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Gyrokinetic simulation of fusion plasma turbulence

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European
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Applications

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Outline

I. Numerical methods
II. Benchmarking the code
III. Influence of noise on results.
IV. Transport simulations in toroidal plasmas
V. Resources and Deisa experiences
VI. Conclusions

The ELMFIRE group

Founded in 2000

International group
Finland
Spain
Holland

Main affiliations
VTT
TKK

... but also ...
CSC
Åbo Akademi
UNED (Spain)

Section I
Numerical methods

ELMFIRE code

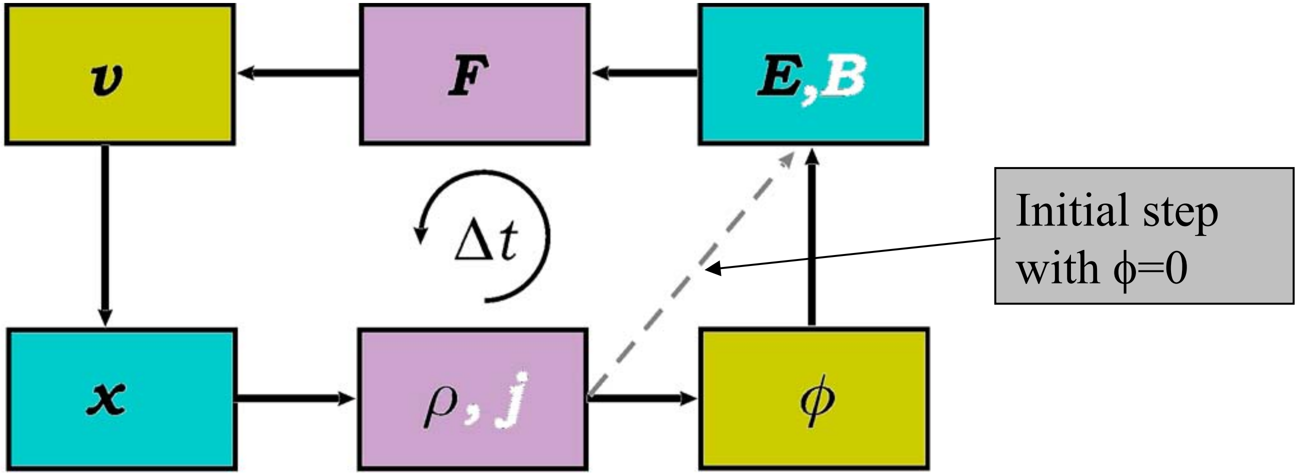
- Full *f* nonlinear gyrokinetic particle-in-cell approach for global plasma simulation (present version electrostatic).
- Magnetic coordinates (ψ,θ,ζ) Boozer '81.
- Guiding-center Hamiltonian White & Chance, '84.
- Gyrokinetics is based on Krylov-Boholiubov averaging method in description of FLR effects (P. Sosenko, '01).
- Adiabatic or kinetic electrons with impurities.
- Parallelized using MPI with very good scalability.
  - Based on free software: PETSc and GSL for math calc.
  - CPP-controlled use of optimized numerical libraries (also PESSL, ACML, MKL, S3L...)

Calculation flux in particle codes

Acceleration and
increment of velocity

Calculation of forces
from fields and
velocity

Computation of electric
field. Magnetic is given.



Initial step
with $\phi=0$

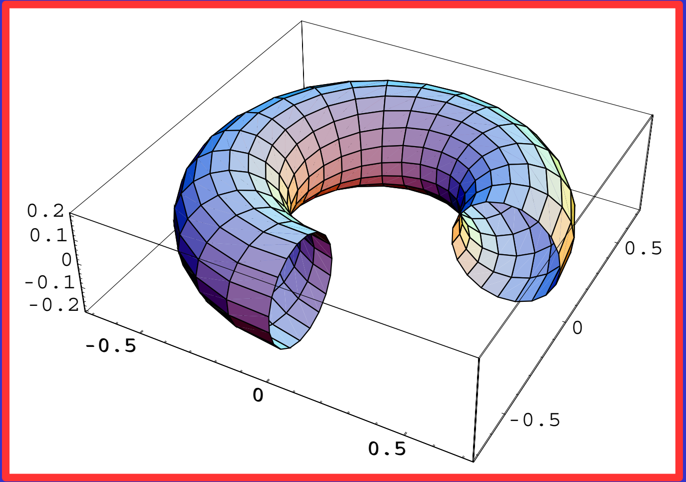
Displacements and
new positions.
Boundary conditions.

Calculation of
density. Current
profile fixed.

Resolution of Poisson
equation for the
electrostatic potential.

ELMFIRE full *f* features

- An initial canonical distribution function avoids the onset of unphysical large scale ExB flows (Heikkinen, ‘01)
- Direct implicit ion polarization (DIP) and electron acceleration (DEP) sampling of coefficients in the gyrokinetic equation
- Quasi-ballooning coordinates to solve the gyrokinetic Poisson equation
- Versatile heat (RF, NBI, Ohmic) sources and particle sources/ recycling
- Full binary collision operator



Delta *f* vs. full *f*

- Delta *f* calculates pertur-bations from an assumed background distribution f_0.
- Powerful for small f-f_0
  - Linear mode analysis
  - “Snapshot” transport analysis
  - Path-breaking global transport studies for large toroidal installations
- Few particles (~10-100) per cell are needed for good results with small f-f_0.

- Full *f* calculates the whole particle distribution.
- Fitting processes that perturbate strongly the particle distribution
  - Strong transient or long time scale transport in core or edge plasmas
  - Strong particle/energy sources
  - Edge plasma (wall losses, recycling, separatrix, flows)
- ~1000 particles per cell for an acceptable noise level

Poisson equation

- W.W. Lee proposed “standard” model with polarization drift included in equation operator.
  - Ion density evaluated from ion motion without polarization drift

$$\nabla^2\Phi + \frac{q^2}{mB\epsilon_0}\int(\Phi - \langle\Phi\rangle)\frac{\partial\langle f\rangle}{\partial\mu}\mathrm{d}\vec{v} = -\frac{1}{\epsilon_0}(q\tilde{n}_i(\vec{r}) - en_e(\vec{r}))$$

- P. Sosenko proposes including polarization in the ion density.
  - Ion density evaluated from ion motion with polarization drift. Circular gyro-orbits.

