Total-f Fully Nonlinear Electromagnetic Gyrokinetic Computation

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Gyrokinetic Field Theory

- original GK Poisson equation in terms of representations (Lee 1983)
- gyrokinetics becomes Lie transform theory (Littlejohn & Cary 1980-3)
  - ◦ potential obtained via "pull-back" transform
    (Dubin 1983, Hahm 1988-96, Brizard 1989-95)
- gyrokinetics becomes field theory (Sugama 2000, Brizard 2000)
  - ◦ both motion and potential obtained via Euler-Lagrange equations
  - ◦ Noether theorem gives conserved energy
- field theory and pull-back methods identical (Brizard & Hahm 2007)
- Lie transform and Poisson bracket transform methods also identical (Brizard 2004)

underlying symmetry: mathematical operations in Euler-Lagrange equations, Lie transform, Poisson bracket transform are all the same

- GK field theory guarantees energy/momentum conservation (Scott & Smirnov 2010)
  - ◦ vector→scalar conservation under low-frequency reduction (Brizard 2011)

Meaning of Energetic Consistency

- as in, eg, Landau-Lifshitz (*Classical Theory of Fields*)
  - ◦ quasineutrality: neglect $E^2/8\pi$ (small versus ExB energy if $v_A^2 \ll c^2$)
  - ◦ low-frequency: keep only shear-Alfvén disturbances ($A_\parallel$)

- full system Lagrangian involves **both** particle coords **and** field potential
  - ◦ particle coords move according to their Euler-Lagrange eqs
  - ◦ field potentials given according to **their** Euler-Lagrange eqs

- gyrokinetic equation built according to Liouville theorem

- any version is consistent as long as approximations are taken solely in the Lagrangian
  - ◦ gyrokinetic theory: low-frequency gauge transform, not "orbit averaging"

symmetry between field terms in L and the E-L eqs for fields automatic conservation of energy and (tokamaks) toroidal momentum

FEFI Model

- longwave limit, keep full nonlinearity in Hamiltonian, polarisation

$$L_p = \left(\frac{e}{c}\mathbf{A} + p_z\mathbf{b}\right)\cdot\dot{\mathbf{R}} + \frac{mc}{e}\mu\dot{\vartheta} - H \qquad L = \sum_{\mathrm{sp}}\int d\Lambda\, L_p\, f - \int dV\, \frac{B_\perp^2}{8\pi}$$

$$H = m\frac{U^2}{2} + \mu B + e\phi - m\frac{v_E^2}{2} \qquad v_E^2 = \left|\frac{c}{B}\nabla_\perp\phi\right|^2 \qquad mU = p_z - \frac{e}{c}A_\parallel$$

- Gyrokinetic equation (with collisions)

$$B_\parallel^*\frac{\partial f}{\partial t} + \nabla H\cdot\frac{c\mathbf{F}}{eB}\cdot\nabla f + \mathbf{B}^*\cdot\left(\frac{\partial H}{\partial p_z}\nabla f - \frac{\partial f}{\partial p_z}\nabla H\right) = B_\parallel^* C(f)$$

- Polarisation/Induction equations (Euler-Lagrange equations for potentials)

$$\sum_{\mathrm{sp}}\int dW\left[ef + \frac{1}{B_\parallel^*}\nabla\cdot B_\parallel^*\frac{fmc^2}{B^2}\nabla_\perp\phi\right] = 0 \qquad \nabla_\perp^2 A_\parallel = -\frac{4\pi}{c}\sum_{\mathrm{sp}}\int dW\, e(fU)$$

FEFI4 Model for Gyrokinetic Equilibrium

- total-f FEFI model, axisymmetric version
  - ◦ longwave limits, fully nonlinear Hamiltonian, polarisation
  - ◦ reference: B Scott et al, Contrib Plasma Phys 2010

- scenario: pedestal "equilibrium" (steady state)
  - ◦ longer than oscillation scales, shorter than transport

- nominal parameters

$$n_0 = 3 \times 10^{19}\,\mathrm{m}^{-3} \qquad T_0 = 200\,\mathrm{eV} \qquad B_0 = 2.5\,\mathrm{T} \qquad a/R = 0.5/1.65\,\mathrm{m}$$

- nominal profiles

$$q = 4\,r_a^2 \qquad R/L_T = 15 + 75\,\mathrm{sech}^2\,\frac{r_a - 0.95}{0.02} \qquad \eta = L_n/L_T = 3$$

- time scale with $c_s^2 = T_0/M_D$ and furthermore always use $m_e/M_D = 1/3670$

$$a/c_s = 5.1\,\mu\mathrm{sec} \qquad c_s\tau_A/a = 1.0 \qquad c_s\tau_G/a = 21 \qquad c_s\tau_S/a = 73$$

Grid

- 4-D distribution function $f = f(x, y, z, w)$ with 2-D potentials $\phi, A_{\|}(x, y)$
- all grids equidistant in actual coordinates (x, y, z, w)

Spatial Grid

- conformal coordinates in poloidal plane (x_c, y_c) with $r_a = \exp x_c$
- radial grid 128 pts in x_c over $0.71 < r_a < 0.99$
- poloidal (parallel) grid 64 pts in y_c on $[-\pi, \pi]$
- on the graphs, y_c is labelled s
- on some of the graphs, $x = (r_a - 0.85)/\rho_s$ with ρ_s eval at $T_e/B = T_0/B_0$

Velocity Grid (for each species, $v_0^2 = T_0/m_0$)

- parallel canonical momentum basis, 32 pts, inhomogeneous spacing $p_z = m_0 v_0 \times \sinh z$
- magnetic moment basis, 16 pts, inhomogeneous spacing $\mu = (T_0/B_0) \times \sinh^2 w/2$

Numerics

Geometry

- conformal coordinate system (x_c, y_c) with volume element $\sqrt{g} = R/g^{xx}$
  ◦ property $g^{xx} g_{yy} = 1$ is exact (in a cylinder $x_c \to \log r$ and $y_c \to \theta$)

- drift tensor $\mathbf{F} = (BR/I_0)\mathbf{F}_0$ with $\nabla \cdot \mathbf{F}_0 = 0$ so that $B^*_{\|} = B$ since $\mathbf{B} \cdot \nabla \cdot \mathbf{F} = 0$

- note that the flux surfaces (const-$A_{\|}$) move off of the const-r_a lines

- requirement $\nabla \cdot (c\mathbf{F}/eB) + \partial \mathbf{B}^*/\partial p_z = 0$ satisfied exactly by bracket formulation

Scheme

- 4th-order Arakawa for all bracket pieces, RK4/Karniadakis3 for time step

Initial State

- Maxwellians with nominal profiles, ramped from flat to gradient over $0 < c_s t/a < 20$

Bracket Structures

- collisionless part of the GK eqn is a single bracket

$$\frac{1}{B_{\parallel}^{*}}\left[\nabla H\cdot\frac{c\mathbf{F}}{eB}\cdot\nabla f+\mathbf{B}^{*}\cdot\left(\frac{\partial H}{\partial p_z}\nabla f-\frac{\partial f}{\partial p_z}\nabla H\right)\right]=\mathcal{E}^{abcd}\,H_{,a}\,f_{,b}\,A^{*}_{c,d}$$

- double/triple brackets

$$[H,f]_{ab}=H_{,a}\,f_{,b}-f_{,a}\,H_{,b}$$

$$[H,f,G]_{abc}=[H,f]_{ab}\,G_{,c}+[H,f]_{bc}\,G_{,a}+[H,f]_{ca}\,G_{,b}$$

- methods: Arakawa (*JCP* 1966), implemented: Naulin/Nielsen (*SIAM JNA* 2003)
- methods: Morinishi (*JCP* 1998), implemented: Idomura (*JCP* 2007)
- as used here: Scott/Kendl/Ribeiro (*Contrib Plasma Phys* 2010)

Time Step

- RK4 was used in the axisymmetric work
- better scheme for waves: Karniadakis (*JCP* 1991)

$$\frac{\partial f}{\partial t} = S \qquad \sum_{j=1}^{3} \alpha_j \frac{f_0 - f_j}{\Delta t} = \sum_{j=1}^{3} \beta_j \, S_j \qquad f_j = f(t - j\Delta t)$$

- coefficients for order 3:

$$\alpha_{1,2,3} = \quad 3 \quad -3/2 \quad 1/3 \qquad \beta_{1,2,3} = \quad 3 \quad -3 \quad 1$$

- solve for f_0 with f_j and S_j known for $j > 0$
- implemented:
  - ◦ Hasegawa-Wakatani equations: Naulin/Nielsen (*SIAM JNA* 2003)
  - ◦ gyrofluid GEM: Scott (*Phys Plasmas* 10/2005)

Energetic Quantities

- electron and ion contributions to ExB energy

$$E_p = \int d\Lambda \left(-e\phi - m_e \frac{v_E^2}{2}\right) f_e \qquad E_P = \int d\Lambda \left(e\phi - M_i \frac{v_E^2}{2}\right) f_i$$

- electron and ion contributions to magnetic energy

$$E_j = \int d\Lambda \left(-\frac{e}{c} U_e f_e\right) A_\parallel \qquad E_J = \int d\Lambda \left(\frac{e}{c} U_i f_i\right) A_\parallel$$

- electron and ion contributions to thermal energy

$$E_n = \int d\Lambda \left(m \frac{U_e^2}{2} + \mu B\right) f_e \qquad E_N = \int d\Lambda \left(m \frac{U_i^2}{2} + \mu B\right) f_i$$

