Fusion Results within EGEE

F. Castejón (CIEMAT)
francisco.castejon@ciemat.es

Egee08, Clermont-Ferrand
11-14 February 2008

www.eu-egee.org

Information Society and Media

Co-authors

- Dr. CAMPOS, Isabel (IFCA. CSIC. Spain)
- Dr. CAPPA, Álvaro(CIEMAT. Spain)
- Dr. GUILLERMINET, Bernard (CEA, France)
- Dr. ROSSI, Luca (BIFI. Universidad de Zaragoza. Spain)
- Dr. TARANCÓN, Alfonso (BIFI. Universidad de Zaragoza. Spain)
- Dr. TERESHCHENKO, Maxim (General Physics Institute, Russian Academy of Sciences)
- Mr. VÁZQUEZ-POLETTI, José Luis (Universidad Complutense de Madrid. Spain)
- Mr. VOZNESENSKY, Vladimir (Inst. of Information Systems, RRC "Kurchatov Inst.", Russia)
- Mr. VELASCO, José Luis (BIFI. Universidad de Zaragoza. Spain)

Contents

- **Introduction: Serial Fusion Problems.**
- **EGEE Experience:**
  - Fusion VO.
  - Running Applications & Results.
- **New Applications and upgrades.**
- **Future Plans:**
  - More complex Workflows: Kepler
  - Euforia Project.
- **Final Remarks**

Contents

- **Introduction: Serial Fusion Problems.**
- **EGEE Experience:**
  - Fusion VO.
  - Running Applications & Results.
- **New Applications and upgrades.**
- **Future Plans:**
  - More complex Workflows: Kepler
  - Euforia Project.
- **Final Remarks**

Grids and distributed problems

- **Monte Carlo codes (Langevin Equation):**
  - Plasma-wall interaction; neutral particle orbits.
  - Kinetic transport: Particle orbits in toks. and stell.
- **Parameter Variation:**
  - Stellarator Optimization
  - Neoclassical Transport estimates (DKES).
  - Simulation of Heating by Microwaves: Massive Ray Tracing.
- **Two main strategies:**
  - Rendering all the simulated data.
  - Choosing the best among all of them by a genetic algorithm.

Contents

- Introduction: Serial Fusion Problems.
- EGEE Experience:
  - Fusion VO.
  - Running Applications & Results.
- New Applications and upgrades.
- Future Plans:
  - More complex Workflows: Kepler
  - Euforia Project.
- Final Remarks

Fusion VO Working

http://grid.bifi.unizar.es/egee/fusion-vo/

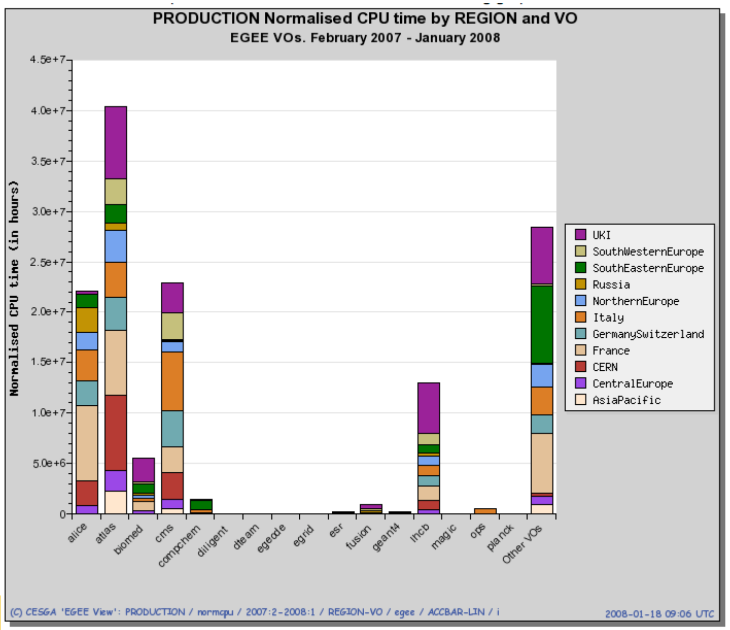
http://www.fusion.ciemat.es/collaboration/egee/

- **14 Partners ~ 4500 CPUs ~ 45 Tflops**

project-eu-egee-na4-fusion-applications@cern.ch

Fusion:

The most demanding after HEP and Biomed.

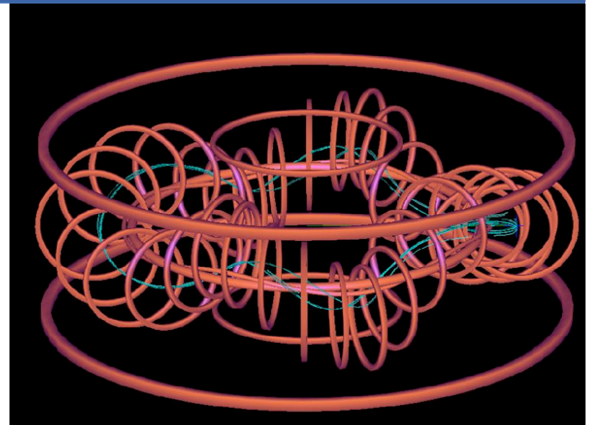


Contents

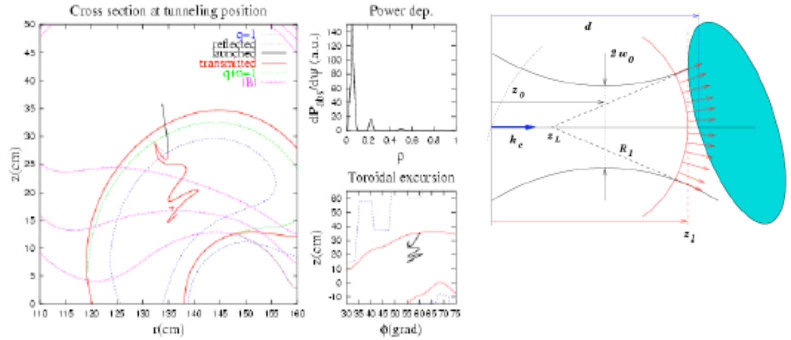
- Introduction: Serial Fusion Problems.
- EGEE Experience:
  - Fusion VO.
  - Running Applications & Results.
- New Applications and upgrades.
- Future Plans:
  - More complex Workflows: Kepler
  - Euforia Project.
- Final Remarks