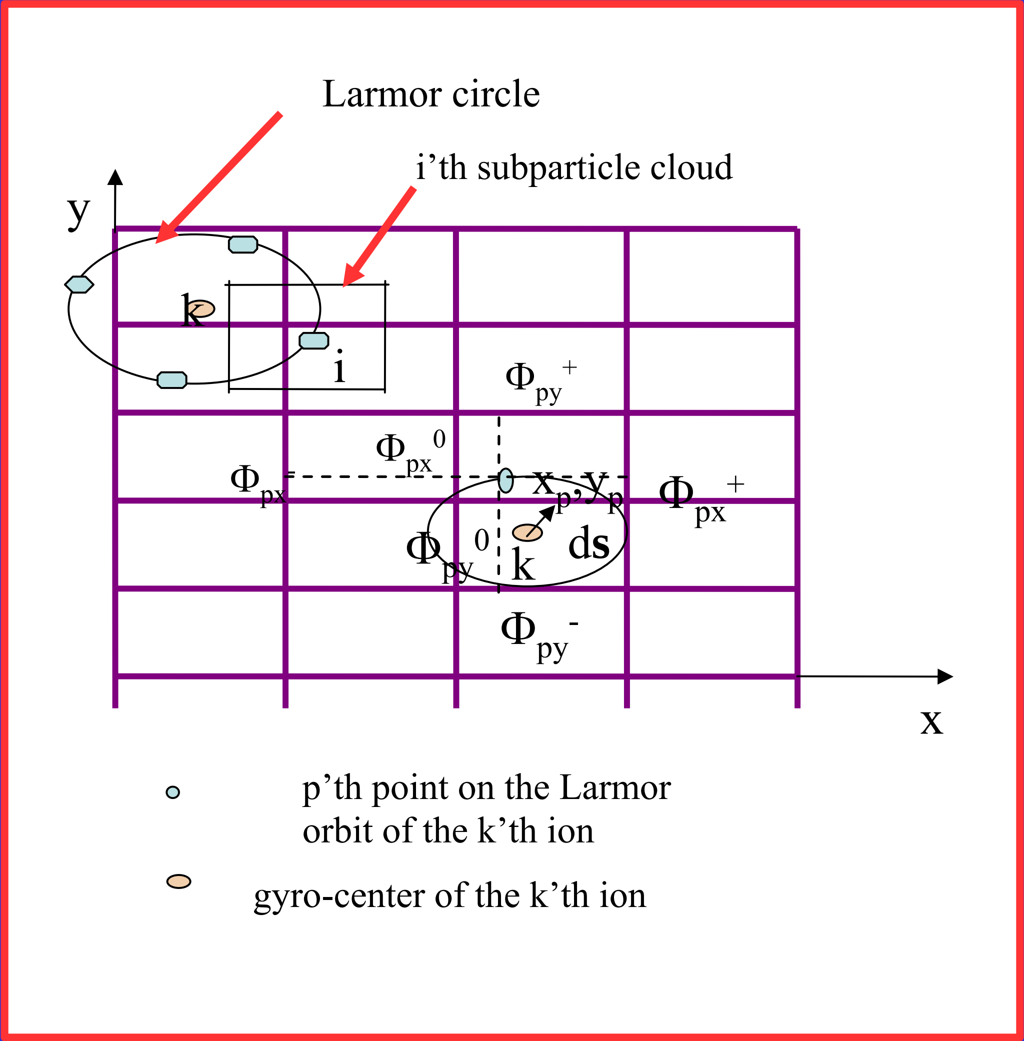
$$\nabla^2\Phi + \frac{q^2}{mB\epsilon_0}\int\left[(\Phi - \langle\Phi\rangle)\frac{\partial\langle f\rangle}{\partial\mu} + \frac{m}{q\Omega}\langle f\rangle\nabla_\perp^2\langle\Phi\rangle\right]\mathrm{d}v = -\frac{1}{\epsilon_0}(q\tilde{n}_i(\vec{r}) - en_e(\vec{r}))$$

GK-Poisson problem in ELMFIRE

- Particle movement is first calculated without ion polarization or E_z acceleration of electrons.
- The code calculates the electrostatic field so that the remaining implicitly calculated drifts return the plasma to neutrality.
- Matrix element A_{ij} contains the effect of j-cell potential into i-cell density ($A_{ij} = dn_i/d\Phi_j$).
- ELMFIRE builds the GK-Poisson problem matrix from particle data every timestep.

Implementation into ELMFIRE

- Solve Φ by isolating ion polarization drift contribution to density.
- That contribution is calculated implicitely every timestep using also previous values of Φ.
- The gyroaveraged electric field is interpolated from grid potential values for the ion polarization drift.

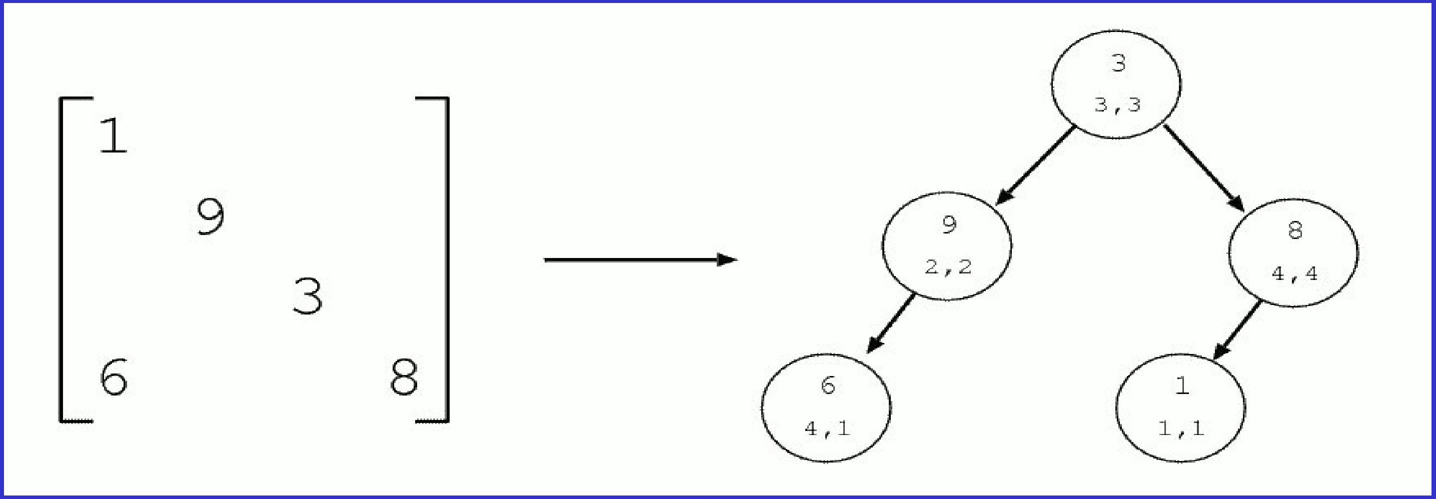


AVL tree method

- Result of optimization under project FinHPC, with collaboration of ÅA and CSC.
- Reduced memory consumption significantly
- AVL method reduces memory consumption and even network overall traffic by increasing communication steps.
- in slower ethernet network relative advantage to AVL while in infiniband faster network AVL not so profitable → AVL system introduced as optional module.

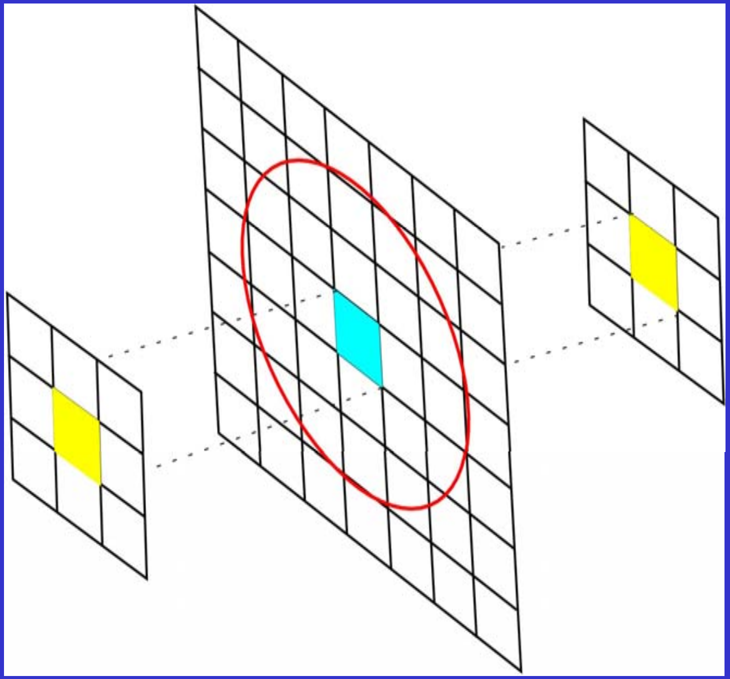
What is this AVL method?

- AVL is a self-balancing search tree structure.
- It is designed to store sparse matrix elements that need frequent updating, with fast search algorithm.
- Trees don't store nonzero elements, can be accessed quickly and interchanged among procs.