- totals

$$E_E = E_p + E_P \qquad E_B = E_j + E_J \qquad E_T = E_E + E_B + E_n + E_N$$

Other Conserved Quantities

- conserved densities

$$N_e = \int d\Lambda\, f_e \qquad\qquad N_i = \int d\Lambda\, f_i$$

- conserved entropies

$$S_e = -T_0 \int d\Lambda\, f_e \log f_e \qquad\qquad S_i = -T_0 \int d\Lambda\, f_i \log f_i$$

- conserved toroidal canonical momenta

$$P_e = \int d\Lambda\, f_e \mathcal{P}_{e\varphi} \qquad\qquad N_i = \int d\Lambda\, f_i \mathcal{P}_{i\varphi}$$

- these are $O(1)$, but the total is $O(10^{-4})$

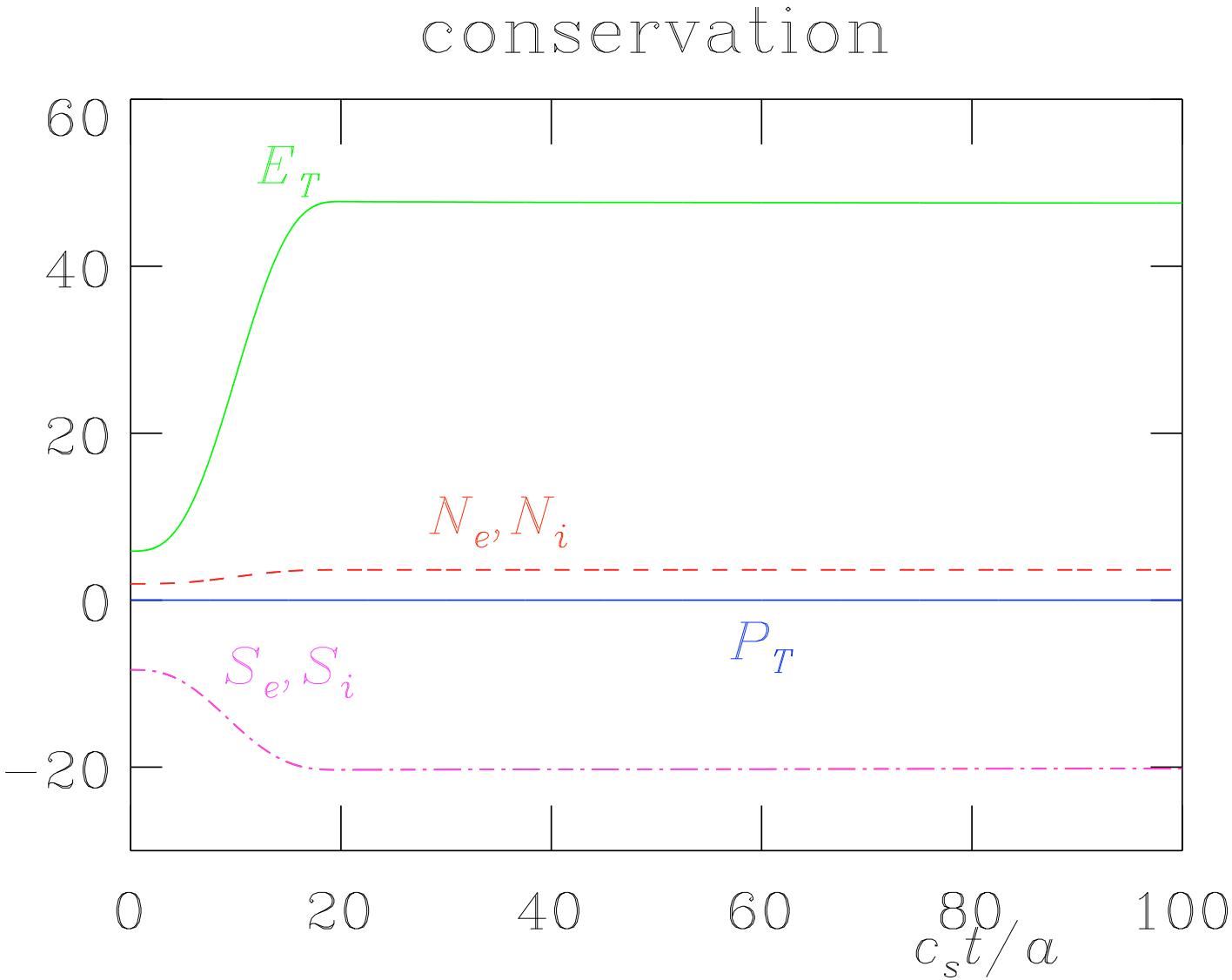
- note role of ExB component to toroidal momentum (longwave MHD limit)

$$\sum_{\text{sp}} \int d\Lambda\, f \mathcal{P}_\varphi \approx \rho_M \left(u_\parallel \frac{I}{B} + R^2 \mathbf{v}_E \cdot \nabla\varphi \right)$$

