Grid Computing for Fusion Research (Applications running under EGEE and EUFORIA Projects)

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Egee 2009, Barcelona

www.eu-egee.org

Information Society and Media

Contents

- **Introduction & Strategy.**
- **Application Ported (in the frame of EUFORIA & EGEE):**
  - ISDEP (EGEE & EUFORIA); Fafner (EGEE); MaRaTra (EGEE); Stellarator Optimization thru GA (EGEE); DKES (EGEE); EIRENE (EUFORIA); BIT1 (EUFORIA); GEM (EUFORIA).
- **Workflows**
- **Conclusions**

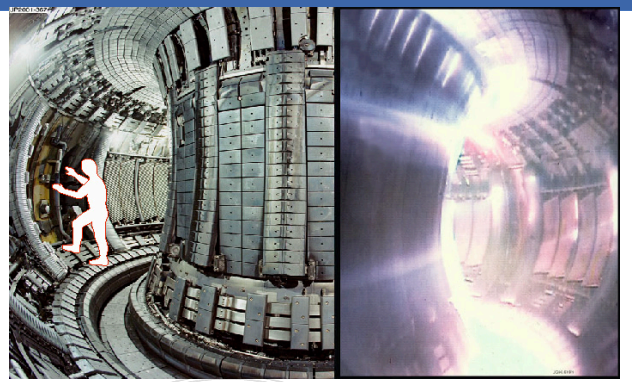
Introduction: Fusion Applications

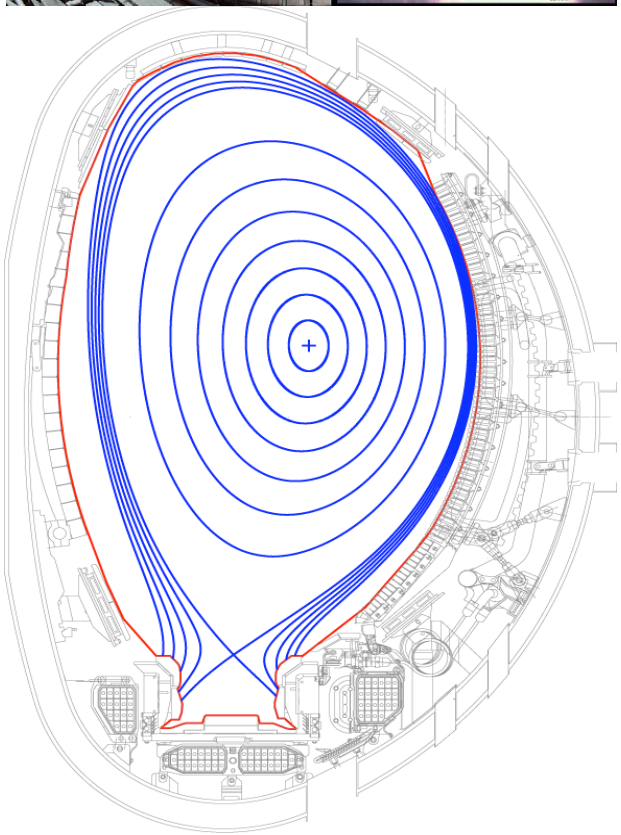
- High Computation Capability needed.
- A large Diversity of Disciplines in Plasma Physics: Complex Systems, Kinetic Theory, Fluid Theory, Waves, Non-linear problems,…
- Therefore: A wide Diversity of Applications.
- Some of them Suitable for the Grid:
  - Embarrasingly Parallel Problems.
  - MC codes.
  - Parameter Scan.

Introduction: The Strategy

- **BUT:**
  - **No use of the Grid before 2005.**
  - **2009: Limited use of the grid by fusion community.**
- **1) Port Applications that can be easily ported and produce results.**
- **2) Choose applications that act on different research fields with different porting techniques.**
- **3) Establish complex Workflows to show the grid Flexibility.**
- **PRODUCE RELEVANT PHYSCIS RESULTS THAT GIVE VALUE TO THE WORK.**

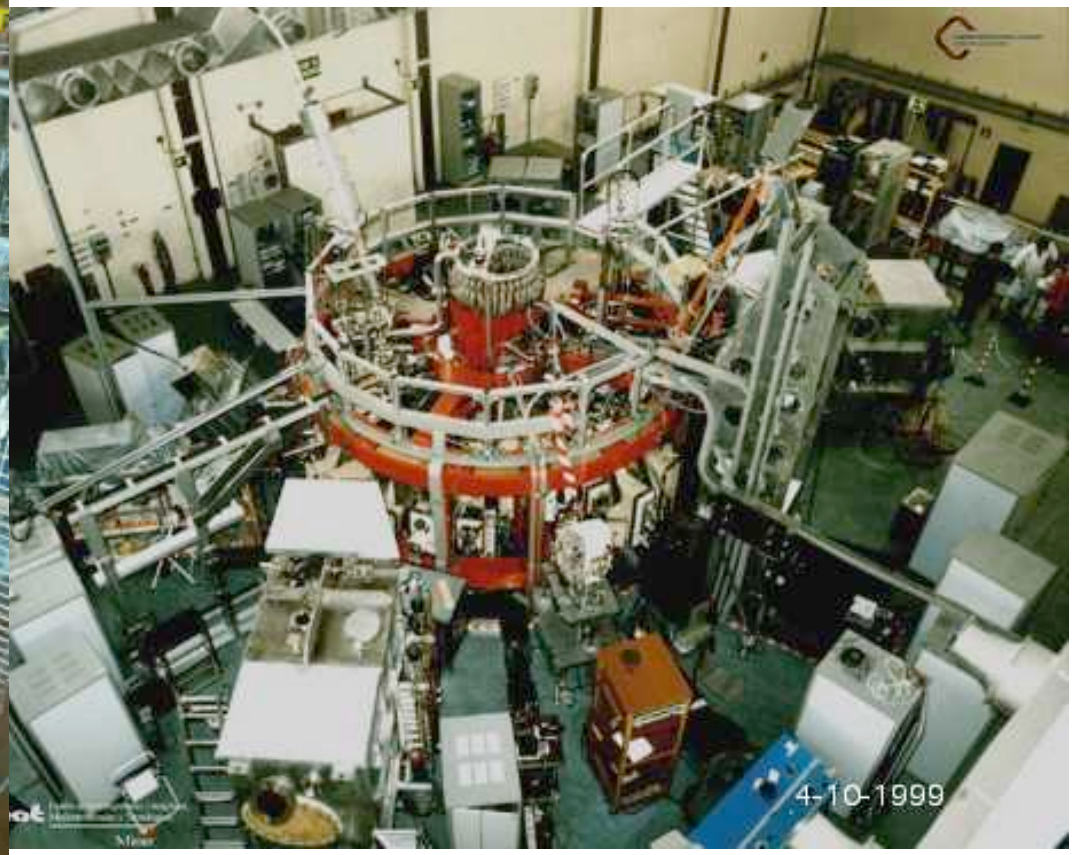
Introduction: Research Topics





- **Plasma-Wall Interaction and Edge Physics** (EIRENE, BIT1)
- **Transport:**
  - Collisional (ISDEP, DKES)
  - Turbulent (GEM)
- **Heating**
  - Microwaves (MaRaTra)
  - NBI (FAFNER)
- **Equilibrium and MHD** (VMEC, GA)

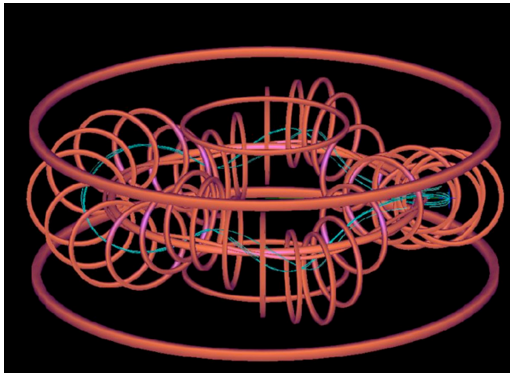
EXISTING DEVICES: Tokamaks & Stellarators.



- **Integrator of Stocahstic Differential Equations in Plasmas.**

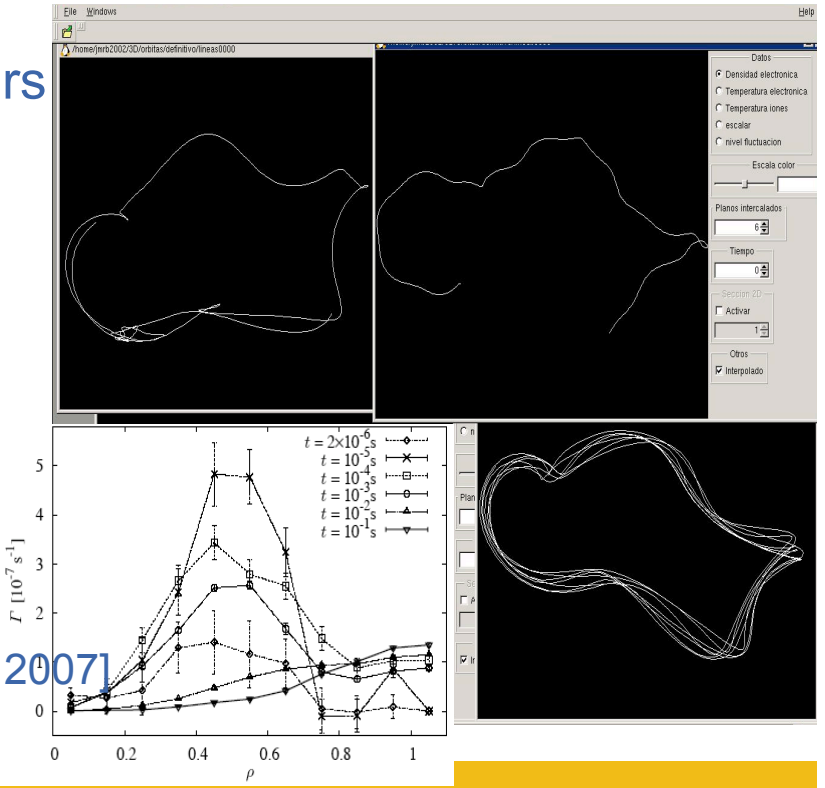
MC: Following independent particle orbits in a fixed plasma background (Geometry+density+temperature+electric field).

Background Plasma → To the Data Catalog



- 10^7 orbits(=jobs) x10 - 20 min≈10 CPU-years
- Based on gLite scripts.
- Launched also with Ganga&Diane
- Random parameters for every orbit.
- i-i & i-e Collisions plus electric field.
- No matter if some jobs are missed.
- Results: Statistical measurements.

[F. Castejón et al. Plasma Physcs and Controlled Fusion, 2007]



ISDEP: Further Developments

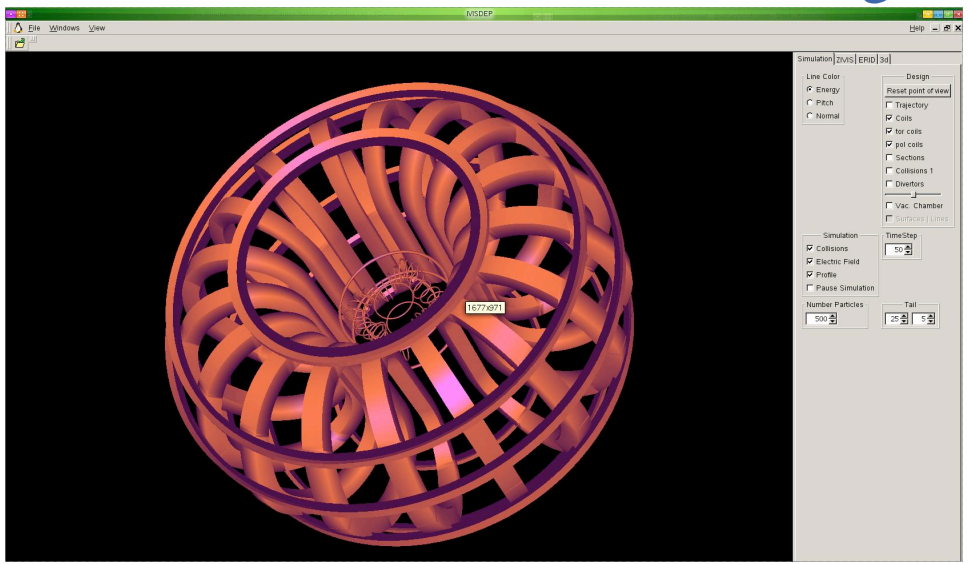
- ISDEP Developments:

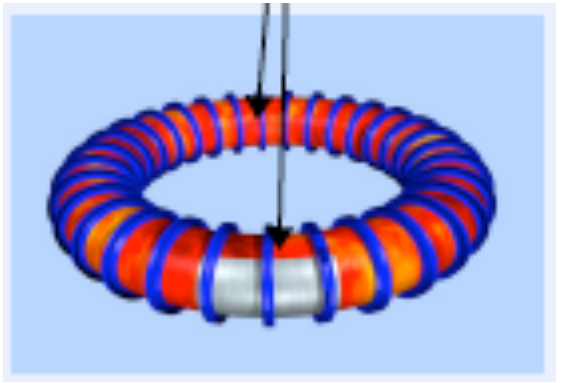
  Self consistent Plasma Profiles: Introduction of Non-linear effects.

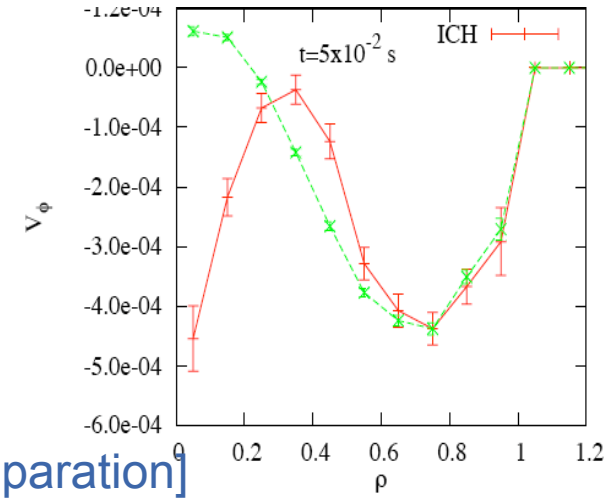
  Tokamak Geometry. (ASDEX, ITER)

  Ion Heating (ICRH).

  Benchmark with NC codes envisaged.