Domain decomposition (1)

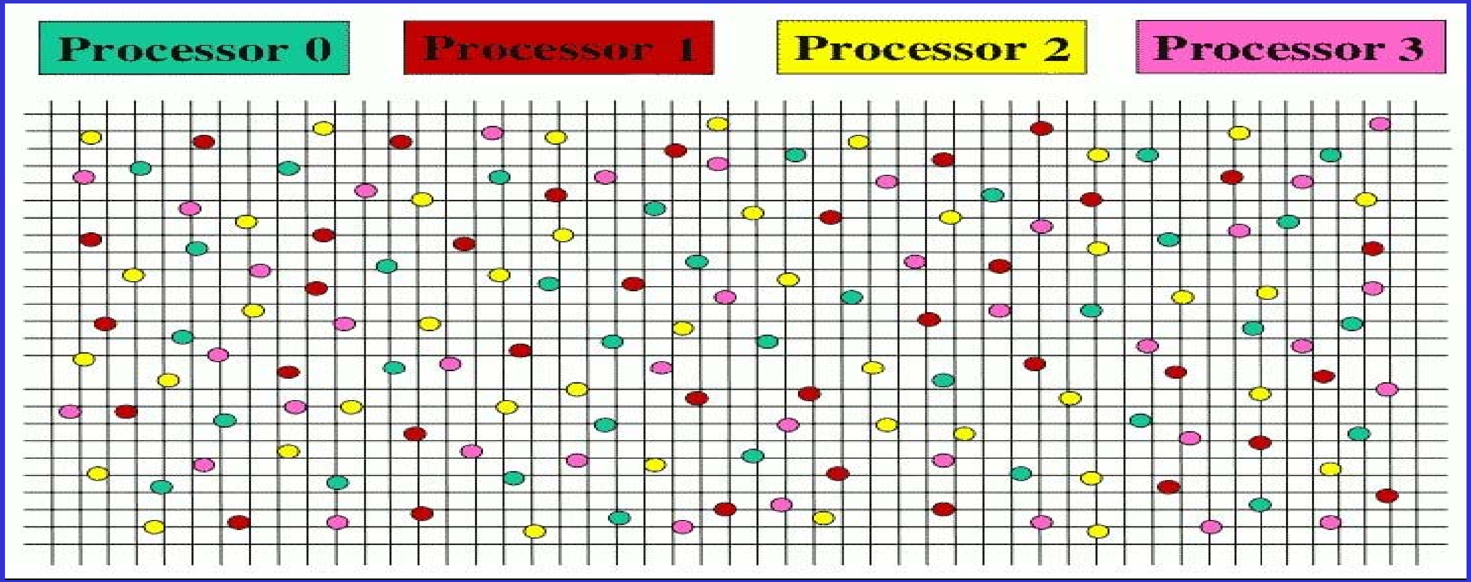
- Goal is to further reduce memory consumption
- A certain particle only affects its toroidal plane and locally the neighbouring ones.

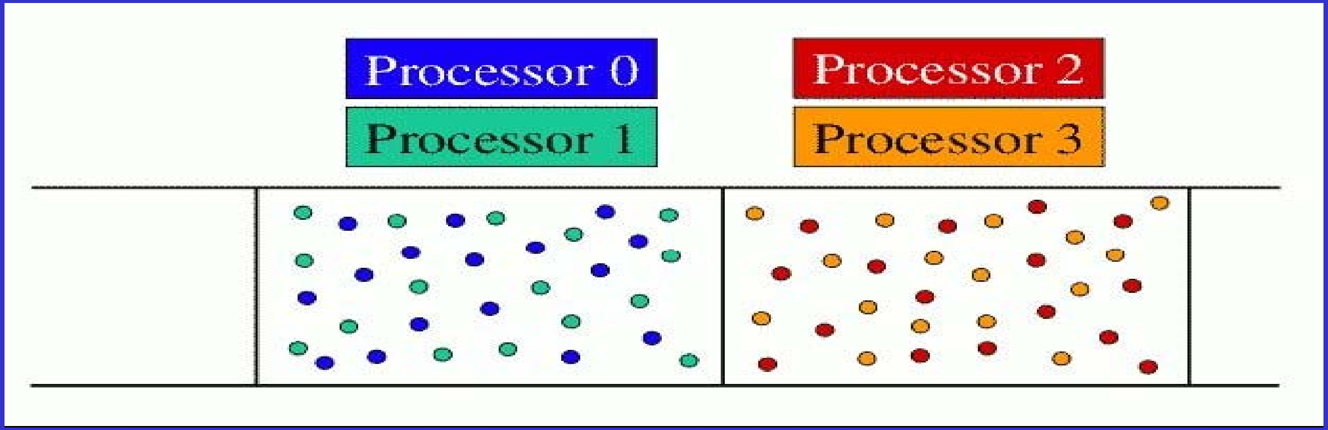


- If we keep process particles inside a toroidal domain, their coefficients will NOT span the whole torus.
- Particles have to be transferred to the proper domain every time they cross toroidal domain boundaries.

Domain decomposition (2)

- Original particle distribution





- Distribution under toroidal domain decomposition

Section II
Benchmarking of ELMFIRE

Testing ELMFIRE

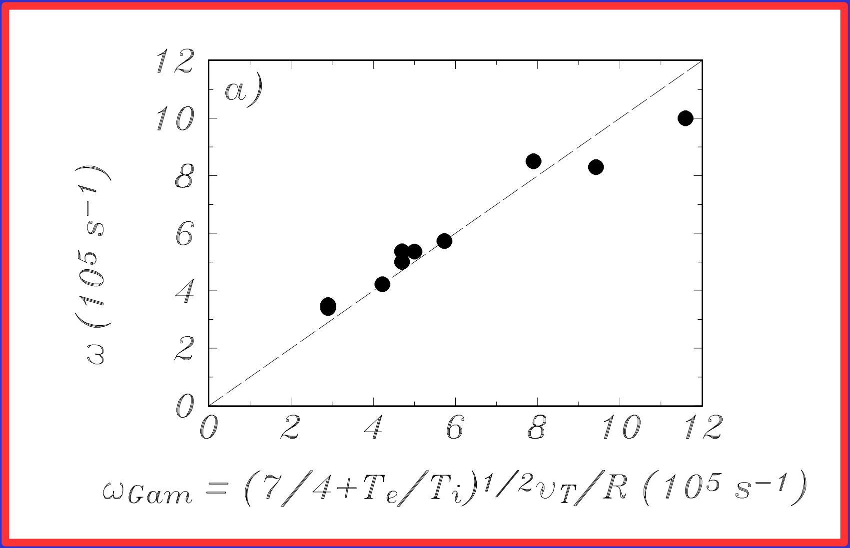
- Comparison to neoclassical theory in the presence of turbulence.
  - Frequency of GAM and Rosenbluth residual.
  - Neoclassical radial electric field.
- Comparison to other codes has been done in the well-known Cyclone Base cases.
  - Linear growth of unstable modes and their phase.
  - Nonlinear saturation of transport
- Comparison to experimental results.
  - Collaboration with IOFFE Institute and St. Petersburg Polytechnic working with the FT-2 tokamak.

