Status of Fusion activities in the Grid

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Outline

- Motivation: Computing in Plasma Physics.
- Parallel vs. distributed problems.
  - Supercomputers and parallel problems.
- Grids and distributed problems.
- Fusion VO
  - Ported applications.
  - Possible future Applications.

Computing in Plasma Physics (I).

- Plasmas:
  - Complex systems, with a lot of non-linear processes, with all the time and space scales playing a role (selfsimilarities, self-organization,...): Advances in chaos and selforganisation problems
  - Out of the equilibrium, open systems: Challenging for Statistical Physics.
  - They are in the intermediate range between Fluid and Kinetic Theories. Both of them are at work at given plasma ranges.

Computing in Plasma Physics (II).

- Plasma Physics is, of course, useful for Fusion, but it has interest itself.
- There are still open problems. Their solutions can help in commercial fusion achievement.
- Computing is a key element for solving complex problems in Plasma Physics.
- Computational Plasma Physics: A motivation for developing powerful computers and grid technologies.

Stellarators & Tokamaks: Complex Systems

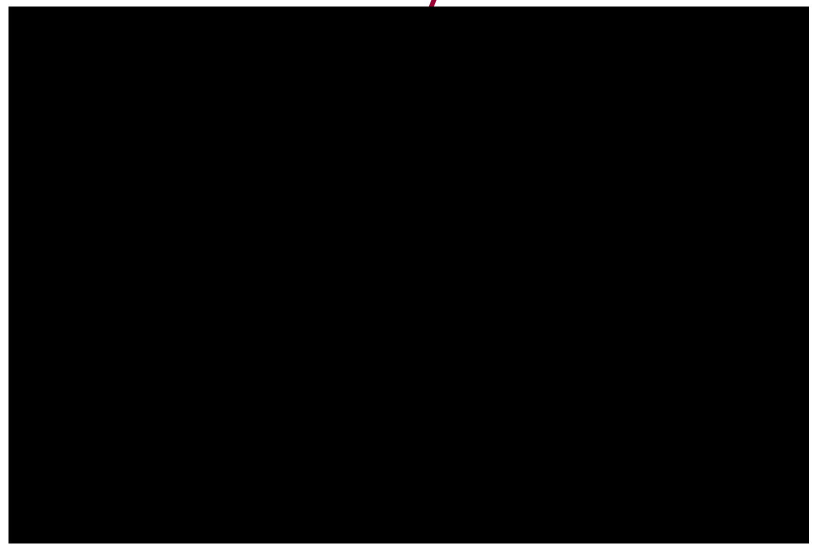
Stellarators: Fully 3D.

Consider exactly the geometry in almost all the problems.

Tokamaks:

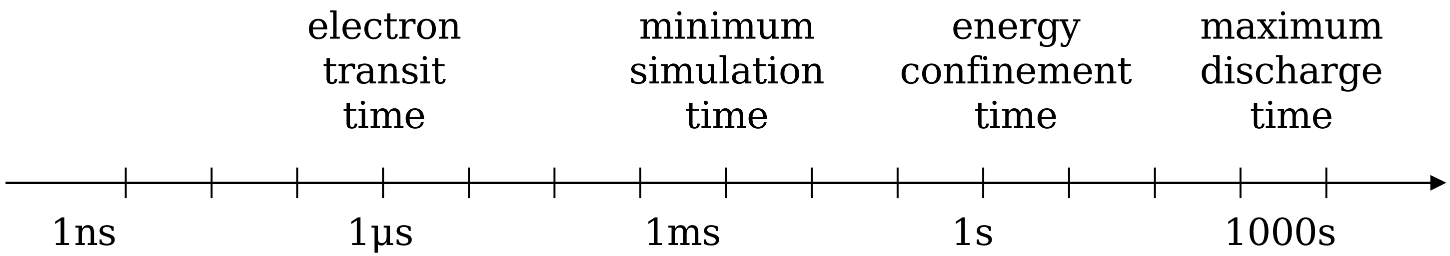
Usually 2D.

Fully 3D



Challenging Simulation: Numerical Tokamak and Stellarator. Gyrokinetic

Time scales and run time estimates



- Today, one could perform a 1 ms simulation within several days on
  the Mare Nostrum (a 100 TFlop/s machine)

- In 2014, a transport-time-scale simulation will take several week[redacted]
  a 4 PFlop[redacted]
  18 month[redacted]

Parallel vs. Distributed problems.

- Two main kinds of problems, depending on the interaction between their elements:
  - Parallel: those that require a lot of communication. The collective behaviour is dominant.
    - Fluid Theory. Gyrokinetic codes. Turbulence. Equilibrium and Stability…
  - Distributed: a large fraction of the problem can be treated solving for its independent elements.
    - Kinetic theory. Massively repeated

Supercomputers and parallel problems.

- Gyrokinetic codes: Continous and PIC.
- Turbulence and Transport.
- MHD.
- Fokker-Planck codes and Kinetic Theory.
- Equilibrium in Stellarators.
- Stellarator Optimization.
- Global NC Transport in Stellarators

Grids and distributed problems.