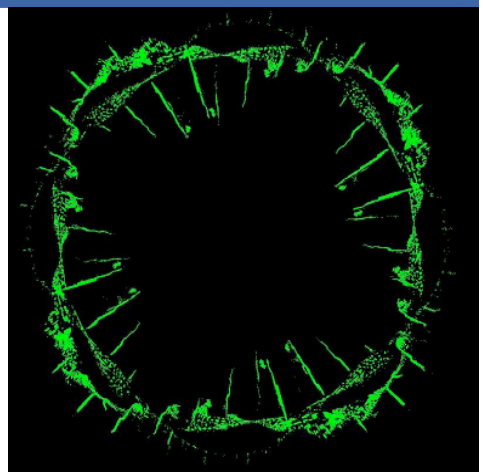
[A. Bustos et al. Fusion Science and Technology. In preparation]

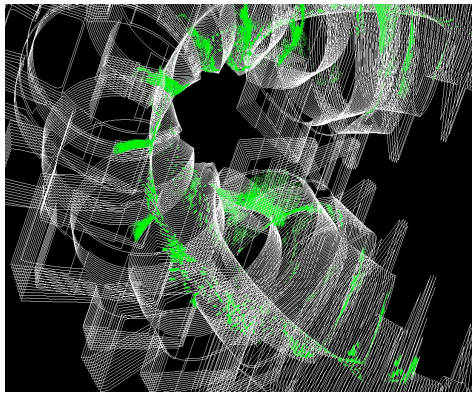
ISDEP: Divertor Studies

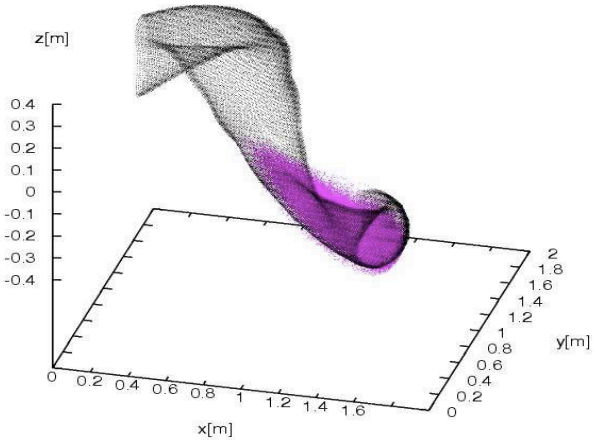
- **Divertor Studies: Study the fluxes on the vacuum vessel and try stop them.**
- Following ions until the vessel: 3D Map of Flux.
- Thermal and fast ions: Link with FAFNER.

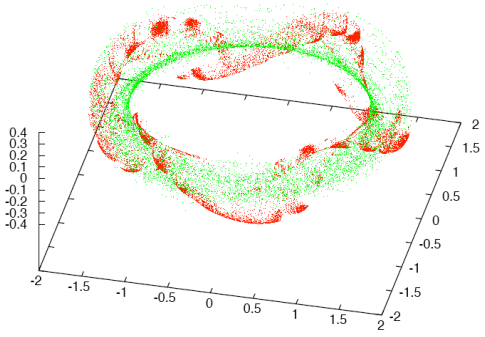
  Hit points on vacuum vessel.

[F. Castejón et al. Nuclear Fusion, 2009]









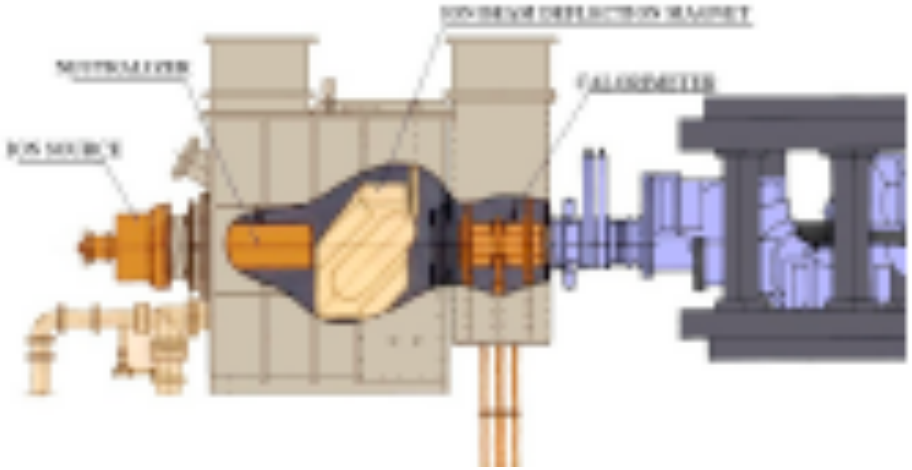
FAFNER

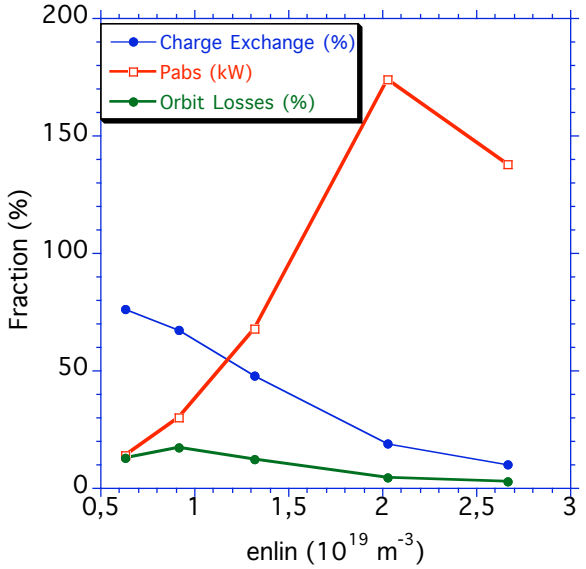
- **FAFNER2: MC code for NBI Heating.**

Launching hot atoms on the plasma.

Following trajectories of he energetic neutral atoms.

Gridway used.





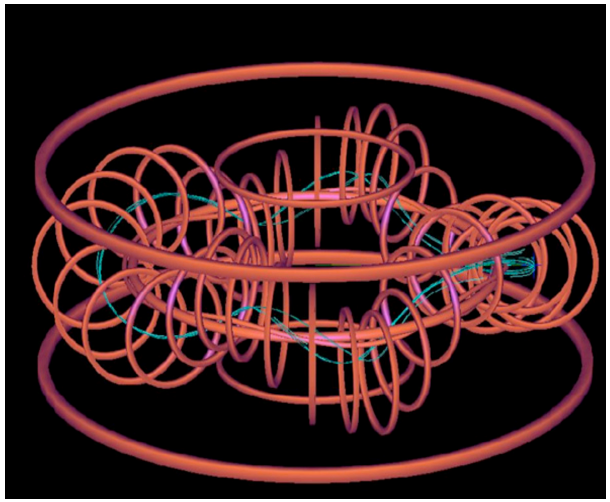
ISDEP: Non-Linear Calculations

- Kinetic 5D code (3D space + 2D velocity).
- Self consistent Plasma Profiles: Introduction of Non-linear effects.
- Update the plasma background with the results of the running.

30 times more CPU time consuming than the single case.

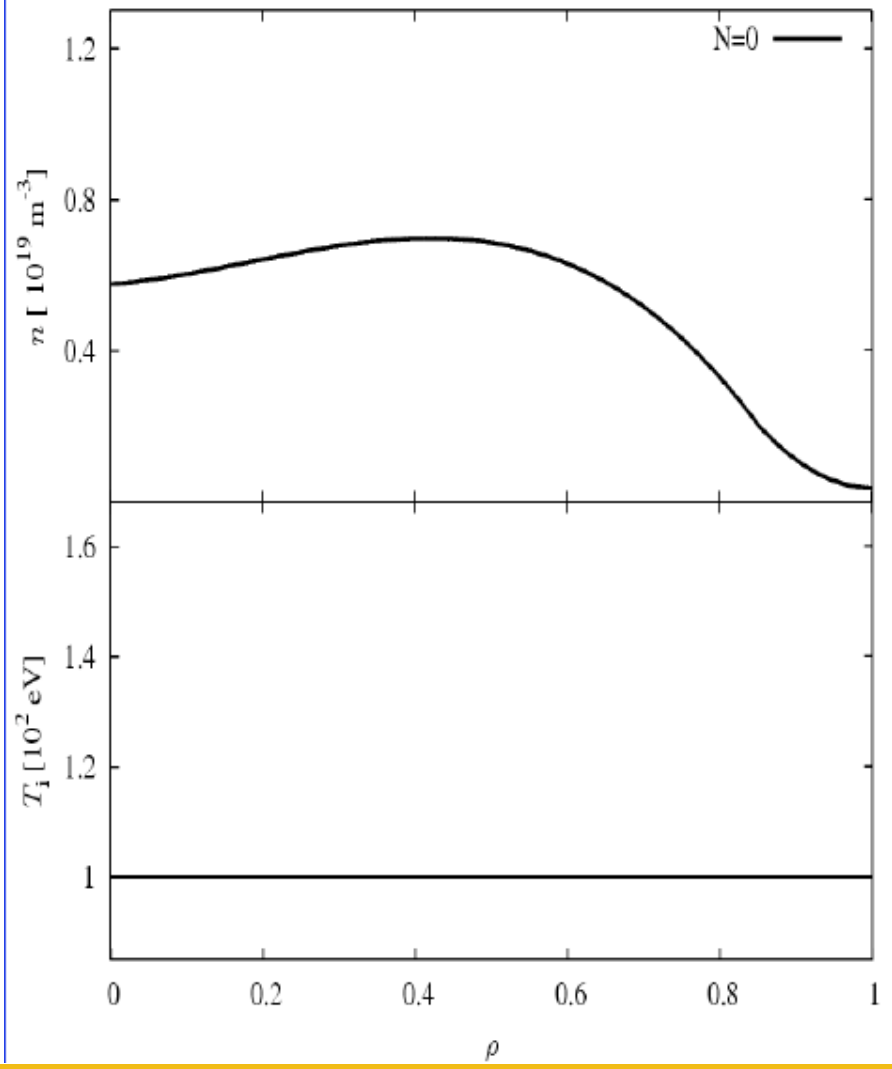
- Plasma Evolution obtained under changes.

[J. L. Velasco, et al. Nuclear Fusion, 2008]

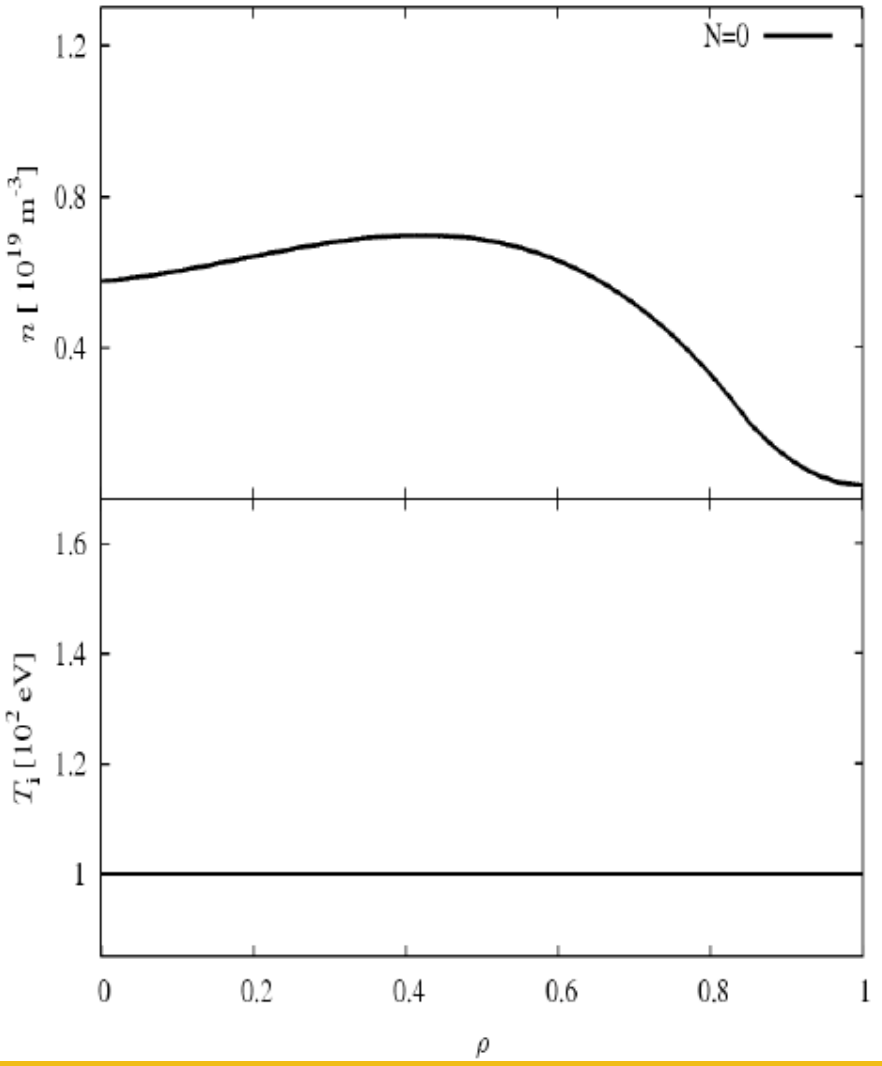


Self-consistent Scheme

$t=10^{-4}s$



$t=10^{-3}s$



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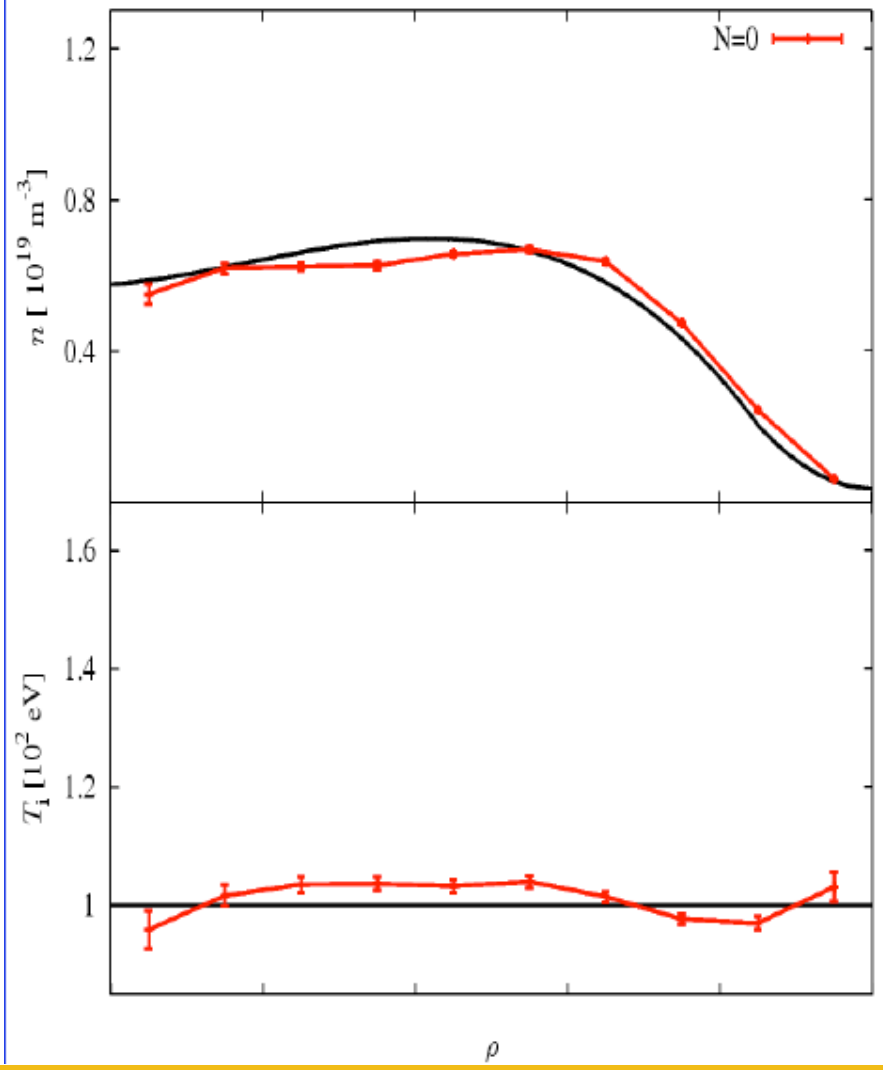

