Numerical treatment of stiff transport in the ASTRA code

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based on the work of G. V. Pereverzev and G. Corrigan

ESF-EW, 13-16 October 2013, Garching, Germany

Motivations for this talk

• Predicting dynamical evolution of plasmas for fusion application is of central importance to design feasible scenarios in ITER

• Dynamics is strongly non-linear (micro-macro coupling, stiffness of profiles, bifurcation phenomena, transport barriers, periodic or aperiodic relaxations, etc.)

• At the level of macroscopic time/length scale, it would be desirable to have a tool to perform transport simulations in view of designing real "discharges", that is robust against disparate type of numerical instabilities arising from the aforementioned non-linearities

the ASTRA code being the transport simulator

Outline

- The problem of stiff transport in turbulence-dominated plasmas
- Numerical scheme for stiff diffusive/convective transport equations
- Applications in the ASTRA code

Origin of stiff transport in turbulent plasmas

* Focus on turbulence-driven transport (dominant in axisymmetric plasmas)

* Follow evolution of short time/length scale fluctuations

$$\frac{\partial \tilde{f}}{\partial t} + V_0 \cdot \nabla \tilde{f} + \tilde{\boldsymbol{V}} \cdot \nabla \tilde{f} + \frac{d\tilde{E}}{dt}\frac{\partial \tilde{f}}{\partial E} = -\tilde{\boldsymbol{V}} \cdot \nabla F_0 + \frac{d\tilde{E}}{dt}\frac{\partial F_0}{\partial E}$$

resonant damping/ excitation — mode coupling — **free-energy drive**

* Which impact long time/length scale equilibrium (quadratic process):

$$\frac{\partial F_0}{\partial t} + \langle \tilde{\boldsymbol{V}} \cdot \nabla \tilde{f} \rangle_{(\delta t, \delta \vec{x})} + \langle \frac{d\tilde{E}}{dt}\frac{\partial \tilde{f}}{\partial E} \rangle = 0$$

diffusion/convection transport — turbulent heating exchange

* Fluctuating velocity $\tilde{\boldsymbol{V}}$ is provided by (gyro-averaged) **E** x **B** drift

Origin of stiff transport in turbulent plasmas

* Moment-integrate to get, e.g. transport of thermal energy (averaged over 2D):

$$\frac{3}{2}\left[\frac{\partial p_0}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\langle\tilde{V}_r\tilde{p}\rangle\right)\right]=P_{aux}$$

* Substituting the formal solution of the equation for the fluctuations

$$\frac{3}{2}\left[\frac{\partial p_0}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}r\left(-D\left(\boxed{\frac{\partial p_0}{\partial r}},p_0,\ldots\right)\frac{\partial p_0}{\partial r}+V\left(\frac{\partial p_0}{\partial r},p_0,\ldots\right)p_0\right)\right]=P_{aux}$$

diffusion **convection**

* This is a local-limit (Fick-type diffusion/convection representation)

* Dependence of D, V on **pressure slope** is due to its role as drive of turbulence

* Usual situation: turbulence is a threshold phenomenon with some critical gradient value $\left[\partial_r p_0\right]_{crit}$. Above threshold: D ~ $\left[\partial_r p_0-\left[\partial_r p_0\right]_{crit}\right]^{\alpha}$

An example from magnetized plasmas: the ITG instability

* Taking the fluid first two even moments of the kinetic equation:

$$\frac{\partial \tilde{n}}{\partial t} - i\, 2\omega_D(\tilde{n}+\tilde{T}) = -\vec{V}_{ExB}\cdot\nabla\log(n_0) - \nabla\cdot\vec{V}_{ExB}$$

$$\frac{\partial \tilde{T}}{\partial t} - i\,\omega_D\left(\frac{4}{3}\tilde{n}+\frac{14}{3}\tilde{T}\right) = -\vec{V}_{ExB}\cdot\nabla\log(T_0) - \frac{2}{3}\nabla\cdot\vec{V}_{ExB}$$

$$\tilde{n}=\tilde{\phi} \quad ; \quad \vec{V}_{ExB} = -\frac{\nabla\tilde{\phi}\times\vec{B}}{B^2}$$

* ω_D terms arise from magnetic field curvature, i.e. centrifugal force

* The resulting instability to grow requires:

$\omega_D \partial_r T_0 > 0$ - Unfavourable curvature

$\partial_r \log(T_0) > \partial_r \log(T_0)_{crit}$ - Threshold gradient

Quasi-linear estimate

* The mode growth rate will be like:

$$\gamma \propto \sqrt{\frac{R}{L_T} - \frac{R}{L_{T\,crit}}}$$

* The induced radial transport can be estimated via quasi-linear mixing-length estimate:

$$\chi \sim \rho_s^2 \frac{c_s}{R} \left[\hat{\gamma}^{\alpha} \hat{\lambda}^{\beta} \right] \qquad \hat{\gamma} = \gamma \frac{R}{c_s} \quad ; \quad \hat{\lambda} = \frac{1}{k_{\perp} \rho_s}$$

* This is usually a valid approximation in a turbulence regime in which the non-linear phase is dominated by the linearly-growing modes, which saturation is then imposed by mode-mode coupling, i.e. cascade in wave-number space.

Quasi-linear estimate

* Thus we obtain the estimated diffusivity:

$$\chi \sim \rho_s^2 \frac{c_s}{R} \left[\hat{\lambda}^{\beta}\right] F(\ldots) \left[\frac{R}{L_T} - \frac{R}{L_{T\,crit}} \right]^{\alpha/2}$$

A mock-up model to study numerical schemes

* Simplified 1D model [taken from Pereverzev & Corrigan, CPC 2008]:

$$u_t = (Du_x - Vu)_x + S, \quad 0 < x < 1, \; t > 0.$$

* Apply standard semi-implicit finite-volume scheme:

$$\frac{\hat{u}_i - u_i}{\tau} + \frac{q_{i+1/2} - q_{i-1/2}}{h} = S_i, \quad i = 0, 1, \ldots, N,$$

$$q_{i+1/2} = -D_{i+1/2} \frac{\alpha_{i+1/2}\hat{u}_{i+1} - \beta_{i+1/2}\hat{u}_i}{h},$$

$$\left[O(h^2), \;\; O(t)\right]$$

* With the following definitions for the diffusive/convective components:

$$\alpha(\xi) = \frac{\xi}{1 - e^{-\xi}}, \quad \xi = -\frac{hV}{D},$$

$$\alpha_{i+1/2} = \alpha(\xi_{i+1/2}), \qquad \beta_{i+1/2} = \alpha_{i+1/2} - \xi_{i+1/2},$$

* Notice that the exponential scheme is used to avoid convection-driven numerical instabilities when $|\xi| > 1$