where the contribution from $(m_e/e)J_\parallel$ is neglected

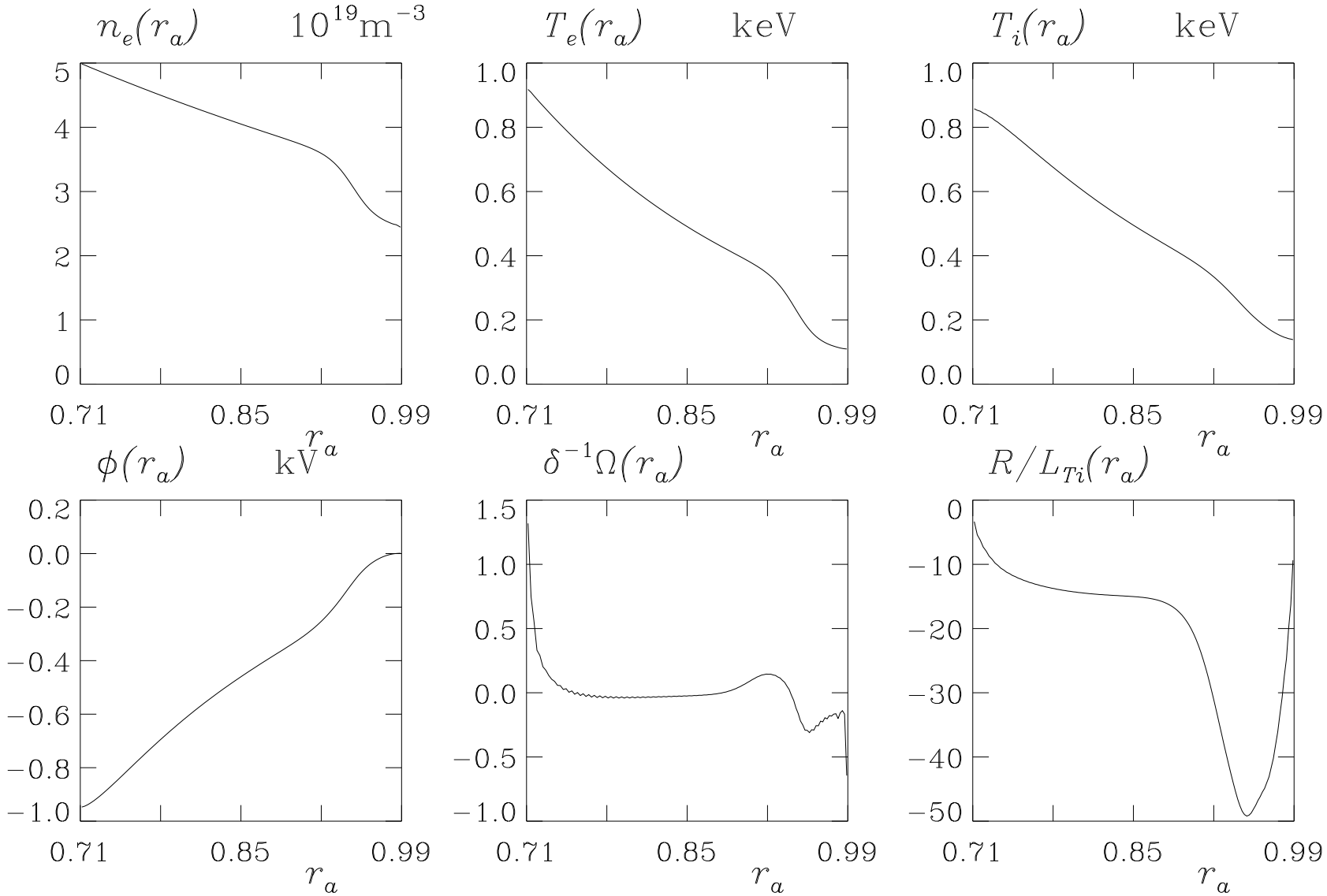
evolution of conserved quantities

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



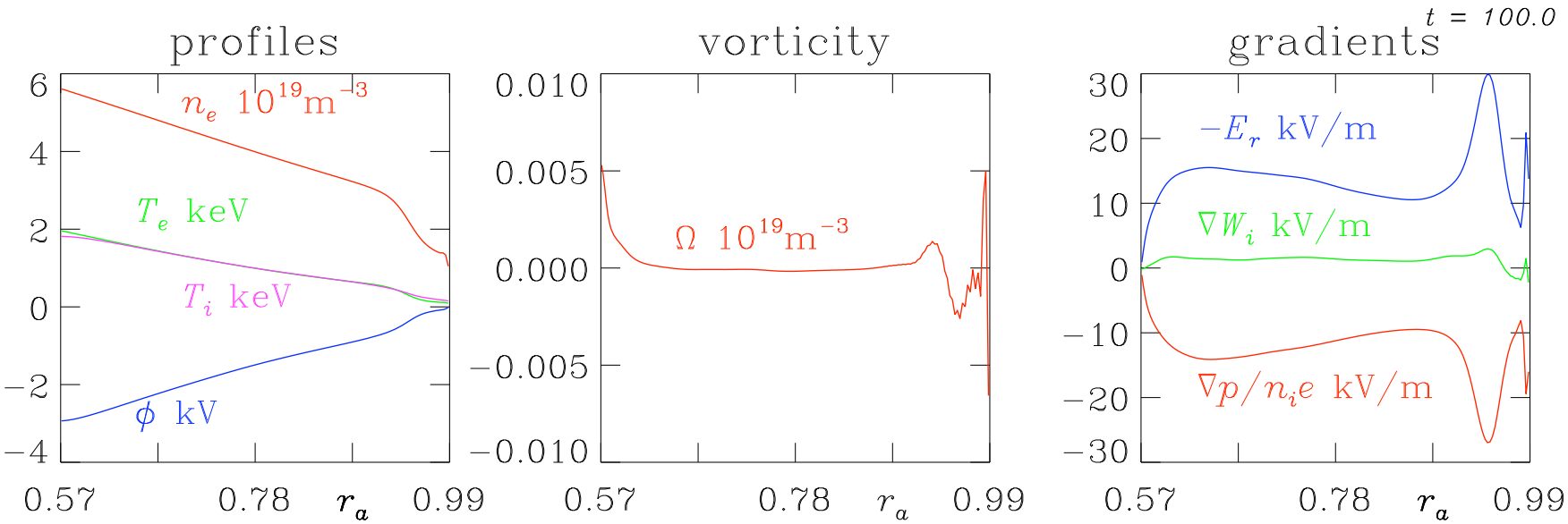
zonal profiles

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



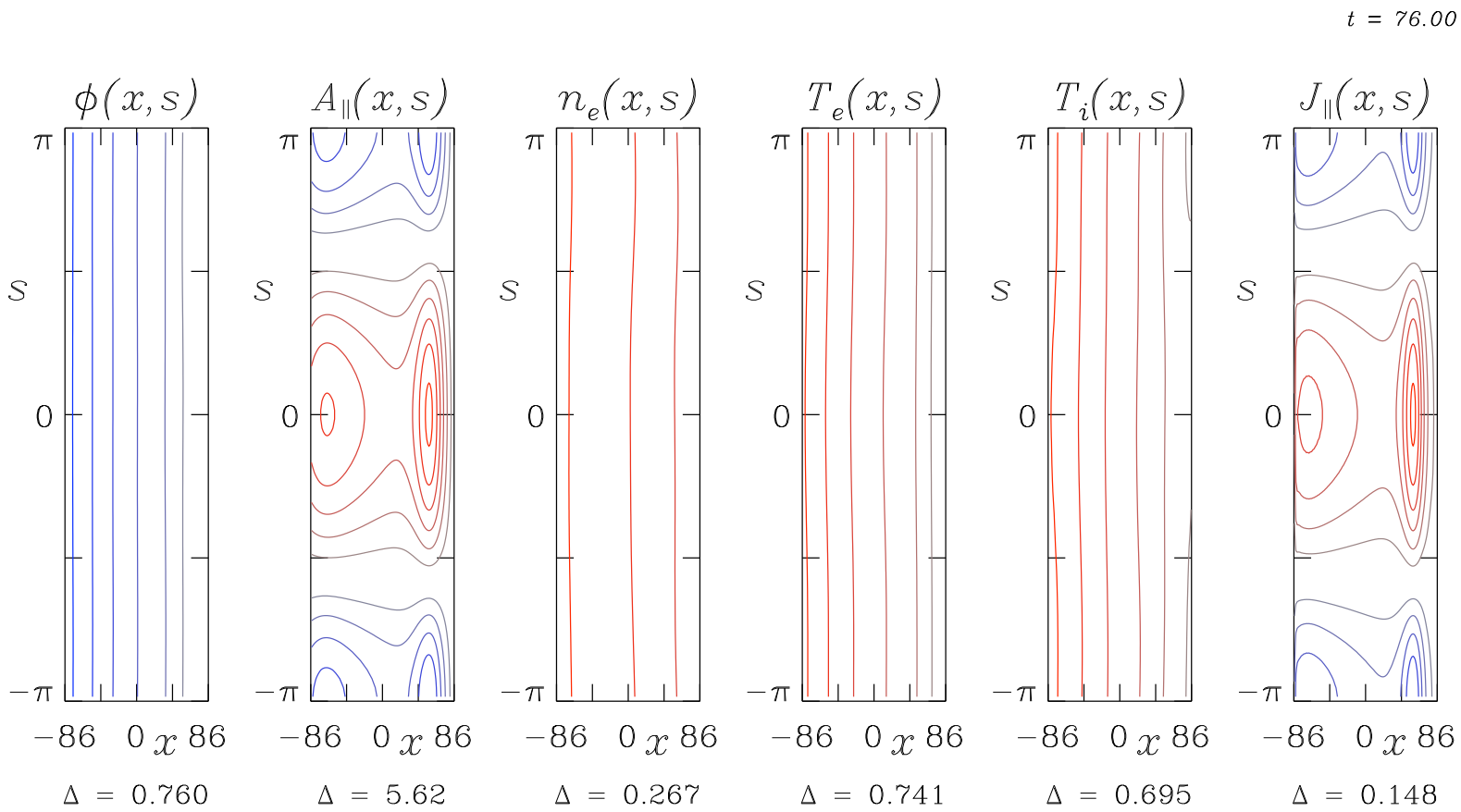
zonal profiles, force balance

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



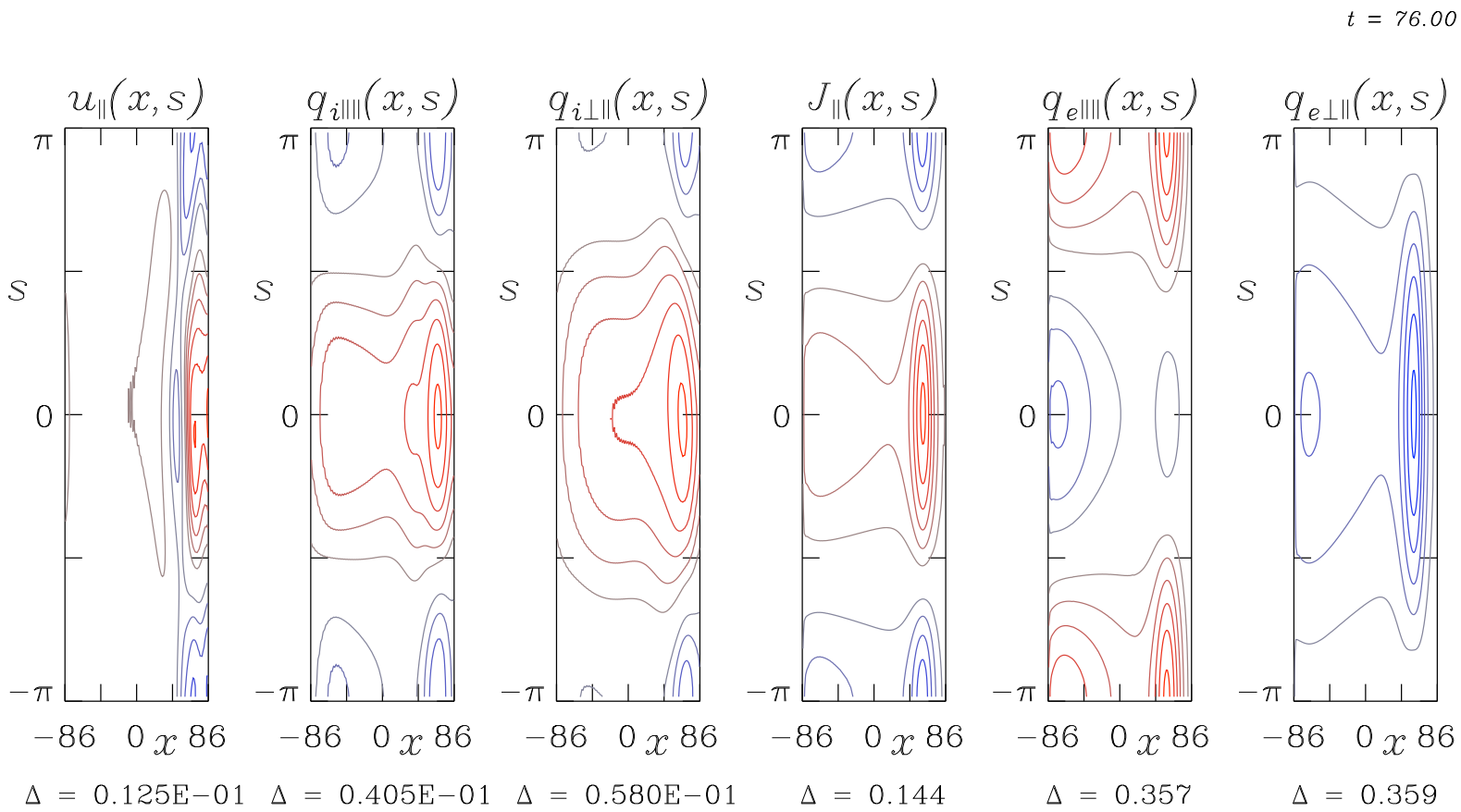
spatial morphology

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



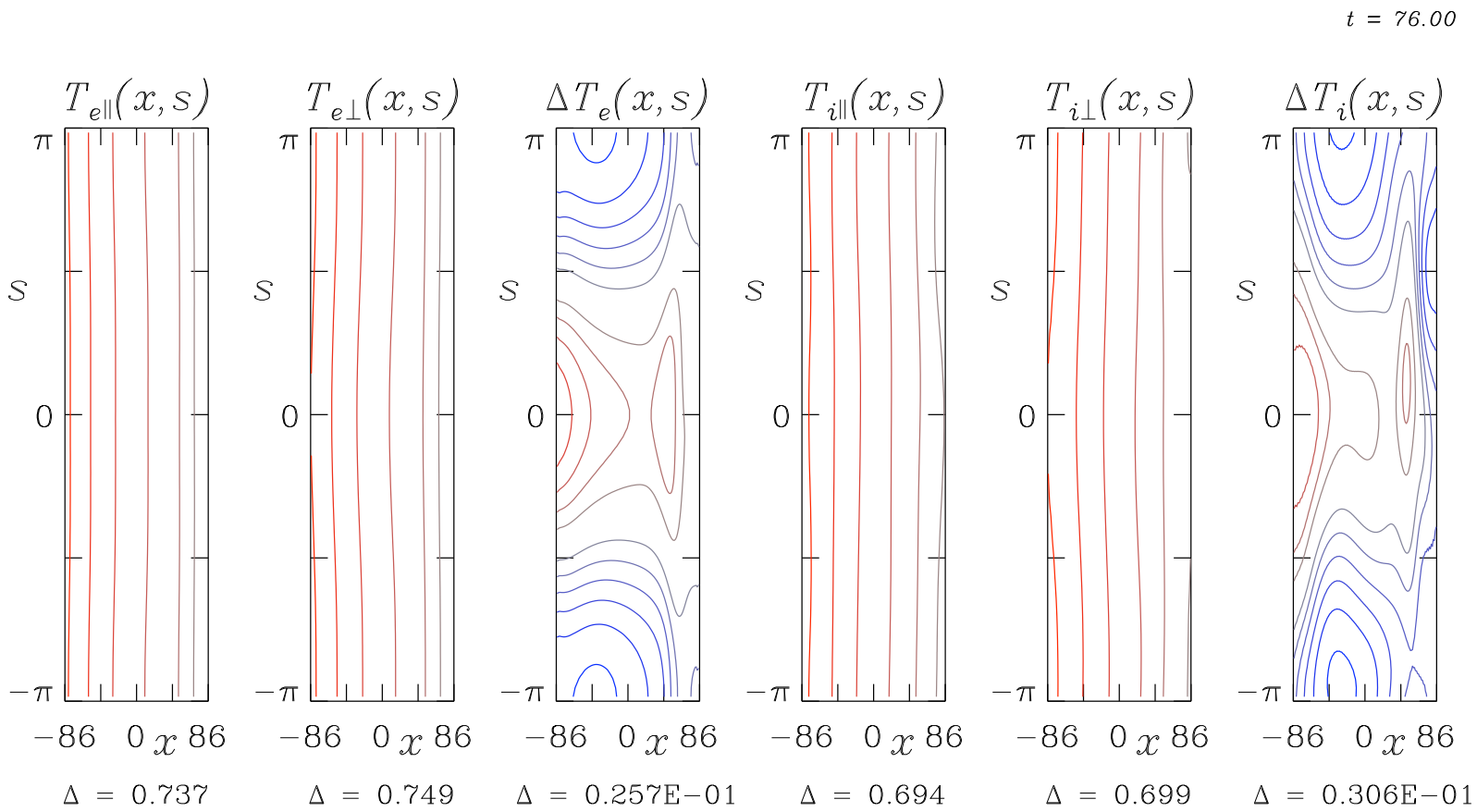
parallel flows and heat fluxes