Running applications

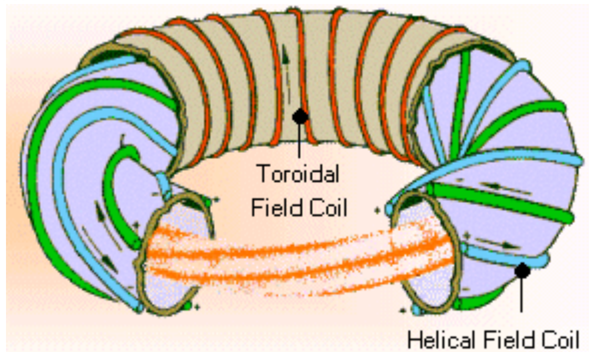
- **Ion Kinetic Transport (ISDEP)**



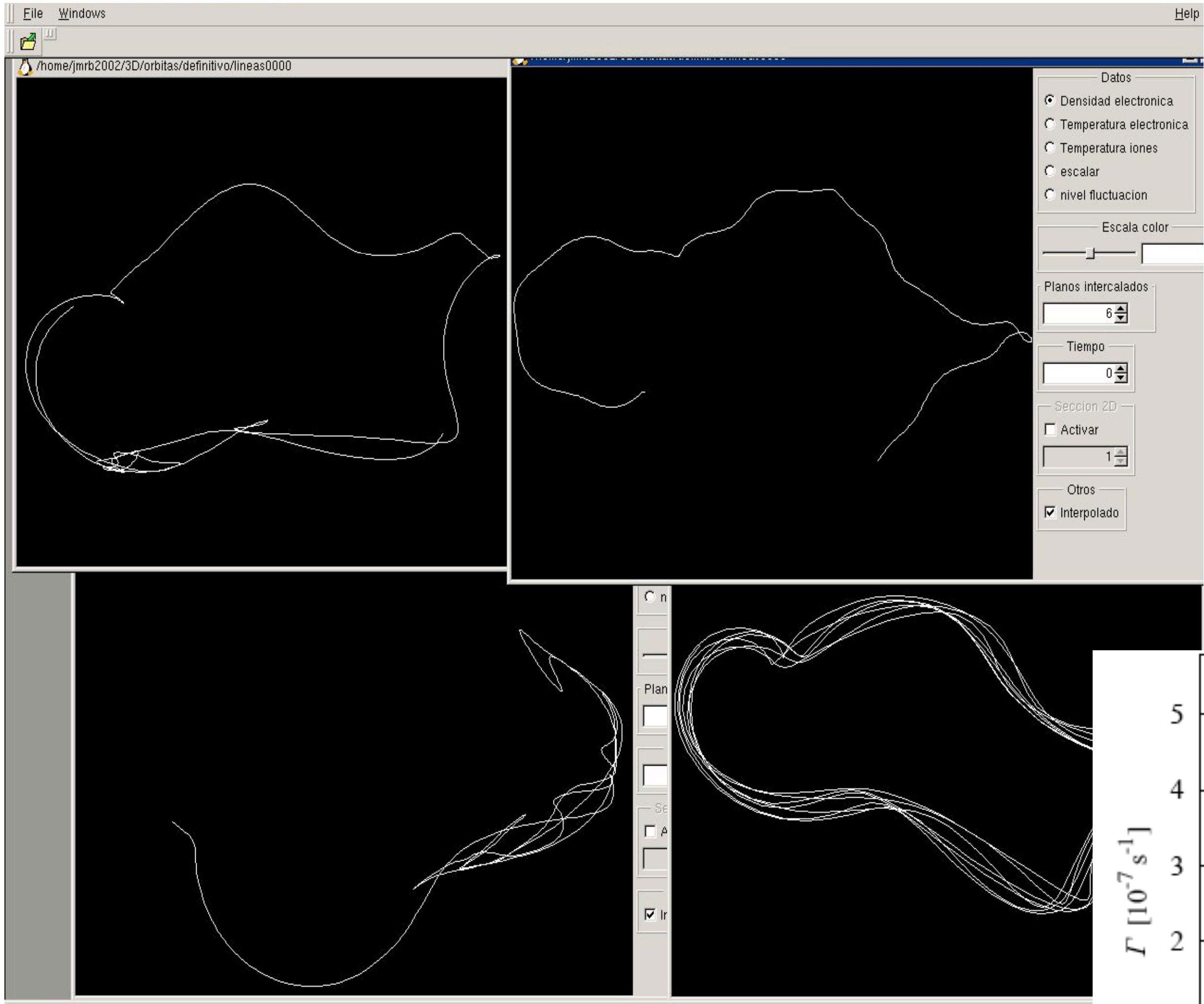
- **Massive Ray Tracing (MaRaTra).**



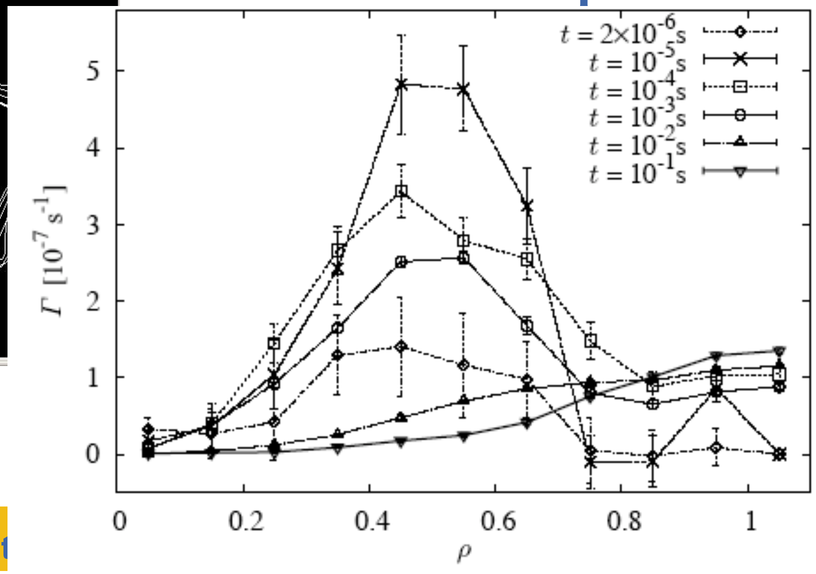
- **Stellarator Optimization.**



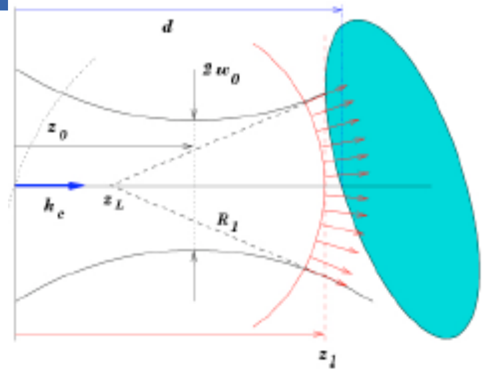
ISDEP code: 3D orbits



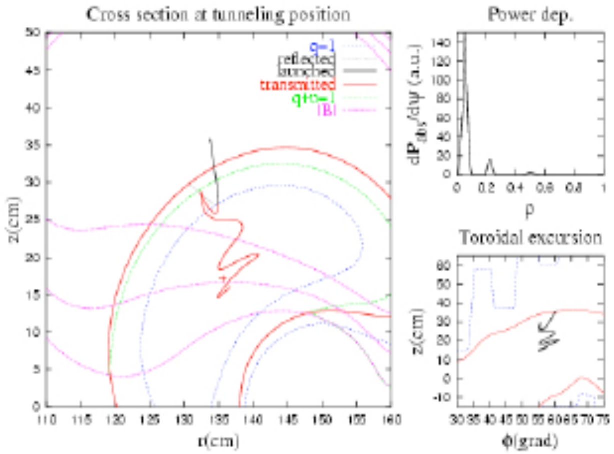
- Following ion trajectories (10^5-10^6 particles).
- Guiding centre approximation.
- i-i & i-e Coulomb collisions.
- Considering electrostatic potential.
- No assumptions on orbit size or diffusive transport.

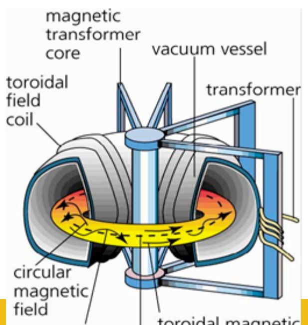


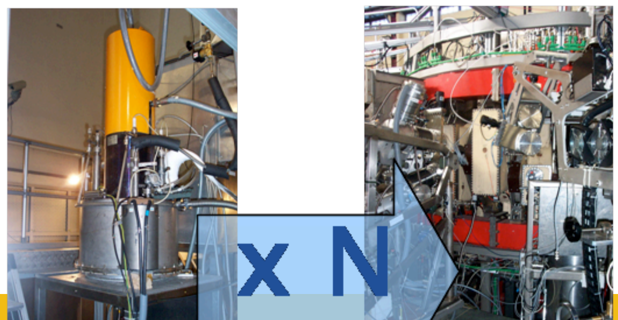
MARAT MaRaTra: Massive Ray Tracing RA

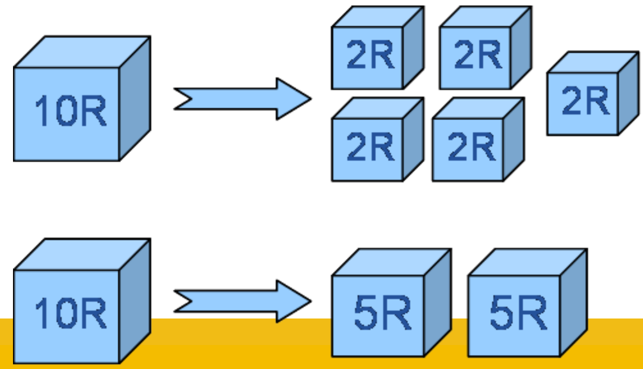


- Combination of MARATRA jobs in chunks
- Dynamic distribution of chunks using GRIDSelf-Scheduler
- GRIDSelf-Scheduler is a distributed and dynamic self-scheduler algorithm:
  - **Framework used: GridWay Metascheduler (GridWay.org)**
  - **Considers dynamic resource information**
  - **Dynamic and adaptative chunk size in each node**
- Advantages: Reduction of time execution and load balancing
- More details in “Distributed Task Scheduling for Physics Fusion Applications” talk









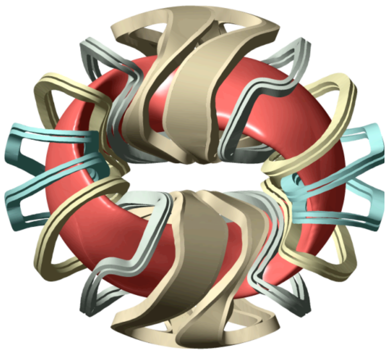
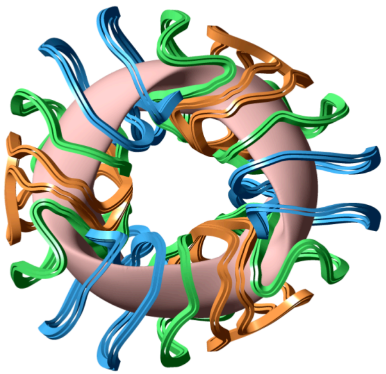
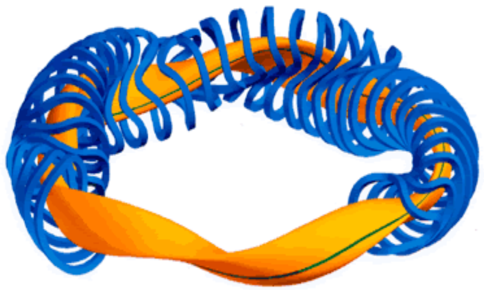
STELLARATORS: A lot of different Magnetic Configurations operating nowadays.

-OPTIMIZATION NECESARY BASED ON KNOWLEDGE OF STELLARATOR PHYSICS.
Plasma configuration may be optimised numerically by variation of the field parameters.
Every variant computed on a separate processor (~10')
VMEC (Variational Momentum Equilibrium Code)
See V. Voznesensky's this afternoon talk.
120 Fourier parameters are varied.

$$\vec{B}(\psi,\theta,\varphi) = \sum_{m,n} \vec{B}_{m,n}(\psi) e^{i(m\theta - n\varphi)}$$

$$R(\psi) = \sum_{m,n} R_{m,n}(\psi)\cos(m\theta - n\varphi)$$

$$Z(\psi) = \sum_{m,n} Z_{m,n}(\psi)\sin(m\theta - n\varphi)$$

Contents

- Introduction: Serial Fusion Problems.
- EGEE Experience:
  - Fusion VO.
  - Running Applications & Results.
- **New Applications and upgrades.**
- Future Plans:
  - More complex Workflows: Kepler
  - Euforia Project.
- Final Remarks