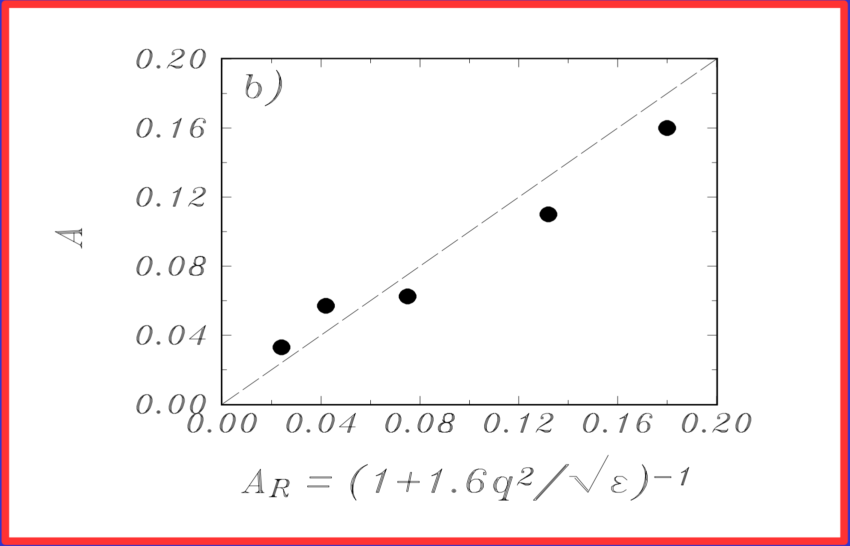
Geodesic Acoustic Modes

- Neoclassical theory predicts GAM frequency and Rosenbluth residual.

$$w_{Gam} = \frac{v_{Ti}}{R}\sqrt{7/4+T_e/T_i} \qquad A_R = \left(1+\frac{1.6q_s^2}{\sqrt{r/R}}\right)^{-1}$$

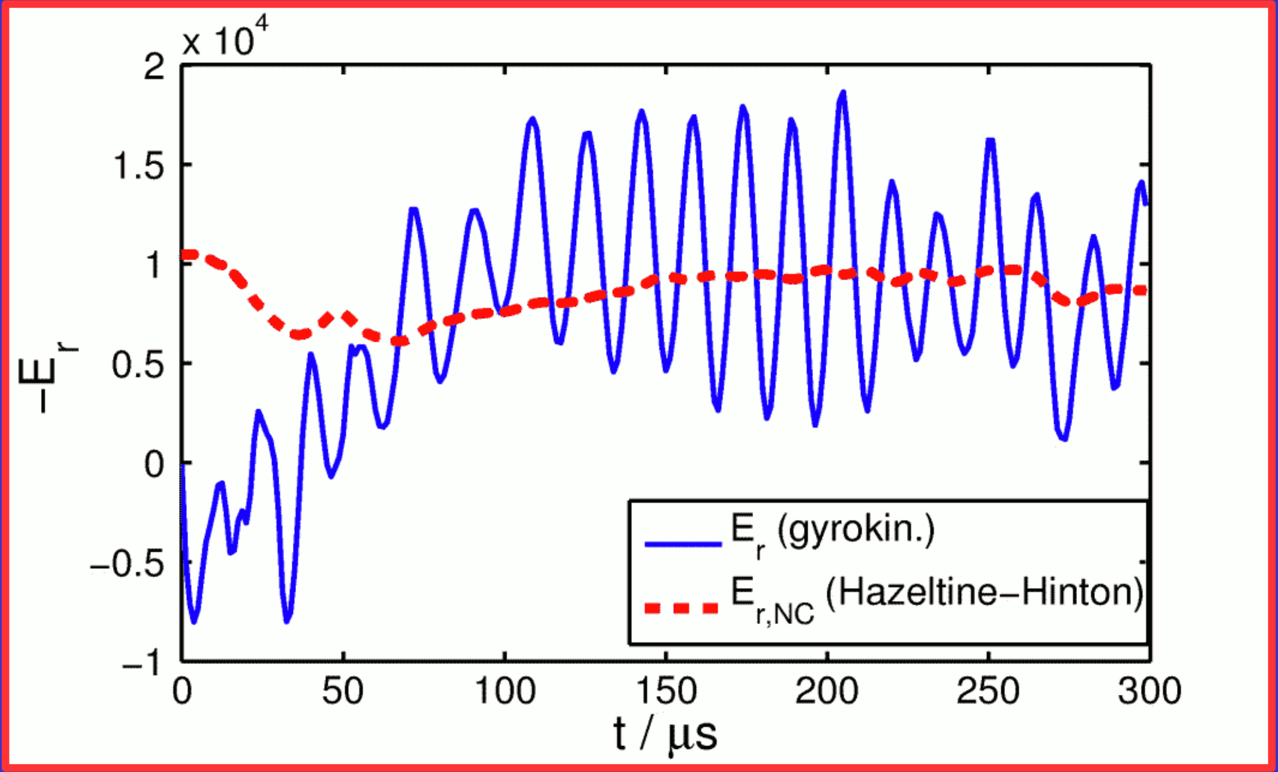
- Results show good wide agreement with theory.
- Simulations done on a plasma annulus.
  - R=0.3-0.9 m, a=0.08 m, B=0.6-2.45 T, q=1.28-2.91, Ti=90-360 eV, ni=5.1×10^{19}m^{-3} (r/a=0.75)





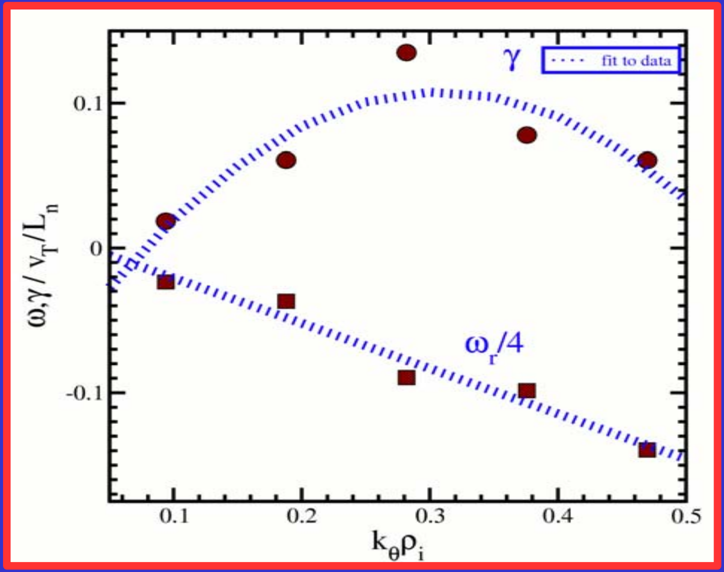
Neoclassical radial electric field

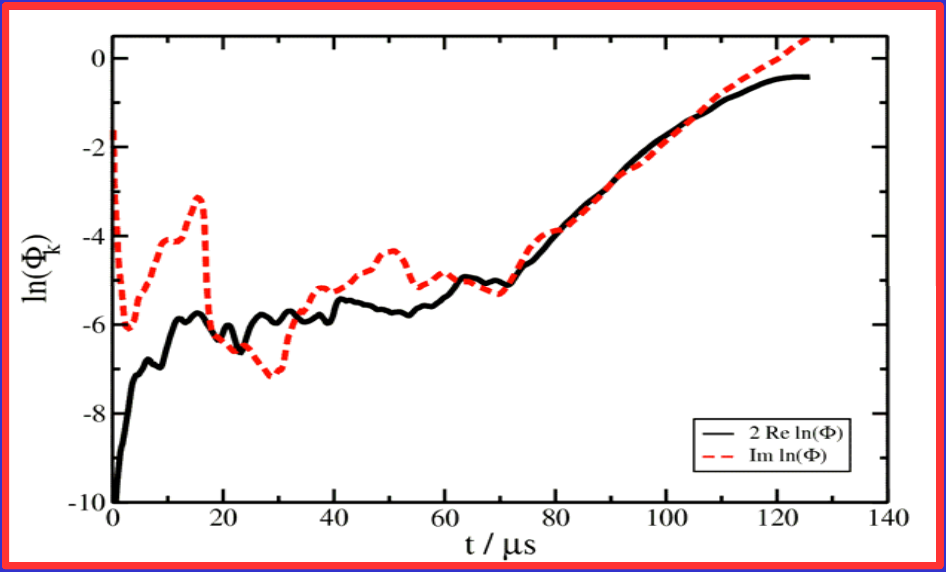
- Neoclassical radial electric field is well followed in conventional (L-mode) turbulent simulations both in radius and in time
  - R=1.1 m, a=0.08 m, B=2.1 T, I=22 kA, parabolic ion heated n,Ti,e profiles (r=0.04m).