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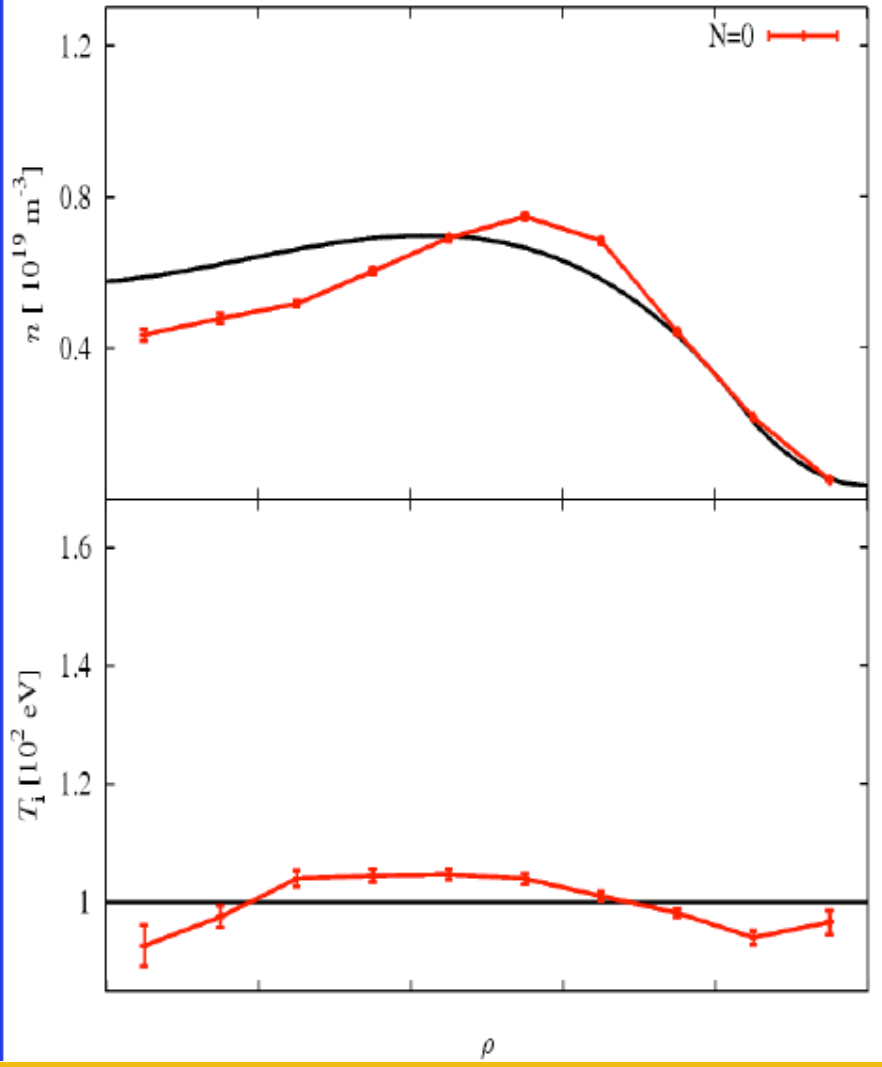

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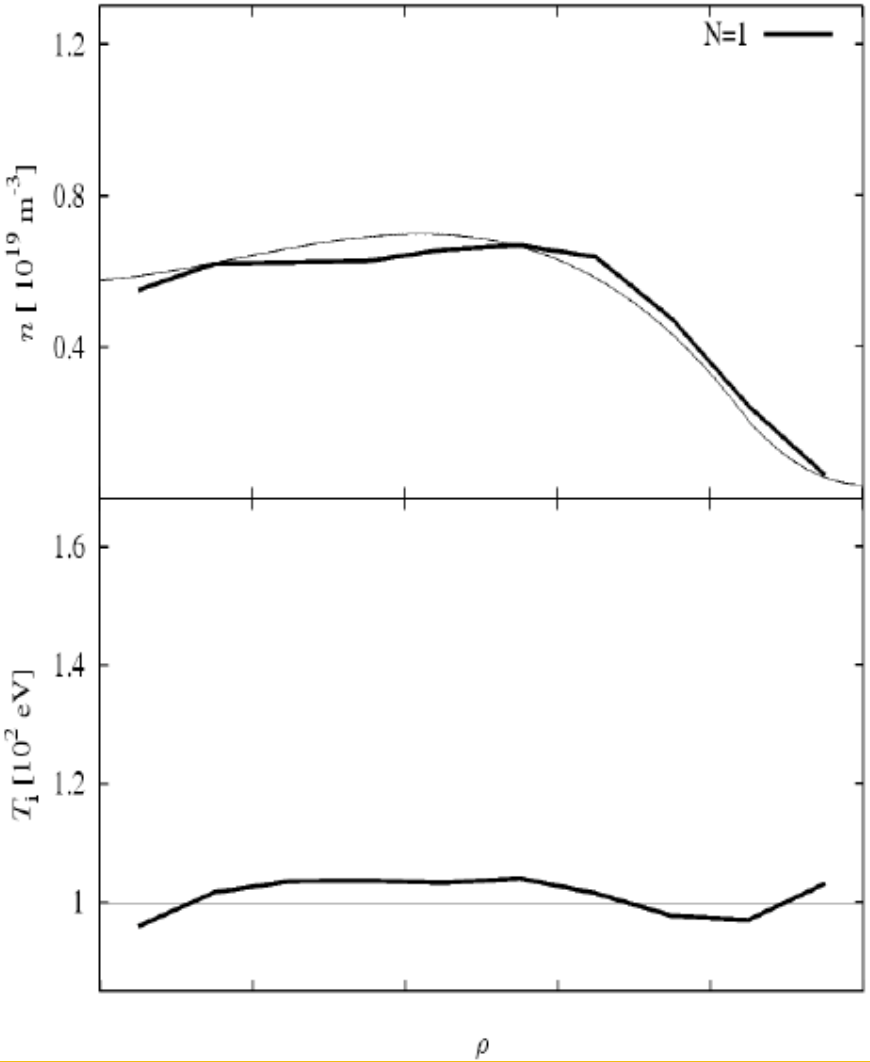

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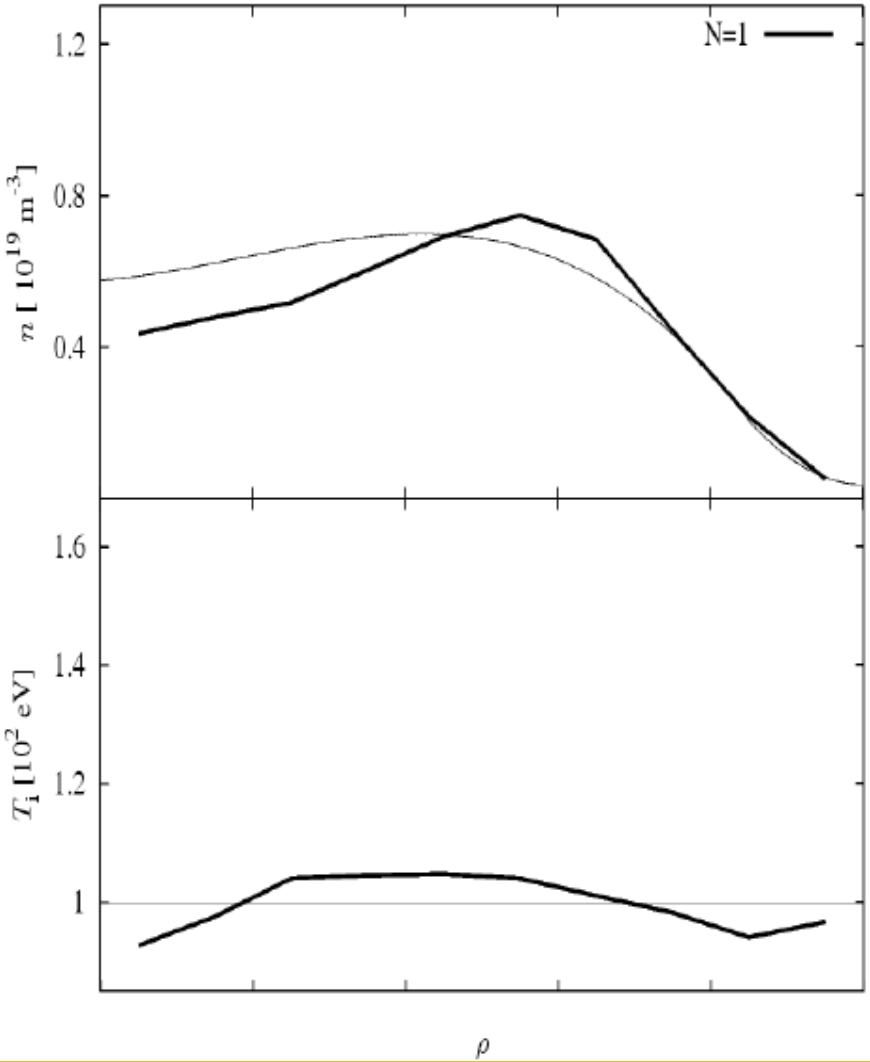