- Monte Carlo codes:
  - Plasma-wall interaction; neutral particle orbits.
  - Kinetic transport: guiding centre orbits in toks. and stell.
  - Langevin equations.
- Parameter Variation:
  - Neoclassical Transport estimates (DKES).
  - Massive Transport analysis.
- Simulation of Heating by Microwaves: Massive Ray Tracing.
- Stellarator Optimization.

Fusion VO Working

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

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

- **14 Partners, >1000 CPUs: CIEMAT: 27 KSpecInts; BIFI: 8 KSpecInts; INTA: 6 KSpecInts; 70 KSpecInts; BIFI: 64 KSpecInts**

~10 Tflops

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

Open Problem: Global NC Transport

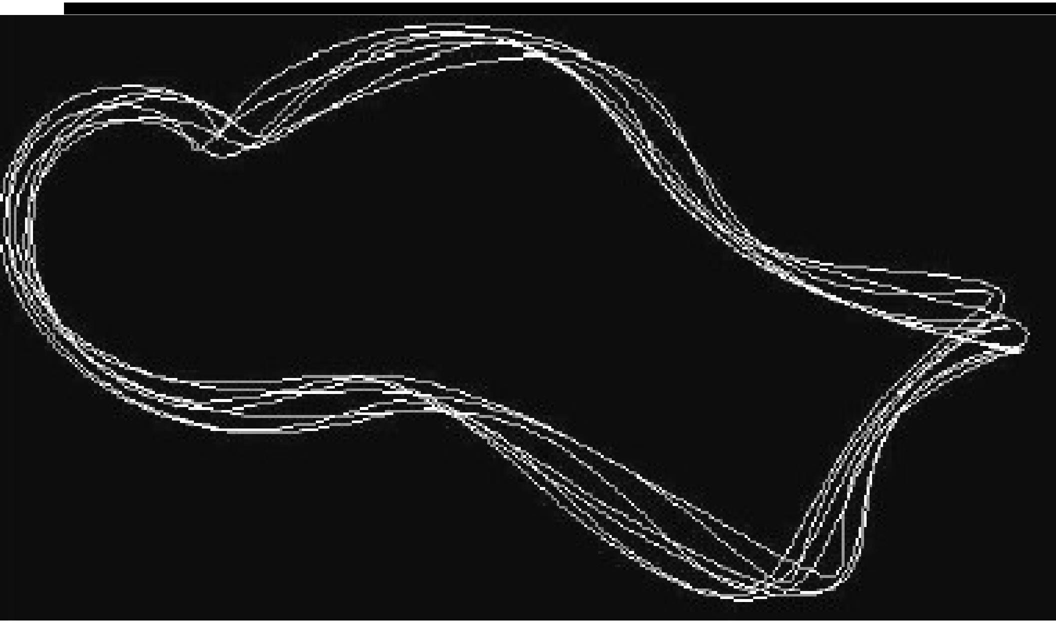
Time consuming MC Codes in the LMFP regime .
Suitable for Grids.

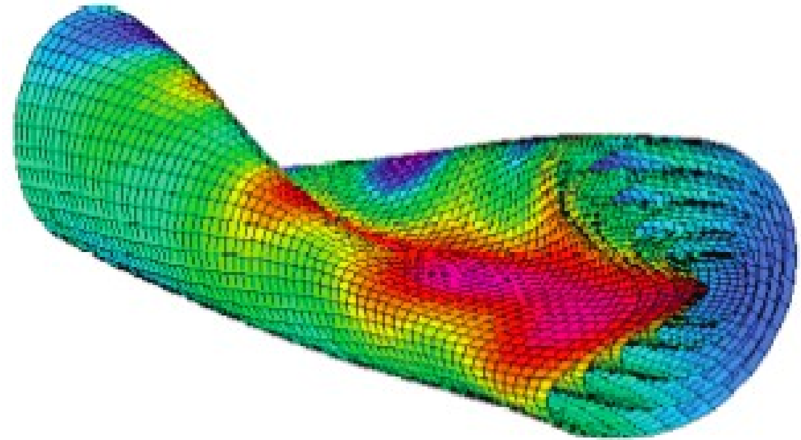
In optimised stellarators: Poloidal Drifts close to magnetic surfaces.