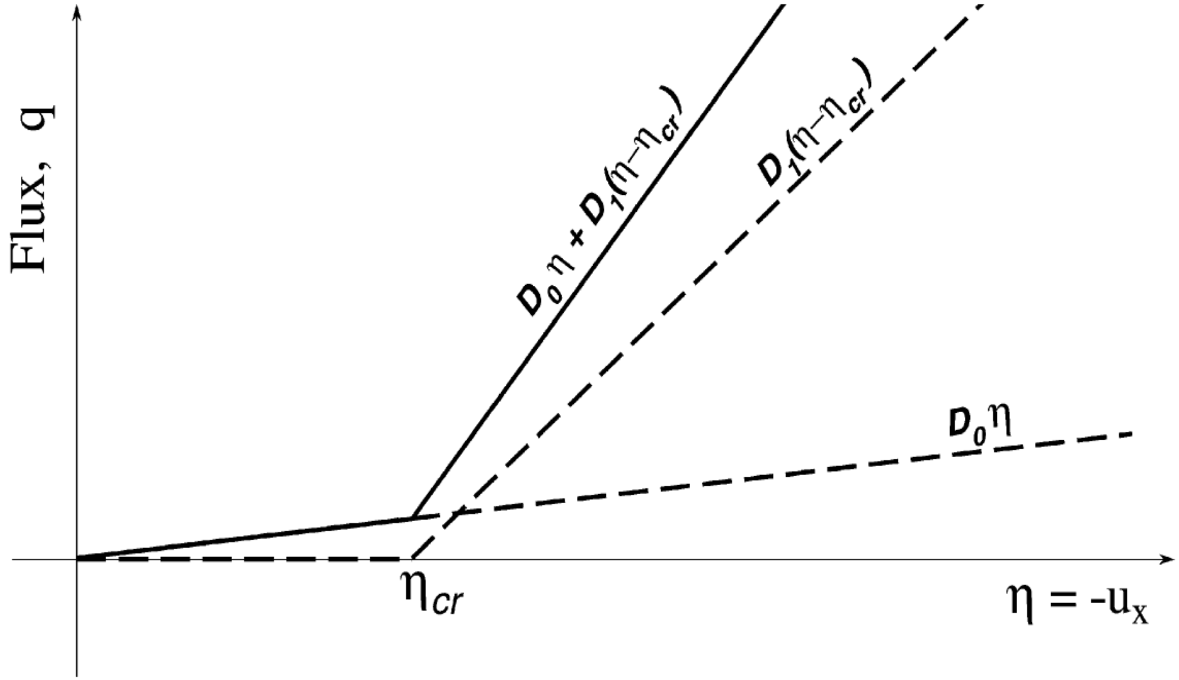
The model for "stiff" diffusive transport

* Choose the simplest example of critical-gradient model:

$$q = -\left[D_0(x,u) + D_{an}(x,u,u_x)\right]u_x \quad ; \quad D_0 \ll D_{an}$$

$$D_{an} = \begin{cases} D_1(\eta - \eta_{cr})/\eta, & \text{if } \eta > \eta_{cr} > 0, \\ 0, & \text{if } \eta < \eta_{cr}, \end{cases} \quad ; \quad \eta = -u_x$$

* How it looks like:
* Resulting flux q is piece-wise **linear** in the gradient u_x with two distinct slopes



Numerical properties as a function of τ

* Defining: $D^{eff} = D_0 + D_{an}$

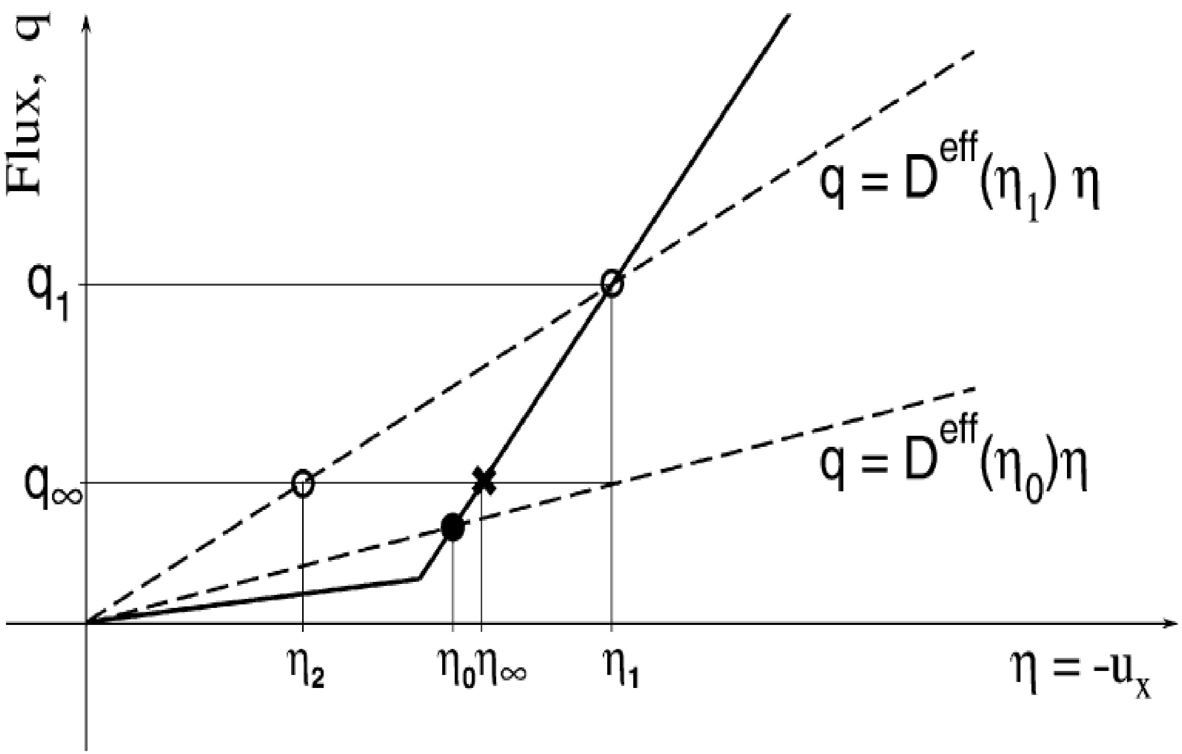
$$\frac{\hat{u}_i - u_i}{\tau} = D^{\text{eff}}_{i+1/2}\frac{\hat{u}_{i+1} - \hat{u}_i}{h^2} - D^{\text{eff}}_{i-1/2}\frac{\hat{u}_i - \hat{u}_{i-1}}{h^2} + S_i,$$

* Subsequent time steps:
$\eta_0, \eta_1, \eta_2, \ldots$

* Stationary solution η_∞

* For not-small-enough τ, solution jumps wildly

due to $D^{\text{eff}}(\eta_1)/D^{\text{eff}}(\eta_0) \gg 1$



A new scheme to treat the "instability"

* Modify flux expression in this way:

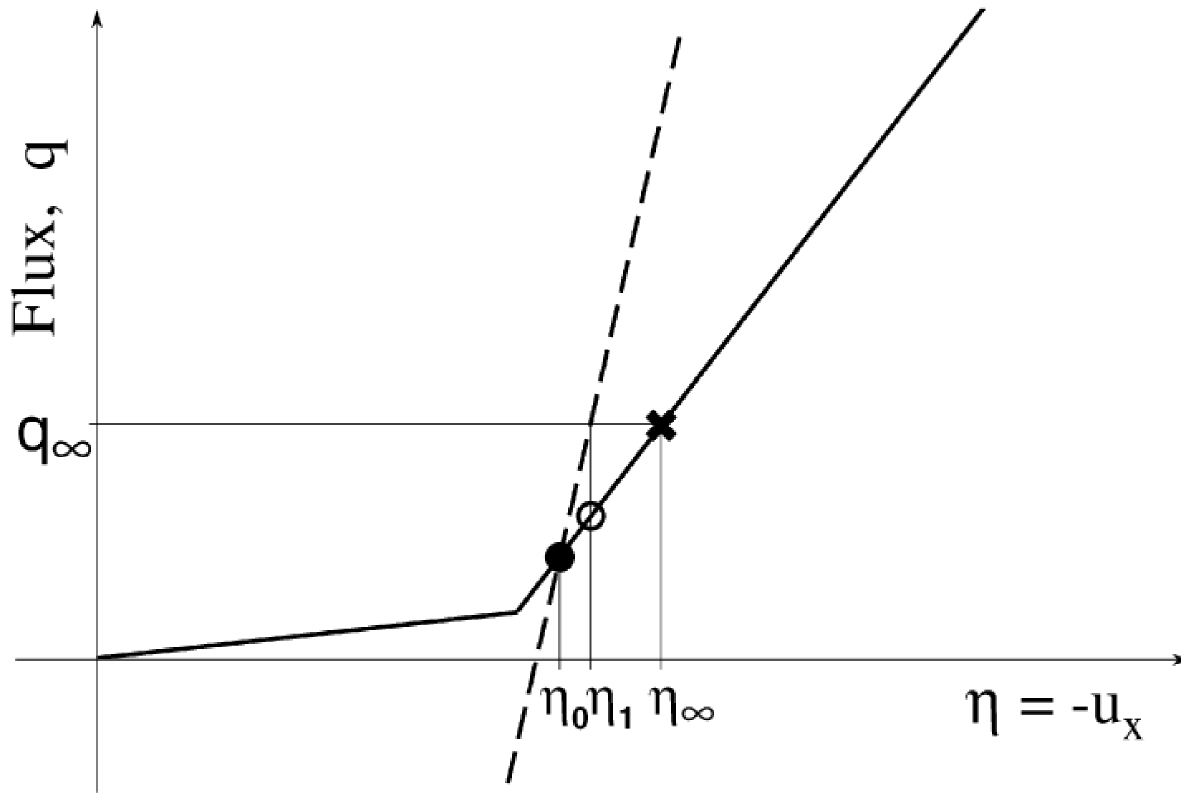
$$q = D^{eff}\,\hat{u}_x + \overline{D}\,\hat{u}_x - \overline{V}\,\hat{u} \qquad , \qquad \overline{V} = \overline{D}\,\frac{u_x}{u}$$