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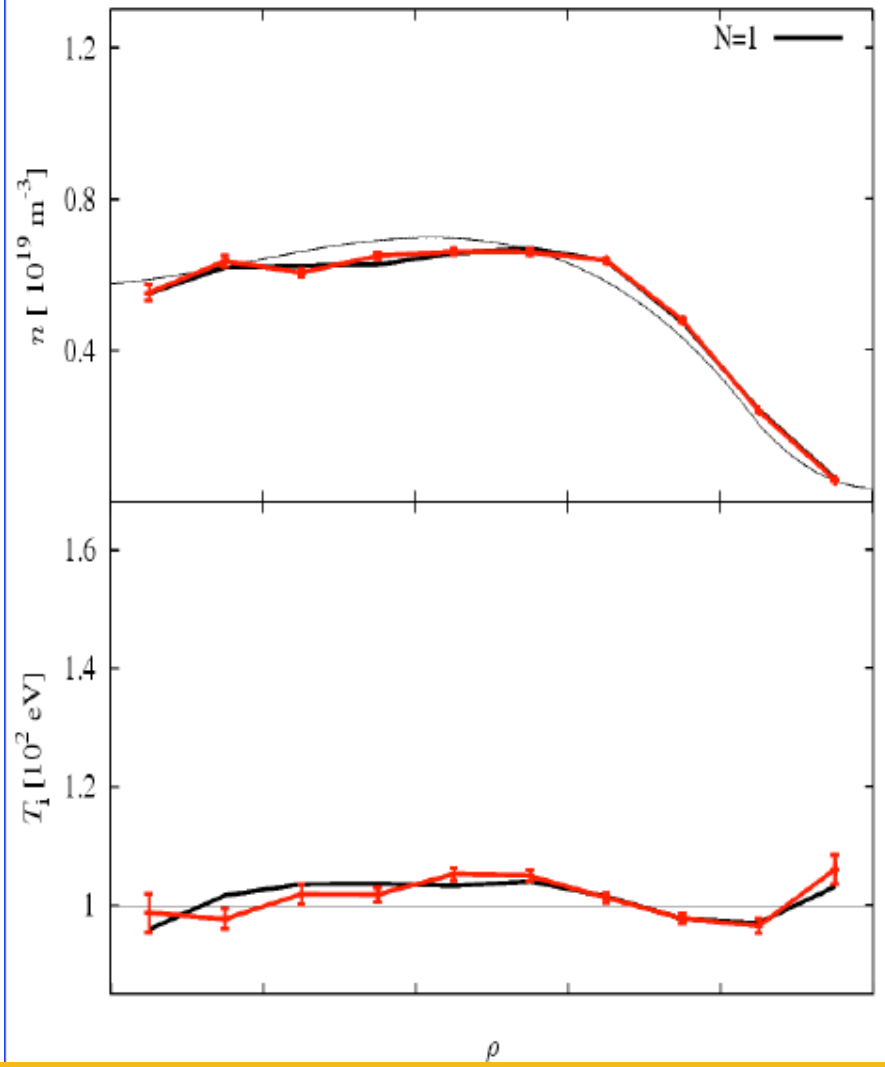
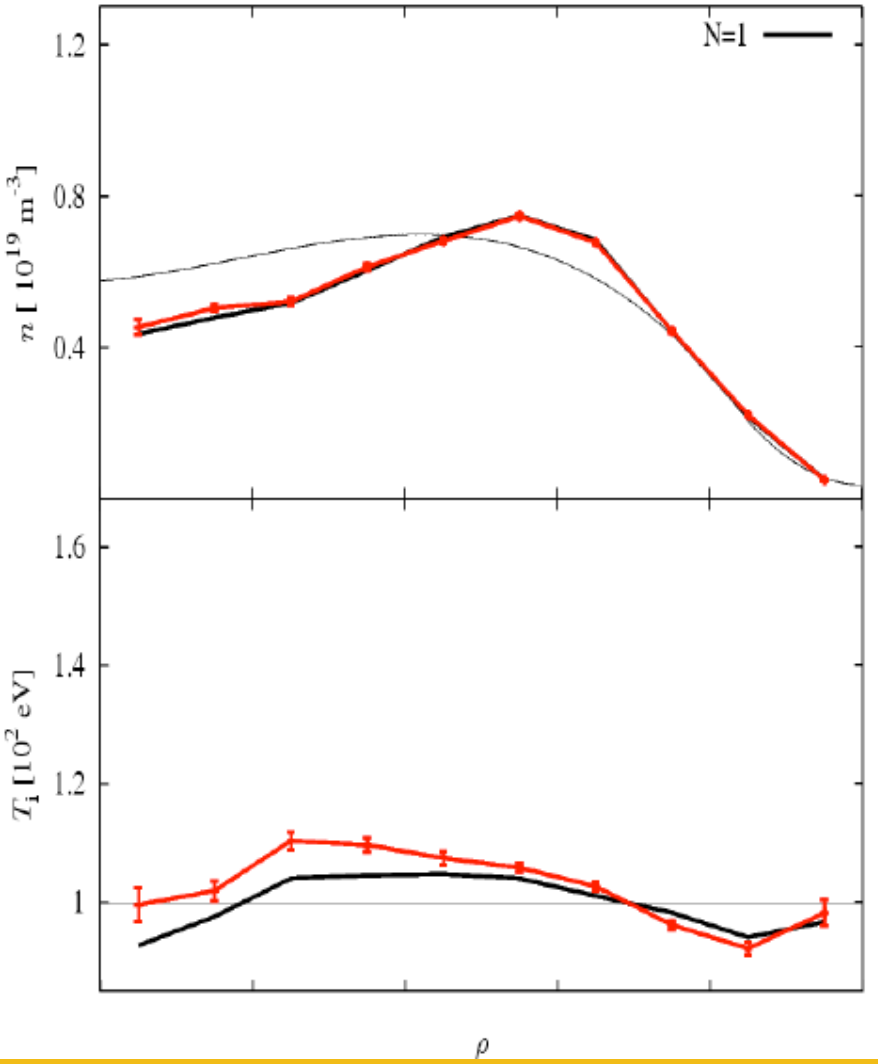
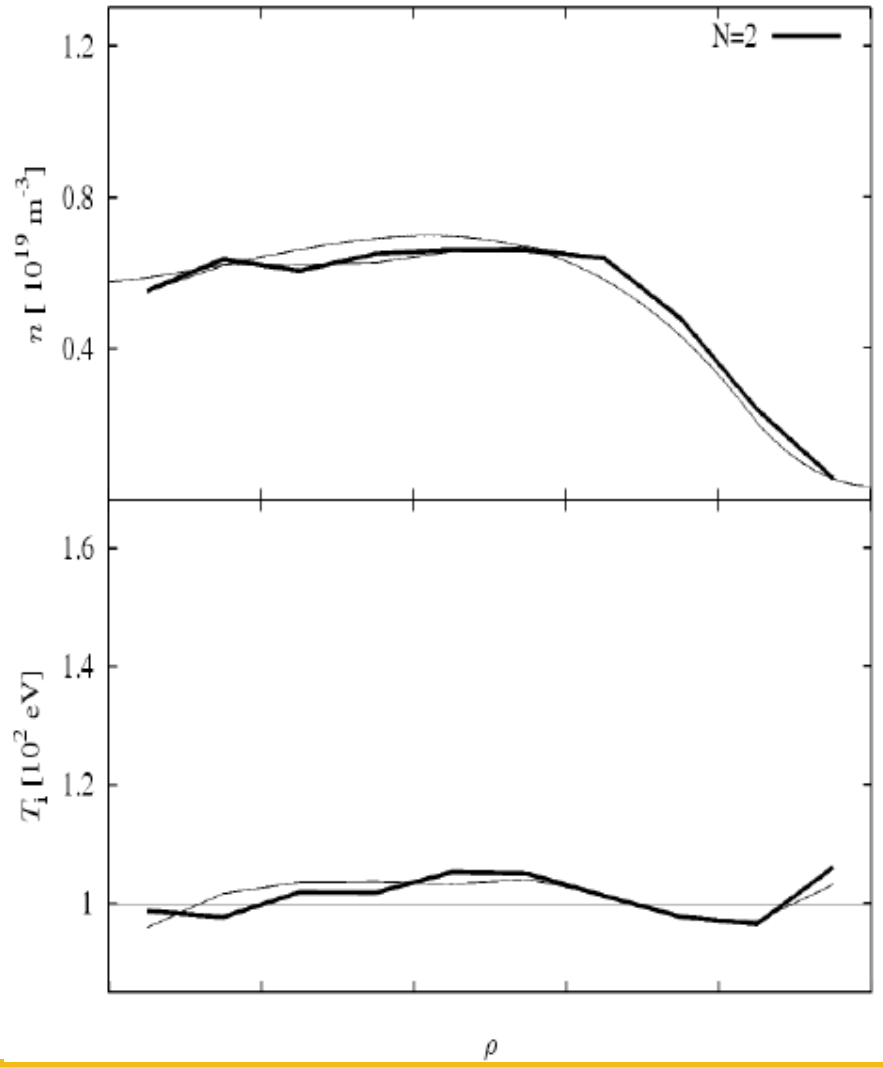