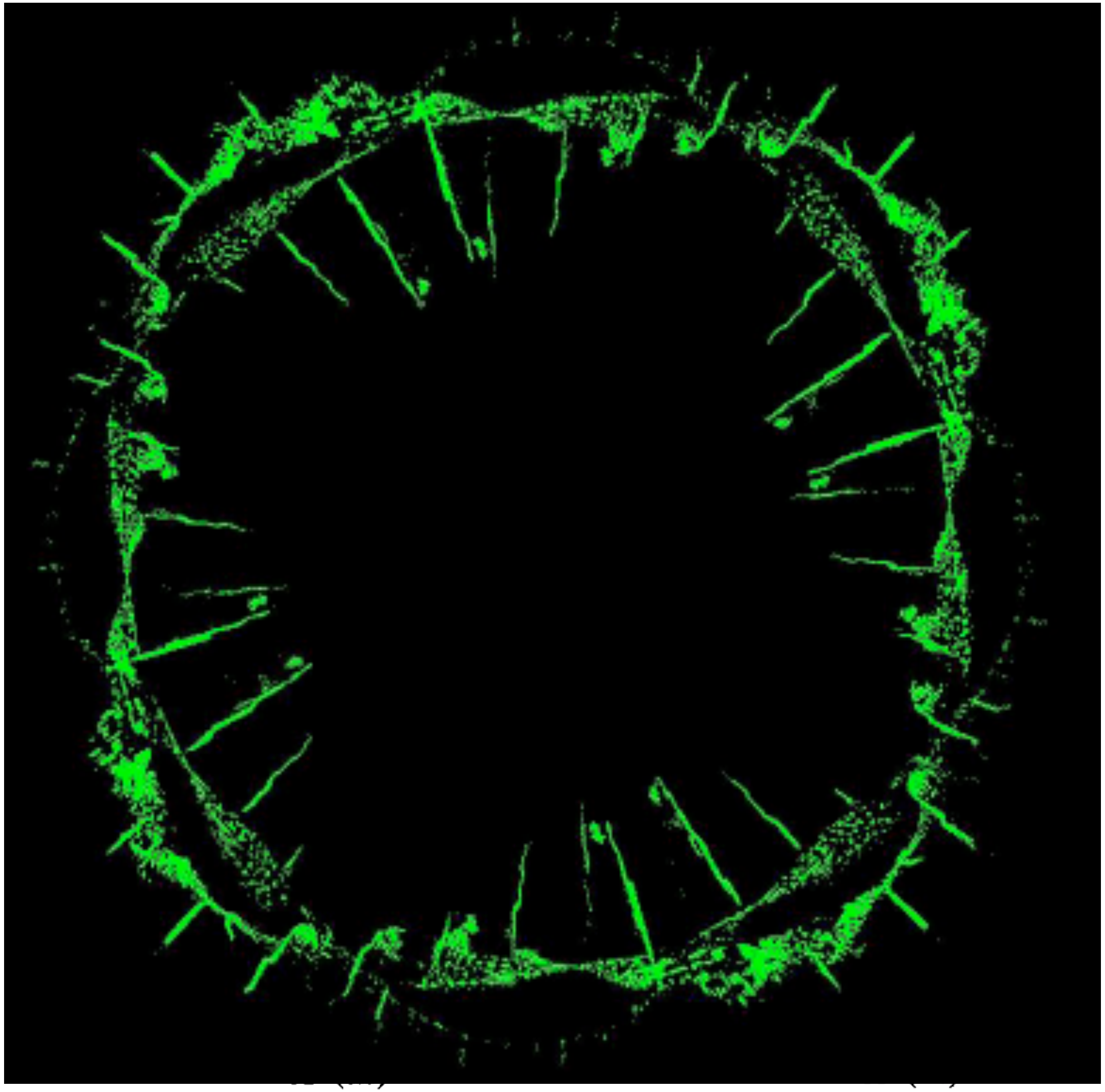
New applications & Improvement

- **Ion Kinetic Transport: Divertor Studies (3D Map of Flux)**
- **ISDEP:**
  - Self consistent Plasma Profiles
  - Tokamak Geometry. (ASDEX, ITER)
  - Ion Heating (ICRH).
- **NBInjector simulation**
- **DKES (Drift Kinetic Equation Solver)**

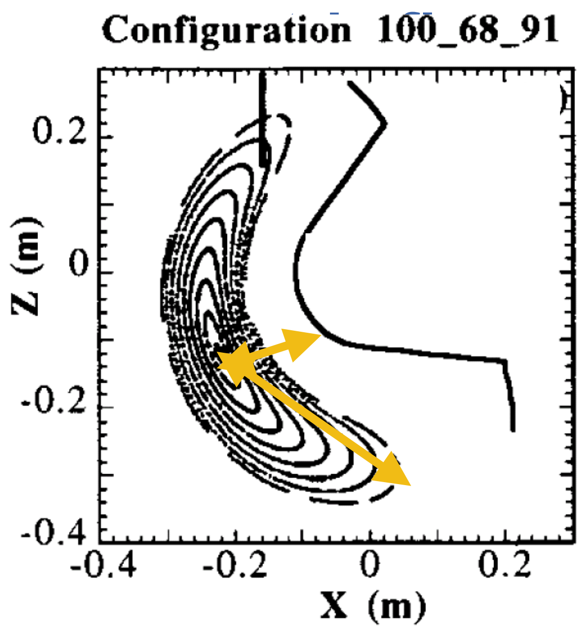
New applications & Improvement

- **Ion Kinetic Transport: Divertor Studies (3D Map of Flux)**
- **ISDEP:**
  - Self consistent Plasma Profiles
  - Tokamak Geometry. (ASDEX, ITER)
  - Ion Heating (ICRH).
- **NBInjector simulation**
- **DKES (Drift Kinetic Equation Solver)**
- **Massive Ray Tracing (MaRaTra): CD**

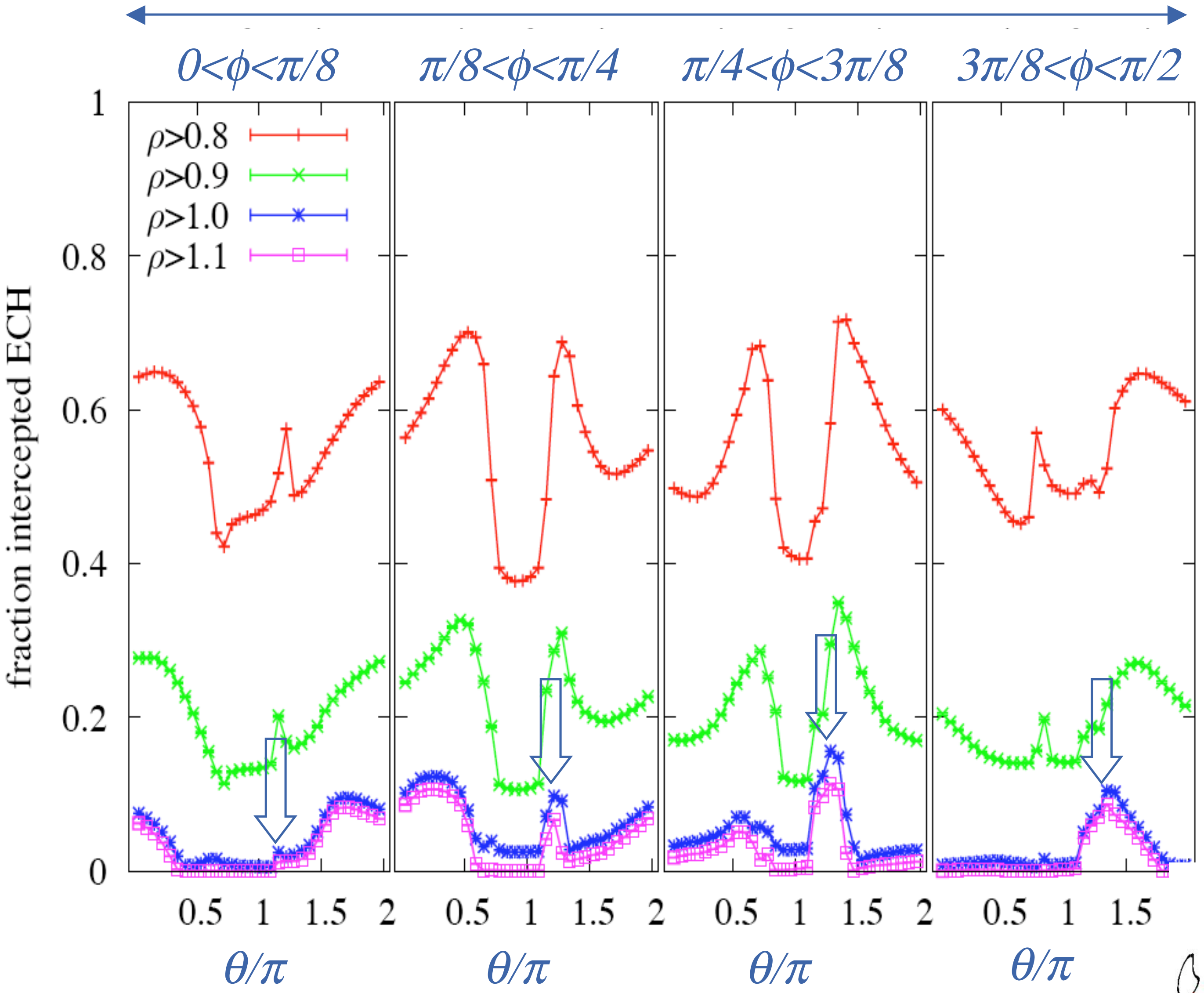
The Map of Losses in TJ-II



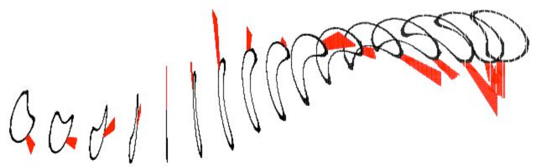
- Maximum plasma-wall interaction on the groove.
- PWI close to the plasma bulk.
- Up-down



Asymmetric Flux Map



- TJ-II Period
  - Clear poloidal and toroidal structure.
  - Plates located on the arrows.
  - Fraction of trajectories on the plates: **50%.**
  - Fraction of collisions on the groove: **from 60% to 35%**