* Subsequent time steps:

$\eta_0, \eta_1, \ldots, \eta_\infty$

* Stationary solution η_∞

* Now the solution converges rapidly to η_∞ without jumping



Numerical properties of the new scheme

* After having split the flux in the original and correction contributions:

$$q_{i+1/2} \longrightarrow q_{i+1/2} + \bar{q}_{i+1/2}$$

* Where:

$$\bar{q}_{i+1/2} = -\bar{D}_{i+1/2} \frac{u_i \hat{u}_{i+1} - u_{i+1} \hat{u}_i}{h u_{i+1/2}} = \mathcal{O}(\tau) + \mathcal{O}(h^2)$$

* This quantity can be computed at each time step to check for the accuracy of the solution

* To have a more transparent computation of the error, one can also decribe the correcting term in this way:

$$q = D^{eff}\, \hat{u}_x + \overline{D}\left(\hat{u}_x - u_x\right)$$

* So that an effective source term is computed: $\bar{S}_i = \frac{1}{h}(\bar{q}_{i+1/2} - \bar{q}_{i-1/2}) = \mathcal{O}(\tau)$

that can be compared with the real source term S_i

Advantage of the second choice

* Choosing this form:

$$q = D^{eff}\,\hat{u}_x + \overline{D}\left(\hat{u}_x - u_x\right)$$

with respect to:

$$q = D^{eff}\,\hat{u}_x + \overline{D}\,\hat{u}_x - \overline{V}\,\hat{u} \quad , \qquad \overline{V} = \overline{D}\,\frac{u_x}{u}$$

has the advantage that the latter becomes *O(dx)* when convection is large, while the former is $O(dx^2)$

Steady-state simulations

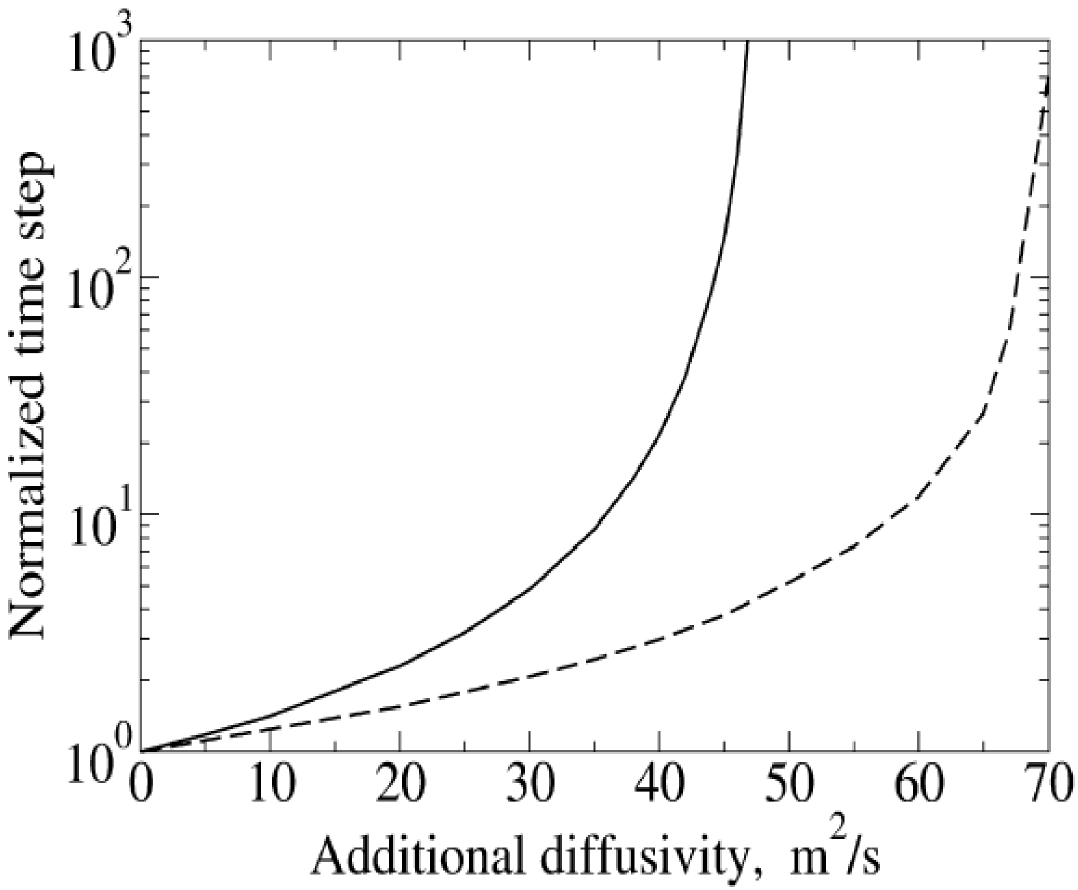
* The new scheme allows to perform much faster simulations to obtain a converged steady-state solution

* The normalized time step is defined as:

$$\hat{\tau} = \frac{\tau_{tol}}{\tau_0}$$

* τ_{tol} is the time step required to maintain the flux oscillations inside a specific tolerance