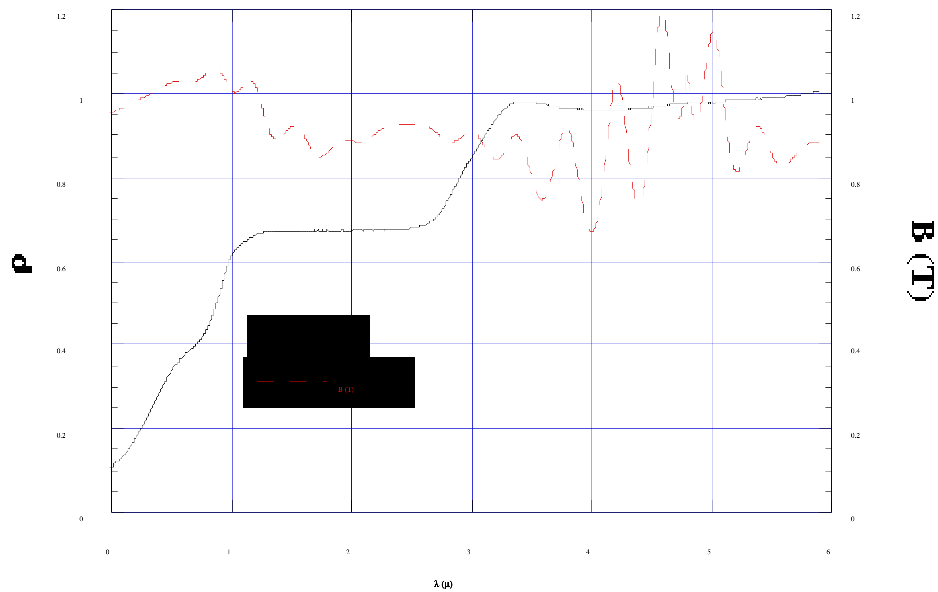
In no optimised ones: large radial excursions.

10^6-10^7 markers or particles. Tflops.

Kinetic Transport







Example of orbit in the real 3D TJ-II Geometry (single PE).
Collisions included: 1 ms of trajectory takes 4 sec CPU.
Particle life: 150 - 200 ms. Single particle ~ 10 - 20 min.
10^6 - 10^7 particles needed.

Kinetic Transport

- **Monte Carlo code that solves microscopic Langevin Equations for every ion, including:**
  - the movement inside the magnetic and electric fields created by the magnetic confinement device and the plasma.
  - random term to simulate collisions with the background plasma.
- **The particles are distributed randomly in the plasma according to experimental results:**
  - The spatial distribution of particles is done accordingly to plasma density.
  - The distribution of particles in momentum space follows a Maxwellian distribution function according to the measured temperature (which astonishingly happens to be almost constant).
- **Estimate every trajectory independently in a single CPU (about 10 - 20 min of elapsed time).**

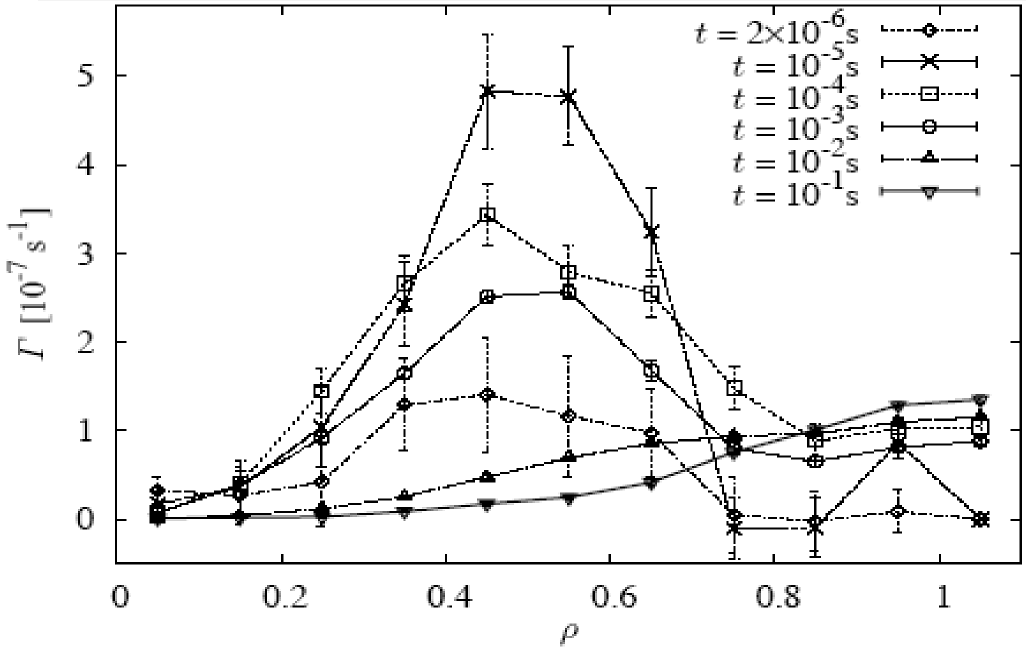
Kinetic Transport

- **Every case (particle) needs:**
  - A seed for random space distribution.
  - A seed for random momentum distribution.
  - An initial seed for collisions.
- **The background plasma is common for every particle, therefore is located at the catalog:**
  - Background density and temperature, i. e., collisionality.
  - Background electric field.
  - Background magnetic field and magnetic configuration.
- **~10^7 particles launched in bunches of about 10^3 to be run in every CPU.**
- **Post process. Statistical measures: Fluxes, velocity distribution, space distribution, etc.**
- **No problem if some (few) cases are lost.**