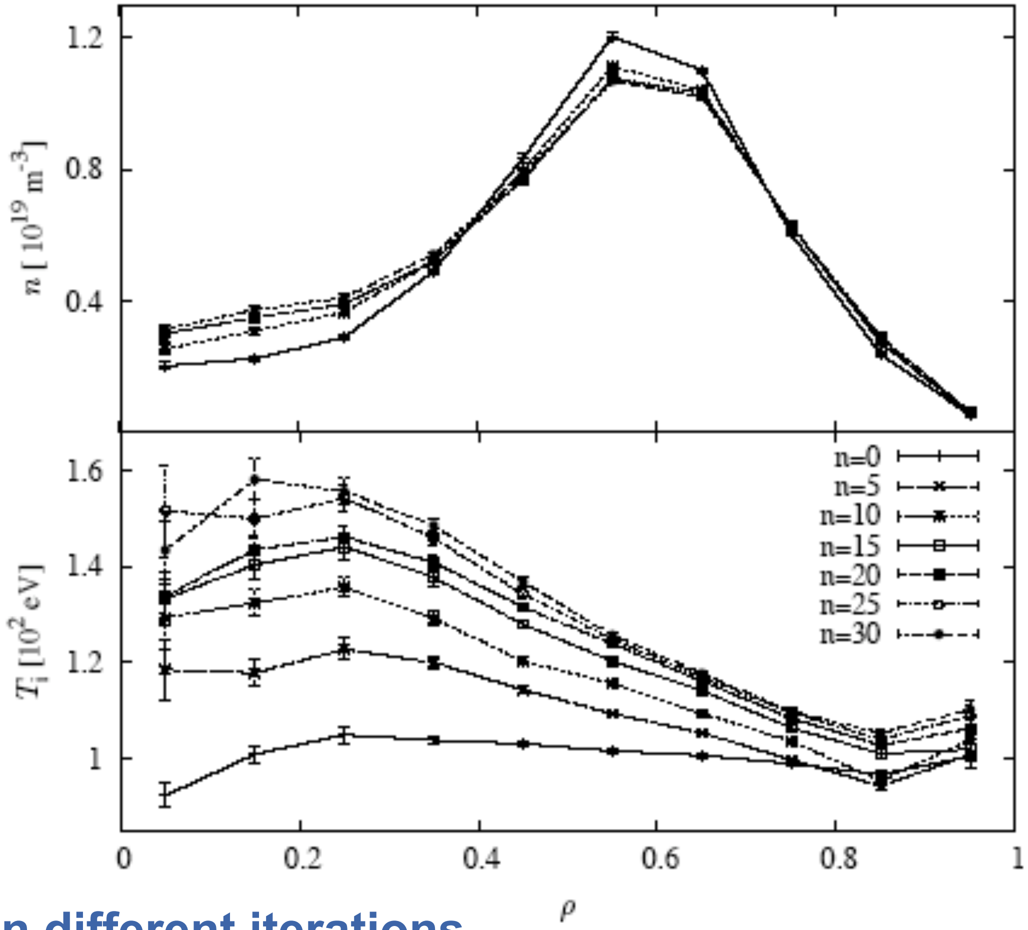
New applications & Improvement

- **Ion Kinetic Transport: Divertor Studies (3D Map of Flux)**
- **ISDEP:**
  - Self consistent Plasma Profiles
  - Tokamak Geometry. (ASDEX, ITER)
  - Ion Heating (ICRH).
- **NBInjector simulation**
- **DKES (Drift Kinetic Equation Solver)**
- **Massive Ray Tracing (MaRaTra): CD**

ISDEP Improvement

- **Selfconsistent Profiles (Quasi-linear Evolution)**

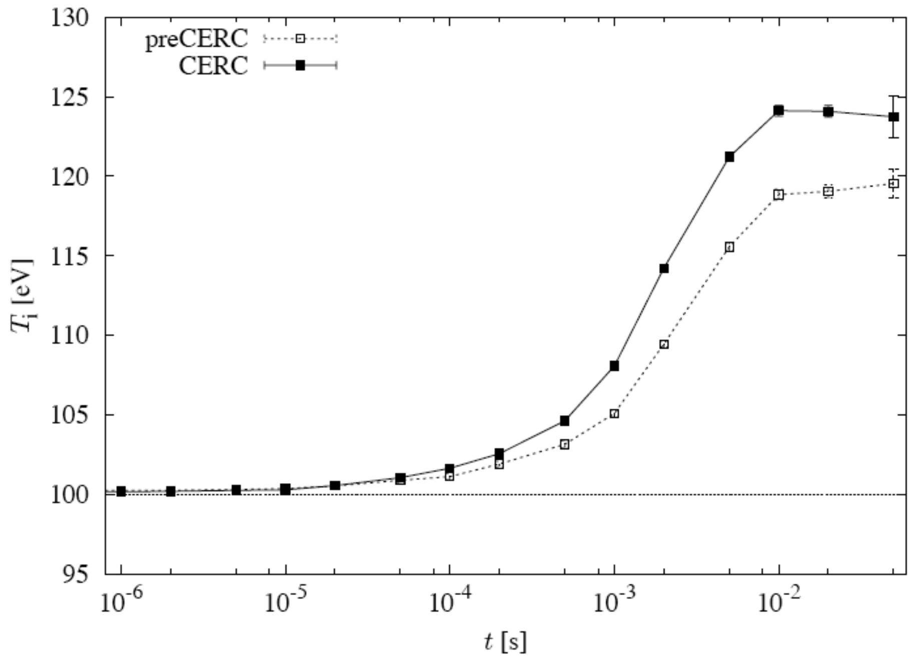
- **Single Profile: Following a large number of independent trajectories.**
- **New Profile: Update the background at every time-step with the test particle results.**
- **Iterate until steady state is achieved.**
- **Every iteration launches a huge set of jobs to the grid.**

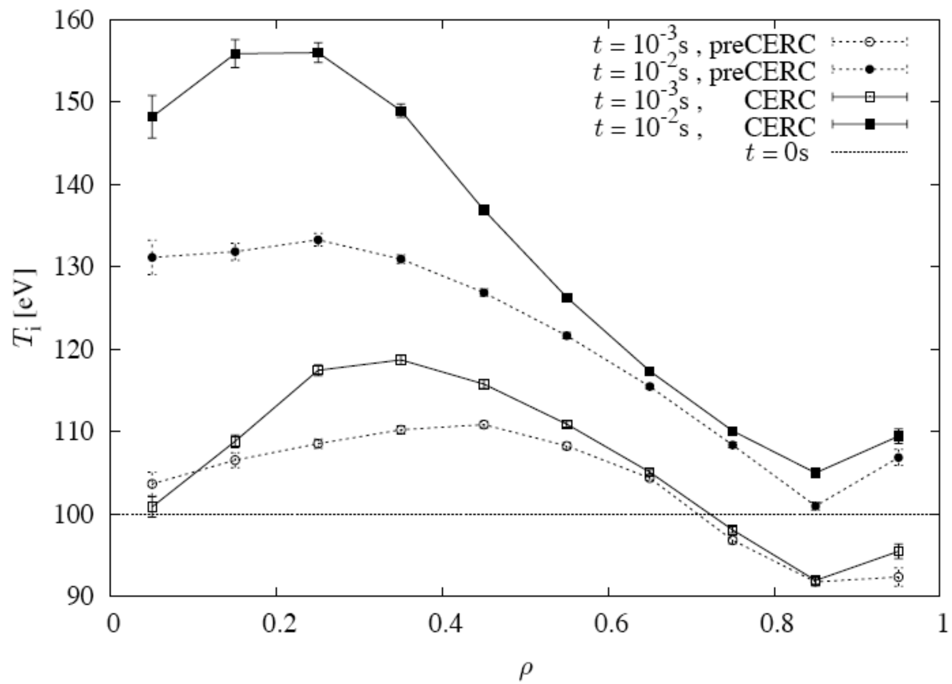


- **Density & temperature profiles in different iterations.**
- **30 iterations are needed for every time step.**

Temperature Evolution

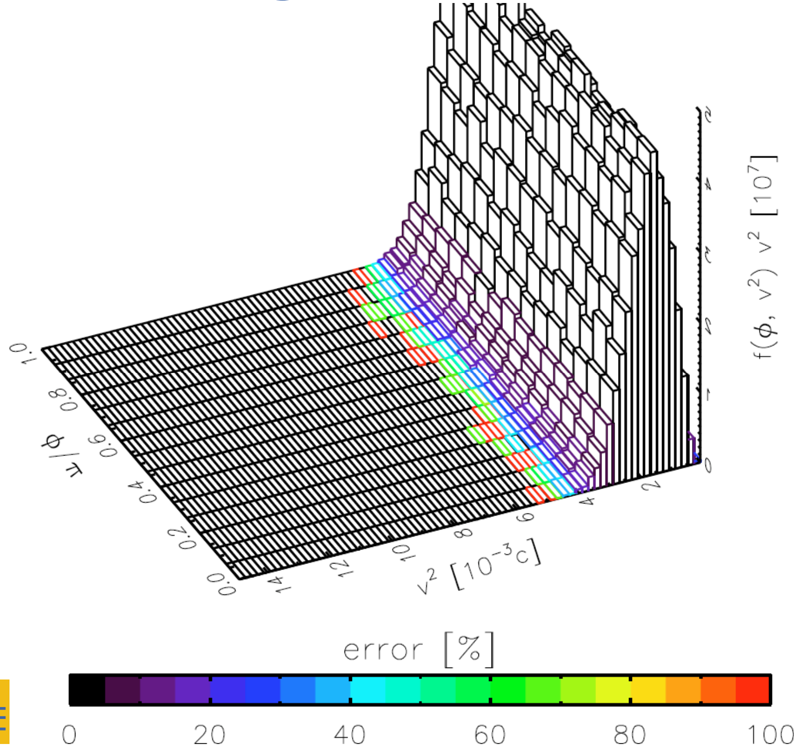
- **The Non-linear terms allow one to introduce the evolution of the plasma (Temperature and density) in different experimental conditions.**