* τ_0 is the time step required when



* There is a large gain in computational time when increasing $\bar{D}$

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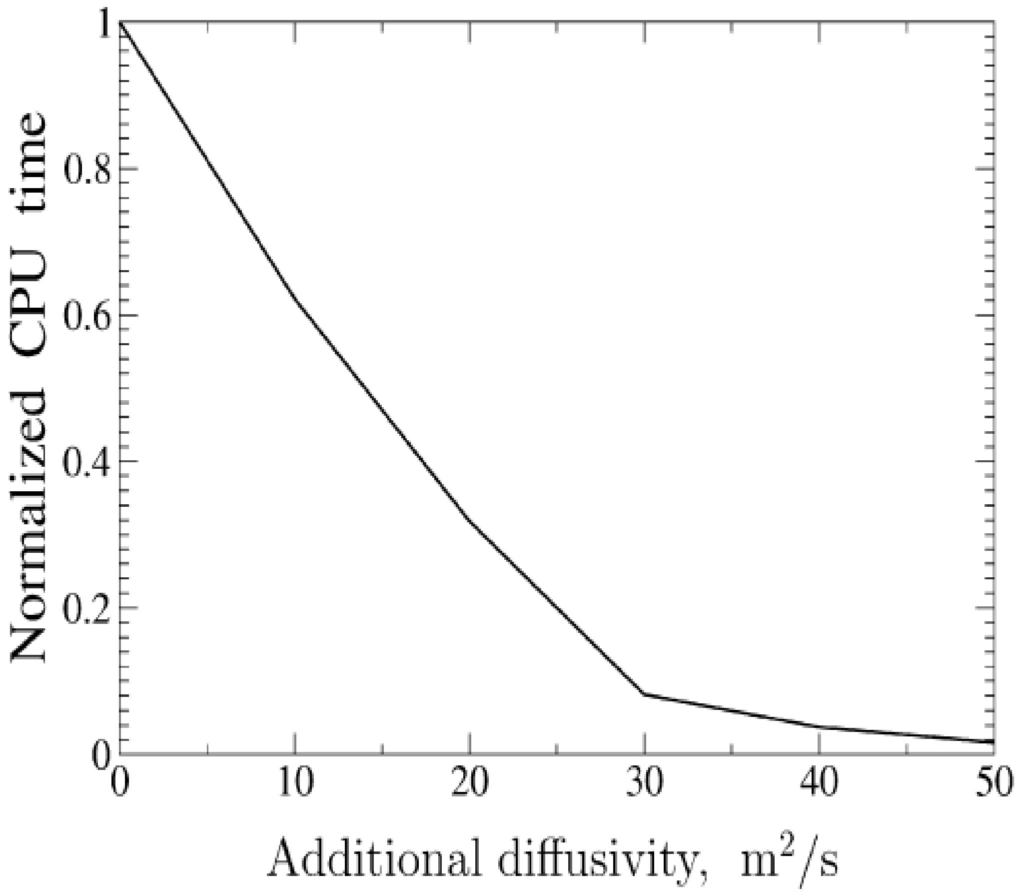

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Transient phases

* The numerical scheme introduced before can be applied also during transient phases

* However there the choice of the artificial diffusivity can have some consequence on the dynamics, for example if it is too large

* To estimate its impact it is instructive to transform $q = D^{eff}\,\hat{u}_x + \overline{D}\left(\hat{u}_x - u_x\right)$

into an equivalent continuous differential equation with a 'discrete time parameter' τ:

$$q = D^{eff}\,u_x + \tau\,\overline{D}\,u_{xt}$$

so that the full equation becomes: $u_t - \left[D^{eff}\,u_x + \tau\,\overline{D}\,u_{xt}\right]_x = S$

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* It is clear that the artificial term in **red** will not impact the dynamic if

$$\tau\,\overline{D} \ll \tau_E\,D^{eff} \qquad \left[\tau\,\overline{D} \ll \left|\frac{u}{u_{xx}}\right|\right]$$

Transient phases

* The condition $\tau \overline{D} \ll \tau_E D^{eff}$ can be translated in the possible choice of the time step:

$$\tau \ll \tau_E \frac{D^{eff}}{\overline{D}} \qquad (1)$$

* To avoid the artificial diffusivity having an impact on the dynamics. On the other hand, as we discussed before, this parameter should be large enough to suppress the instability associated with stiff transport:

$$\overline{D} > D^{eff}$$

* When the artificial diffusivity is zero, then the time step has to fulfill:

$$\tau D_{an} \left| \eta - \eta_{cr} \right| \ll dx^2 \eta_{cr} \qquad (2, ?)$$

* So it is clear that the new scheme is very beneficial. Moreover the condition (1) above is probably an overestimate.

Example of profiles evolution using the ASTRA code

* To show into more details the evolution of the profiles in presence of stiff transport, the following system of equations is solved:

$$\begin{cases} \frac{3}{2}\frac{\partial T_e}{\partial t} - \frac{1}{V'}\frac{\partial}{\partial \rho}\left(V' g_\rho^2 \chi_e \frac{\partial T_e}{\partial \rho} \right) = \frac{\left(P_{EC} - P_{ei} \right)}{n_e} \\ \frac{3}{2}\frac{\partial T_i}{\partial t} - \frac{1}{V'}\frac{\partial}{\partial \rho}\left(V' g_\rho^2 \chi_i \frac{\partial T_i}{\partial \rho} \right) = \frac{P_{ei}}{n_e} \end{cases}$$

$$\begin{cases} \chi_e = 0.001 + 15.\, H\left(\frac{R}{L_{Te}} - 5. \right) \left[\frac{R}{L_{Te}} - 5. \right] \\ \chi_i = \chi_{i,neo} + 15.\, H\left(\frac{R}{L_{Ti}} - 5. \right) \left[\frac{R}{L_{Ti}} - 5. \right] \end{cases}$$

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* Plasma thermal energy with constant density: $E_{th} = 3/2\, n_e\, (T_e + T_i)$

* Heating source on electrons (e.g. electron cyclotron 'EC')

* Ions are heated by electrons via collisional exchange e → I

* Ohmic power OH arises from current-carrying electrons colliding on ions

Example of profiles evolution using the ASTRA code

* Heat diffusivities represented via critical-gradient model:

$$\begin{cases} \chi_e = \chi_{e,neo} + 15.\, H\left(\frac{R}{L_{Te}} - 5.\right)\left[\frac{R}{L_{Te}} - 5.\right] \\ \chi_i = \chi_{i,neo} + 15.\, H\left(\frac{R}{L_{Ti}} - 5.\right)\left[\frac{R}{L_{Ti}} - 5.\right] \end{cases}$$

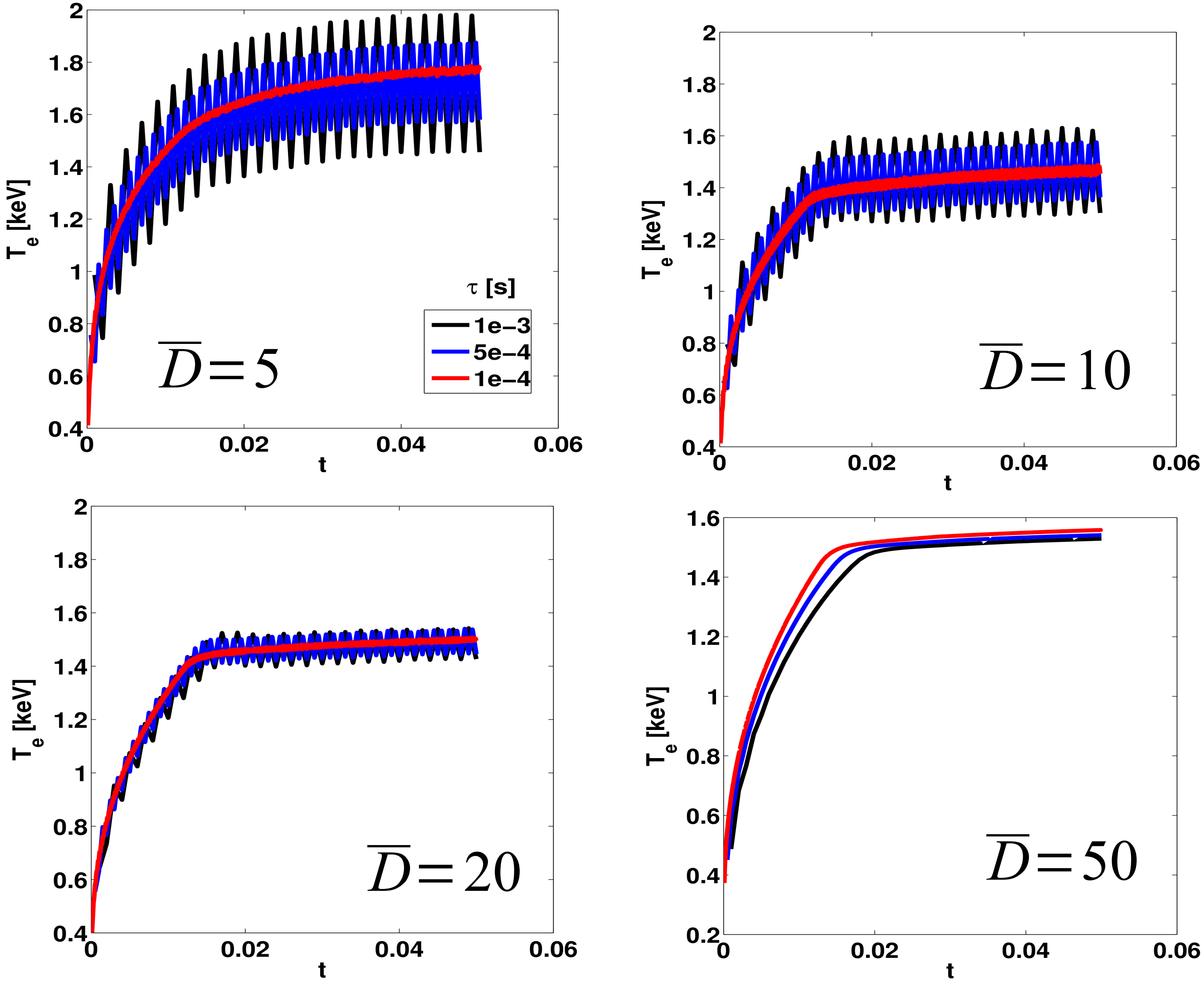
* For both species the critical normalized gradient $\left[\frac{R}{L_T} = -R\frac{\partial \log(T)}{\partial \rho}\right]$ is 5.

