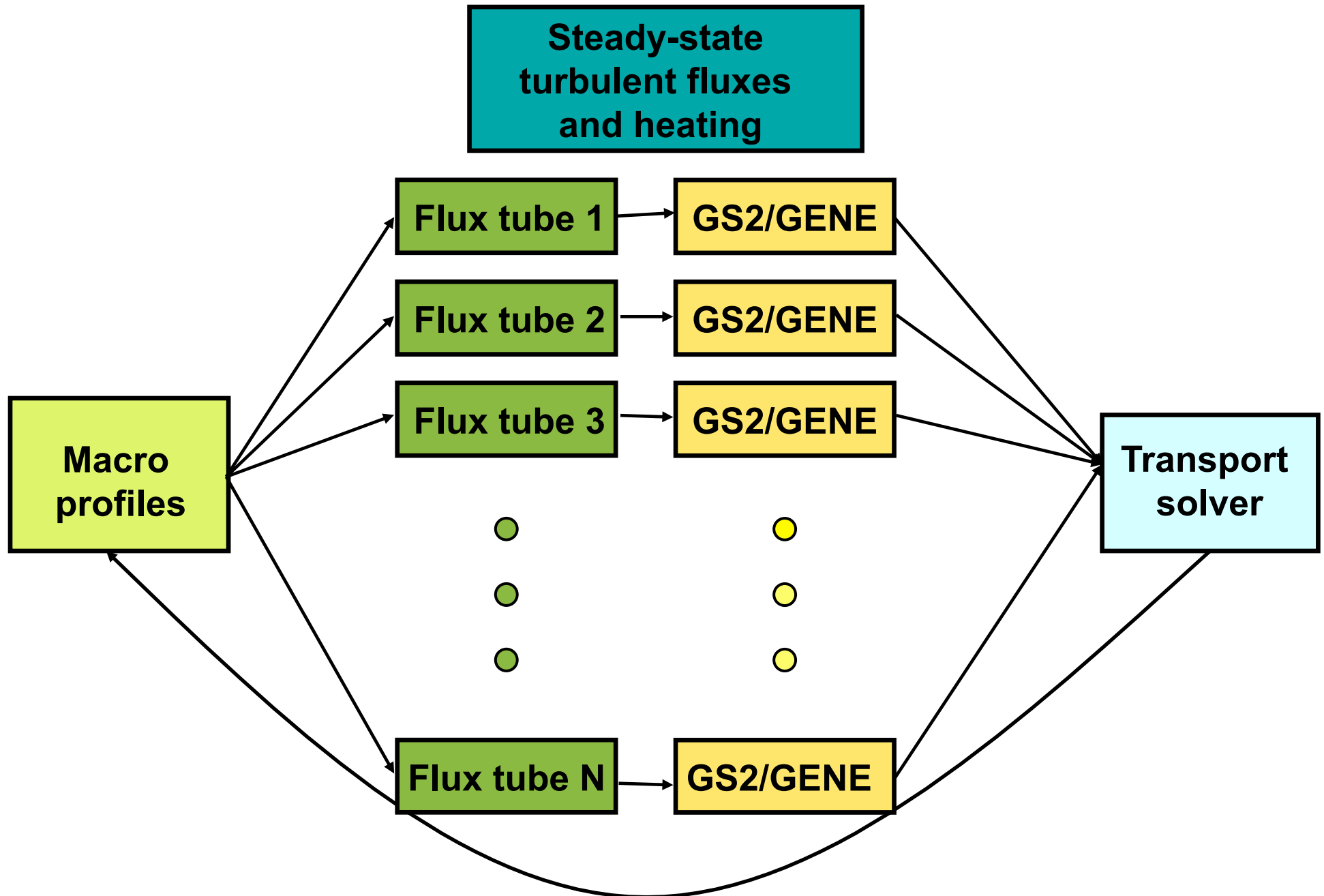
Perpendicular spatial grid: $\sim 10^5$ grid points x 2-D = 10^{10} grid points