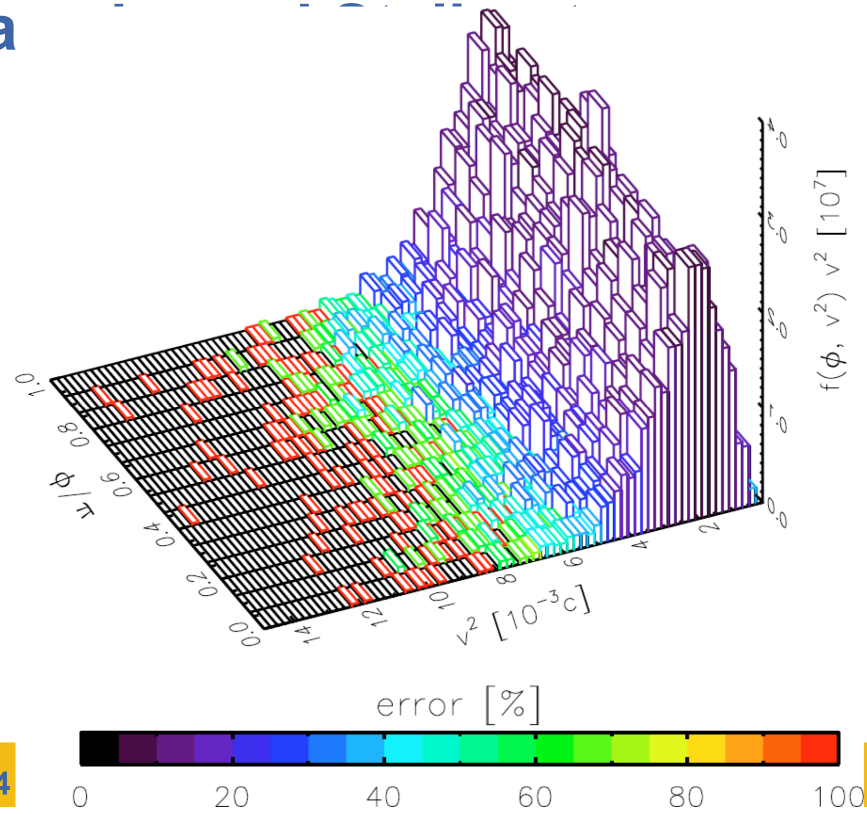




The Distribution Function

- An extra term is introduced in the equations to simulate the particle-wave interaction.
- The heating of the plasma can be estimated using the Grid due to the introduyction of Non-Linear terms.
- The 5D distribution function is obtained with and without Heating Term both in Toka

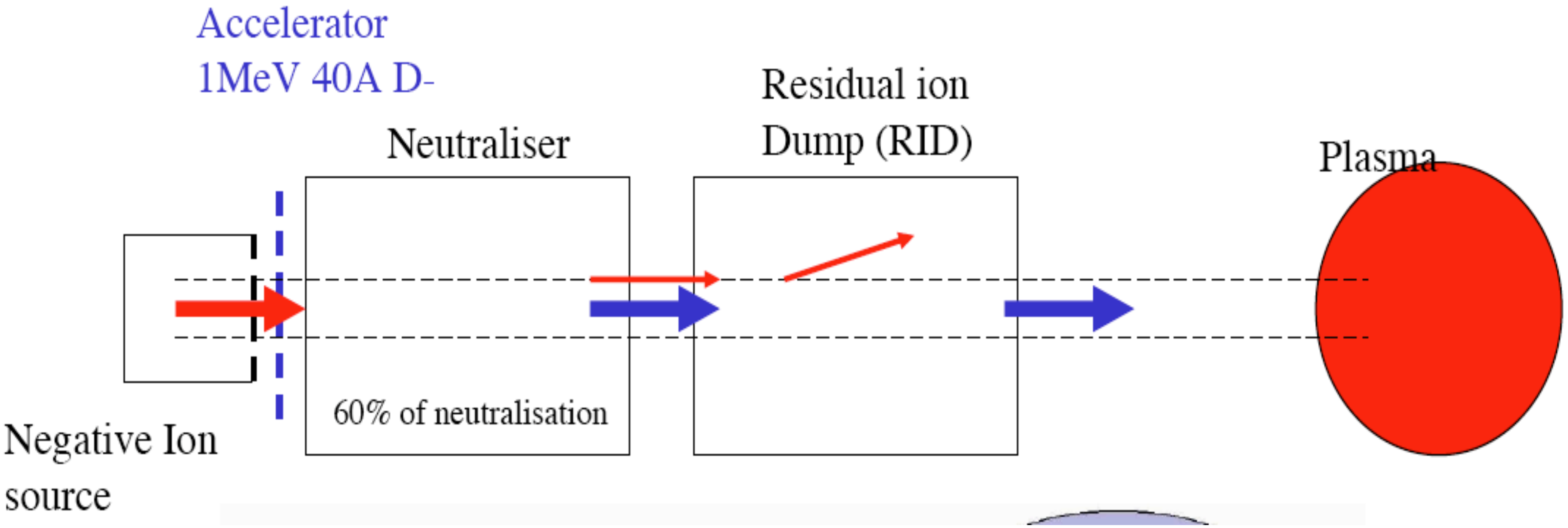




New applications & Improvement

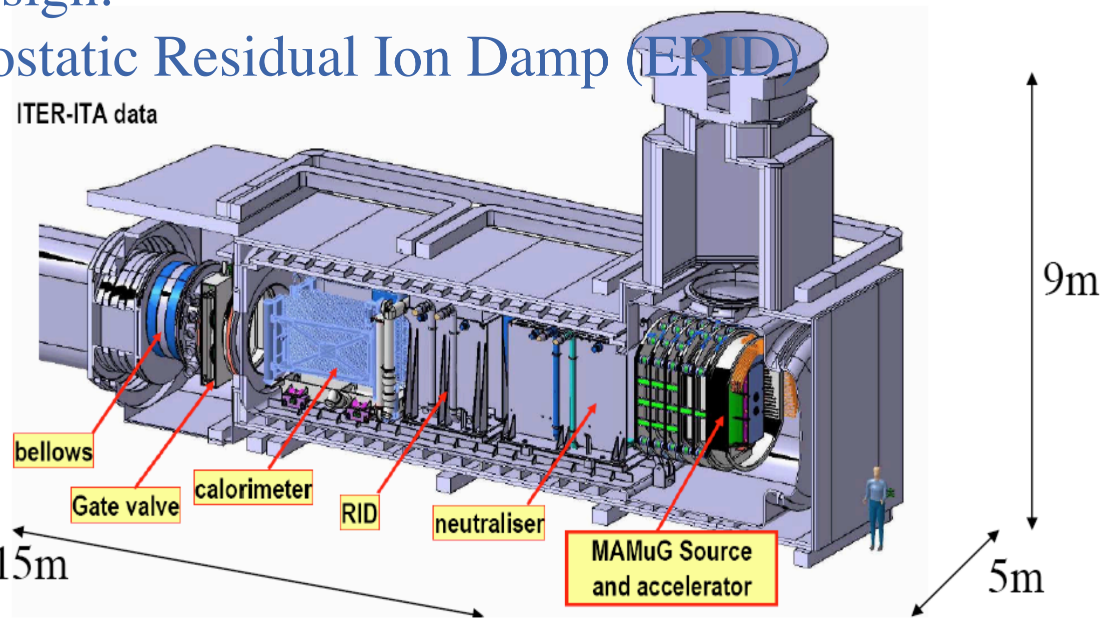
- **Ion Kinetic Transport: Divertor Studies (3D Map of Flux)**
- **ISDEP:**
  - Self consistent Plasma Profiles
  - Tokamak Geometry. (ASDEX, ITER)
  - Ion Heating (ICRH).
- **NBInjector simulation**
- **DKES (Drift Kinetic Equation Solver)**
- **Massive Ray Tracing (MaRaTra): CD**