Linear growth of unstable modes

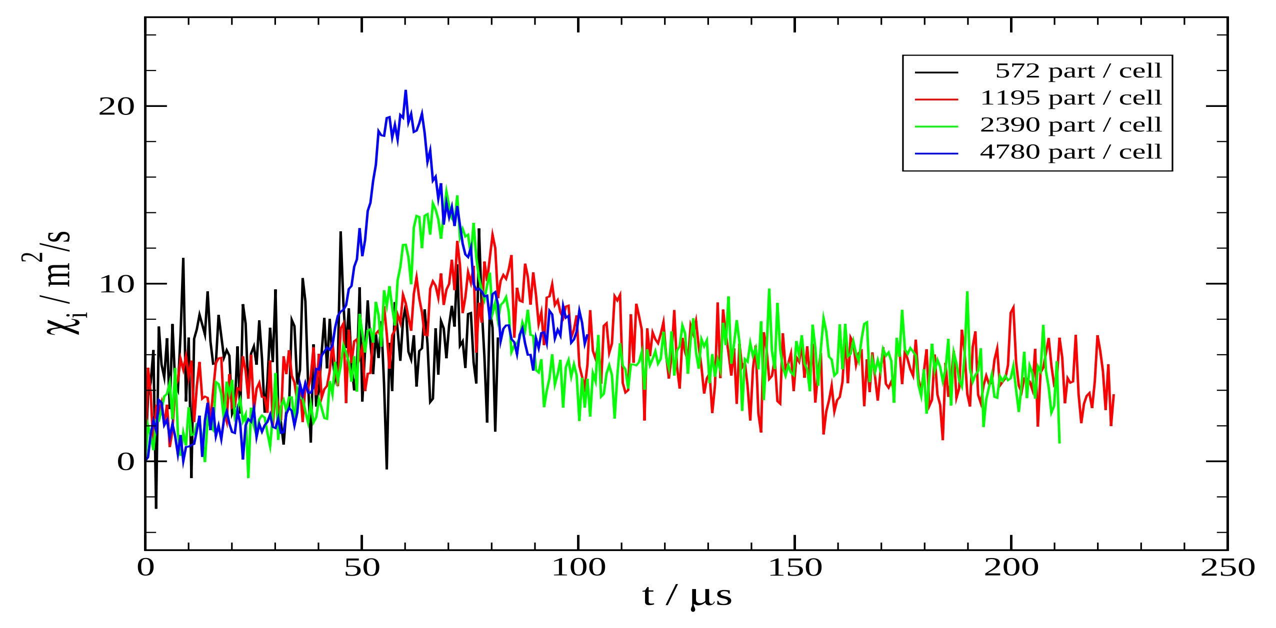
- Test based on adiabatic Cyclone Base Case (Dimits PoP '00)
  - Red points from ELMFIRE, blue line: fit from article.
  - Figures show growth rates and typical time evolution for a mode with $k_\theta\rho_i$=0.3





Evolution of thermal conductivity

- Evolution of χ_i is studied with nonlinear runs of Cyclone Base.
  - Measured at r=a/2 (q=1.4). Using kinetic electrons. $R/L_T=10$. Weak collisionality; T(a/2)=2000 eV, $n=5*10^{17}$ m^{-3}.
- Convergence requires a large number of particles per cell.



Section III
Influence of noise on results

Influence of noise on results

- Caused by finite number of test particles → unphysical density fluctuations, which produce fluxes that perturbate the solution.
- Associated diffusivity can be estimated from the radial particle shift during decorrelation time.

$$dr = \langle\Phi\rangle_{\rm rms}\tau/B\Delta y;\ \tau = \Delta z/v_{Te};\ \langle\Phi\rangle_{\rm rms} \approx \frac{T}{ne}\langle\delta n\rangle_{\rm rms} \ \rightarrow\ D = \langle dr^2\rangle/\tau \propto T^{3/2}$$

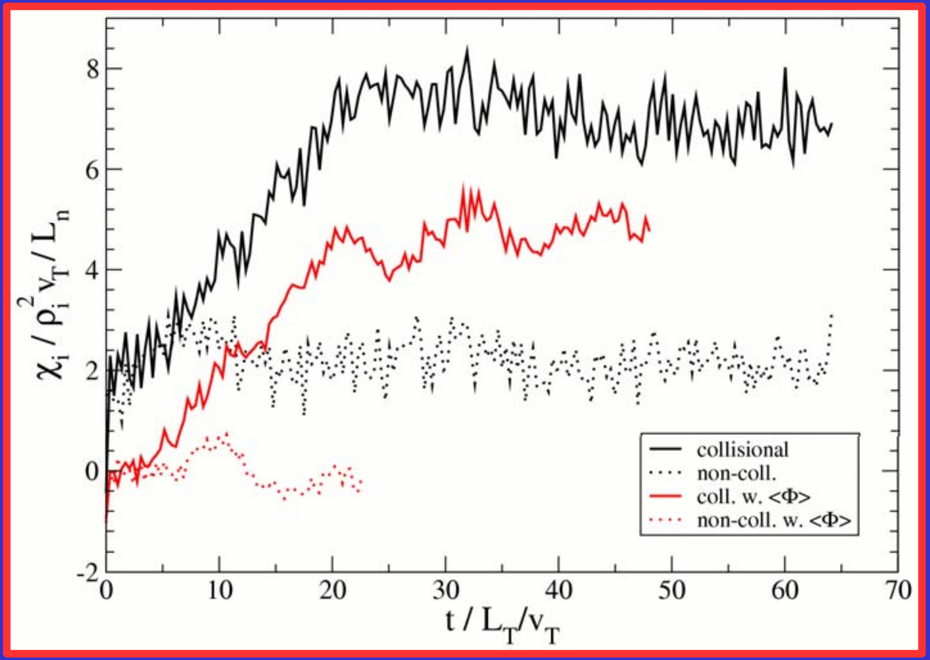
- Physical radial ion heat conductivity can be estimated from mixing-length estimate:

$$\chi = (5/2)(L_T/L_n)(v_{Ti}^2/\Omega_i)(1/k_\perp L_n)g; \quad \delta n = ne\Phi(1-ig)/T$$

Effects on calculated conductivity

- Image shows influence of strong collisionality and potential averaging on ion radial heat conductivity.
  - Collisionless cases show residual noise conductivity.
  - Noise is filtered out by averaging potential over flux surface.
- So far noise is reduced by “brute force” ... *higher N!*