Parallel spatial grid: ~ 10 grid points x 1-D = 10 grid points

Velocity grid: ~ 10 grid points x 2-D v-space = 10^2 grid points

Total: $\sim 10^{18}$ total grid points (10^6 savings)

TRINITY schematic



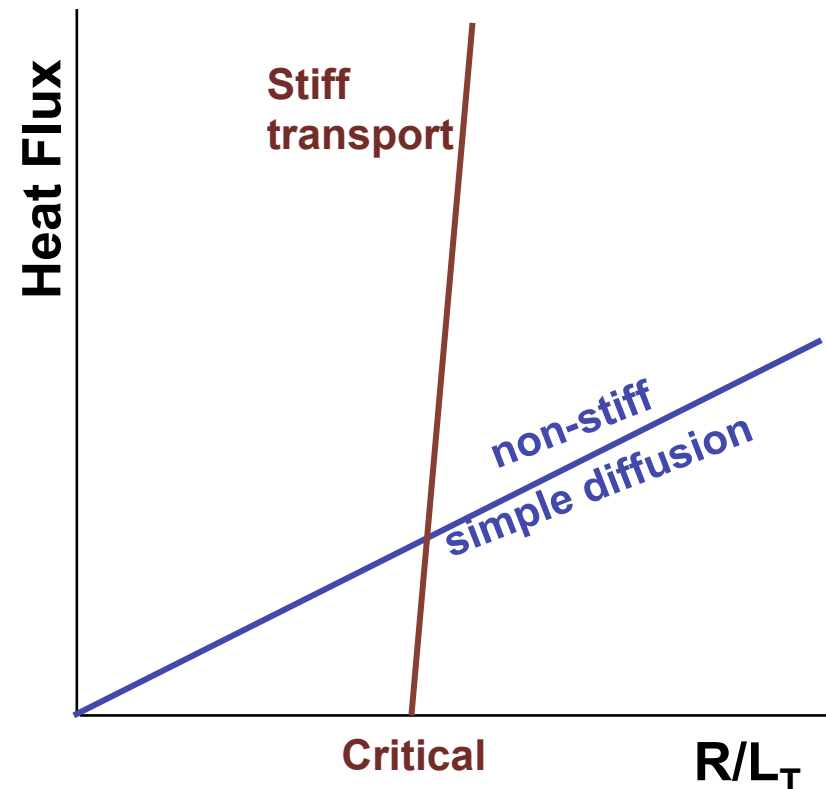
TRINITY transport solver

Transport equations are stiff, nonlinear PDEs:

$$\frac{3}{2} \frac{\partial p_s}{\partial t} = -\frac{1}{V'} \frac{\partial}{\partial \psi} (V' \langle \mathbf{Q}_s \cdot \nabla \psi \rangle) + \dots$$

$$\mathbf{Q}_s = \mathbf{Q}_s [n(\psi, t), T(\psi, t); \psi, t]$$

**Implicit treatment needed
for stiffness**



Newton solve

- Challenge: requires computation of quantities like

$$\Gamma_j^{m+1} \approx \Gamma_j^m + (\mathbf{y}^{m+1} - \mathbf{y}^m) \left. \frac{\partial \Gamma_j}{\partial \mathbf{y}} \right|_{\mathbf{y}^m}$$

$$\mathbf{y} = [\{n_k\}, \{p_{s_k}\}, \{L_k\}]^T$$

- Local approximation: $\frac{\partial \Gamma_j}{\partial n_k} = \frac{\partial \Gamma_j}{\partial n_j} + \frac{\partial \Gamma_j}{\partial (R/L_n)_j} \frac{\partial (R/L_n)_j}{\partial n_k}$
- Simplifying assumption: normalized fluxes depend primarily on gradient scale lengths
- Implicit treatment allows for time steps ~ 0.1 seconds (vs. turbulence sim time ~ 0.001 seconds)

Parallelization

Calculating flux derivative approximations:

- at every radial grid point, simultaneously calculate $\Gamma_j [(R/L_n)_j^m]$ and $\Gamma_j [(R/L_n)_j^m + \delta]$ using 2 different flux tubes
- Possible because flux tubes independent (do not communicate during turbulence calculation)
- Perfect parallelization
- use 2-point finite differences for derivative:

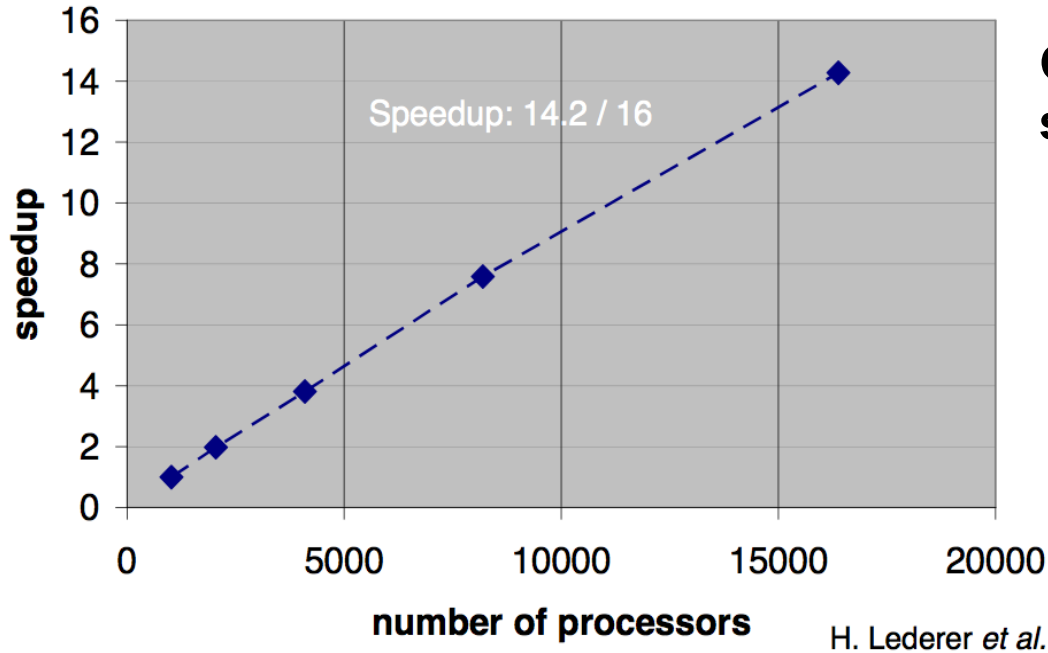
$$\frac{\partial \Gamma_j}{\partial (R/L_n)_j} \approx \frac{\Gamma_j [(R/L_n)_j^m] - \Gamma_j [(R/L_n)_j^m + \delta]}{\delta}$$

Scaling

Example calculation with 10 radial grid points:

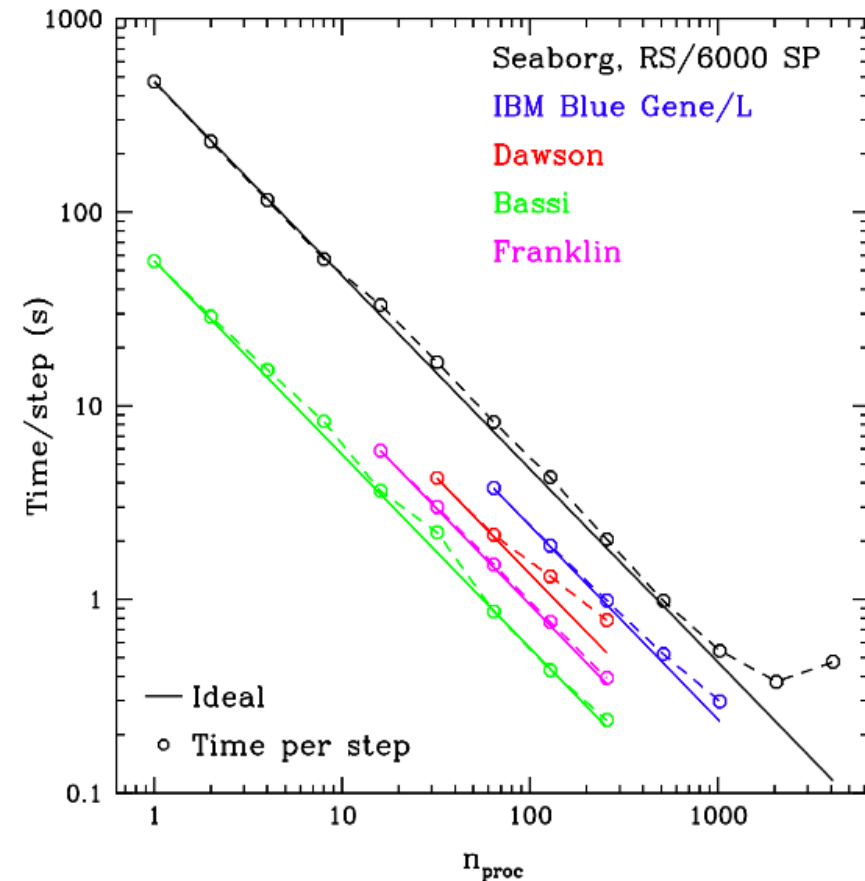
- Evolve electron density, toroidal angular momentum, and ion/electron pressure profiles
- Simultaneously calculate fluxes for equilibrium profile and for perturbed profiles (one for each time-varying gradient scale length, i.e. 4)
- Total of 50 flux tube simulations running in parallel