* The stiffness parameter is 15. (very high diffusivity when gradients over threshold)

* Baseline diffusivities are in the order of 10^{-3} for electrons and 10^{-2} for ions (neoclassical transport).

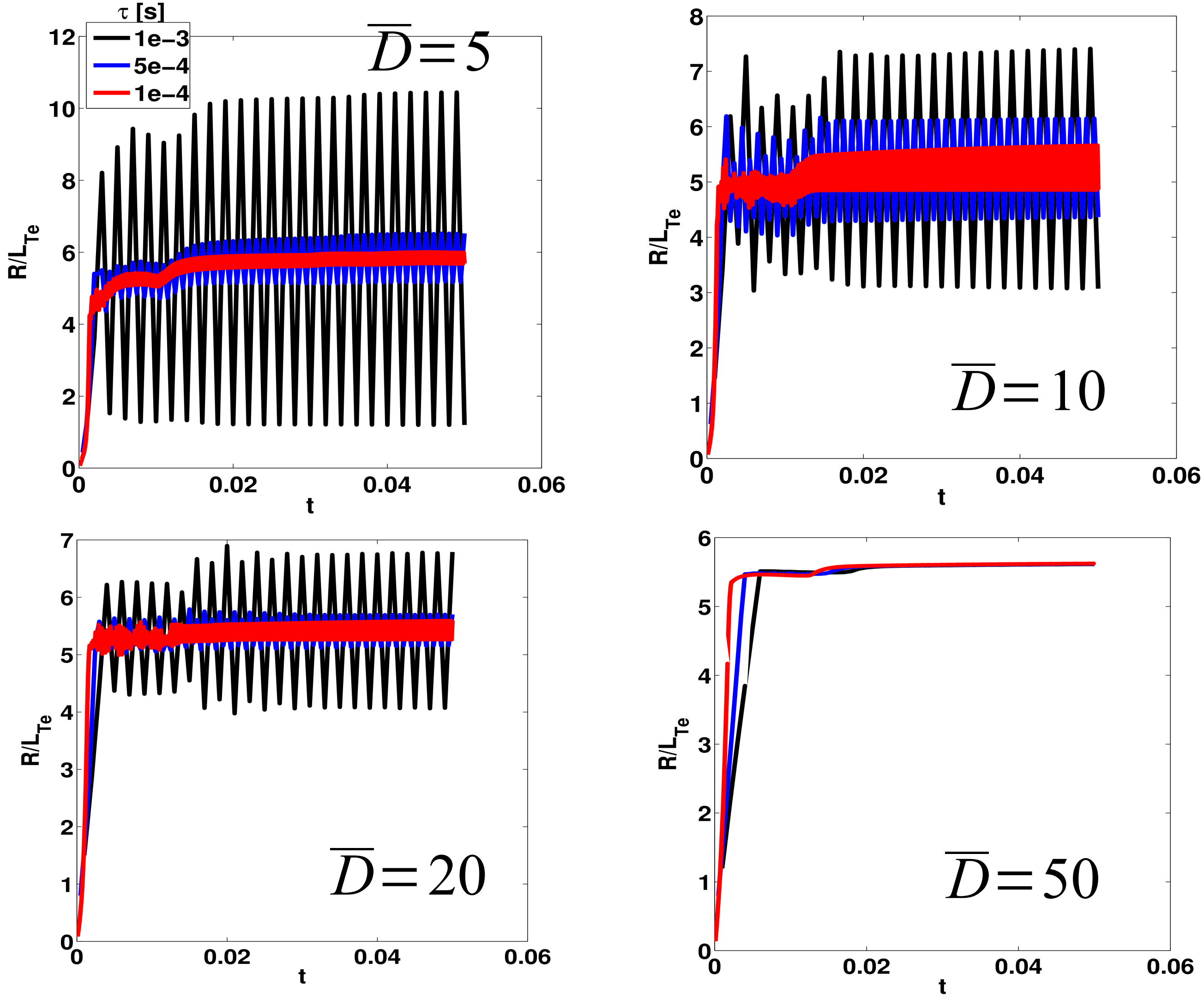
Evolution of central T_e

* The temperature profile evolution at ρ = 0 by varying $\boldsymbol{\tau}$ and $\overline{D}$ is shown below