Input parameters

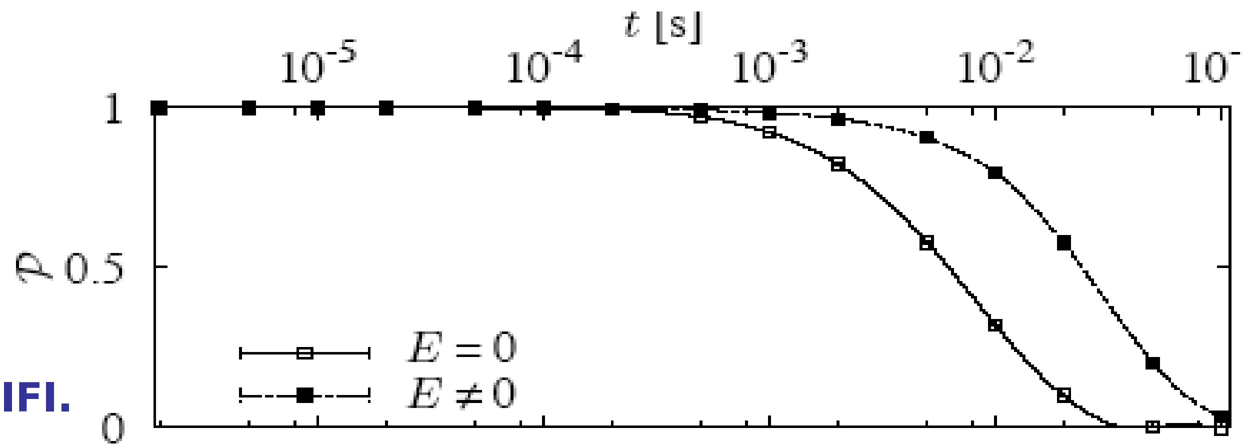
Stored at the FUSION VO catalogue

Relevant Results



Radial Flux evolution: A key quantity for transport.

Persistence of particles: τ=28 ms (to be compared with 21 ms measured)



Collaboration with BIFI.

Standard Neoclassical Transport.

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- APPLICATION IS IN “GRIDIFICATION” PROCESS.
- DKES (Drift Kinetic Equation Solver).
- Diffusive NC Transport. Particle and energy fluxes (s: plasma species):

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

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

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

$$D_j^s = \frac{4}{\sqrt{p}} D_{Tok}^s \quad D_*^s(J^*, E_r, v) \left(\frac{v}{v_{th}} \right)^{+2j} \exp \left(\frac{v}{v_{th}} \right) dv$$

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Standard Neoclassical Transport.

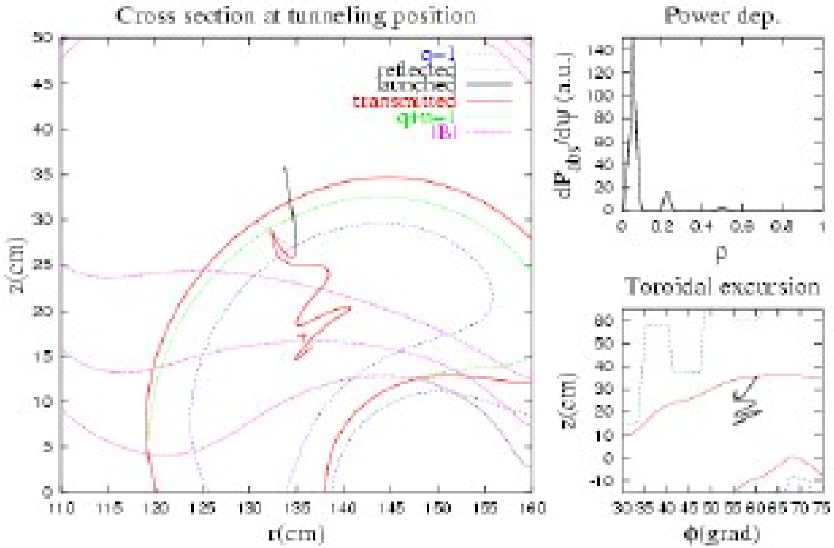
- The monoenergetic coefficient D* is a function of:

  - Device Structure (Magnetic field and equilibrium)
  - Collisionality, i. e., Plasma characteristics: Density and Temperature.

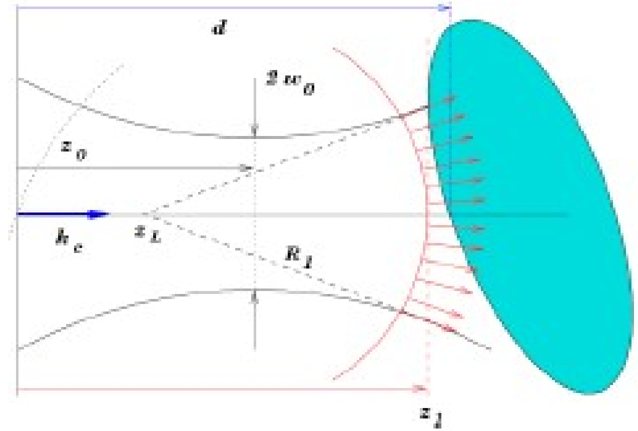
$$D_*^s = D_*^s(J^*, E_r, \nu)$$

  - Electric field.
  - Energy.
  - DKES (Drift Kinetic Equation Solver).
- All of them are independent (10 min a single value).
- STRATEGY: Estimate a table of monoenergeitc coefficients at separate CPUs. THEN Integrate them.