Flux tube scaling

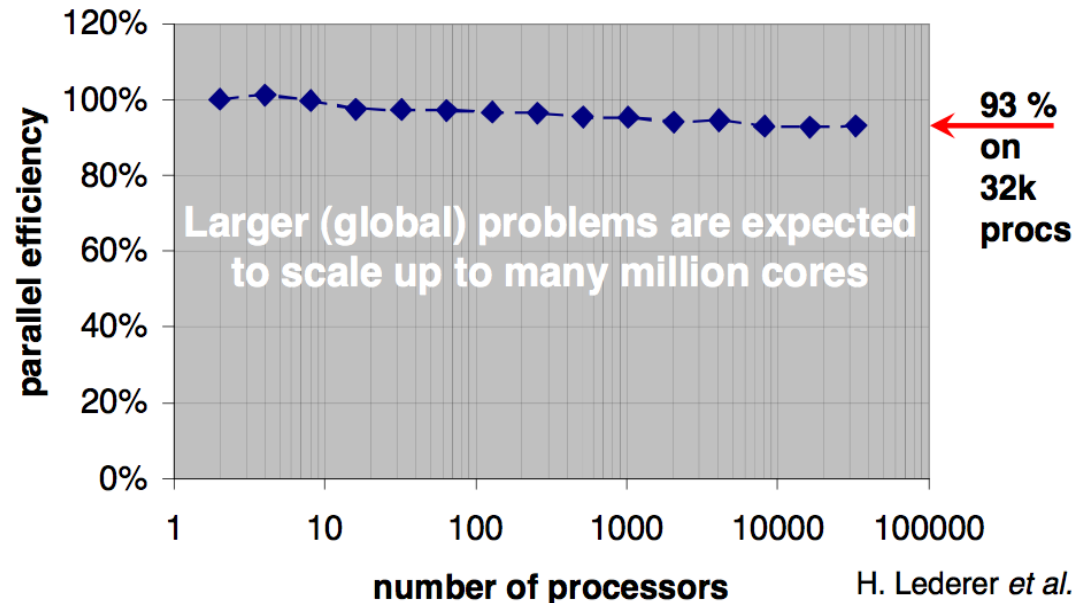


GENE strong scaling

GS2 strong scaling



BG/L at Rochester, Minnesota: 2 – 2k procs BG/L at Watson Research C., NY: 2k – 32k procs