$t=10^{-3}$s

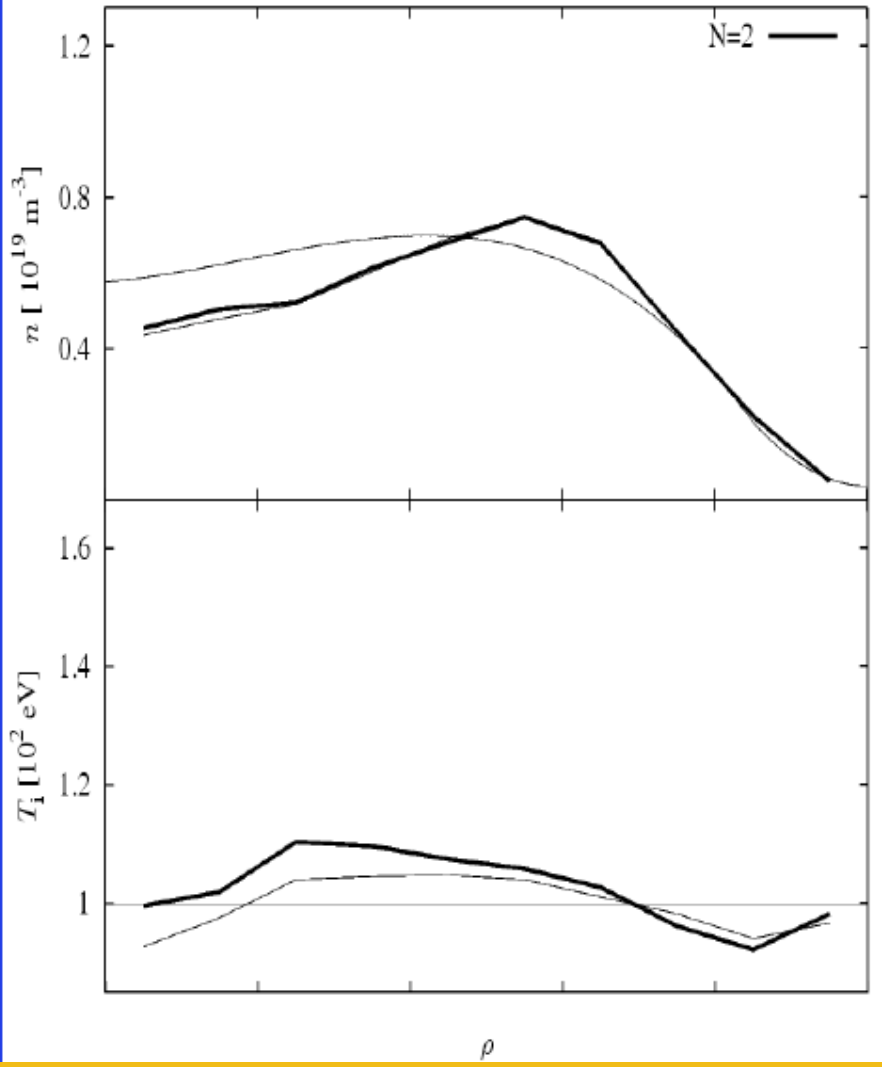


Self-consistent Scheme

t=10^{-4}s

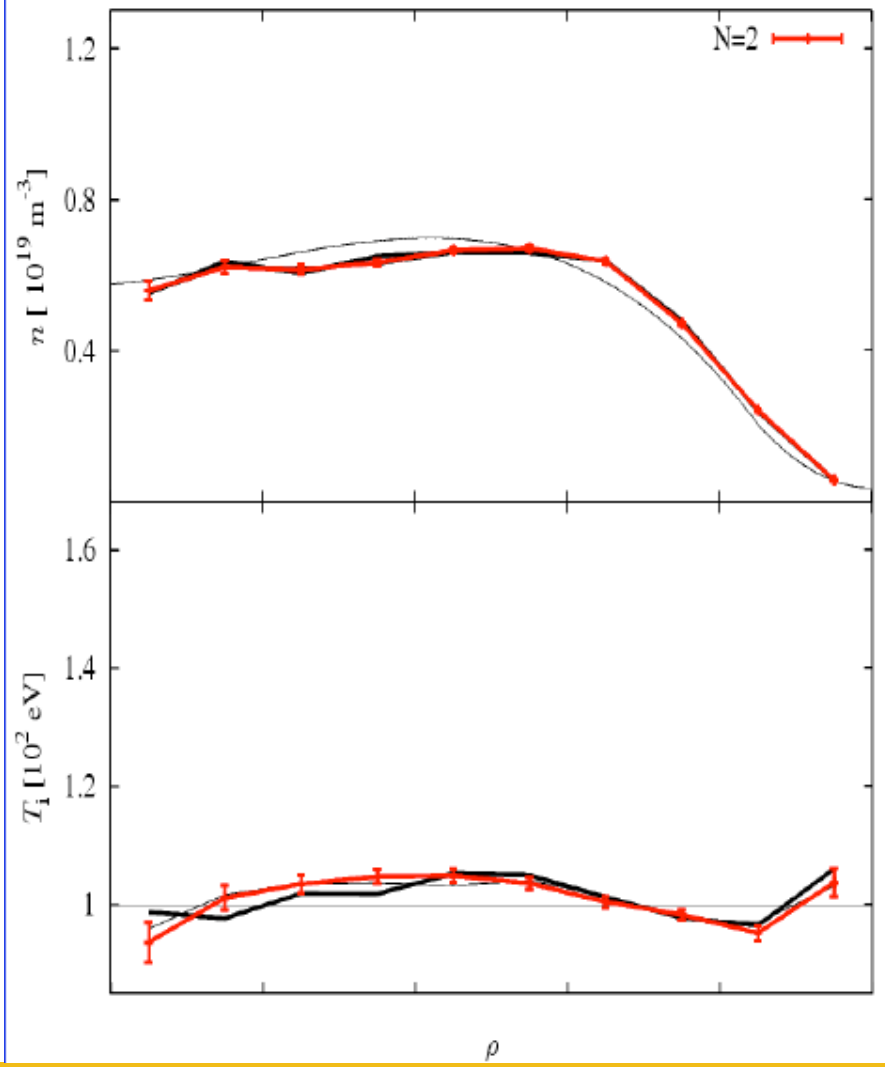


t=10^{-3}s

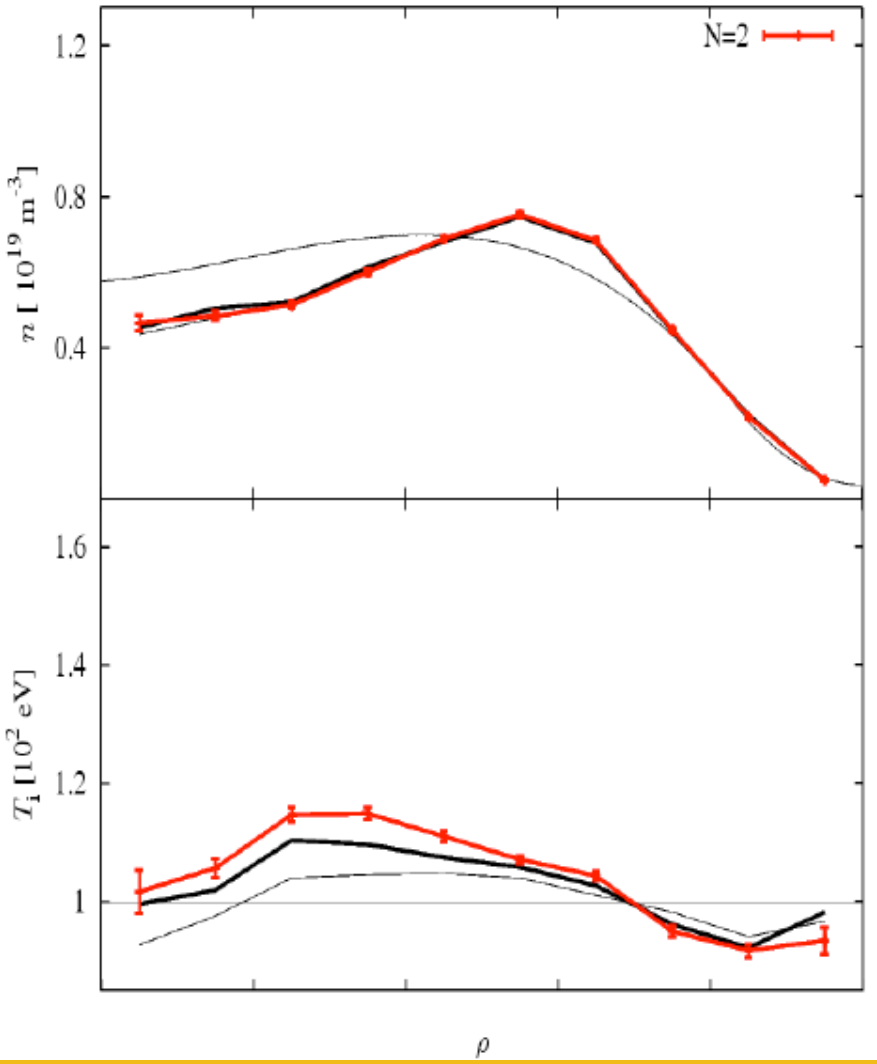


Self-consistent Scheme

t=10^{-4}s



t=10^{-3}s

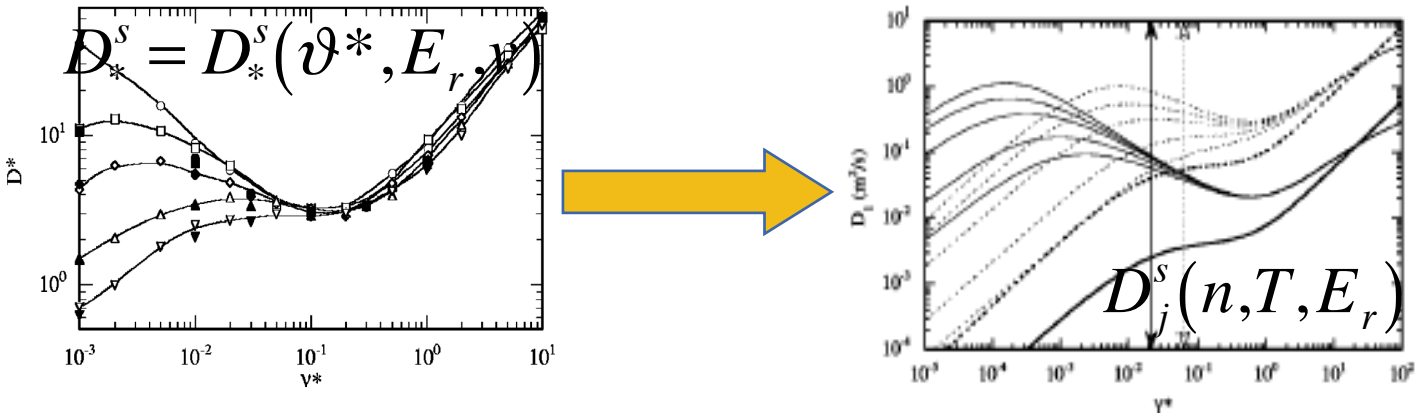


DKES

- **DKES (Drift Kinetic Equation Solver): STANDARD Transport Tool.** [A. J. Rubio. Submitted to PDP, 2010]

$$\Gamma^s = -D_1^s \nabla n + D_2^s \nabla T$$

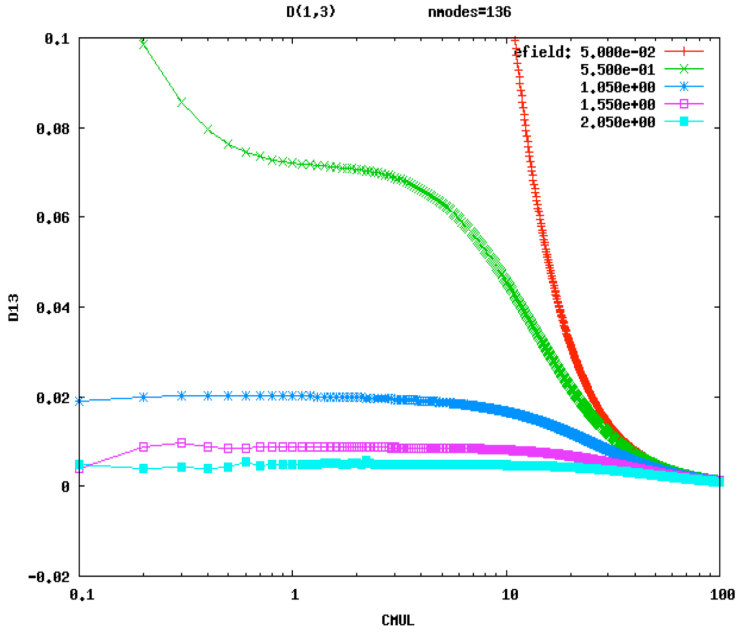
$$D_j^s = \frac{4}{\sqrt{\pi}} D_{Tok}^s \int D_*^s(\vartheta*, E_r, \nu) \left(\frac{\nu}{\nu_{th}}\right)^{3+2j} \exp\left(-\left(\frac{\nu}{\nu_{th}}\right)^2\right) d\nu$$

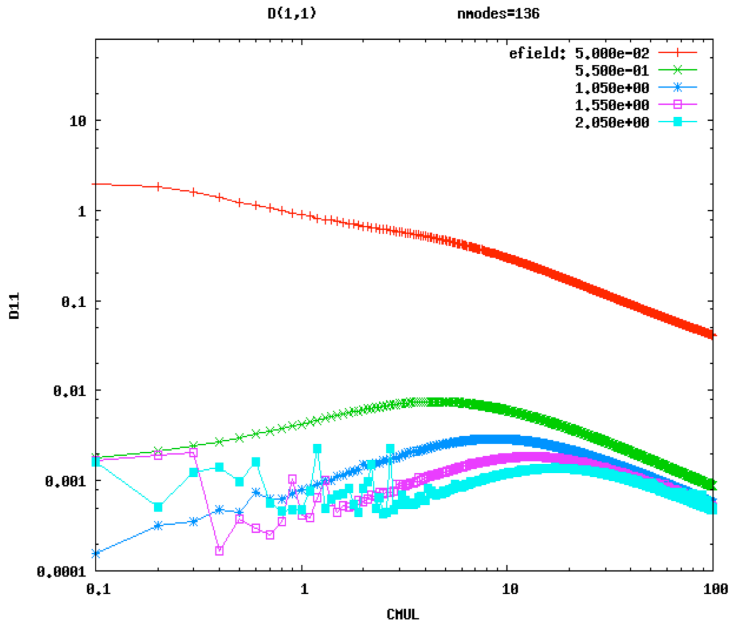


DKES:Results

- **After the Integration:**

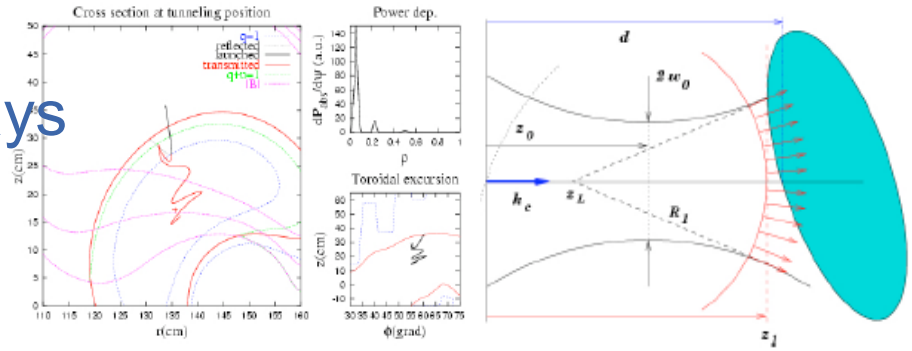
$$D_j^s = \frac{4}{\sqrt{\pi}} D_{Tok}^s \int D_*^s(\vartheta^*, E_r, v) \left(\frac{v}{v_{th}}\right)^{3+2j} \exp\left(-\left(\frac{v}{v_{th}}\right)^2\right) dv$$





MaRaTra

Massive Ray Tracing (MaRaTra).



Simulating microwave beams by rays

(10^5 rays=jobs) x 40 min

Every Ray: Hamiltonian Equation.

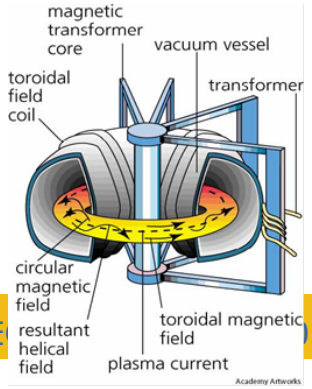
No jobs can be lost.

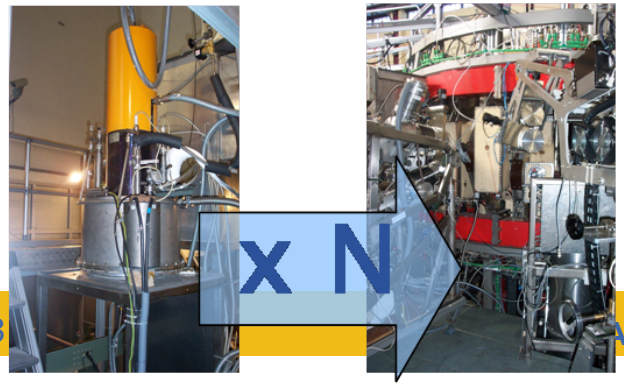
Gridway is used to distribute the jobs.

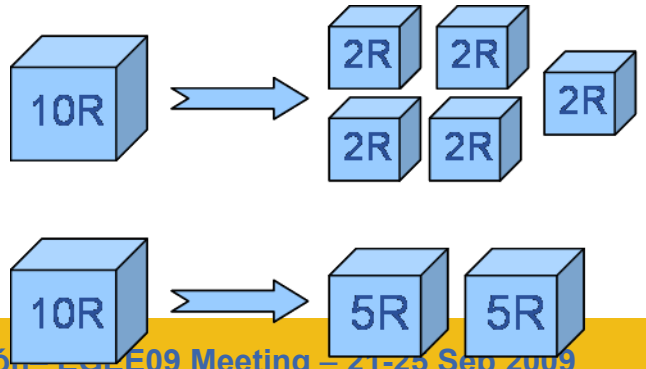
- Dynamic and adaptative chunk size in each node

- Advantages: Reduction of time execution and load balancing

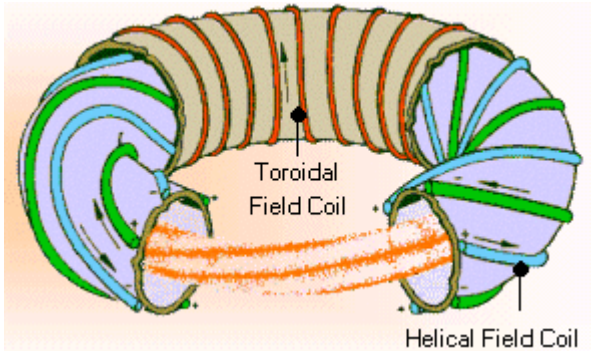
[J. L. Vázquez-Poletti et al. Proc. of EGEE UF, 2008]

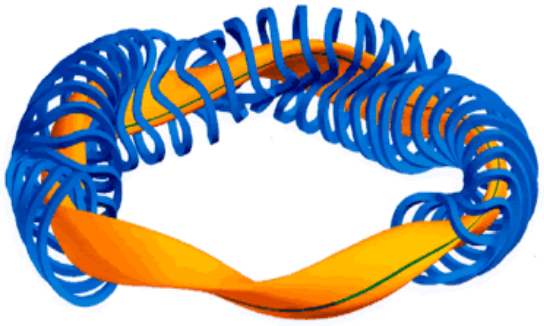






GA & Stellarator Optmization





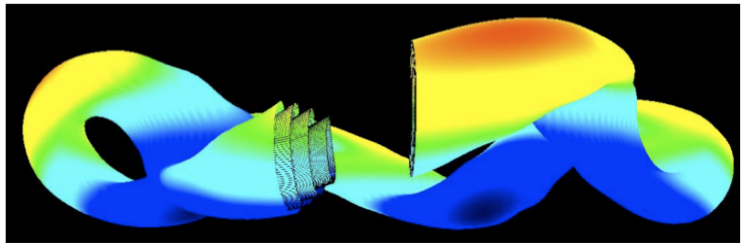
- **Stellarator Optimization.**

Choosing the best configuration according to several targets funtions.

VMEC running thru Genetic Algorithms in the Grid.

(10^5 configurations=jobs) x 40 min

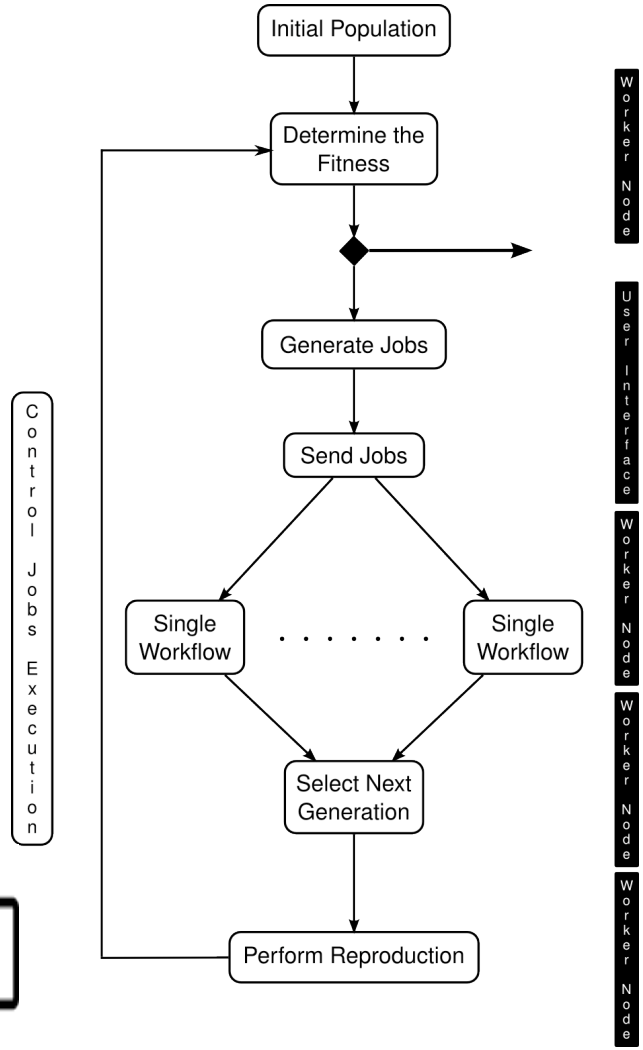
GA & Stellarator Optmization



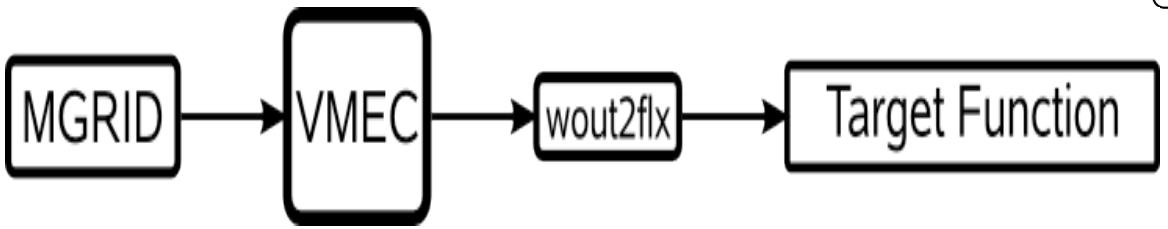
- **Bee algorithm.**

Two Traget functions considered, for the moment.