MaRaTra: Massive Ray Tracing



Single Ray (1 CPU):
Hamiltonian Ray Tracing Equations.



Beam Simulation:

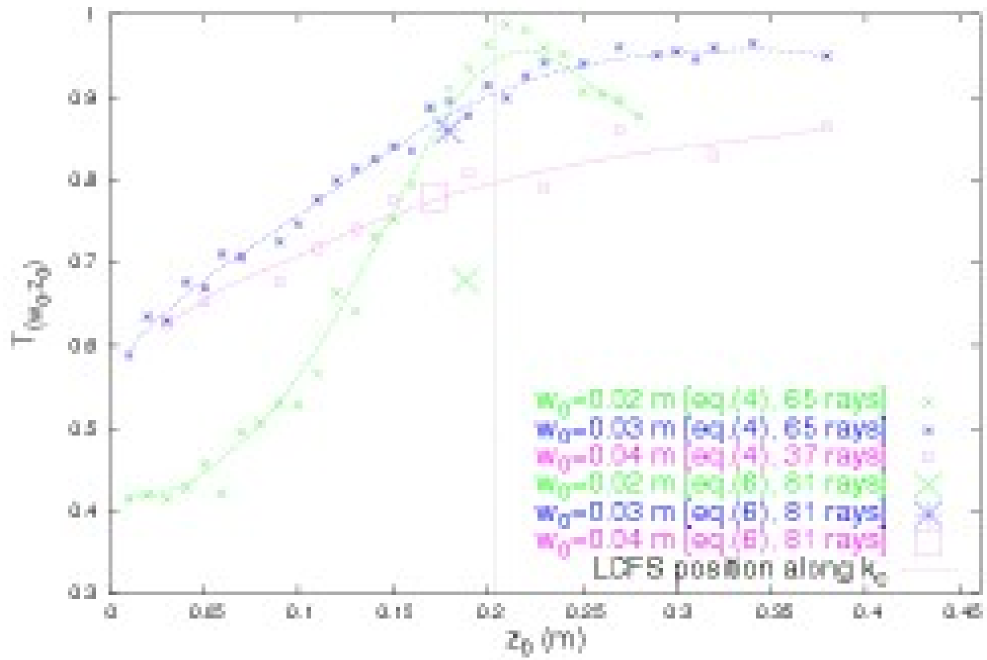
Bunch of rays with beam waist close to the critical layer (100-200 rays) x (100-200 wave numbers) ~10^5

GridWay

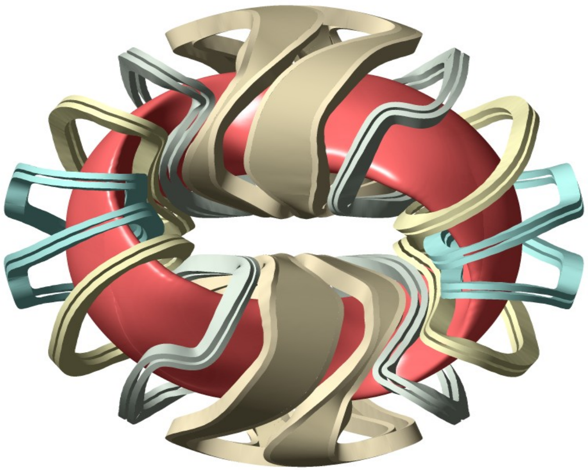
Application in production phase.
Gridification based on Gridway:
EGEE'07
by J.L Vázquez-Poletti et al. UCM (Spain)

MaRaTra

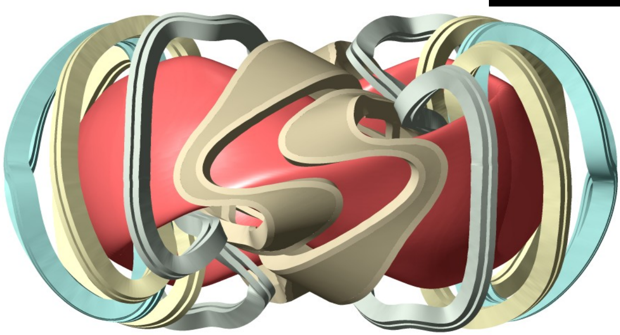
- **A single ray is solved in every CPU: Hamiltonian Equations.**
- **The rays are distributed accordingly to the microwave beam structure: Every case needs Initial space position and Wave vector.**
- **The background plasma is common for every particle, therefore it can be downloaded from a close Storage Element: Background plasma and magnetic configuration.**
- **$\sim 10^5$ rays launched.**
- Post process: Distribution of absorbed power (add all the absorbed powers of the single rays). No case must be lost. This is one reason for using the GridWay metascheduler.