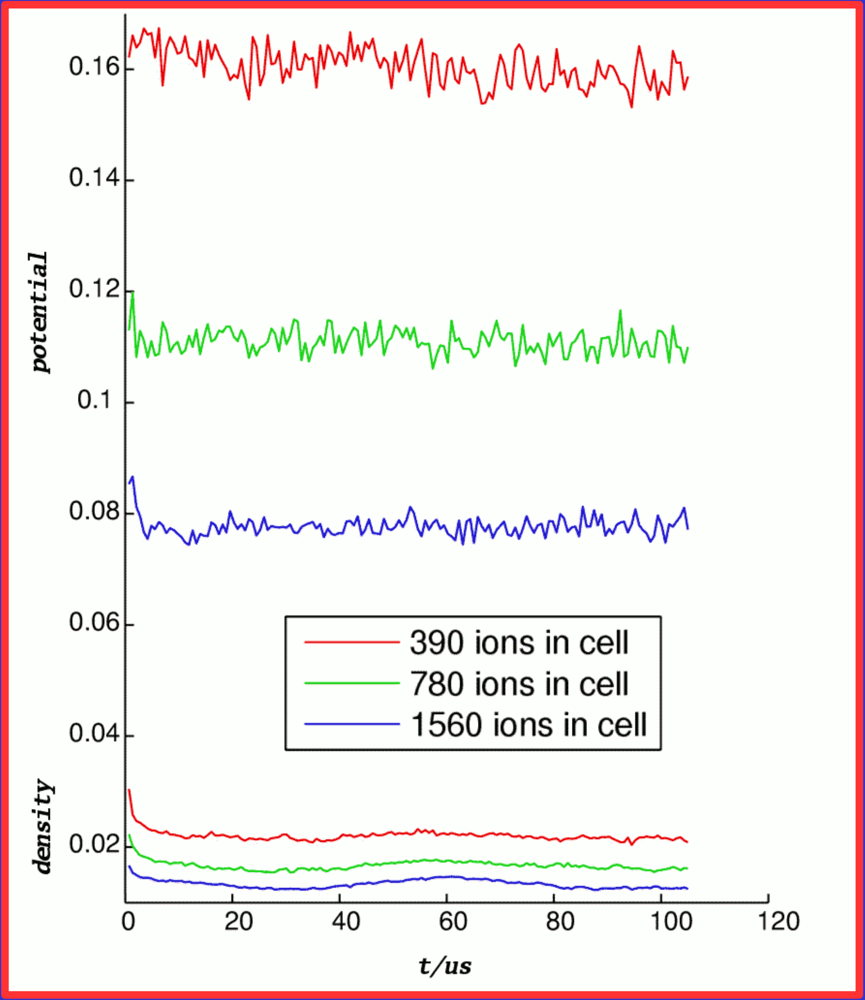
Scaled Cyclone Base Case with kinetic electrons; T=100 eV, n=4.5*10^{19} m^{-3}



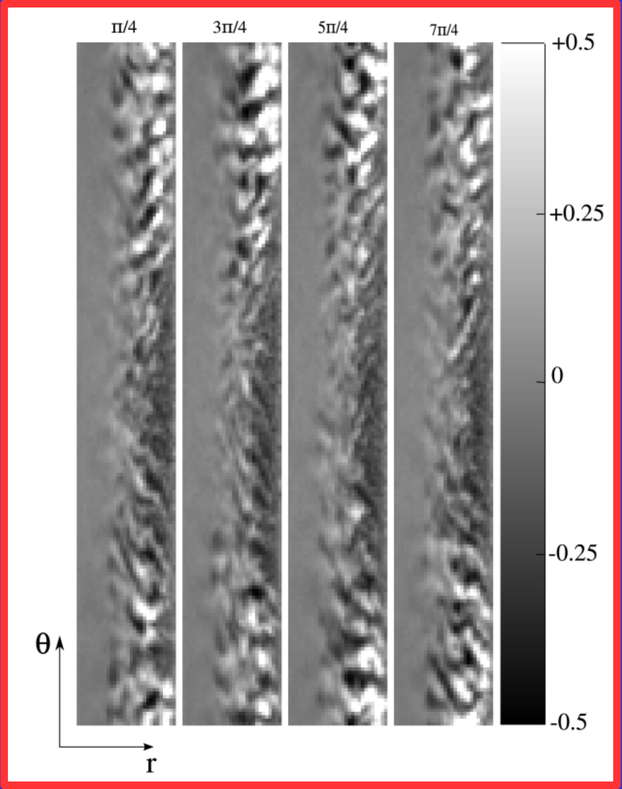
Problematic levels of noise

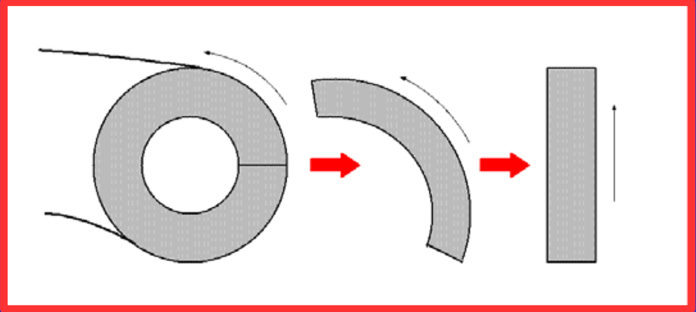
- Highest acceptable level of noise? → optimal use of CPU resources
- Figure show exceptionally bad case regarding noise effects.
- Density fluctuations remain almost constant in time.
- Regression shows almost perfect $N^{-1/2}$ scaling, indicating that results are dominated by noise.

Fluctuations @ r=a/2



but not always problematic...



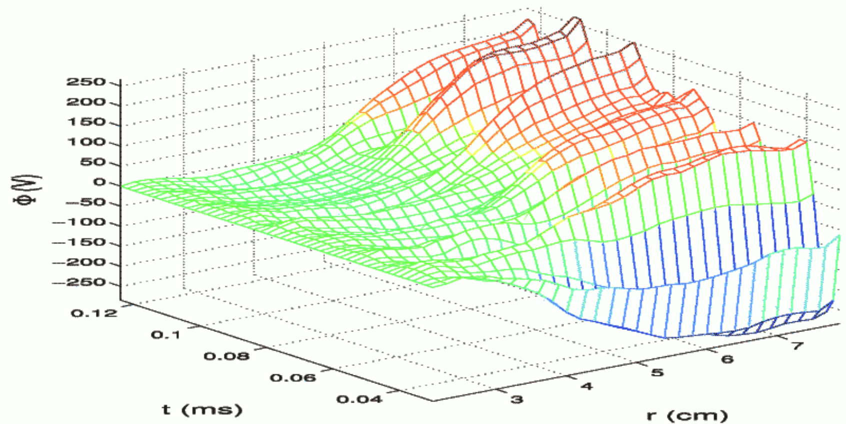


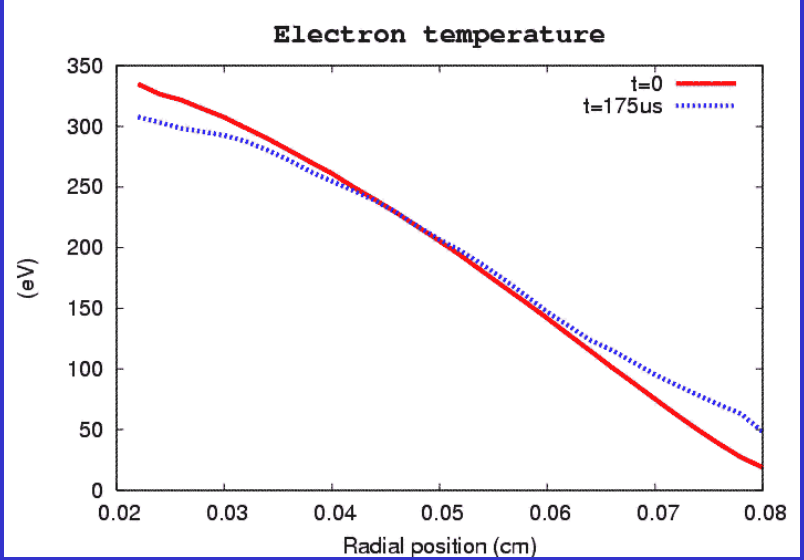
- In FT-2, fluctuation levels are much higher (10-40 %) than in scaled Cyclone Base Case (~ 1%)
  - So high perturbation level warrants the use of a full *f* scheme
- Image shows density fluctuations relative to flux surface average
- Relative importance of noise values can be seen in videos of both cases