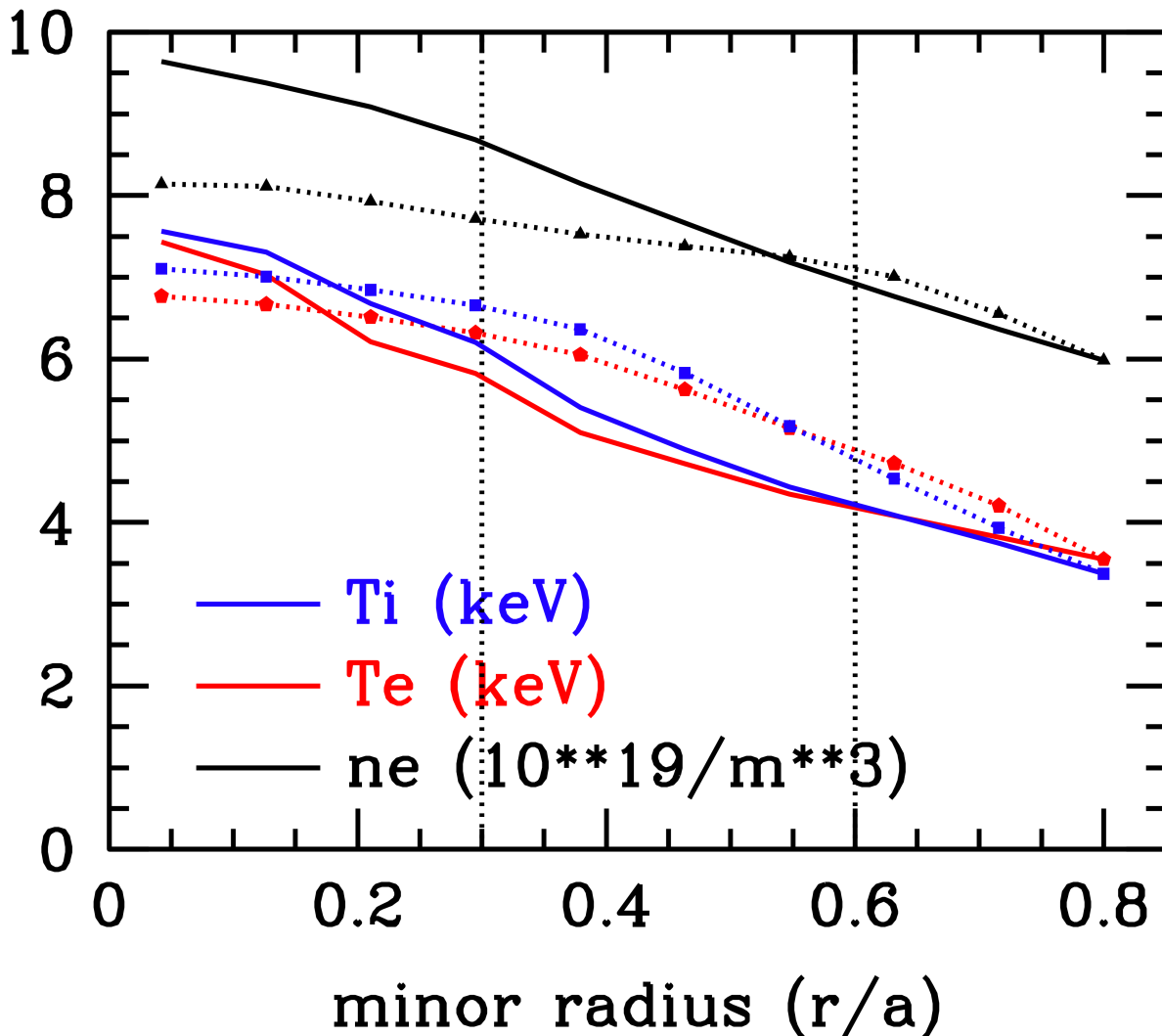
GENE weak scaling

Scaling

Example calculation with 10 radial grid points:

- Evolve electron density, toroidal angular momentum, and ion/electron pressure profiles
- Simultaneously calculate fluxes for equilibrium profile and for perturbed profiles (one for each time-varying gradient scale length, i.e. 4)
- Total of 50 flux tube simulations running in parallel
- ~2-4k cores or more per flux tube => scaling to over 100k's processors with very high efficiency