Evolution of R/L_{Te} at mid radius

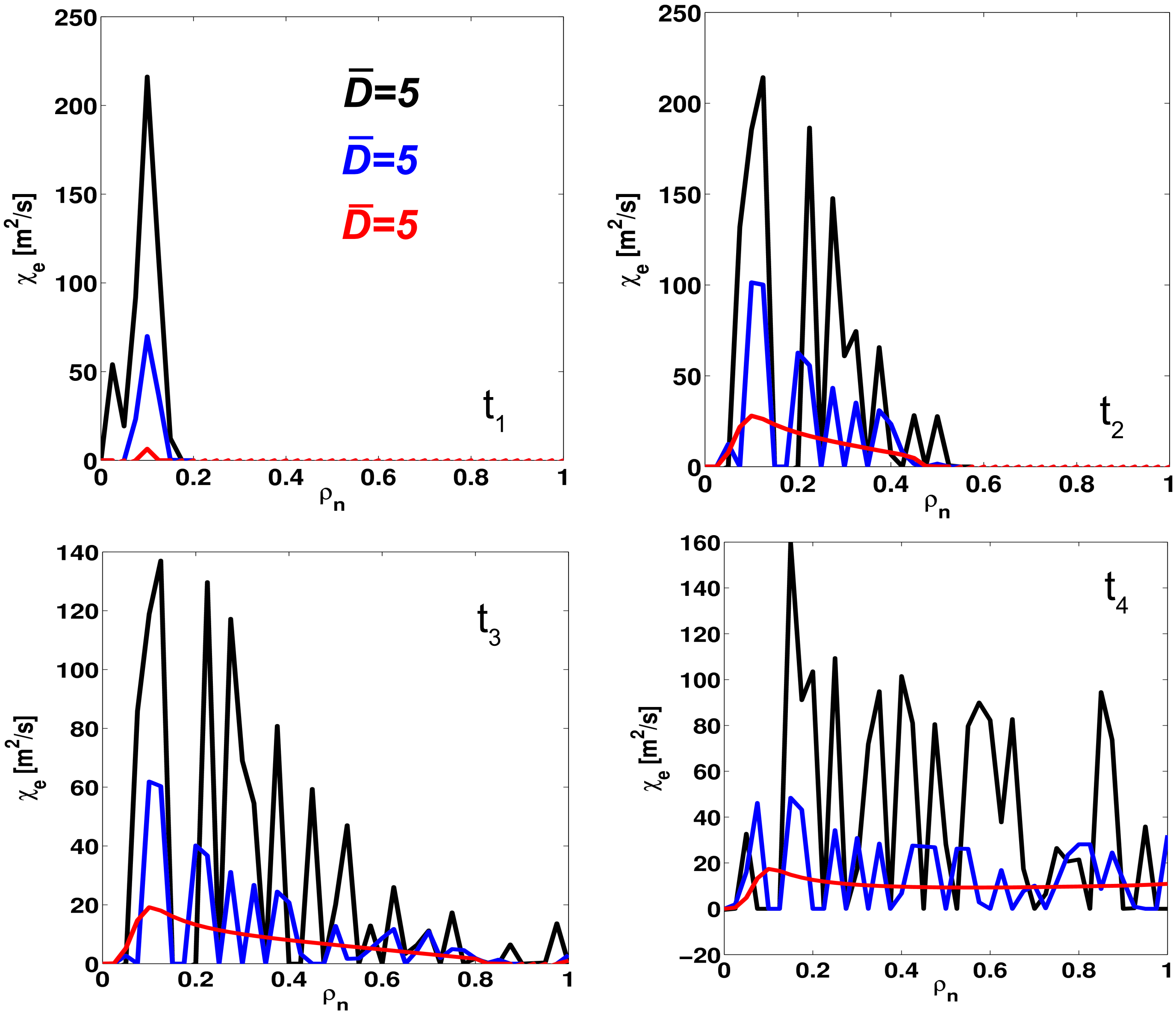
* The normalized logarithmic gradient evolution at mid-radius:



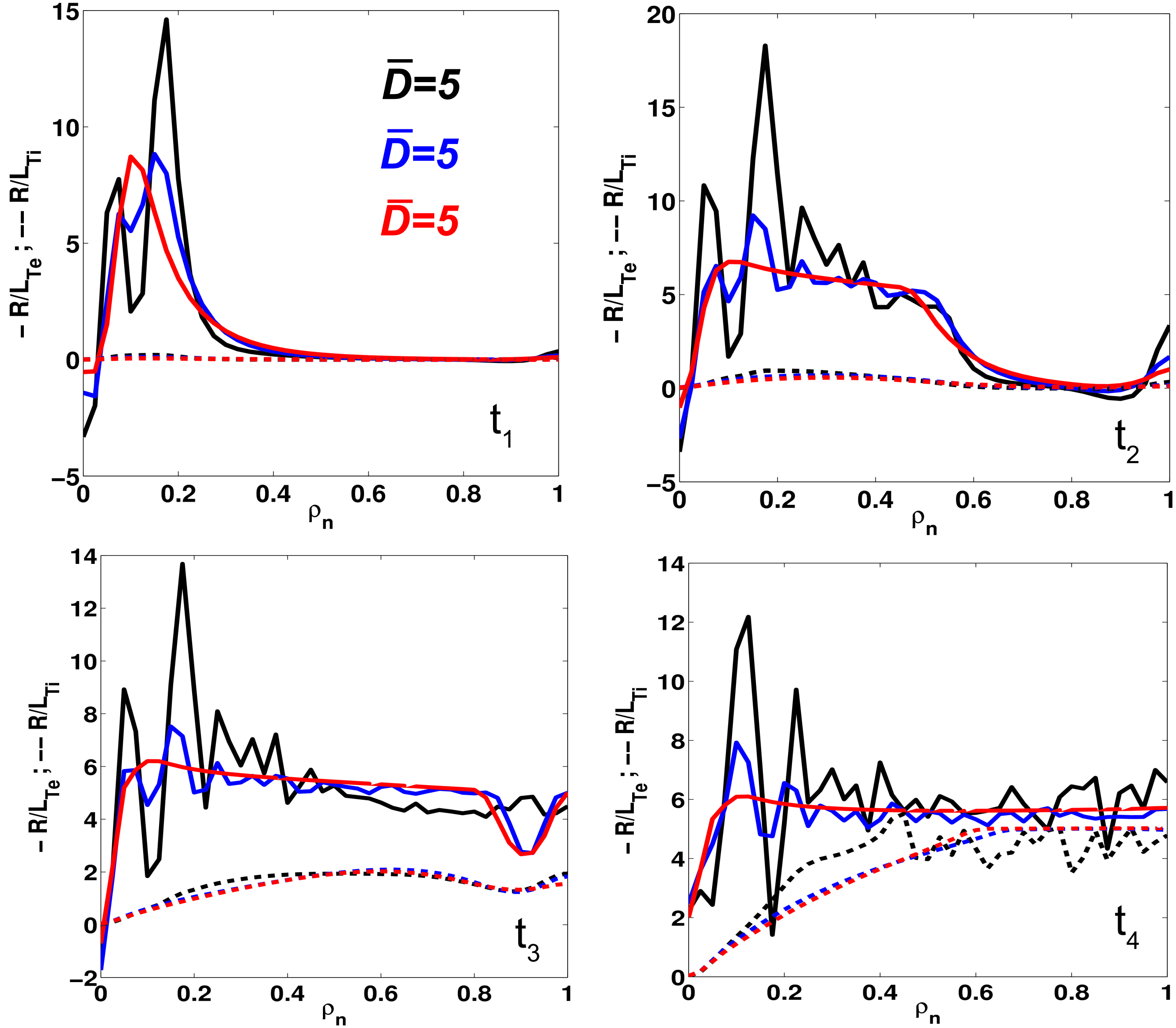
Profile of χ_e during time evolution

* The electron thermal diffusivity as a function of radius shows clearly what is happening during the simulation