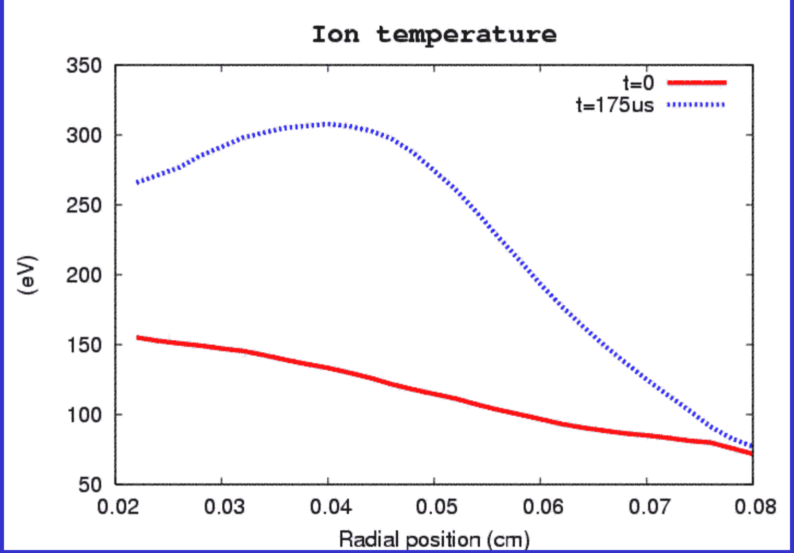
Section IV
Transport simulations

Case 1 under study: LH heated FT-2

- Heating phase for 100 kW LH heated 22 kA FT-2 tokamak (O^{8+} impurities included).