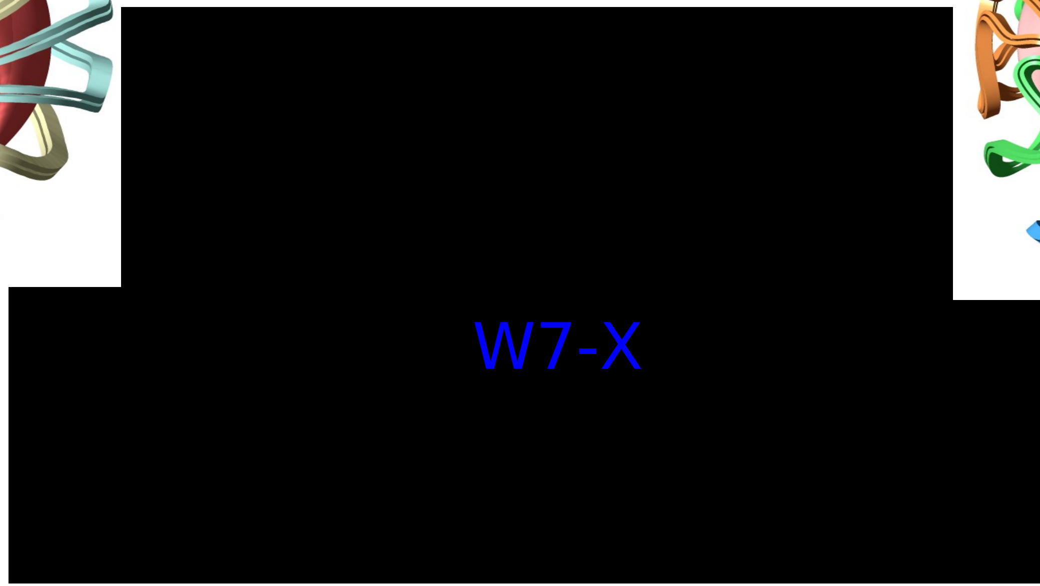


Opt. Stellarators in Supercomputers

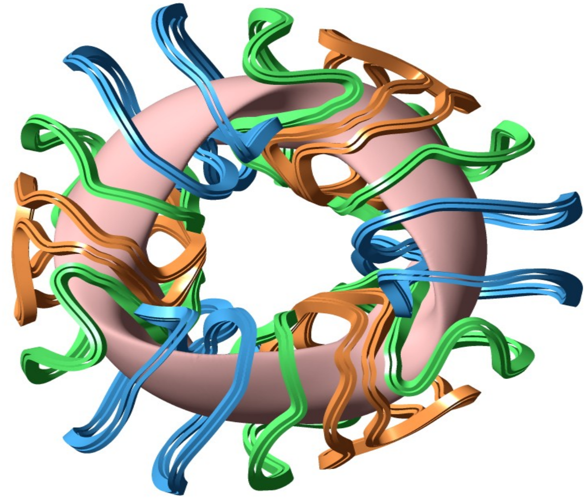


QPS

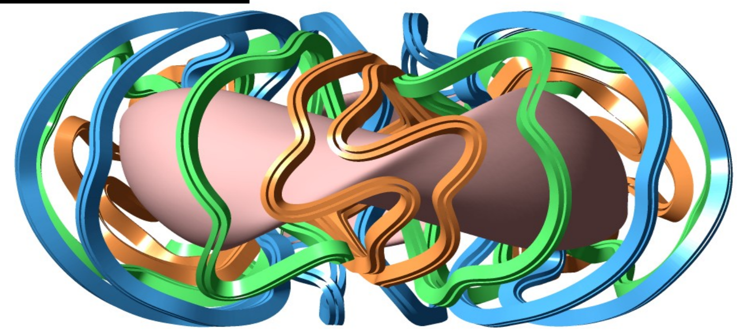




W7-X



NCSX



Stellarator optimization in the Grid

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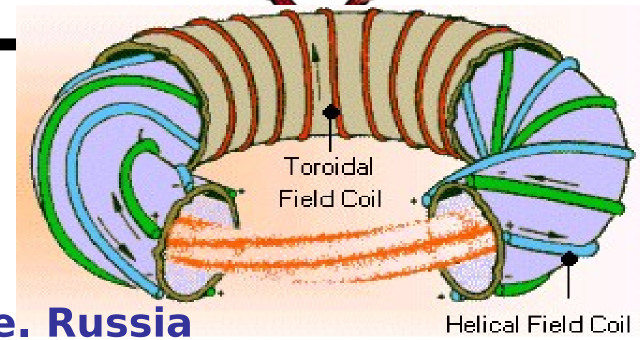


STELLARATORS: A lot of different Magnetic Configurations operating nowadays.