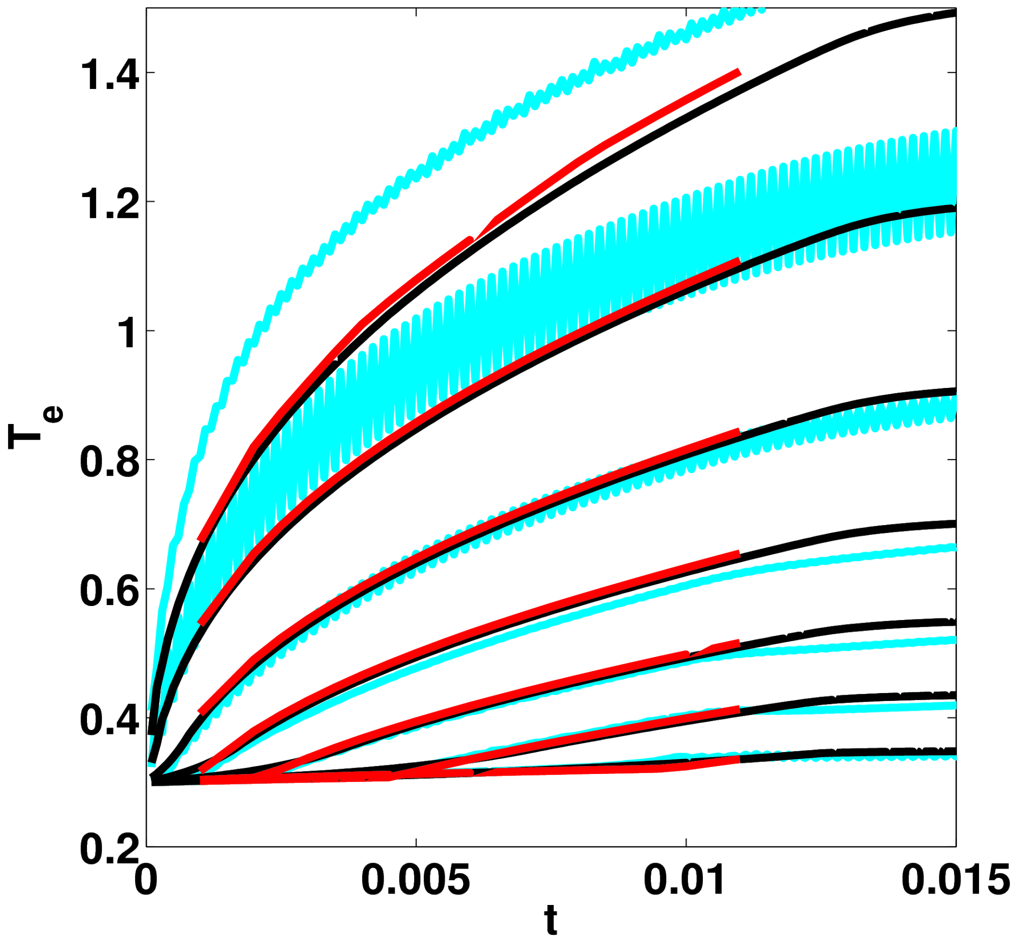
Profile of χ_e during time evolution



Profile of R/L_T during time evolution



What if τ is extremely low



* A case has also been run with

τ = 5e-8 and $\bar{D}$ = 5

compared with:

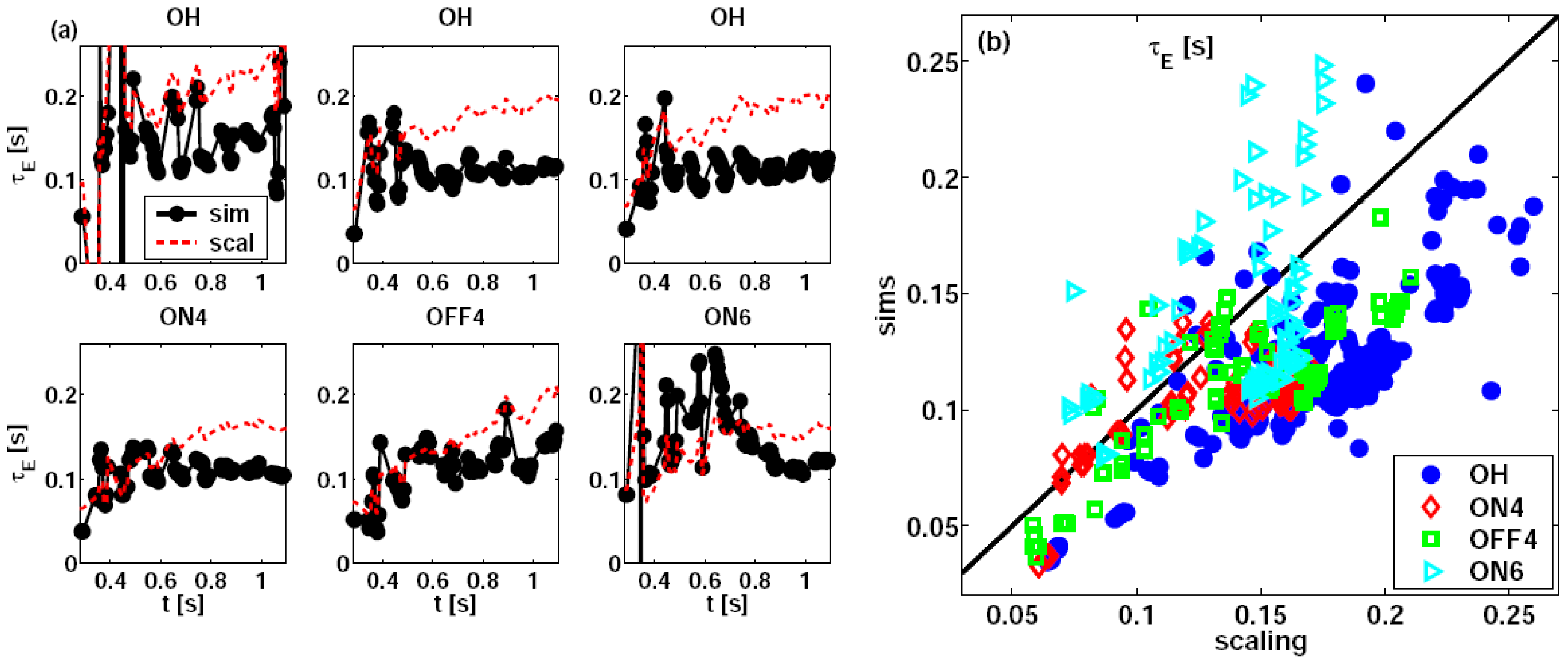
τ = 1e-4 and $\bar{D}$ = 50

τ = 1e-4 and $\bar{D}$ = 5

Applications: prediction of confinement time over current ramp-up phase of a discharge

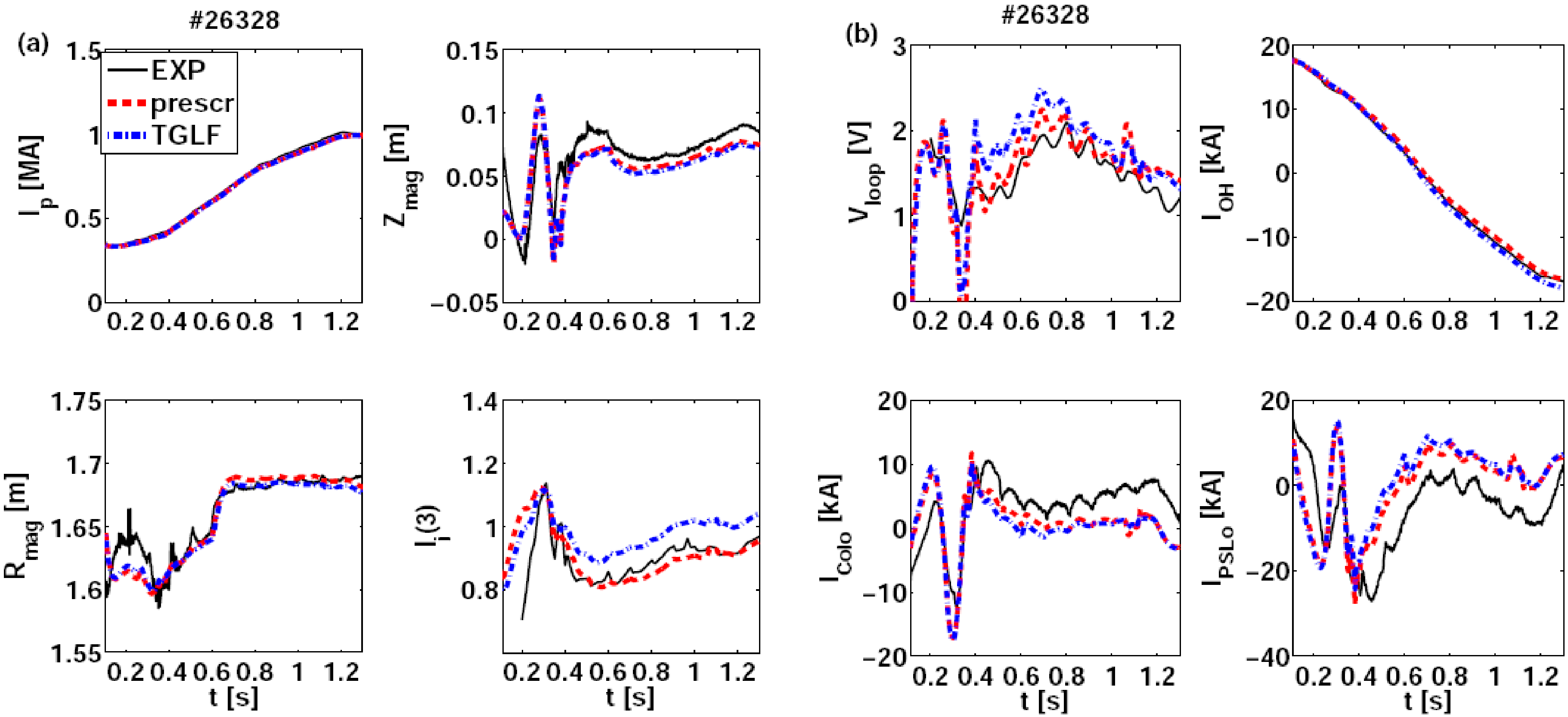
* The numerical scheme is applied to the GLF23 transport model [R. E. Waltz et al., POP 1997], which computed turbulence-driven heat and particle transport