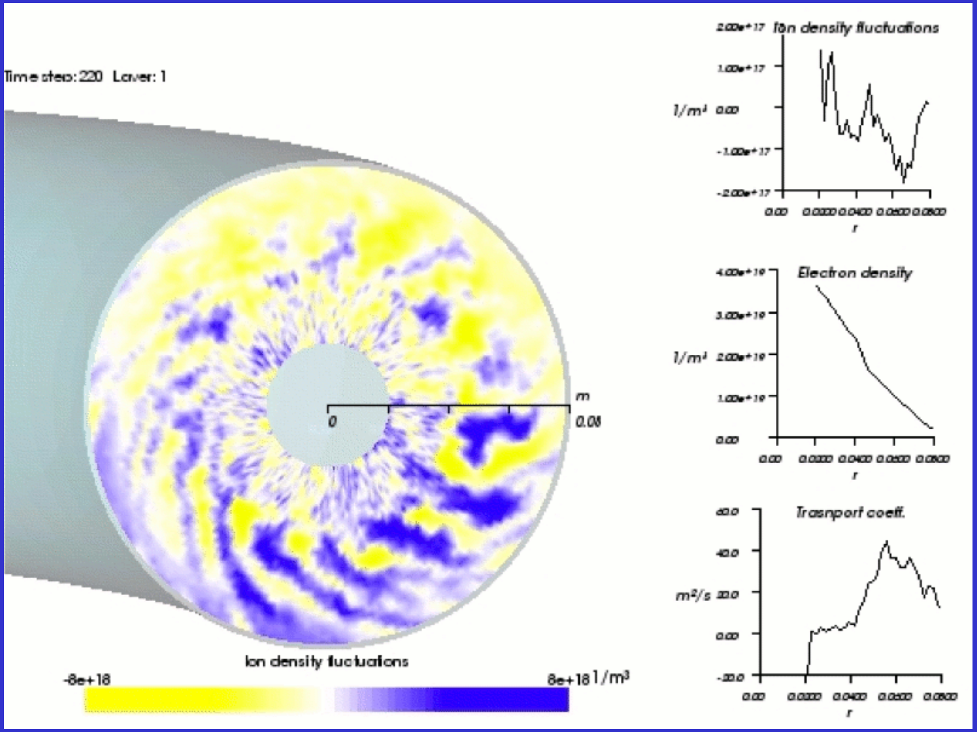


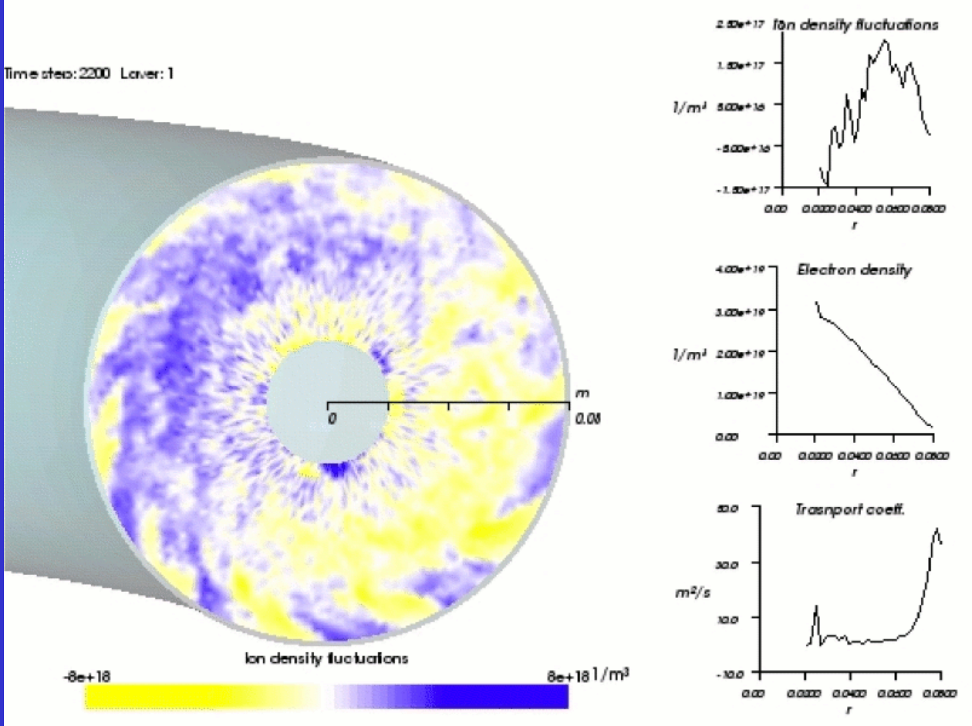




Evolution of large scale fluctuations

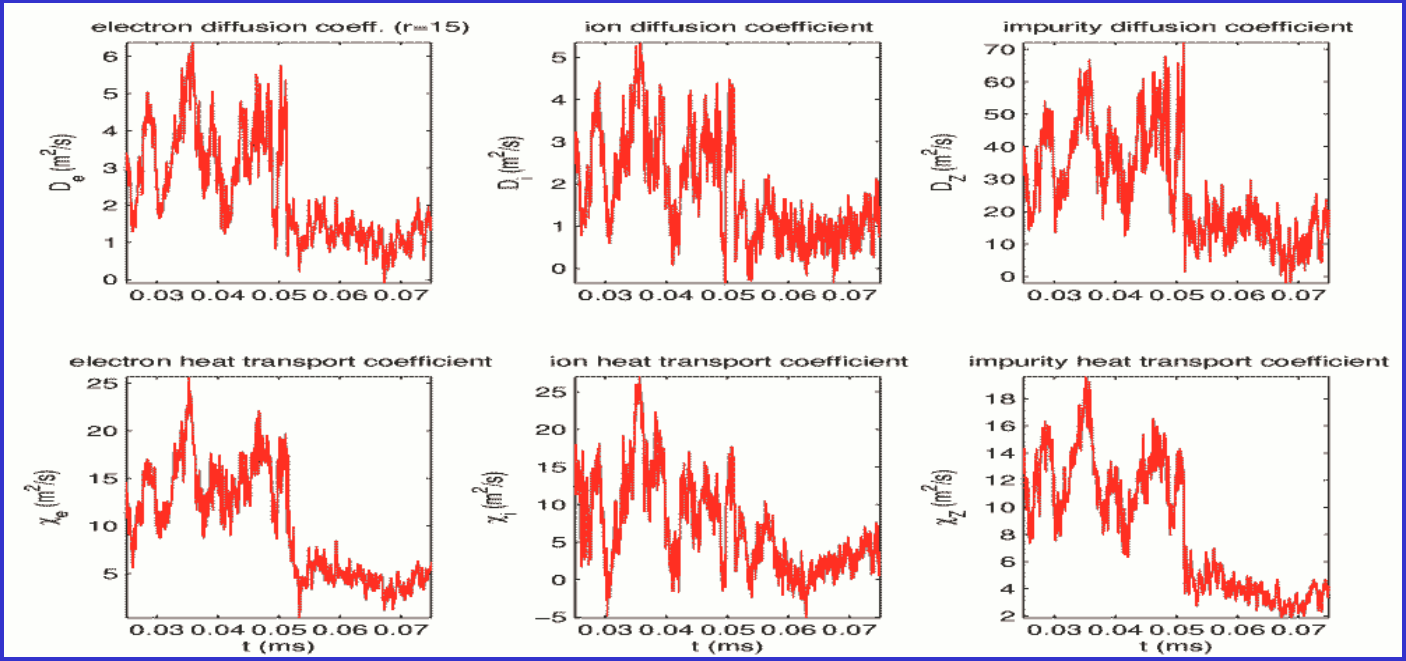
- Density fluctuations plots show the formation and further destruction of macroscopic structures





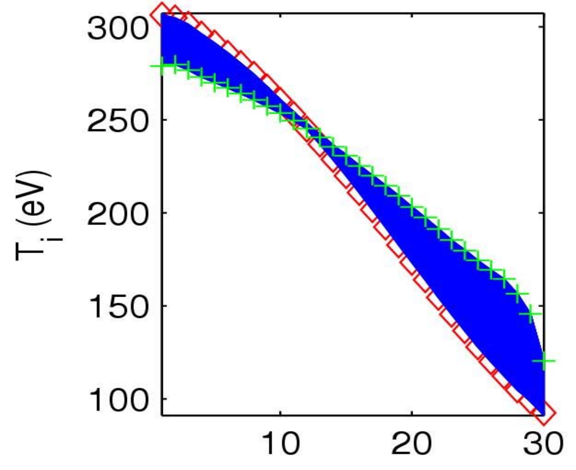
Evolution of diffusivity

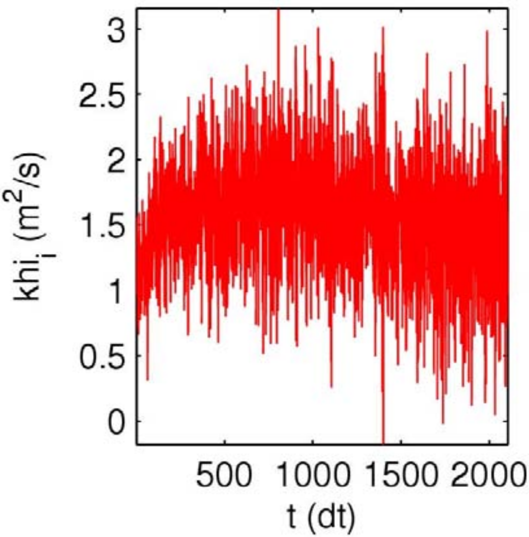
- Both particle diffusivity and heat conductivity drop drastically when poloidal flow shear destroys the turbulent structures
- The figures show values from the middle radius



Case 2 under study: ASDEX Upgrade

- Larger devices are more reactor relevant but also more CPU intensive to simulate → Deisa resources needed





- First results with AUG parameters are obtained (no confinement transition observed yet)

Section V
Resources and Deisa experiences

ELMFIRE requirements

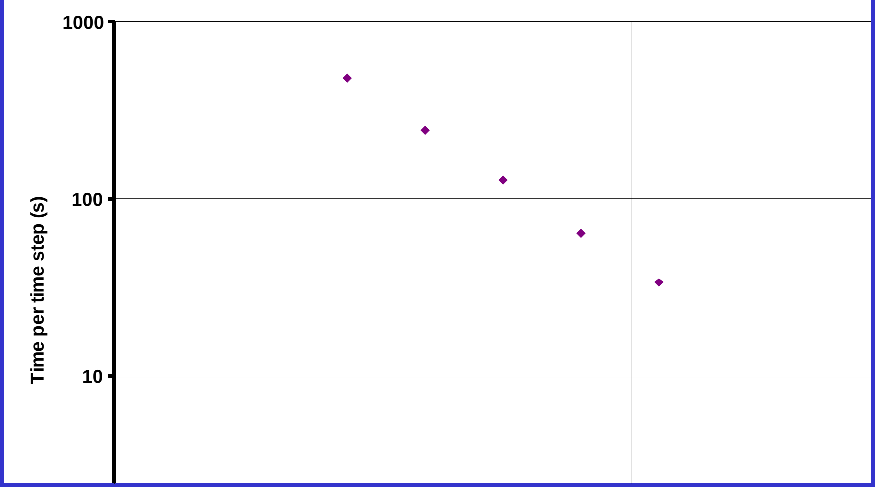
- ELMFIRE is a powerful code with excellent parallelization in most tasks.
- CPUtime (T) is directly related to the number of markers being treated in a single processor (N_p/P).
- Memory usage (M) is proportional to the size of grid (G), since it is not properly splitted among processors.
- The number of particles per cell lies in certain limits.
- $T \sim N_p/P$; $M \sim G$; $N_p \sim G$ -> $M \sim P*T$

Available resources (at CSC)

- CSC (The Finnish IT Center for Science) provides shared use of high-end parallel computers.
  - IBM eServer cluster 1600. 512 processors with 2.2TFlops, 384GB RAM and High Performance Switch communication.
  - Cluster of 768 AMD OpteronTM processors up to 3.2TFlops, 1600GB RAM, Infiniband network.
- Cray XT4 (Hood): 70TFlop, 70TB RAM; HP ProLiant Supercluster, 10.6 Tflop, 100 TB

Scalability

- IB-new = Sepeli with InfiniBand and optimized parallelization
- IB = Sepeli with InfiniBand
- LAM = Sepeli with Gigabit Ethernet
- IBM-new = IBM with optimized parellelization
- CSC (The Finnish IT Center for Science) provides shared use of high-end parallel computers.



DEISA experiences (1)

- ELMFIRE project “fullfgk” was granted computation time in the Distributed European Infrastructure for Supercomputing Applications.
- ELMFIRE has access to a supercomputer in RZG, with up to 512 processors available.
- 165750 normalized CPUh were granted (comparable to total use of ~250000 normalized CPUh for ELMFIRE simulations at CSC during 2006)
- Machine architecture is the same as Ibmsc (CSC), so no big deal to use (compile libraries inside binary etc) → flexible use of both Deisa resources and resources applied from CSC

DEISA experiences (2)

- Characteristic for our simulation: lot of data as an output to be analysed
- Initial troubles with data transfer (which is slow): need to allocate time for this otherwise data is lost. This can be significant fraction of total CPU time allocated.
- Qeueing time sometimes quite long
- Not possible to check how the runs proceed → resources wasted sometimes

Conclusions

- ELMFIRE is a gyrokinetic full *f* particle code for simulation of tokamak electrostatic turbulence suitable for transport both for edge and core plasma
- Huge amounts of resources are however needed when using reactor relevant parameters → DEISA resources are gratefully acknowledged

ACKNOWLEDGEMENTS: Deisa consortium and CSC – The Finnish IT Center of Science for computing facilities.

CSC

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