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



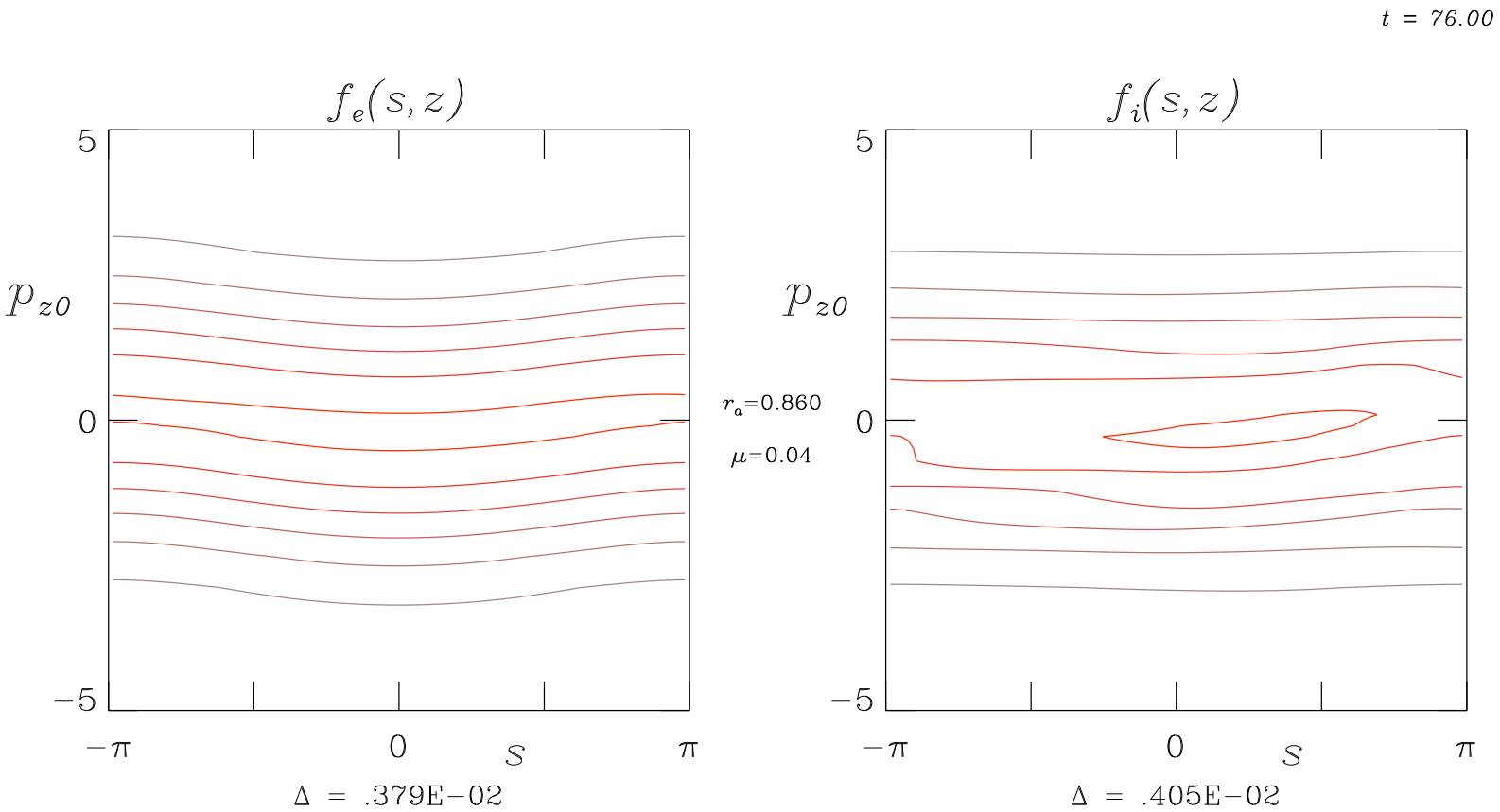
temperatures and anisotropy

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



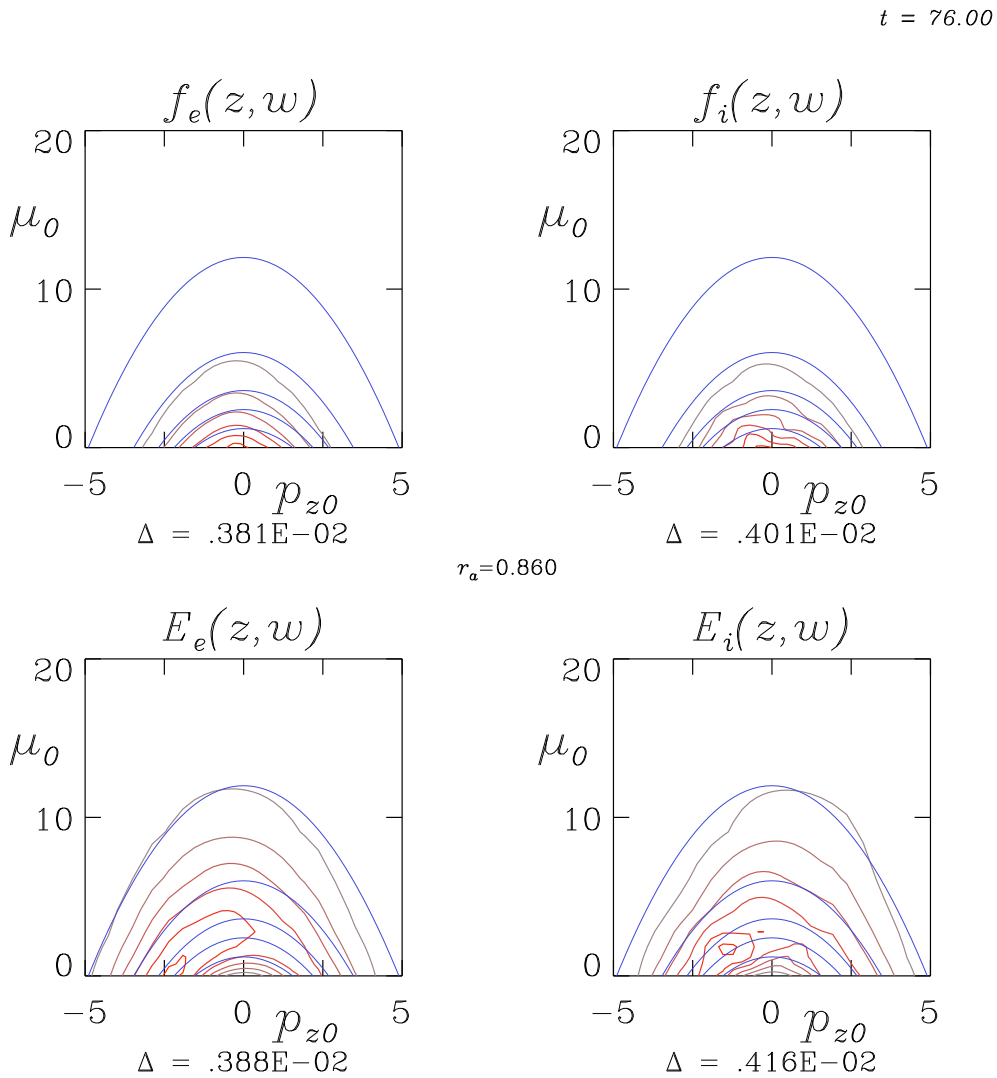
parallel phase space

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



velocity space

FEFI 4D collisionless, Edge Base Case, $0.57 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 2$



Neoclassical Control Case

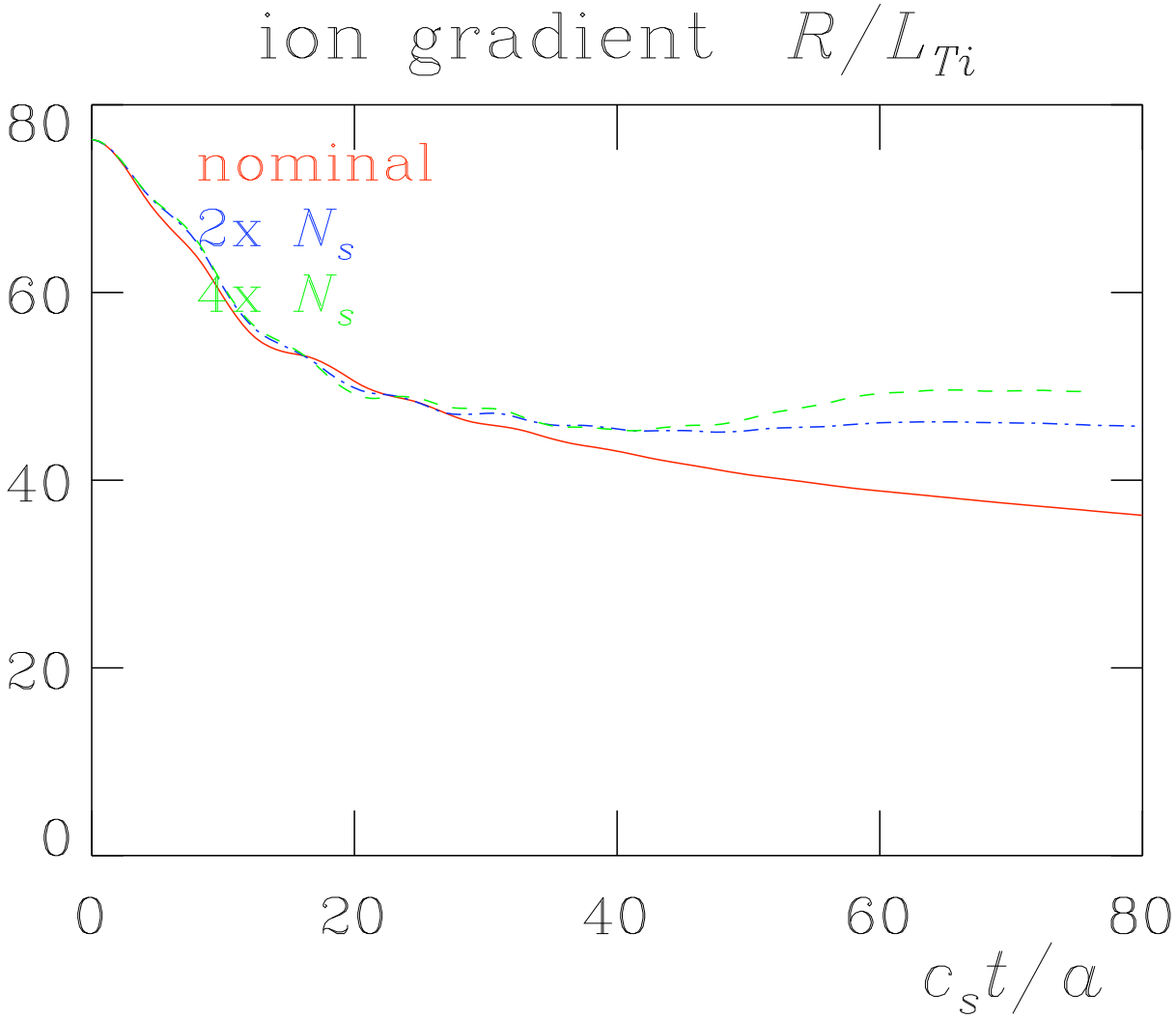
- neoclassical transport theory: no transport if no collisions
- effective "floor" in collisionality given by resolution