* In this example it was applied to several discharges where the initial transient phase (current ramp-up) is studied



Applications: prediction of global "circuit" parameters with TGLF

* Another application envisage the use of TGLF turbulence-transport model [G. M. Staebler et al., POP 2007], to reproduce global controlled plasma evolution and check the behavior of the controller coils, both during current ramp-up and ramp-down



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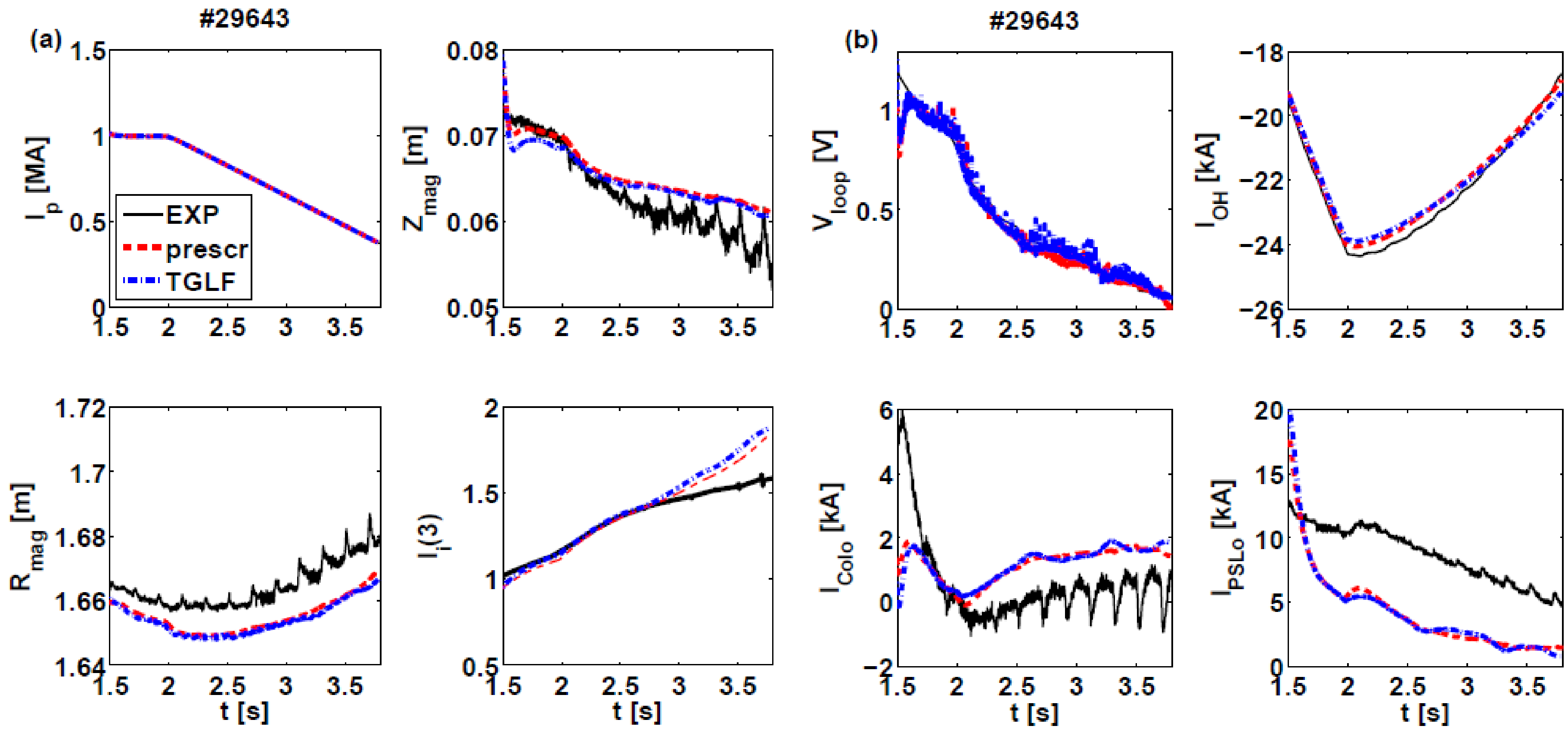

Summary

* Stiff transport resulting from turbulence as a threshold phenomenon with strong dependence on the transported quantity is a common feature in tokamak plasmas (but not only)

* A numerical scheme to treat this into diffusion/convection equations has been presented, which details can be found in G.V. Pereverzev and G. Corrigan, Comp. Phys. Comm. **179**, 579 (2008)

* The numerical stability and accuracy has been discussed, in particular on the details of how the choice of the artificial parameters impact the dynamics

* Test cases run into the ASTRA code has been shown to greatly improve the simulation of plasma profile evolution in presence of turbulence-driven transport

* Application to "real-life" plasmas benefits greatly from the new scheme as ridiculously low time steps would render full-discharge simulations impossible to perform on a reasonable "human" time-scale

Outlook

* It would be desirable to increase the order of the scheme presently implemented in ASTRA, aiming at combining the following ingredients:

- Implicitness of the time stepping, or find a different scheme with higher order of time accuracy

- Treatment of strong convective regimes (e.g. fast plasma expansion/compression, neoclassical transport for impurities)

- High-order spatial accuracy (2^{nd} or 3^{rd} order would be extremely welcome)

- Good conservation properties (e.g. as the finite-volume method employed presently in ASTRA)

Not strictly related

* A presently missing scheme for ASTRA, which I am currently looking at:

$$u_t + C\,x\,u_x + \left(-D\,u_x + V\,u\right)_x = S \qquad ; \qquad C\,,V\,,D = consts \qquad (1)$$

Rewritten as:

$$u_t + \left(-D\,u_x + (V + Cx)\,u\right)_x - C\,u = S \qquad (2)$$

When C >> V and large, still the exponential scheme can be used, however the *-C u* term causes problems if treated either implicitly or explicitly

So the question is: scheme (1) would be implementable with exponential scheme but not in conservative form, while scheme (2) is in conservative form but suffers from numerical problems due to the 'implicit' source term