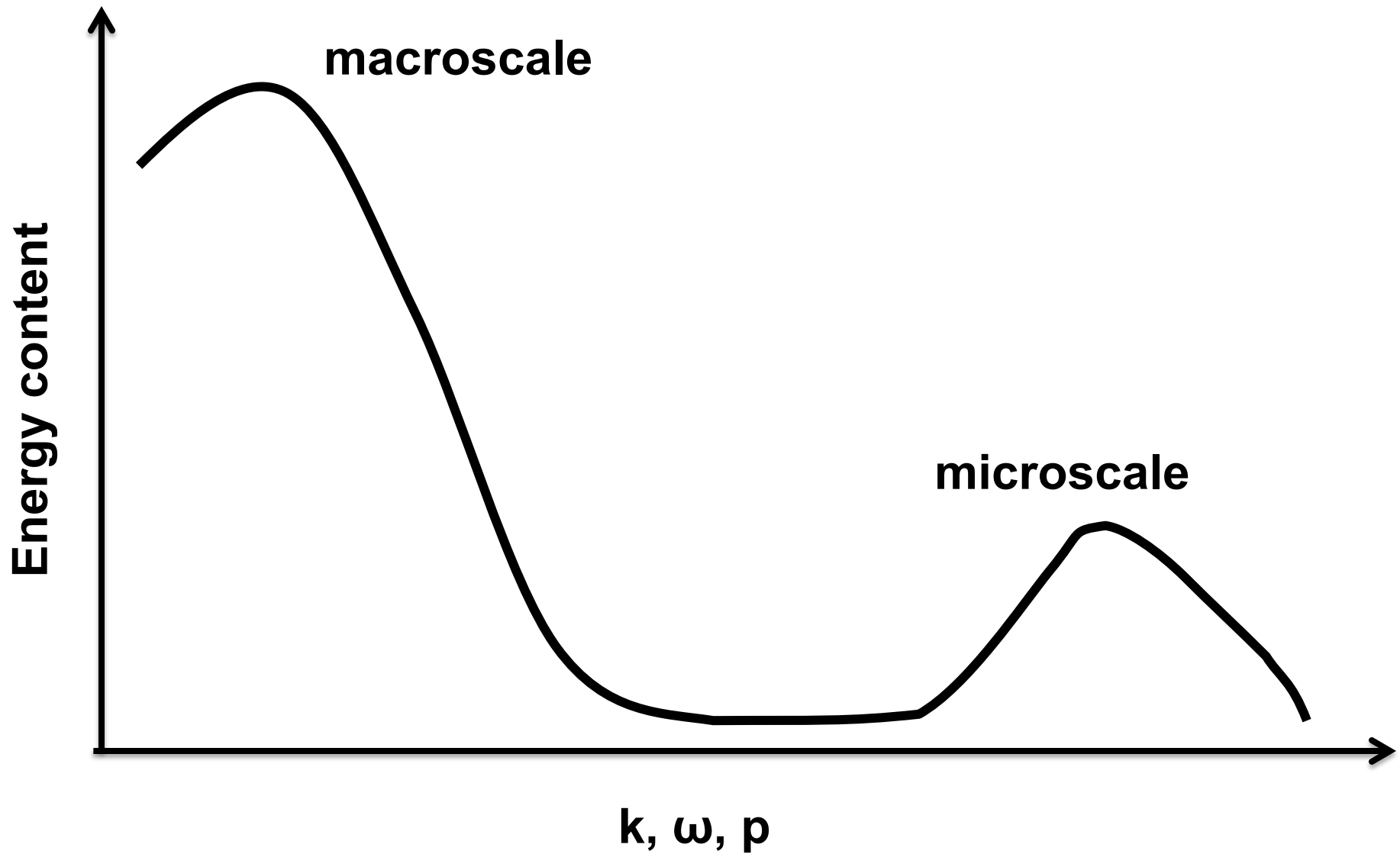
Example: JET H-mode



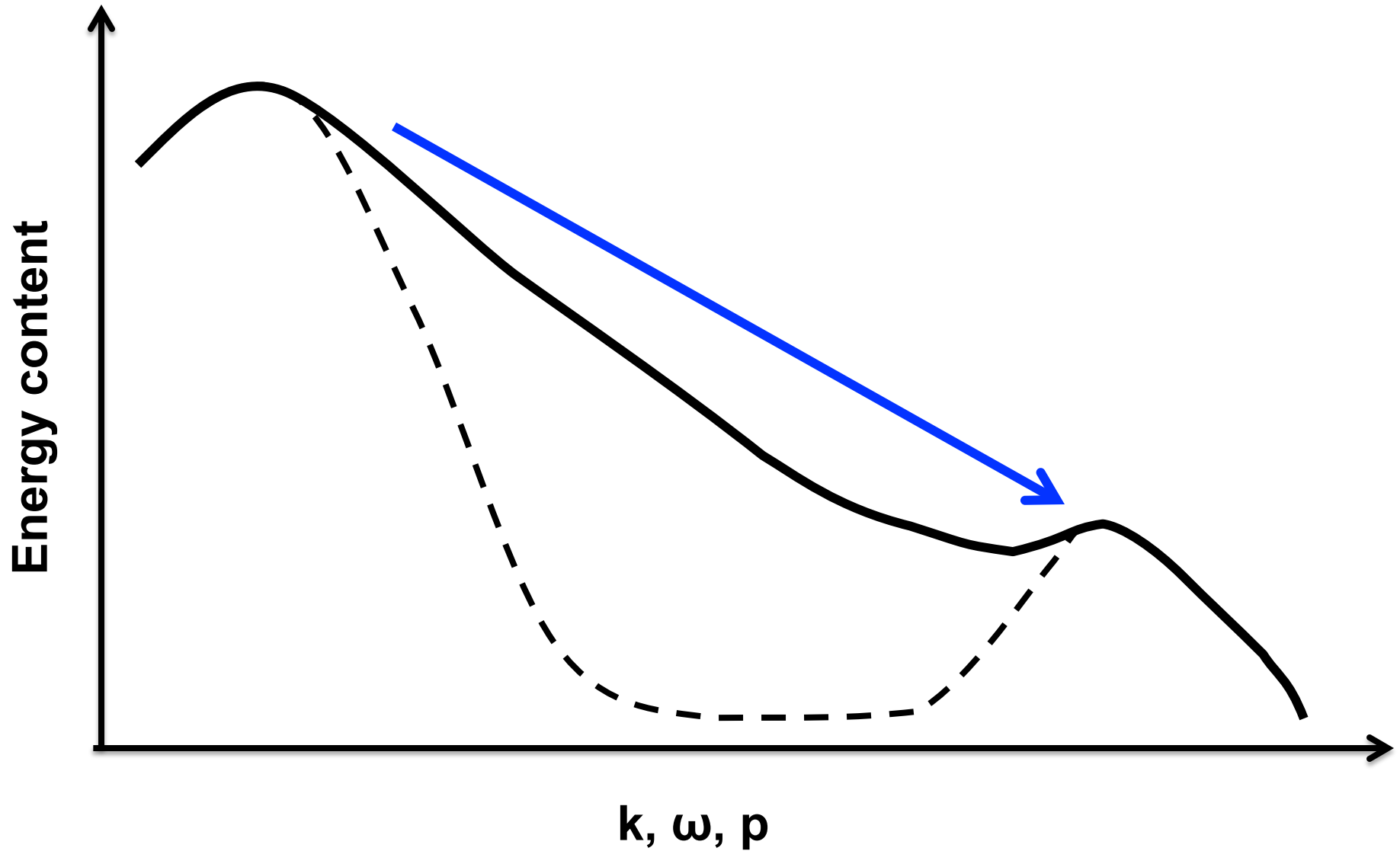
- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%

Issues and opportunities

Issue: Scale separation?



Issue: Scale separation?