  - more resolution $\rightarrow$ less numerical dissipation for stability
- measure evolution of $R\,|\nabla \log T_i|$ in pedestal region
- initial transient arises from "finite-banana" effects
  - radial excursion of ions due to magnetic (curv, grad-B) drift motion
- test to see if measured gradient ceases to evolve

important control case for computation of neoclassical transport

- this is the reason for the effort on collisionless cases

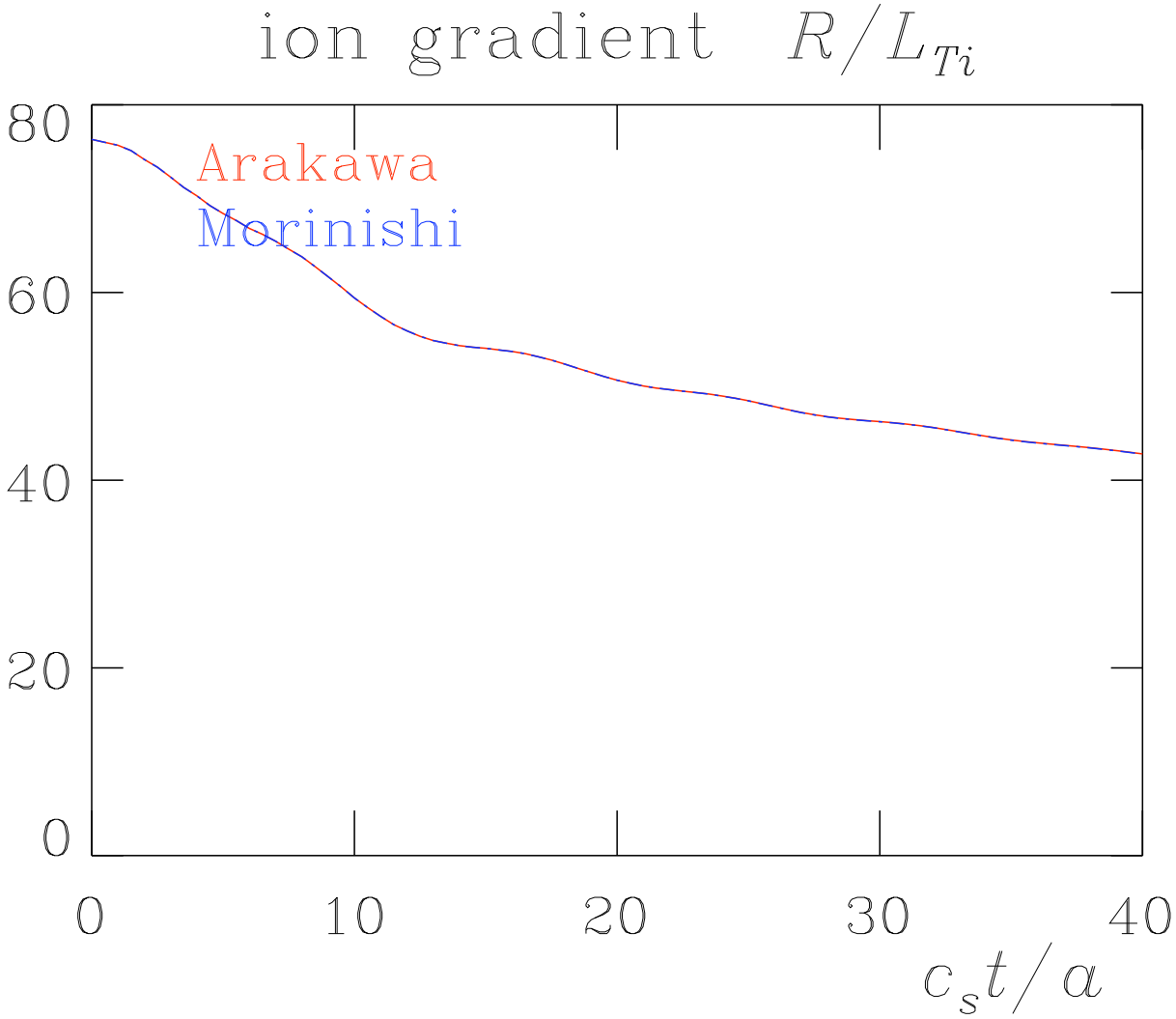
Ion Temperature relaxation, parallel space resolution

earlier case $0.85 < r_a < 0.99$, similar parameters/profiles, "nominal" is $N_s = 32$