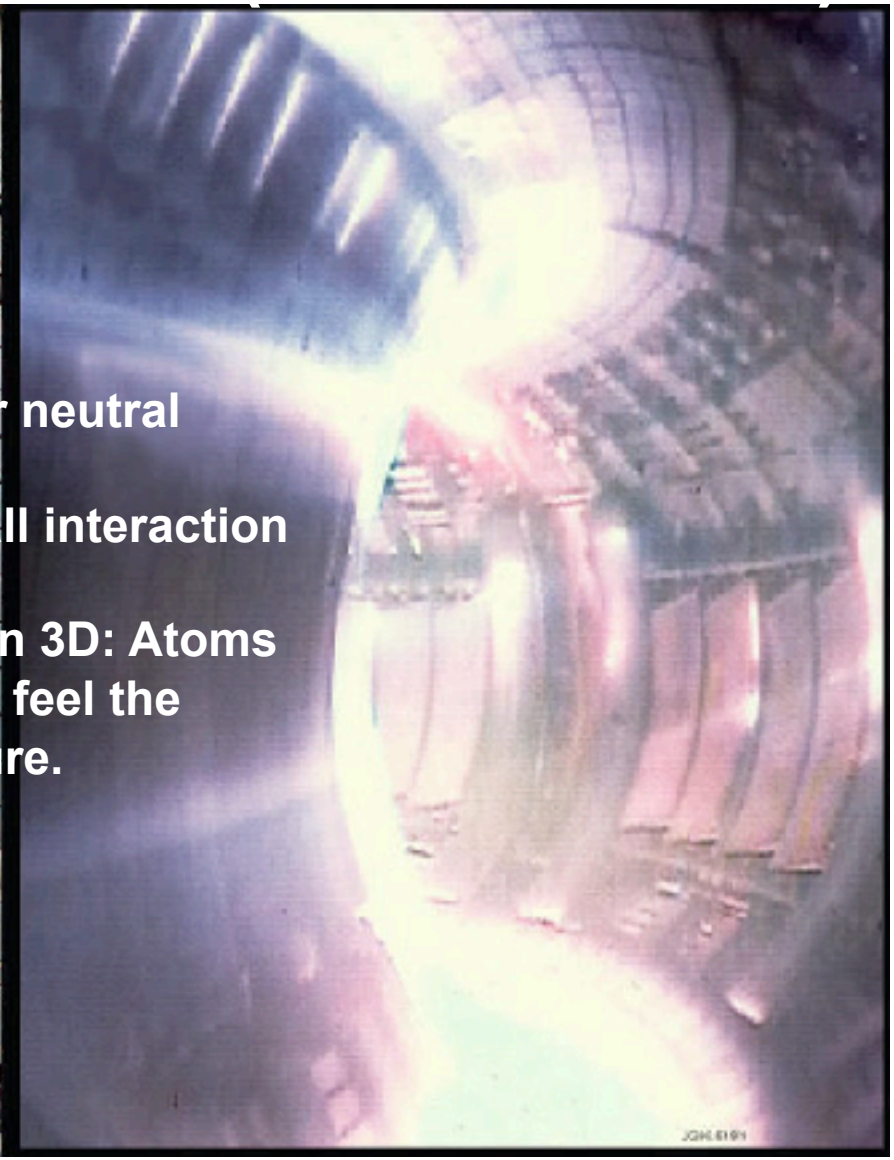
- **Complex workflow in the grid:**



- [A. Gómez-Iglesias. Submitted to PDP, 2010]

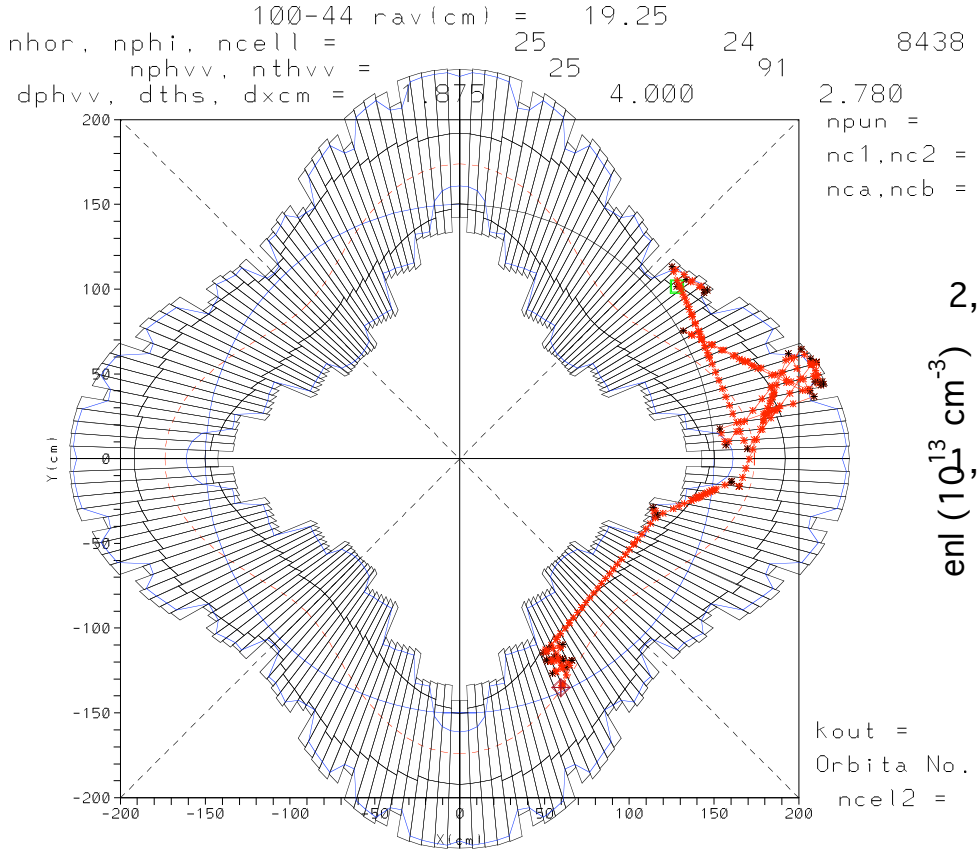


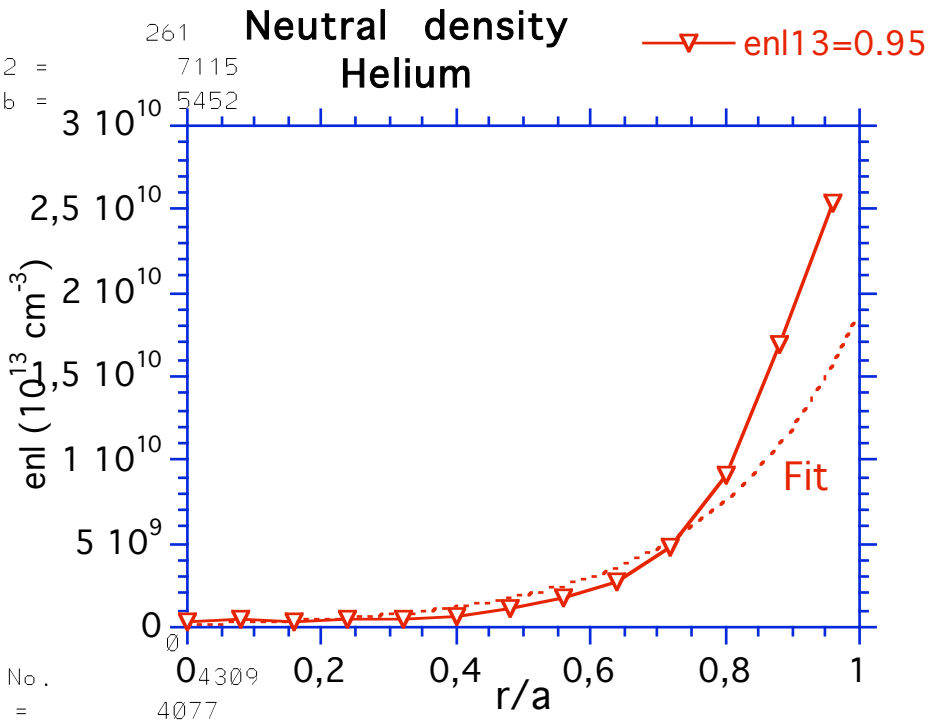
EIRENE: Plasma-Wall Interaction (Toks & Stell.)



-EIRENE: MC code for neutral trandport.
Gives the Plasma- Wall interaction in Toks.& Stells.
-Neutral Distribution in 3D: Atoms and molecules do not feel the magnetic field structure.

EIRENE Code





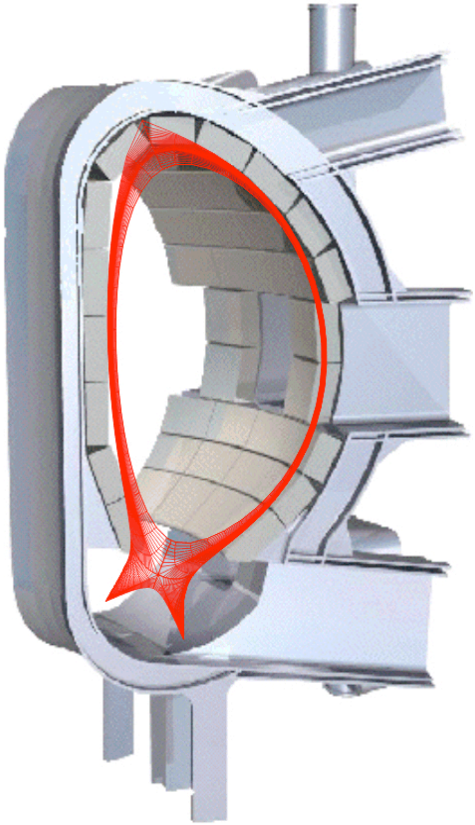
MC Code to estimate neutral density.

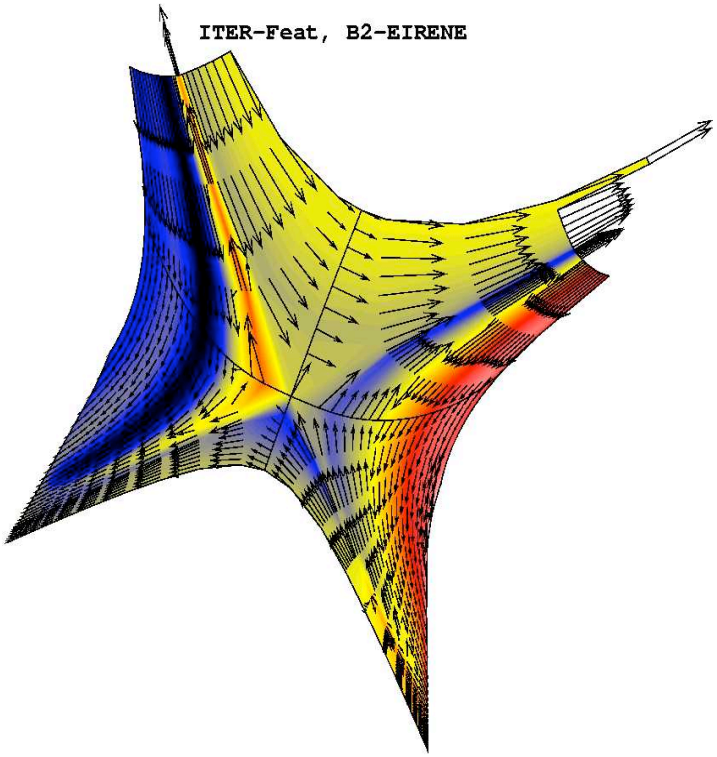
Trajectory of a He atom in TJ-II: starts at the green point and is absorbed in the plasma by an ionization process.

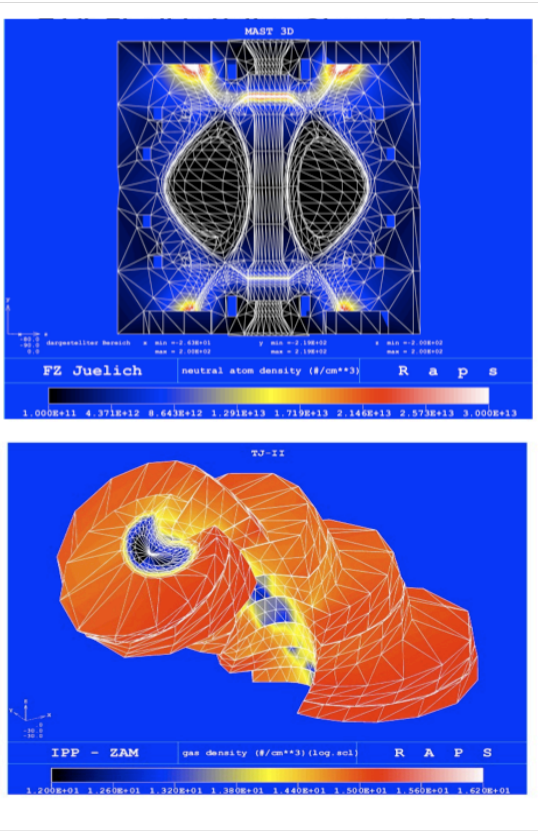
The real 3D geometry of vacuum chamber is considered. RESULT: The Profile

EIRENE

- Integration of physics modules
- Coupling of ISDEP – EIRENE
- ITER 3D geometry
- Read-in of new geometry