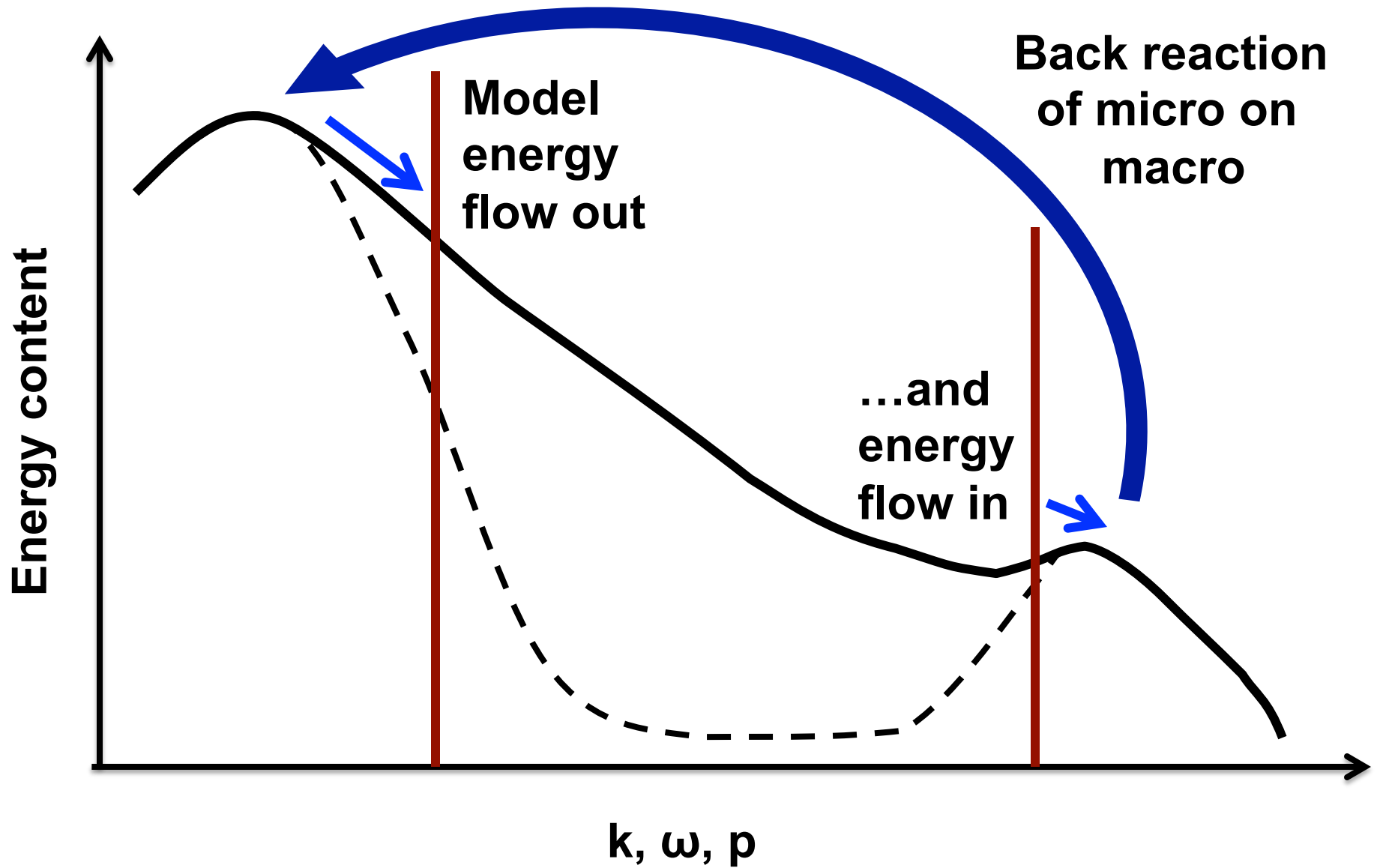


Summary

From T. S. Eliot's *Little Gidding*,

**“We shall not cease from exploration
And the end of all our exploring
Will be to arrive where we started
And know the place for the first time.”**

Opportunity



Issue: Computational expense

- Could reduce computational expense considerably by using a reduced model for the microscale physics
 - fluid model
 - proper orthogonal decomposition
 - LES for kinetics
- These approaches share weakness that they are not universal
- This weakness can be ameliorated by the multiscale approach

Equilibrium macroscale spatial profile