Ion Temperature convergence, two schemes

earlier case $0.85 < r_a < 0.99$, similar parameters/profiles, "nominal" is $N_s = 32$



Collision Operator used in FEFI

- Brizard's (2004) isotropic field particles model
- like-like (parallel velocity scattering "models" energy scattering)

$$C_z = \frac{\partial}{\partial \zeta} \nu_{zp} \frac{1-\zeta^2}{v^3} \frac{\partial}{\partial \zeta} - \frac{\partial}{\partial U} \nu_{ze} \left[(z - \alpha_z) - \beta_z \frac{\partial}{\partial U} \right]$$

transformed coordinates $\quad v^2 = U^2 + 2\mu B \quad \zeta = (U - \gamma_z)/v$

- moments $\alpha_z, \beta_z, \gamma_z$ calculated to conserve energy and momentum
- electron-ion

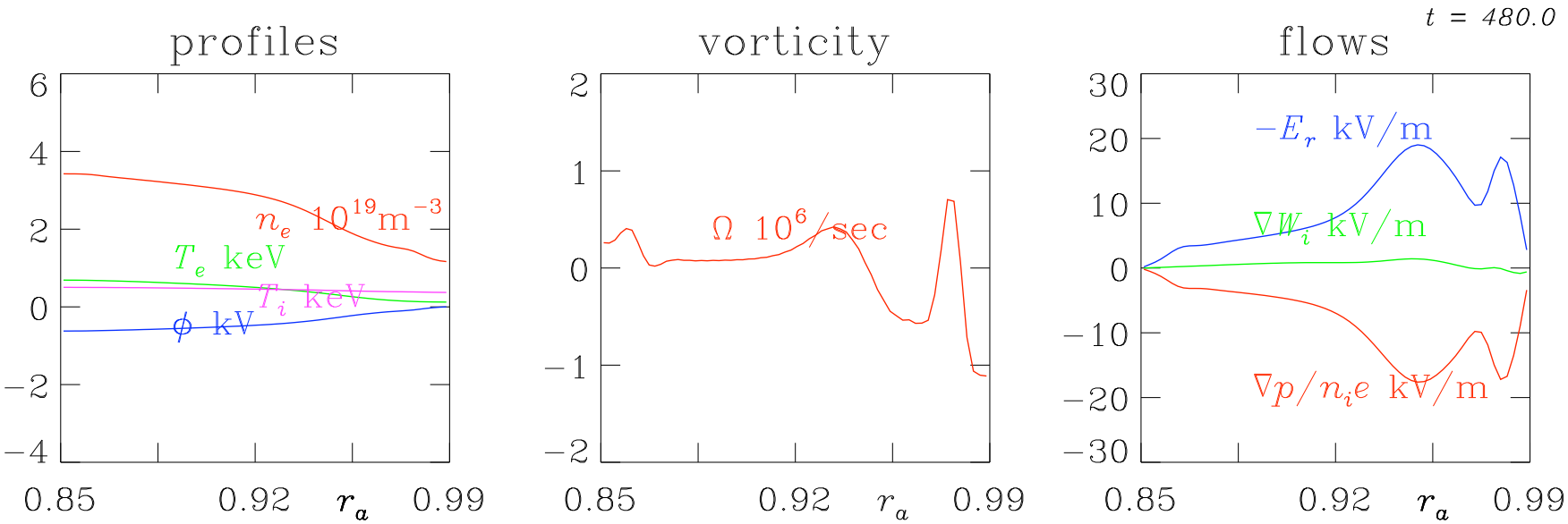
$$C_e = \sum_i \frac{\partial}{\partial \zeta} \nu_{ei} \frac{1-\zeta^2}{v^3} \frac{\partial}{\partial \zeta}$$

transformed coordinates $\quad v^2 = U^2 + 2\mu B \quad \zeta = U/v$

- coefficients are 1.87997 times the Braginskii collision frequency for each species

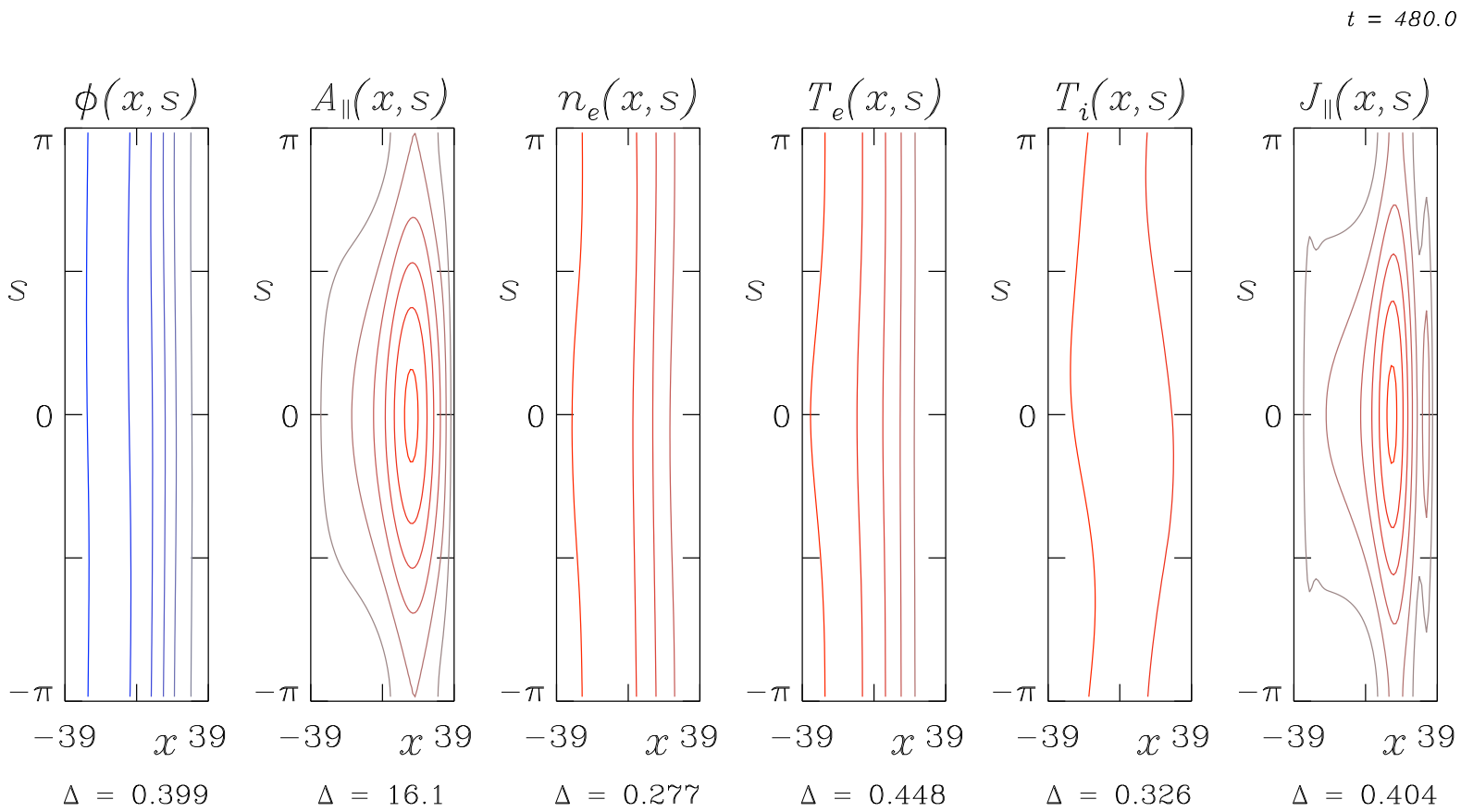
zonal profiles, collisional case

FEFI 4D collisional, Edge Base Case, $0.85 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 1$