V. Voznesensky. Kurchatov Institute. Russia

-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)

120 Fourier parameters are varied.

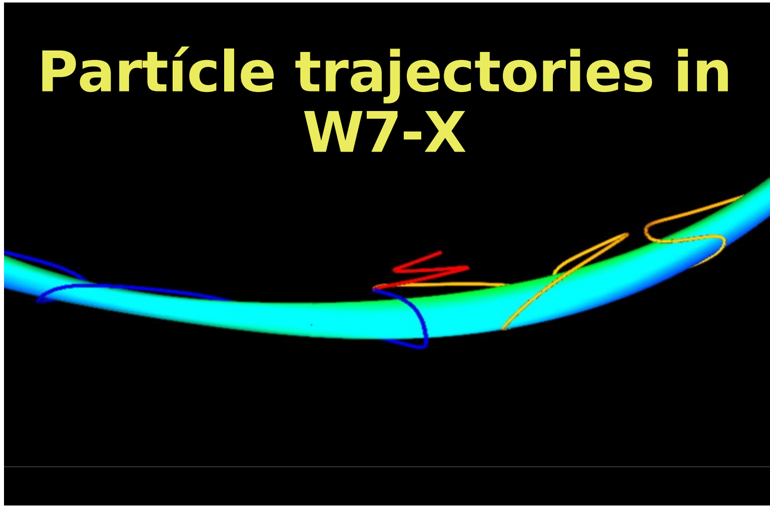
$$\vec{B}(\psi,\theta,\varphi) = \sum_{\mu,\nu} \vec{B}_{\mu,\nu}(\psi)\, e^{i(\mu\theta-\nu\varphi)}$$

$$R(\psi) = \sum_{\mu,\nu} P_{\mu,\nu}(\psi)\cos(\mu\theta-\nu\varphi)$$

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

Optimization Criteria: Target Functions

-Neoclassical Transport.
- Bootstrap current.
- Equilibrium vs. plasma pressure.
- Stability (Balloning, Mercier,...)

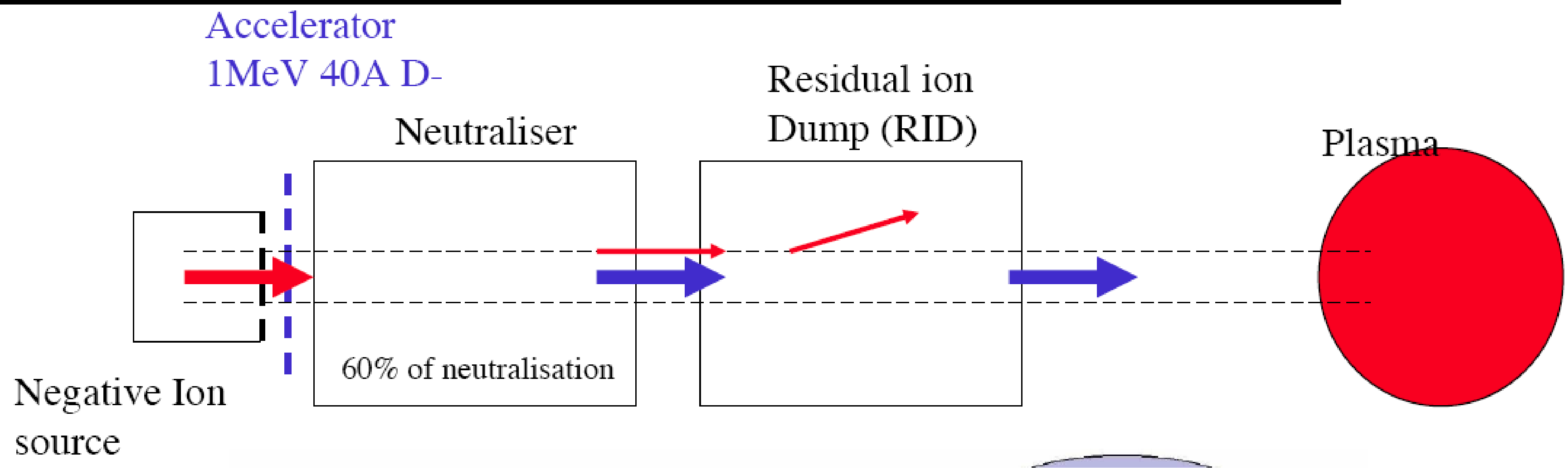


-Genetic Algorithm to select the optimum configuration for given Target Functions.

- LCG-2 - based Russian Data Intensive Grid.
- About 7.500 cases computed (about 1.500 was not VMEC-computable), i.e. no equilibrium).
- Each case took about 20 minutes. Up to 70 simultaneous jobs running in the grid.