Particle trajectories in ITER NBI

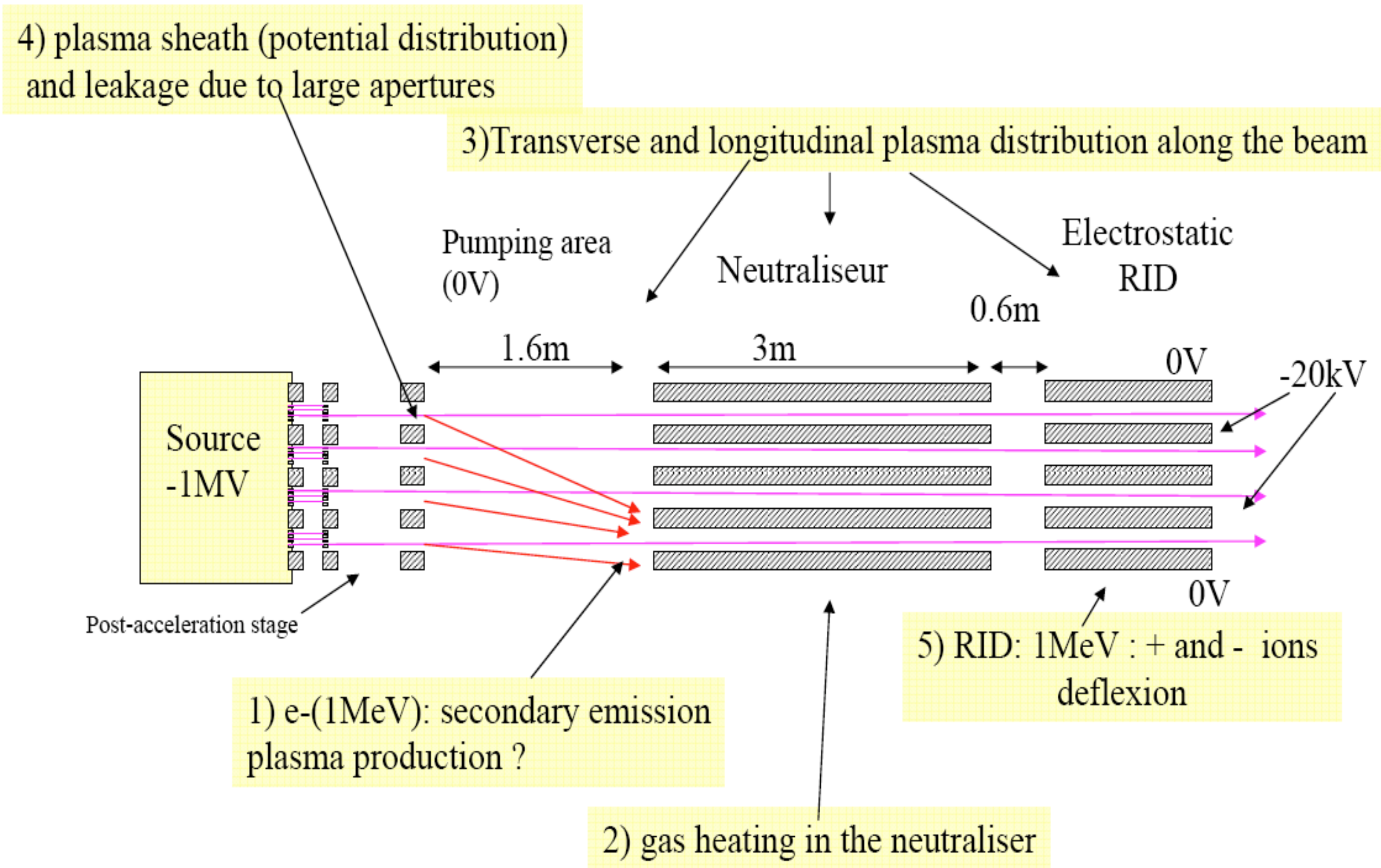


Contribution to the ITER NBI Design:
Particle Trajectories in the Electrostatic Residual Ion Damp (ERID)

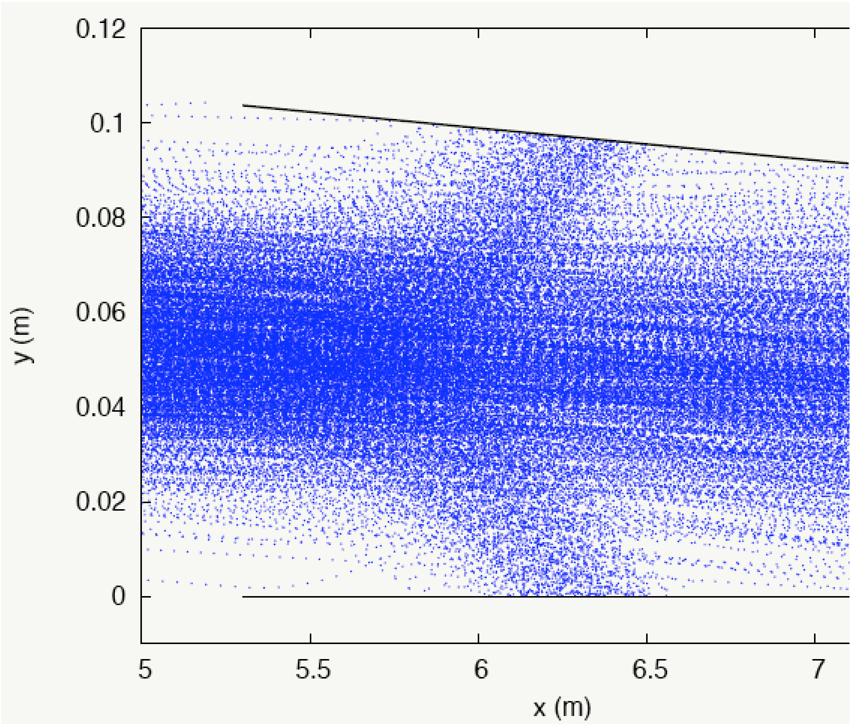
High statistics
Montecarlo calculations:
Independent ion &
neutral trajectories.



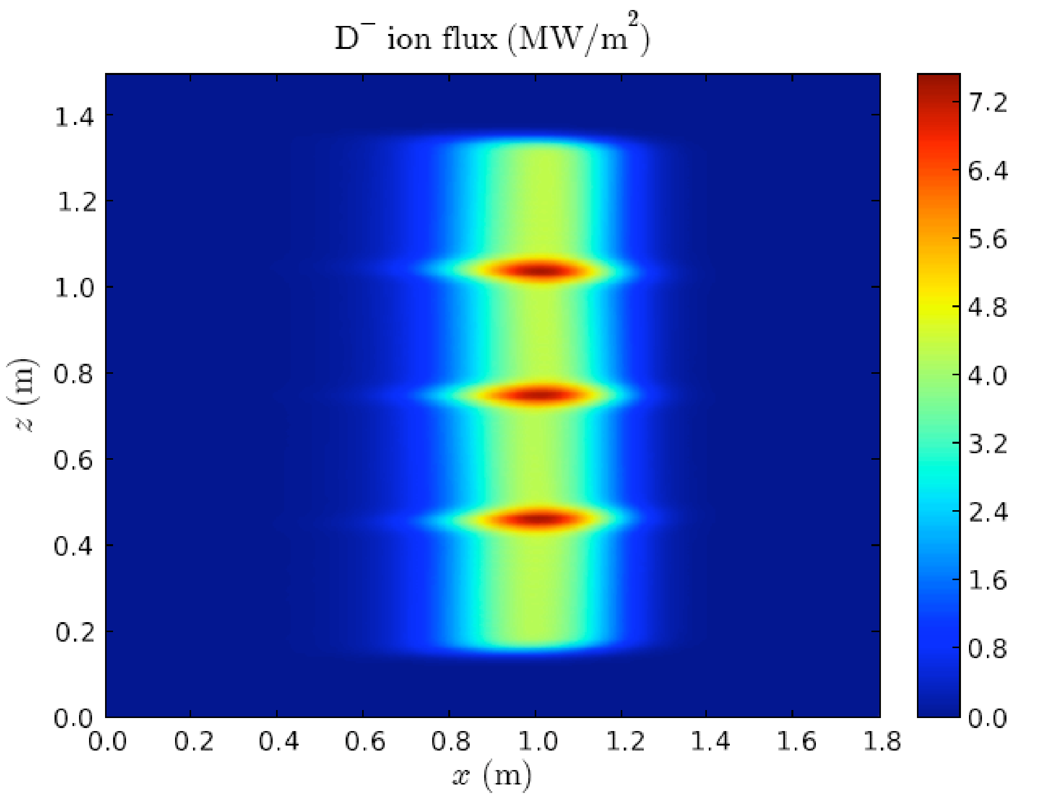
Plasma neutraliser modelling



Resuls of ERID simulations



Trajectories between two plates.



Power Flux on a single plate.

The final result is that the power flux is admisible.
Outgassing and plasma formation are estimated from the flux.

New applications & Improvement

- Ion Kinetic Transport: Divertor Studies (3D Map of Flux)
- ISDEP:
  - Self consistent Plasma Profiles
  - Tokamak Geometry. (ASDEX, ITER)
  - Ion Heating (ICRH).
- NBInjector simulation
- DKES (Drift Kinetic Equation Solver)
- Massive Ray Tracing (MaRaTra): CD

Standard Neoclassical Transport.

- **APPLICATION IN GRID-PORTING PROCESS: DKES (Drift Kinetic Equation Solver).**
- **Diffusive NC Transport. Particle and energy fluxes (s: plasma species):**

$$\Gamma_s = -n_s D_1^s \left(\frac{\nabla n_s}{n_s} - \frac{q_s E_r}{T_s} + \left(\frac{D_2^s}{D_1^s} - \frac{3}{2} \right) \frac{\nabla T_s}{T_s} \right)$$

$$Q_s = -n_s T_s D_2^s \left(\frac{\nabla n_s}{n_s} - \frac{q_s E_r}{T_s} + \left(\frac{D_3^s}{D_2^s} - \frac{3}{2} \right) \frac{\nabla T_s}{T_s} \right)$$

- **The diffusion coefficients are given by the following integrals (j=1,2,3):**

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

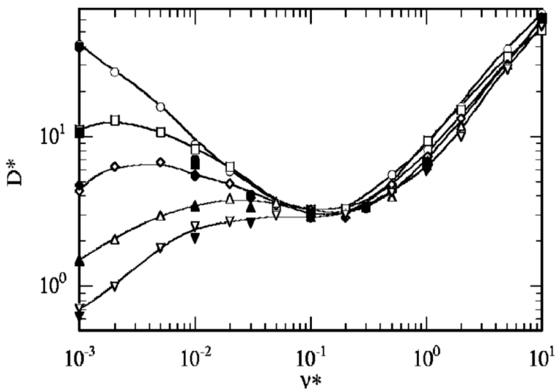
- **STRATEGY: Estimate a table of monoenergeitc coefficients at separate CPUs. THEN Integrate them.**

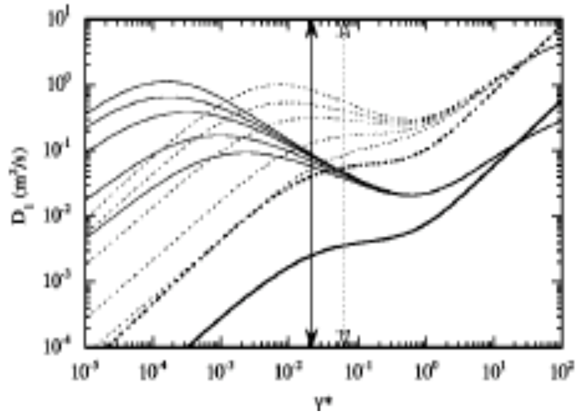
Standard Neoclassical Transport.