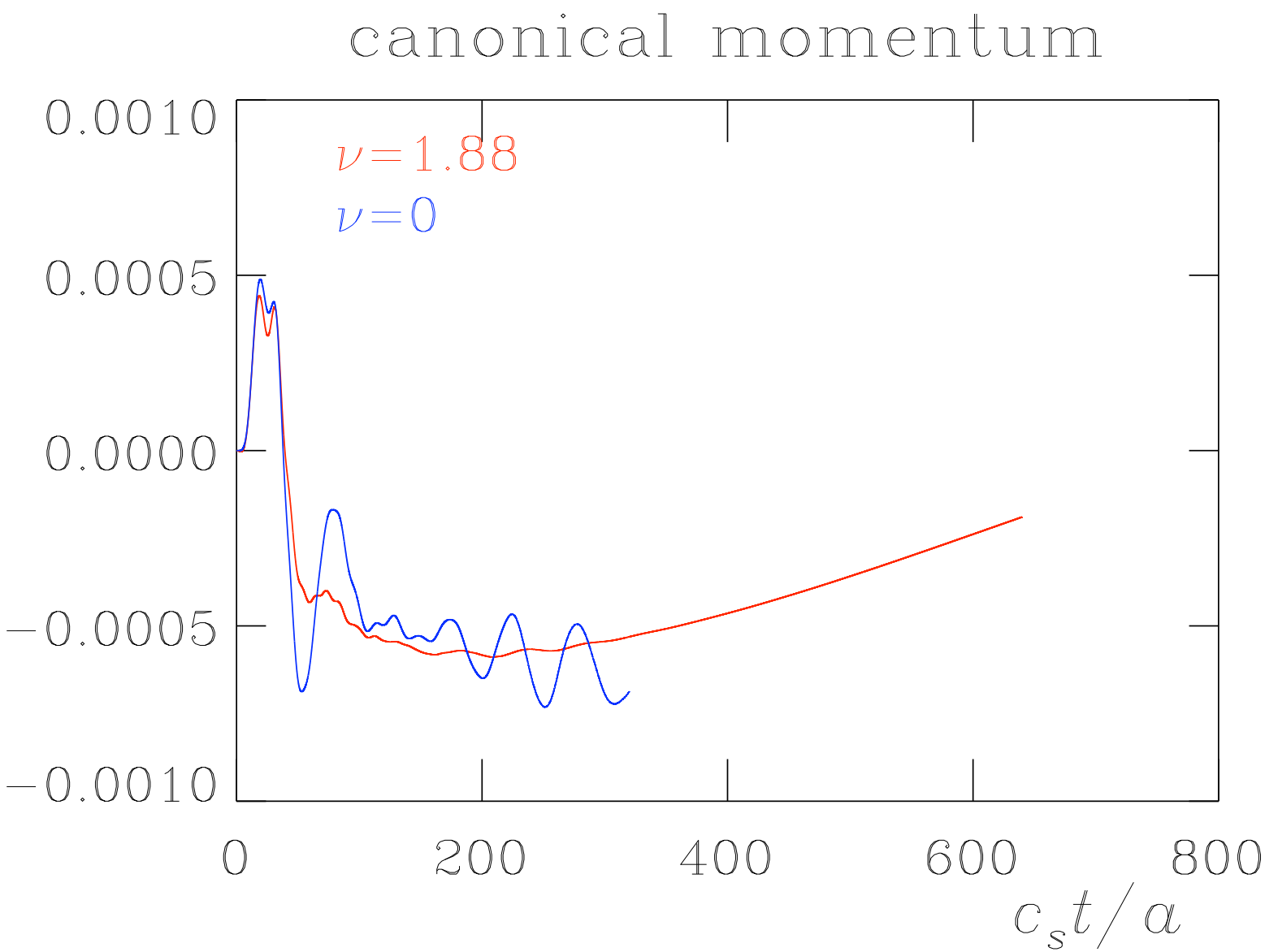
spatial morphology, collisional case

FEFI 4D collisional, Edge Base Case, $0.85 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 1$



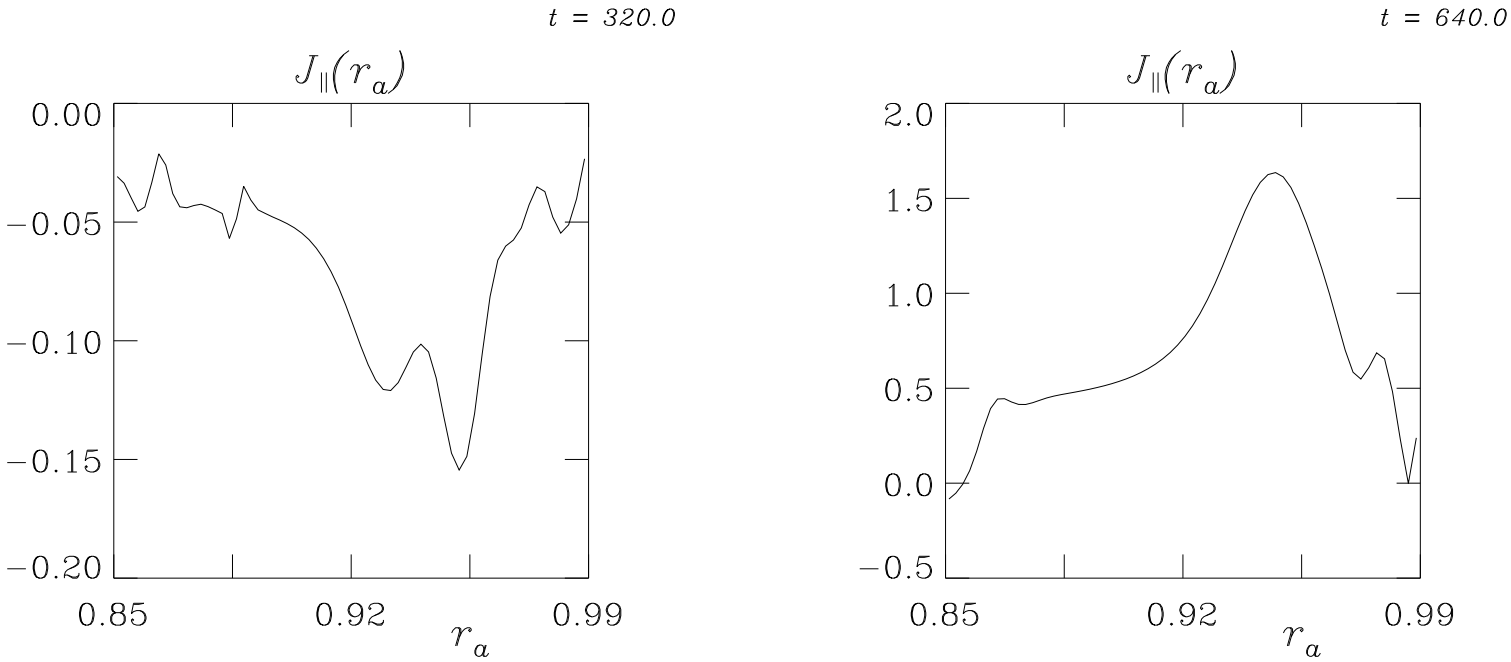
conserved momentum and collisions

FEFI 4D collisional, Edge Base Case, $0.85 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 1$



collisions and zonal current

FEFI 4D collisional, Edge Base Case, $0.85 < r_a < 0.99$ $0.1 < T_{\mathrm{keV}} < 1$



- satisfies control case: no bootstrap current without collisions
- adds weight to the reality of the bootstrap current result

Edge Equilibrium Flows with FEFI

- flows: close to static radial force balance $n_e e \nabla_r \phi + \nabla_r p_i \approx 0$
  - ◦ MHD: Alfvén oscillations occur unless profiles slowly ramped into form

- effect of collisions: bootstrap current
  - ◦ control case: without collisions, no bootstrap current

- **Main Point:** total-f gyrokinetics can recover neoclassical results
  - ◦ demonstrated energy/momentum conservation is essential in establishing them

B Scott/A Kendl/T Ribeiro, Contrib Plasma Phys 50 (2010) 228
Nonlinear Dynamics in the Tokamak Edge

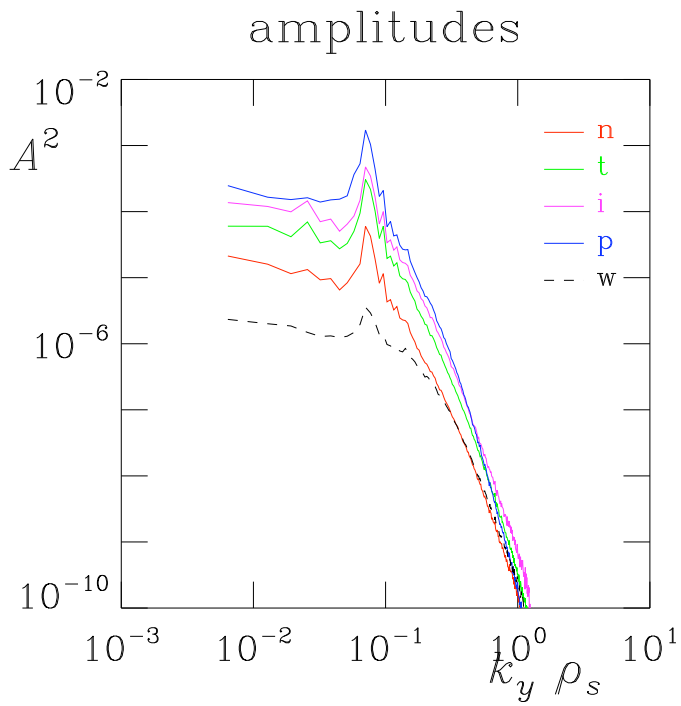
B Scott/J Smirnov, Phys Plasmas 17 (2010) 112302
Energetic Consistency and Momentum Conservation in the Gyrokinetic Description of Tokamak Plasmas