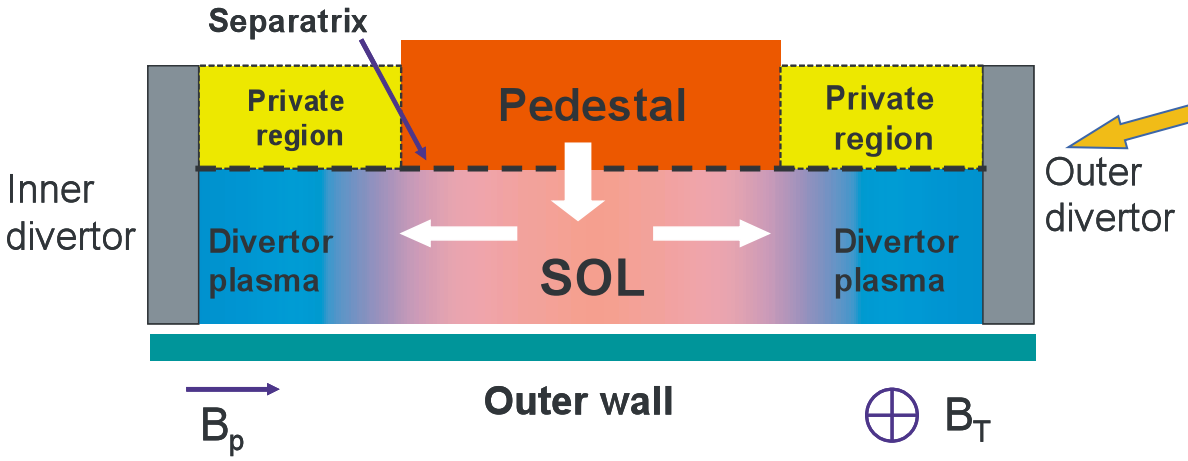


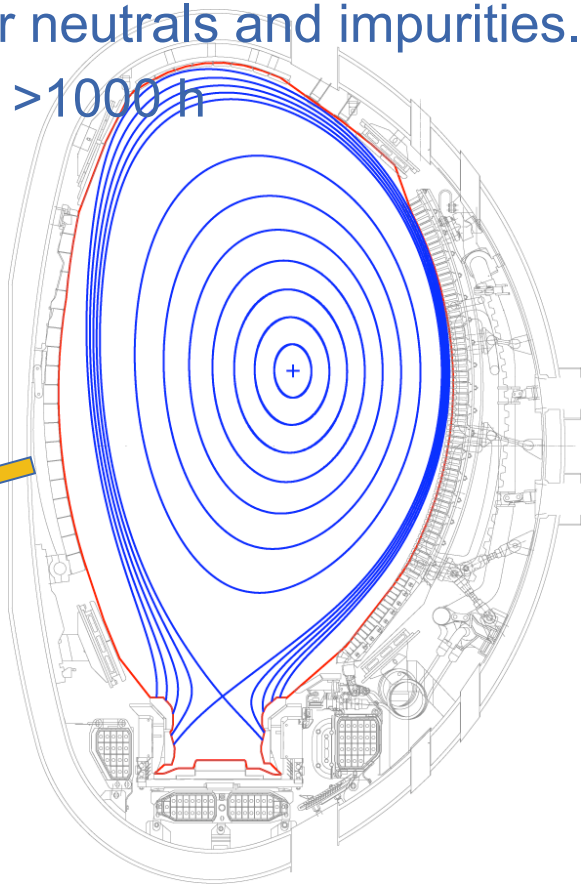


BIT1: Parameter Scan

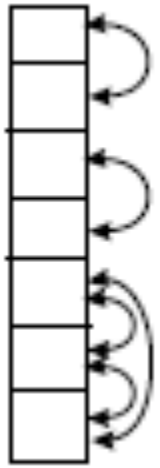
BIT1 is an electrostatic Particle-in-Cell + Monte Carlo (PIC + MC) code for plasma edge simulations. Simplified Plasma Model.
1D in real space.

- **Dimensionality:** 1D+3DV for plasma, 2D+3DV for neutrals and impurities.
- **High Complexity:** about 30.000 lines, **CPU time** >1000 h
- **Resolution:** down to electron gyro-motion





PIC Code

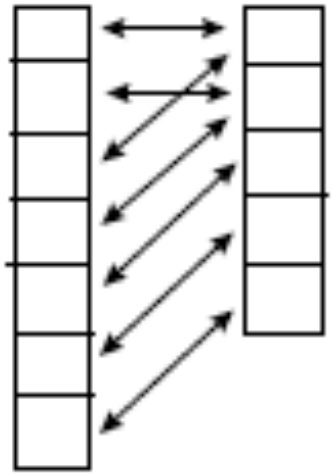


- Typically:

10^5–10^{10} particles in 10^2–10^7 spatial grid cells.

100 – 5000 particles per cell.

- Binary collisions: Particles of the same and different species. COMMUNICATION BETWEEN CPUs.
- A wide range of parameters must be scanned. → TYPICAL PARAMETER SCAN PROBLEM:
- Input file changes for the different cases → The source code and the input sent to the WNs.

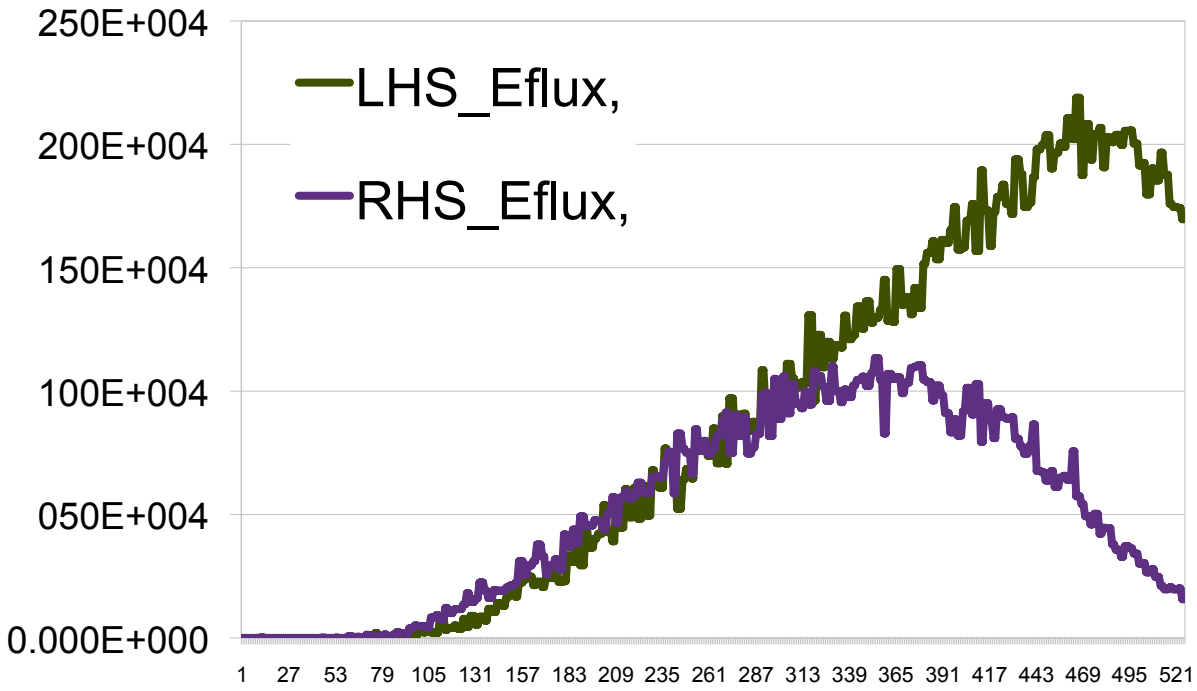


[F. Castejón et al. Proc. of the EGEE UF, 2009]

BT1 Results & Run Statistics

Results: time evolution of several quantities, estimated in the inner and outer walls:

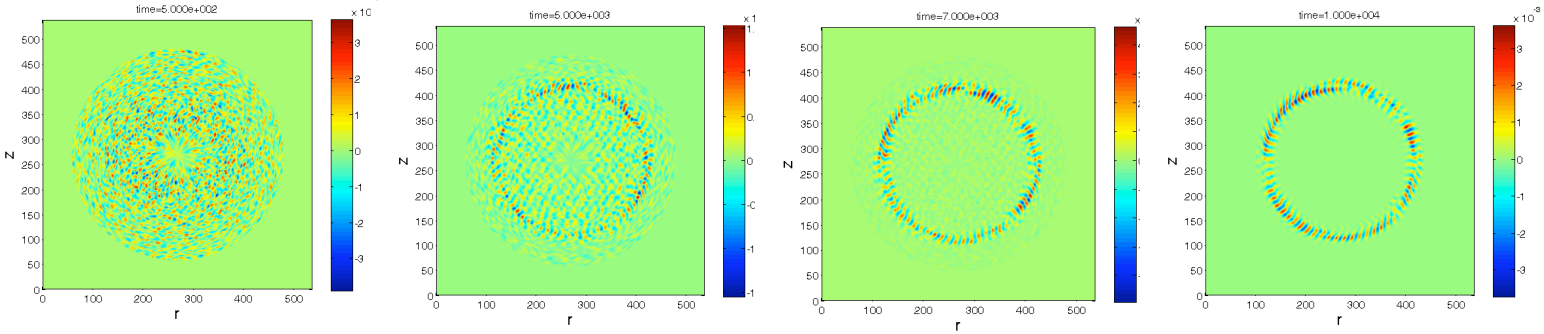
Particle and Energy Fluxes, Temperature.



- Our Present Problem: 8 Scrape-off-Layer widths x 8 impurity concentrations.
- Average CPU time per Job: 6 days, 12 hours and 23 minutes.
- Total (Cumulative) CPU Time: 417 days, 2 h., 32 min., 53 s.

GEM

- GEM: Gyrofluid Turbulence Code.
- GEM will give instabilities behaviour.
- Versions: Serial (small cases) and MPI (High scalability, to hundreds of rpoc.).
- Gaining experience in porting MPI codes.



- (Estimated with EUTERPE by E. Sánchez)

GEM

- **Stauts:**

THE CODE IS RUNNING IN THE GRID NOW.

[M. A. Rodríguez. Submitted to PDP, 2010]

- **Process:**
  - Script to control the remote execution:
    - Uncompress the input data and binaries.
    - Prepare the executon and execute the application.
    - Extract the relevant results and create a .tar.gz with them.

    KEY POINT: CLOSE CONTACT WITH THE CODE OWNER.

GEM

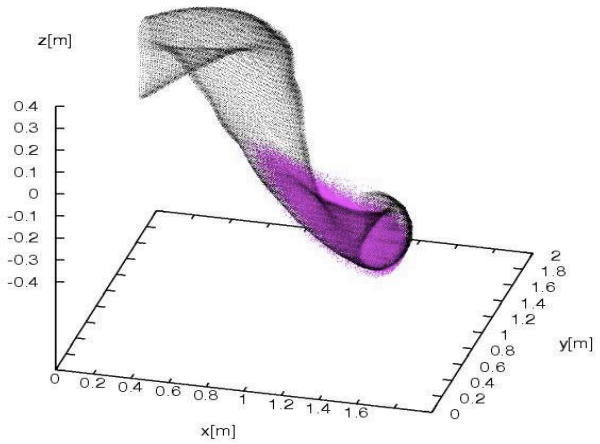
- Possible workflows:
  - Transport coefficients for a Transport code like.
  - Structure of potential: Movement of particles in a turbulent potential (MC code).

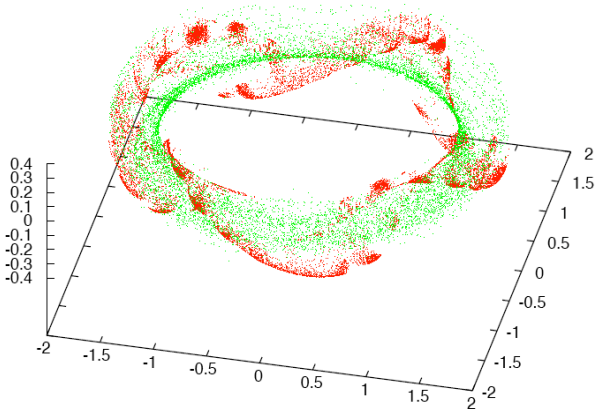
Workflows (I)

- **Interplay between different Physics models**

→ **Linking Applications. Different Possibilities:**

- Linking MC Codes:
  - § EIRENE – ISDEP (Or EMC3,…)
  - § ISDEP – FAFNER: Trajectories of hot ions.





Workflows (II)

- **Using a Transport code for establishing Workflows: Transport Equation:**

$$\frac{dn^s}{dt} + \nabla \Gamma^s = S^s$$

$$\frac{3}{2} n^s \frac{dT^s}{dt} + \nabla q^s = P^s_{in} - P^s_{loss}$$

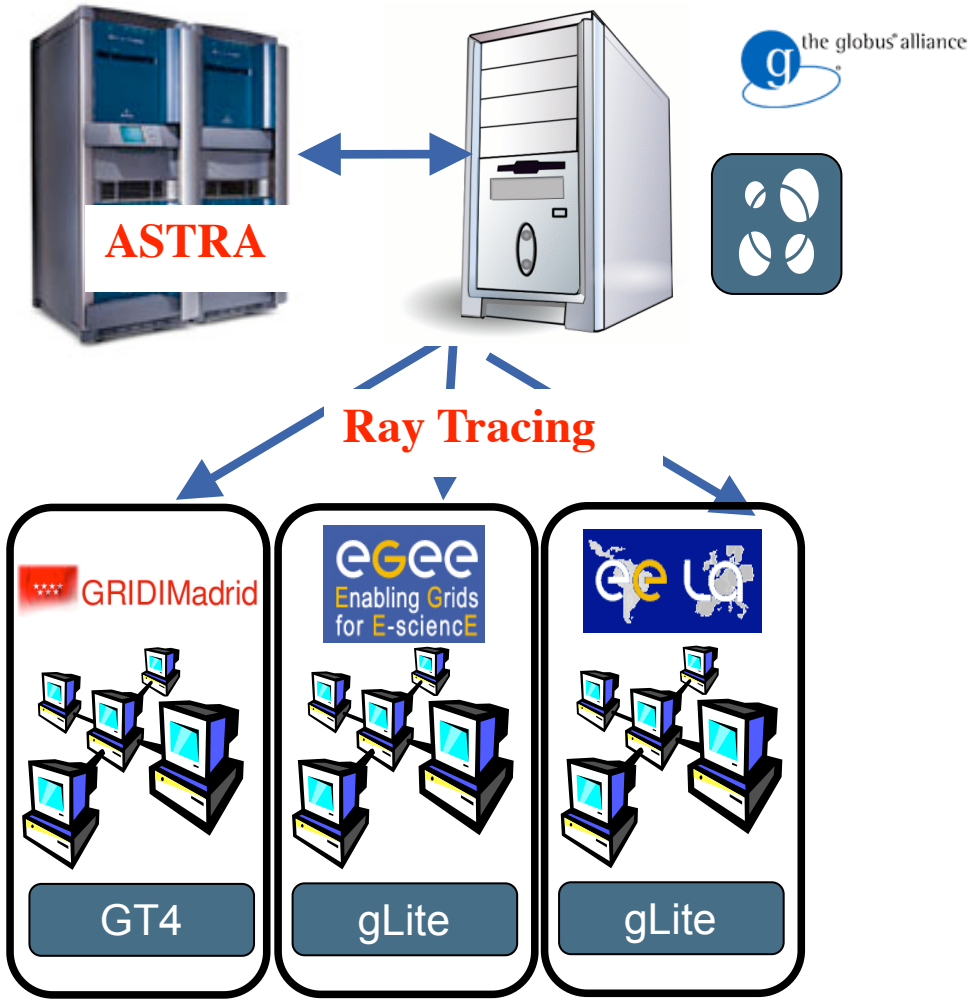
- **Sources and Losses: Complex and heavy functions.**

- **Fluxesd: Given by transport coefficients: Again Complex and heavy functions.**

$$\Gamma^s = -D_1^s \nabla n^s + D_2^s \nabla T^s$$

$$q^s = -\chi^s n^s \nabla T^s + D_3^s \nabla n^s$$

ASTRA-MaRaTra: A complex Workflow



MaRaTra Results depend on Plasma Evolution: TRANSPORT

ASTRA (SGI Application) + MaRaTra (Grid).