- The monoenergetic coefficient D* is a function of:
  - Device Structure (Magnetic field and equilibrium)
  - Collisionality, i. e. plasma characteristics: Density and Temperature.
  - Electric field.
  - Energy.
- All of them are independent (10 min a single value).

$$D_*^s = D_*^s(\vartheta^*, E_r, v)$$

$$D_j^s(n, T, E_r)$$





Contents

- **Introduction: Serial Fusion Problems.**
- **EGEE Experience:**
  - **Fusion VO.**
  - **Running Applications & Results.**
- **New Applications and upgrades.**
- **Future Plans:**
  - More complex Workflows: Kepler
  - Euforia Project.
- **Final Remarks**

Complex Workflows

- **Stellarator Optimization-DKES**
  - The Target Function can be the Minimising DKES Coefficients.
  - Every Case triggers DKES execution in the grid
- **ISDEP - EIRENE**
  - The flux of ions onto the wall (estimated in the grid) is the input for EIRENE (MC code of neutrals).
- **MaRaTra - ISDEP**
  - The power density distribution in the device is given by MaRaTra.

What is KEPLER?

(More Details in this afternoon talk.

Design tool to compose a workflow

- =>graphical: drag & drop the components ("actors")
- =>many actors: database, math, display, web service, grid service, …

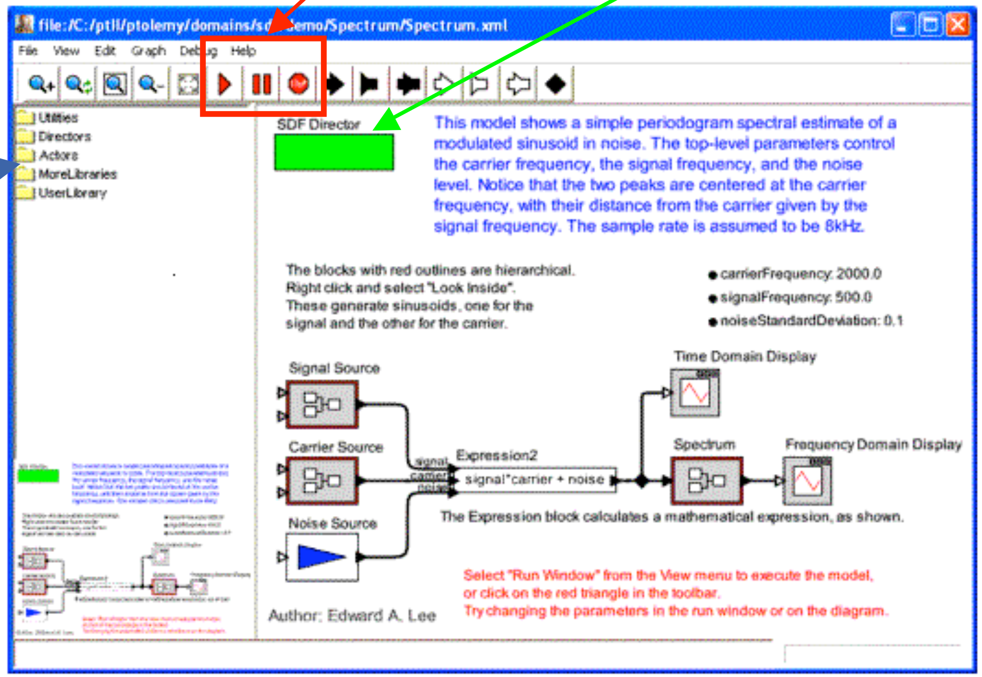
Engine to run a workflow

- =>various model of computations ("directors")
- =>hierarchical design.

Run control buttons

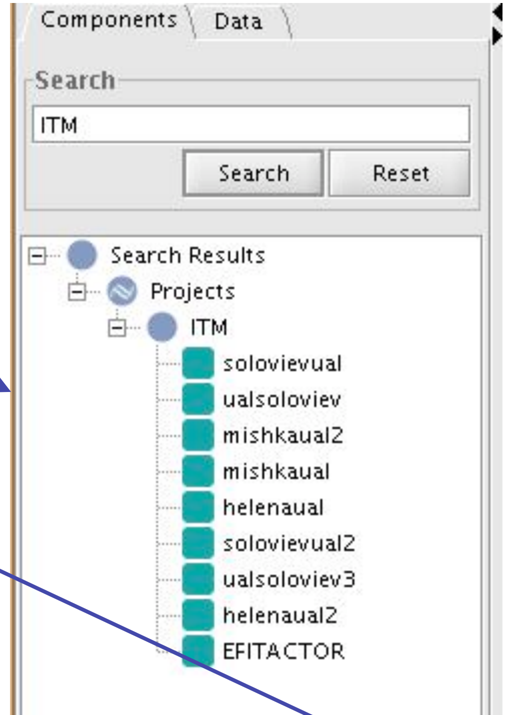
Scheduler: time behavior

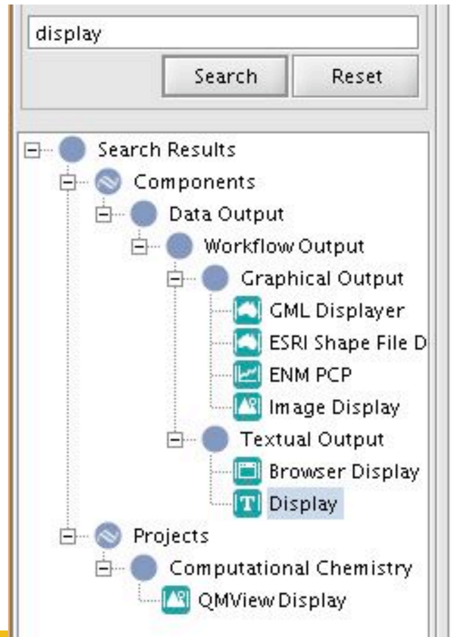
Catalogues of components

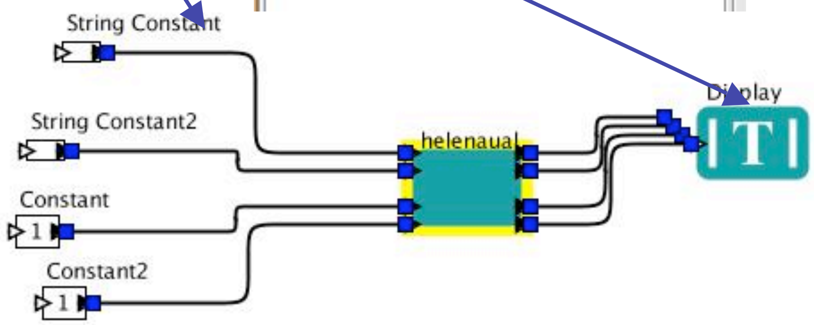


Kepler

- Building a workflow:
- Drag and drop an actor from the catalogues
- Define the input arguments:
- And a display actor: 2D, 3D
- Specify the director







Kepler in the GRID-EGEE Fusion V.O.

GLOBUS → **GLITE** → **ITM**

GLOBUS
- =>C/C++ library
- =>Java library in development

GLITE
- =>Java library in development

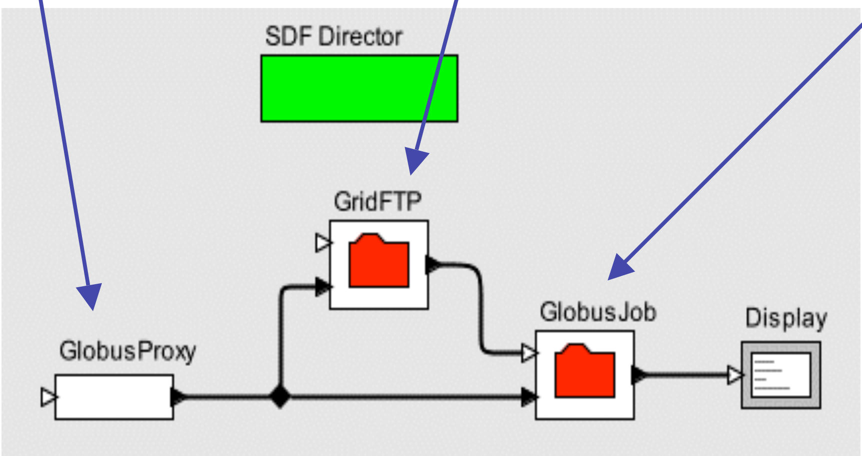
ITM
- =>Codes as WS
- =>UAL data access

Proxy

Job transfer via FTP

Data transfer via FTP

Job scheduling via JCL



Contents

- Introduction: Serial Fusion Problems.
- EGEE Experience:
  - Fusion VO.
  - Running Applications & Results.
- New Applications and upgrades.
- Future Plans:
  - More complex Workflows: Kepler
  - Euforia Project.
- Final Remarks

EUFORIA: EU fusion for ITER Applicatio

- Provide a work & infrastructure frame for fusio simulation, linking fusion, grid and supercomp communities.
- Improve the modelization capacities for ITER through the adaptation, optimization, and integration of a set of applications that can exp and join the core-edge transport.