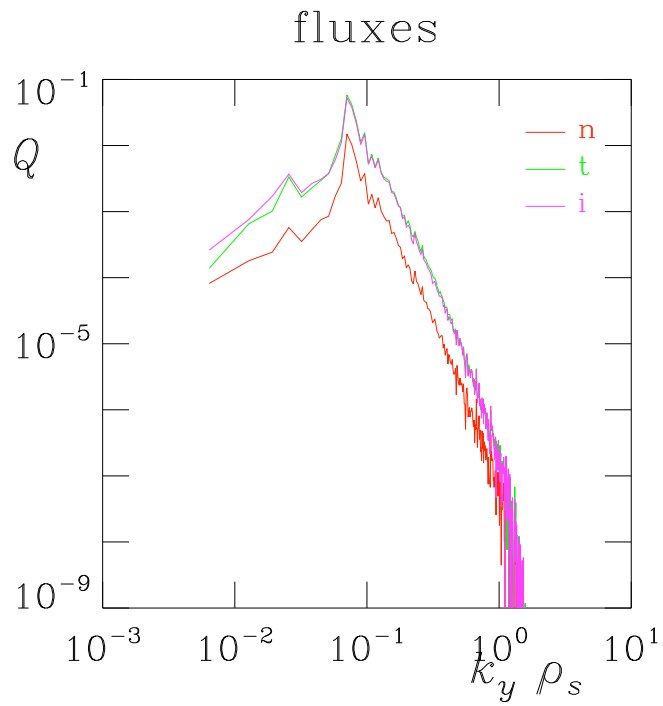
Progress on 5-D FEFI

- FEFI (full electrons, full ions) is a global total-f electromagnetic Vlasov model
- just started, showed in 2008 turbulence plus MHD equilibrium is feasible
  - at least for thin-strip edge cases (small Shafranov shift despite strong $J_{||}$)
- AUG case ($2\rho_s \times 2\rho_s$) on $64 \times 512 \times 32$ grid
  - same parameters as the FEFI4 case, but no pedestal
- spectra are similar to gyrofluid cases, with
  - enhancement of mesoscale MHD range due to trapped electrons
  - same effect of that as seen in fluxtube delta-f gyrokinetic cases
- same shift of the density to top/inside seen as in gyrofluid cases

amplitude and flux spectra

FEFI nominal case: $T_0 = 200\,\mathrm{eV}$, $n_0 = 3 \times 10^{13}\,\mathrm{cm}^{-3}$, $B_0 = 2.5\,\mathrm{T}$

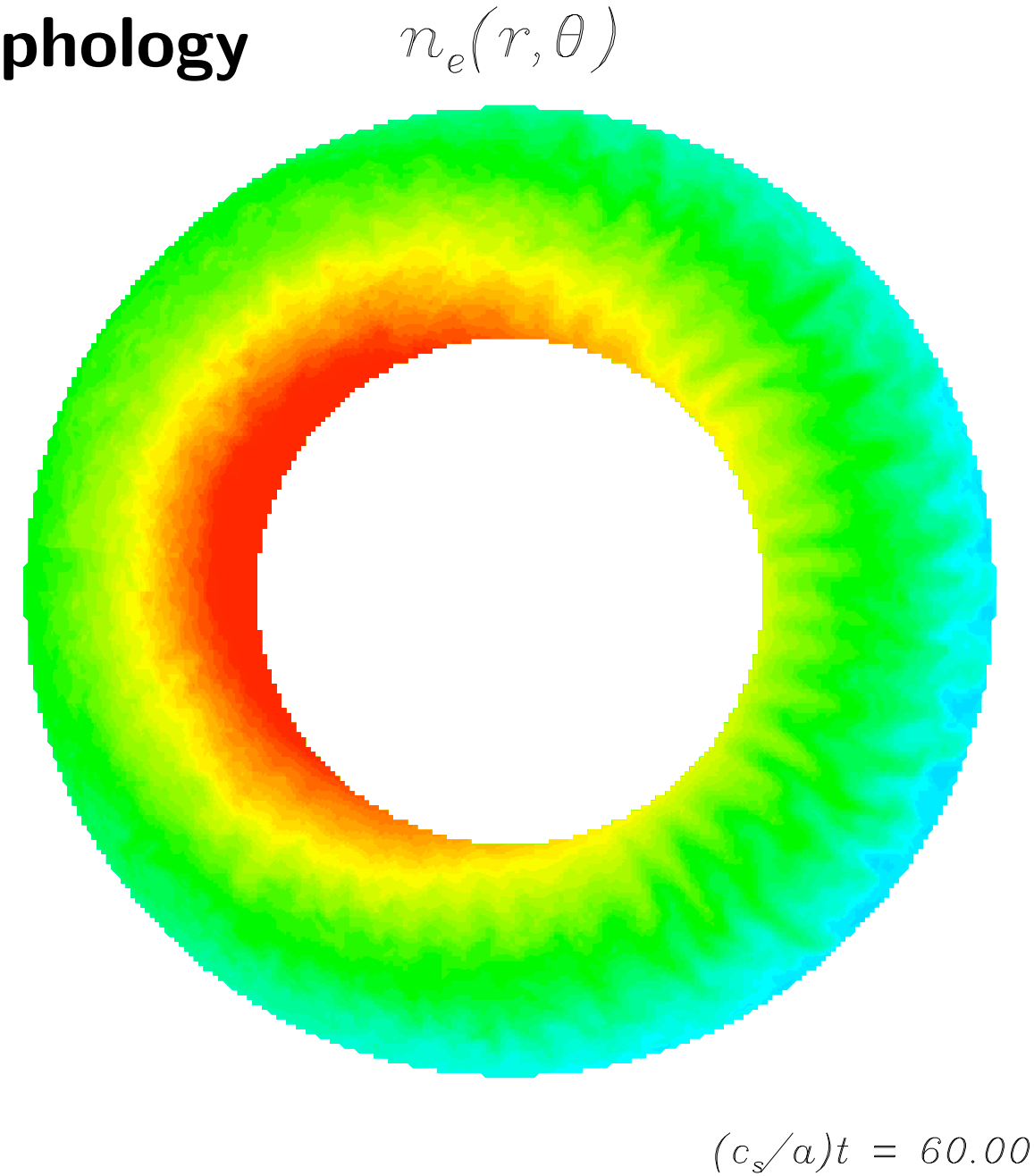




- reflects mesoscale MHD: everything peaks together at large scale

poloidal plane morphology

- strong shift off the flux surface
- radial domain stretch $\times 3$
- filaments visible on outboard side



goal for 5-D total-f computation

- Lagrangian of same form with FLR and finite-flow corrections in H (Miyato/Scott *JPSJ* 2009)

$$H = m\frac{U^2}{2} + \mu B + \left[1 + \frac{1}{4}\left(\rho_L^2 + \rho_E^2\right)\nabla_\perp^2\right] e\phi - m\frac{u_E^2}{2}$$

$$\rho_L^2 = \frac{2\mu B}{m\Omega^2} \qquad\qquad \rho_E^2 = \frac{u_E^2}{\Omega^2}$$

giving finite-vorticity Ω_E/Ω corrections (unusual representation)

$$H = m\frac{U^2}{2} + \mu B\left(1 + \frac{1}{2}\frac{\Omega_E}{\Omega}\right) + e\phi - m\frac{u_E^2}{2}\left(1 - \frac{1}{2}\frac{\Omega_E}{\Omega}\right)$$

- magnetic field term includes the equilibrium (yields Grad-Shafranov equation)

$$\mathcal{L}_B = -\frac{1}{8\pi}\frac{1}{R^2}\left|\nabla_\perp\left(\psi + A_\parallel R\right)\right|^2$$

Nonlinear Nature of the Problem

- short and long wavelengths work together
  - ◦ cascades go both ways, each side is coupled $\phi \leftrightarrow J_{\|} \leftrightarrow p_e$
  - ◦ turbulence scaling does not follow linear growth rates
  - ◦ contact to MHD by microturbulence — self consistent gradient drive

- for MHD instability cases, energetic contact to ion gyroradius scales
  - ◦ saturation occurs via its own self-generated turbulence
  - ◦ microturbulence shorts out MHD self-nonlinearity

- "equilibrium" itself is dynamical
  - ◦ relaxation to perturbation is slower than turbulence saturation
  - ◦ bursty character follows . . . consequences for simulation:

"equilibrium" must work in a time-dependent, electromagnetic model
kinetic: need to capture $O(1)$ rho-banana physics
electromagnetic: all significant responses are electromagnetic

basics of momentum conservation

- Noether theorem: canonical momentum conservation law

$$\frac{\partial}{\partial t} f P_\varphi + \nabla_{\mathbf{Z}} \cdot f P_\varphi \dot{\mathbf{Z}}_{\mathbf{p}} + f \frac{\partial H}{\partial \varphi} = 0$$

- species sum, flux surface average pieces

$$\frac{\partial}{\partial t} \langle f P_\varphi \rangle = \frac{\partial}{\partial t} \langle f p_z R - \mathbf{P} \cdot \nabla \psi \rangle + \frac{\partial}{\partial V} \psi \langle e f \rangle$$

$$\frac{\partial}{\partial V} \left\langle f P_\varphi \dot{Z}_p^V \right\rangle = \frac{\partial}{\partial V} \left\langle f p_z R \dot{Z}_p^V \right\rangle + \frac{\partial}{\partial V} \psi \left\langle e f \dot{Z}_p^V \right\rangle$$

- last terms in each line: exact "polarisation cancellation" leaving

$$\frac{\partial}{\partial t} \langle f p_z R - \mathbf{P} \cdot \nabla \psi \rangle + \frac{\partial}{\partial V} \left\langle f p_z R \dot{Z}_p^V \right\rangle + \left\langle f \frac{\partial H}{\partial \varphi} \right\rangle = 0$$

- last term gives wave-wave transport, others give plasma momentum
  - here, $\mathbf{P} = -\partial L / \partial \nabla \phi$ is the polarisation vector

basics of energy conservation

- Noether theorem: energy conservation law

$$\frac{\partial}{\partial t} f H + \nabla_{\mathbf{Z}} \cdot f H \dot{\mathbf{Z}}_{\mathbf{p}} = f \frac{\partial H}{\partial t}$$

- global conservation: use field equations to eliminate $\partial H / \partial t$
  - same operation as varying field potentials to get their E-L eqs

- this yields field energy term, shear Alfvén disturbances $\mathbf{B}_\perp$

- final result is

$$\frac{\partial}{\partial t} \left(\int d\Lambda \, f H + \int dV \, \frac{B_\perp^2}{8\pi} \right) = 0$$

- local conservation/transport eqn is more involved, not shown here

- reference: B Scott & J Smirnov, Phys Plasmas 17 (2010) 112302