NEW TOOL: VASHRA-T

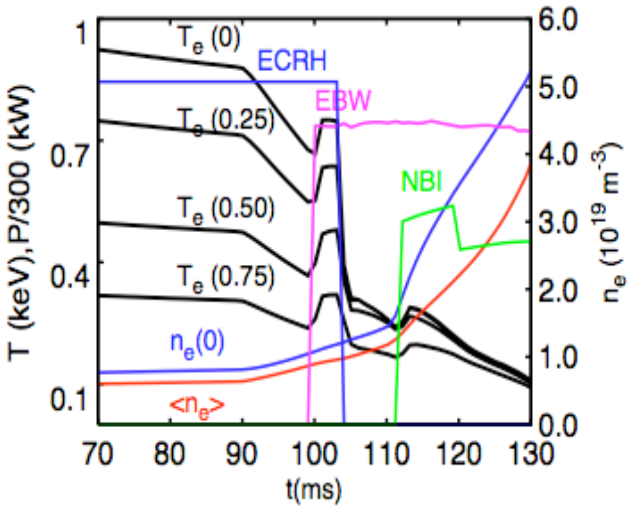
Complex Workflow between applications that run in diferent platforms.

Vashra-T: Results

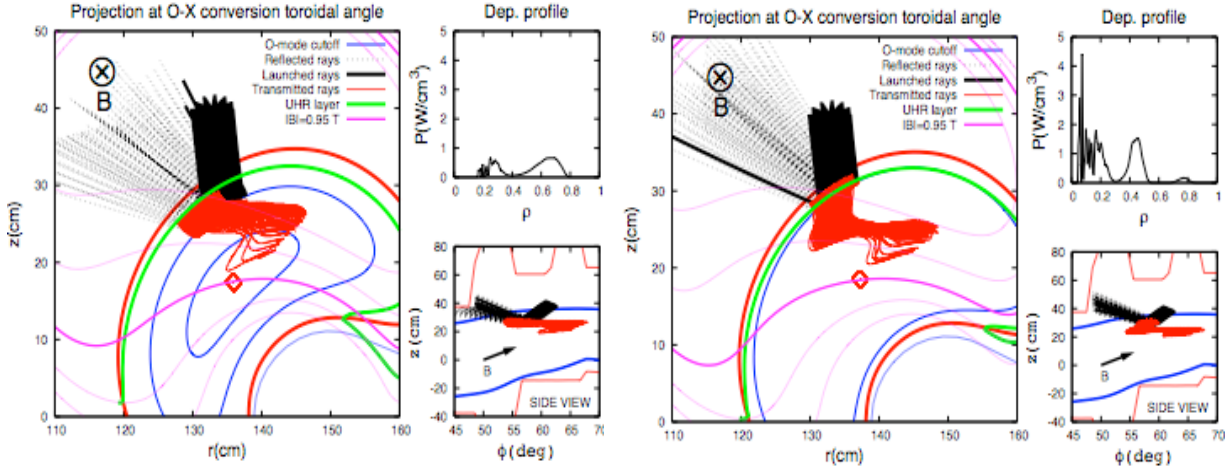
- Evolution of Plasma.

Calculated by ASTRA.

MaRaTra is launched by ASTRA every ms.



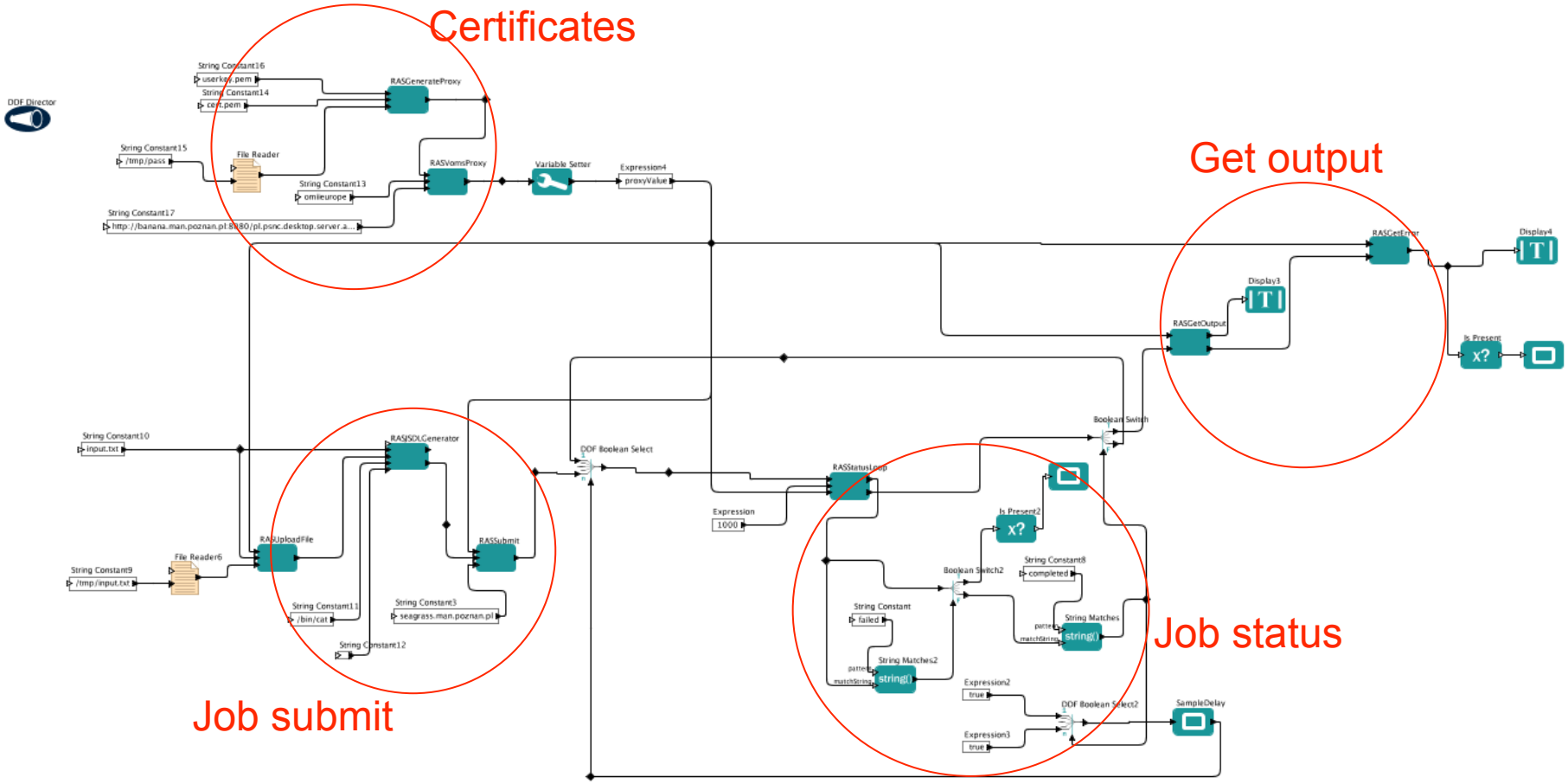
- Evolution of Power Absorption.



[A. Cappa et al. To be sent to Plasma Physcis and Controlled Fusion, 2009]

Kepler: The Workflow Engine in Euforia

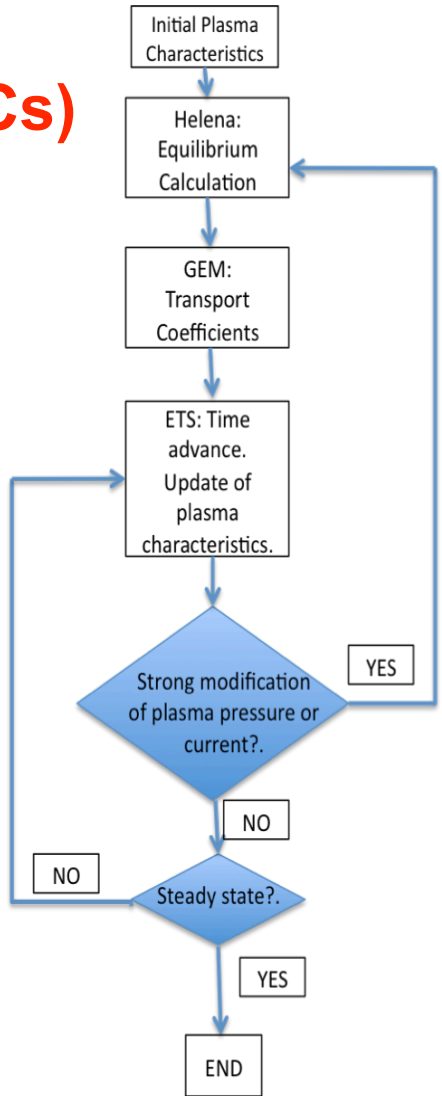
- **All the codes must write CPOs on the UAL.**



Workflow #1

- **ETS, HELENA, GEM**

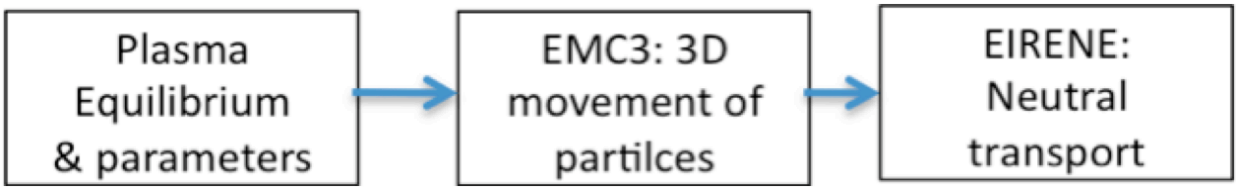
(GEM & Helena run on grids and HPCs)



Workflow #2

- **EMC3 – EIRENE**

(Prepared by FZK)



Workflow #3

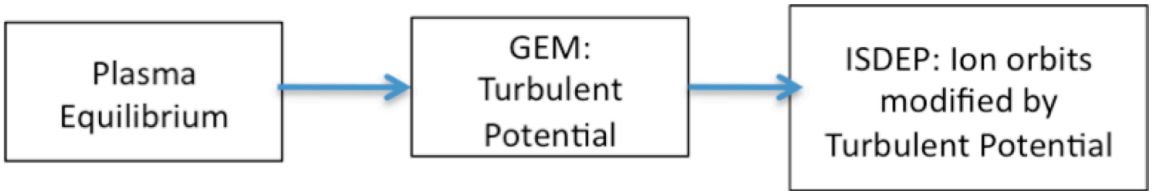
- **BIT1 – TMAP7**

(We have BIT1 ready and we are working on TMAP7)
(Serial code)

Workflow #4

- **HELENA or VMEC, GEM, ISDEP**

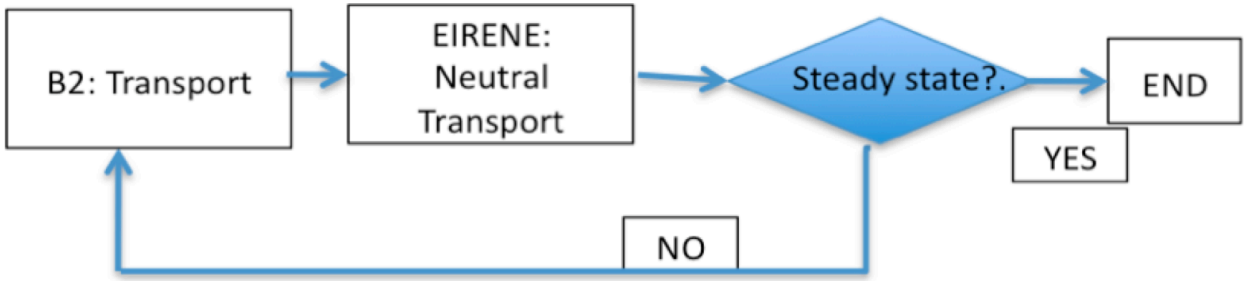
(We have all the codes ready)



Workflow #5

- **B2 – EIRENE (SOLPS)**

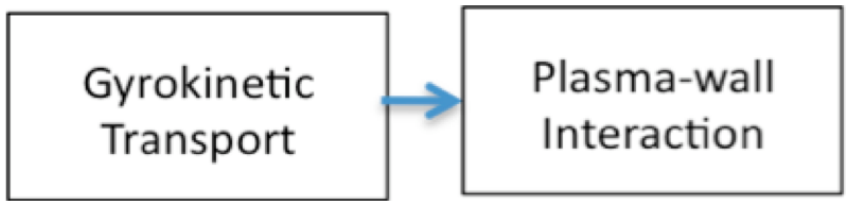
(Codes should be provided by David Coster)



Workflow #6

- **ERO (TWO CODES IN ONE)**

(Codes should be provided by David Coster)



Conclusions

Several Applications have been ported to the grid that:

- Have Diferent Structures: Embarrasingly Parallel, PIC, GA,…
- Solve Different Problems in Fusion. The grid is acting on Different Research Fields.
- Use Different Porting Stratregies: Development of several techniques.
- PRODUCE RELEVANT PHYSCIS RESULTS.

Complex Worflows have been Established among:

- Grid Applications.
- Grid and Share Memory Applications.

DEMONSTRATION EFFECT:

TRY TO INCREASE THE LEVEL OF USE OF THE GRID.

COMING DEVICE: ITER