Physics Codes: GRID (Seri

Code	Physics	Run time
SOLPS	Edge	Multiple * 1 day
Bit1+	divertor-SOL	Weeks to months
ISDEP	Kinetic transport	
TECXY	MC code	
FINITE	MC code	
COREDIV	MC code	
ASCOT	Orbits	

Physics Codes: GRID (Parallel)

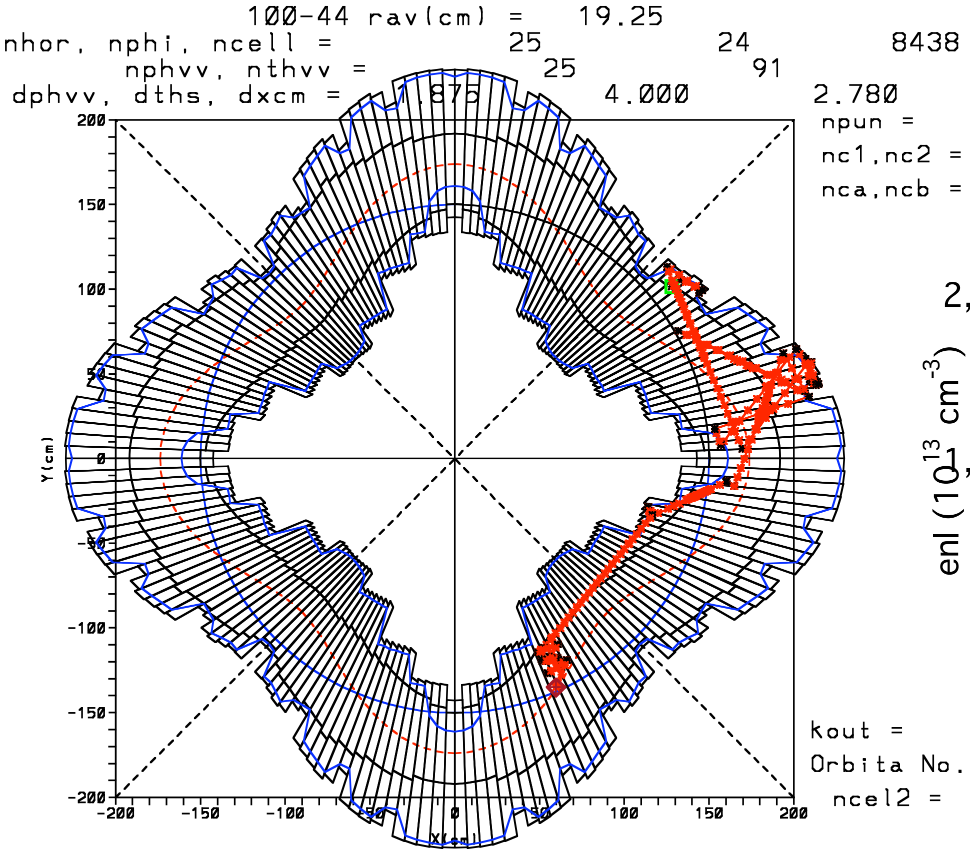
Code	# CPUs
SOLPS	4 --> 8
Bit1+	16 --> 256
ASCOT	16 --> 256
GEM	8 --> 32
ERO/TRIDYN	8 --> 64
TYR	8 --> 64
EIRENE	??
EDGE2D	??

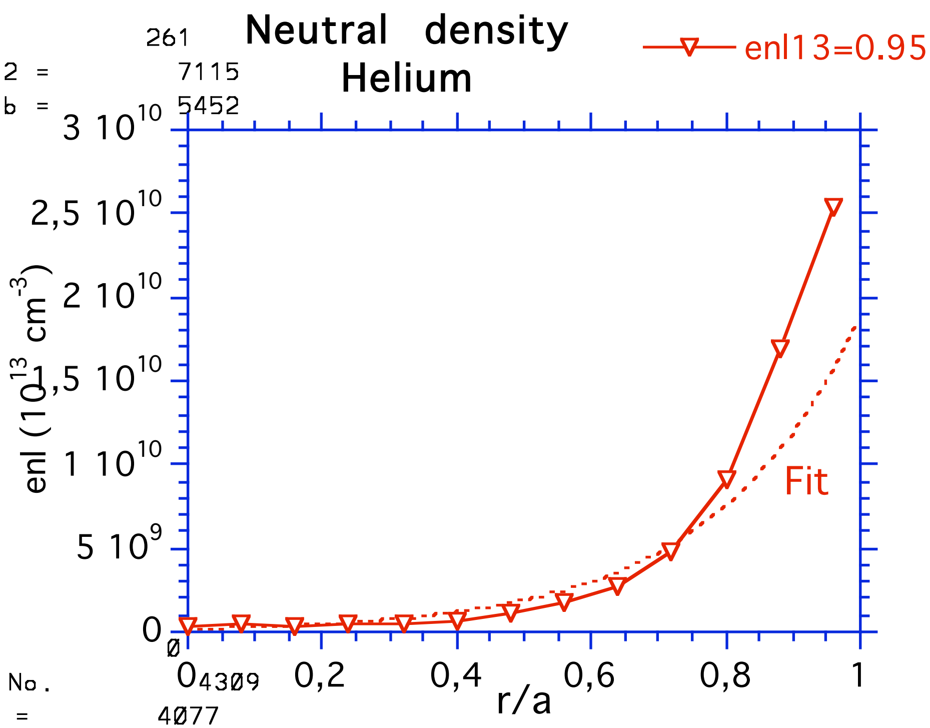
Example: Plasma-Wall Interaction

- EIRENE for tokamaks & Stellarators. Following a large number of neutral particles in a plasma background.
- The real Geometry of the wall and all the elements inside the vessel needed.
- Independent orbits of the neutrals.
- Iteration with a transport code needed.

- BIT1 code: Divertor simulation in toakamaks.

EIRENE Code



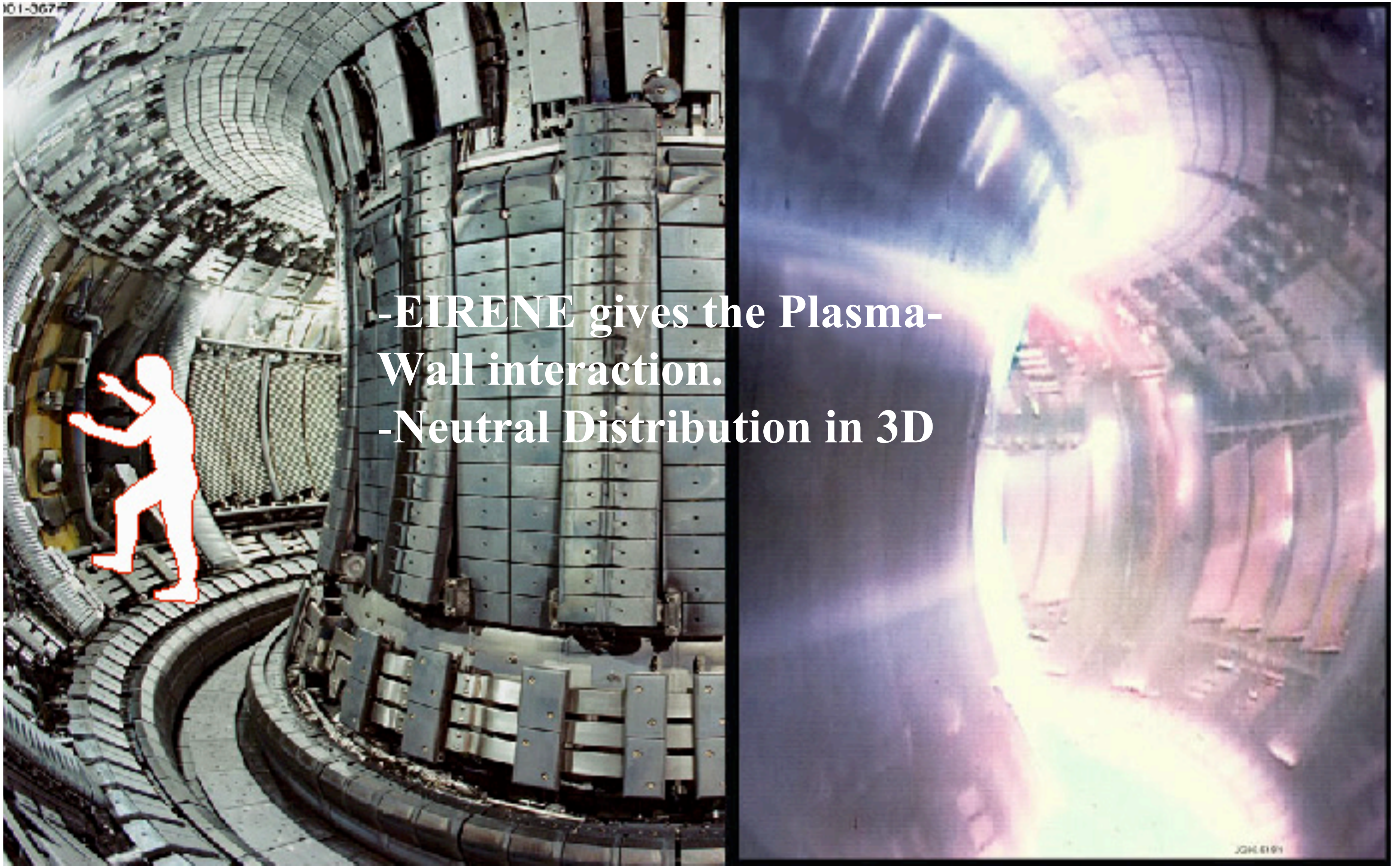


MC Code to estimate atom density.

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 TJ-II vacuum chamber is considered. RESULT: The Profile

EIRENE also works in Tokamaks.



-EIRENE gives the Plasma-Wall interaction.

-Neutral Distribution in 3D

Contents

- Introduction: Serial Fusion Problems.
- EGEE Experience:
  - Fusion VO.
  - Running Applications & Results.
- New Applications and upgrades.
- Future Plans:
  - More complex Workflows
  - Euforia Project.
- Final Remarks

Final Remarks

- Fusion VO in EGEE used for scientific production in Fusion Research.
- New Relevant scientific results obtained with grid capabilities.
- Complex Workflows are being established. Kepler workflow orchestration is a promising tool.
- Euforia: Oportunity for bringing more partners of Fusion Community to Grid Computing.
- Coordination EGEE-EUFORIA guaranteed.
- Workflows between Grid-HPC based on Kepler workflow orchestration is the final goal of EUFORIA.

egee
Enabling Grids for E-sciencE

EUFORIA