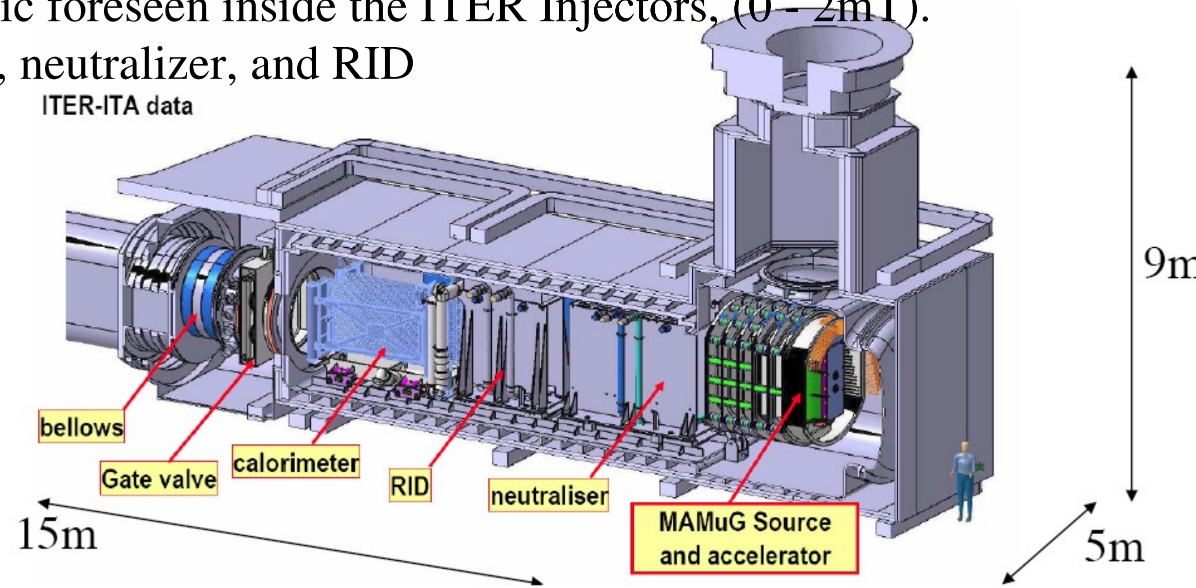
New possible
Fusion applications
to be ported to the grid.

Ion trajectories in ITER NBI



The LNF is contributing to the European Neutral Beam Test Facility: RID Simulation and design of a set of coils to generate the Residual Magnetic foreseen inside the ITER Injectors, (0 - 2mT).
Ion Trajectories: Ion source, extracting grid, neutralizer, and RID

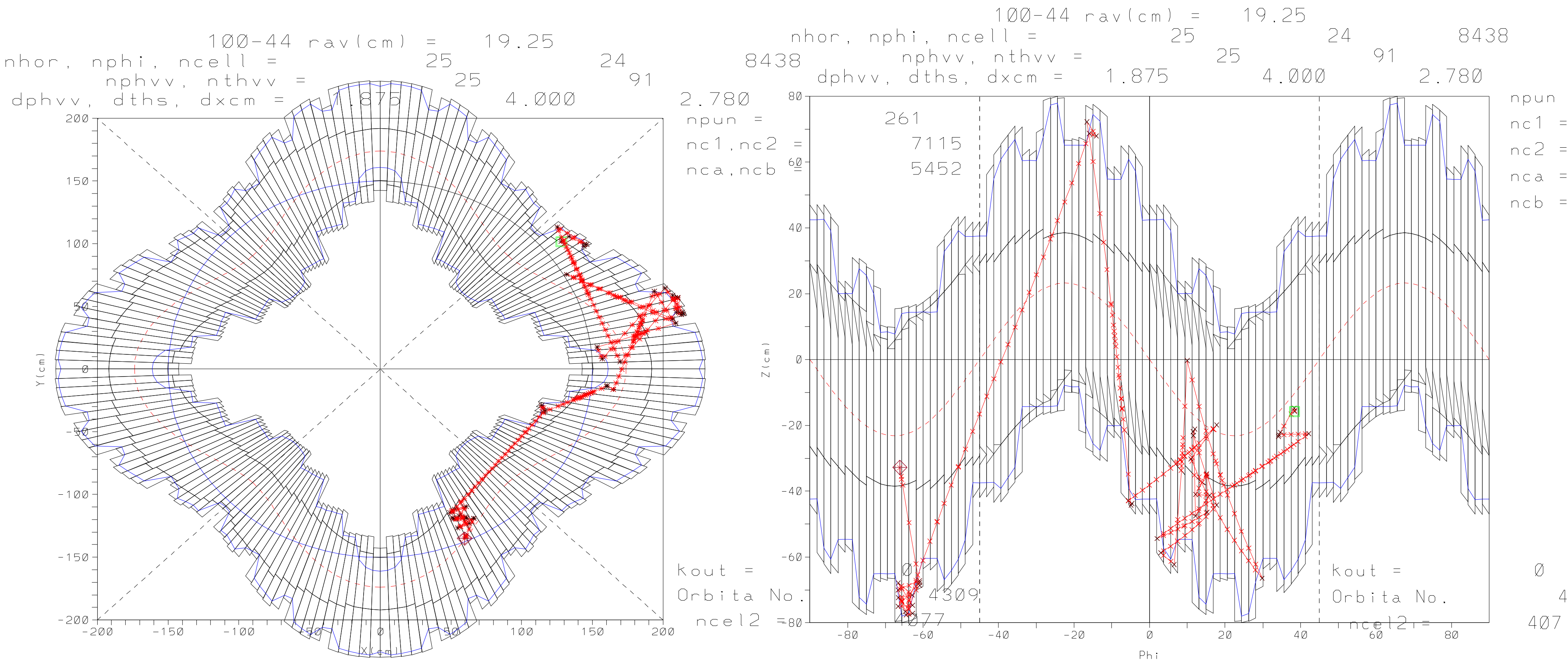
High statistics Montecarlo calculations: High performance computation resources are required.



Plasma-Wall Interaction

- EDGE2D and 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.

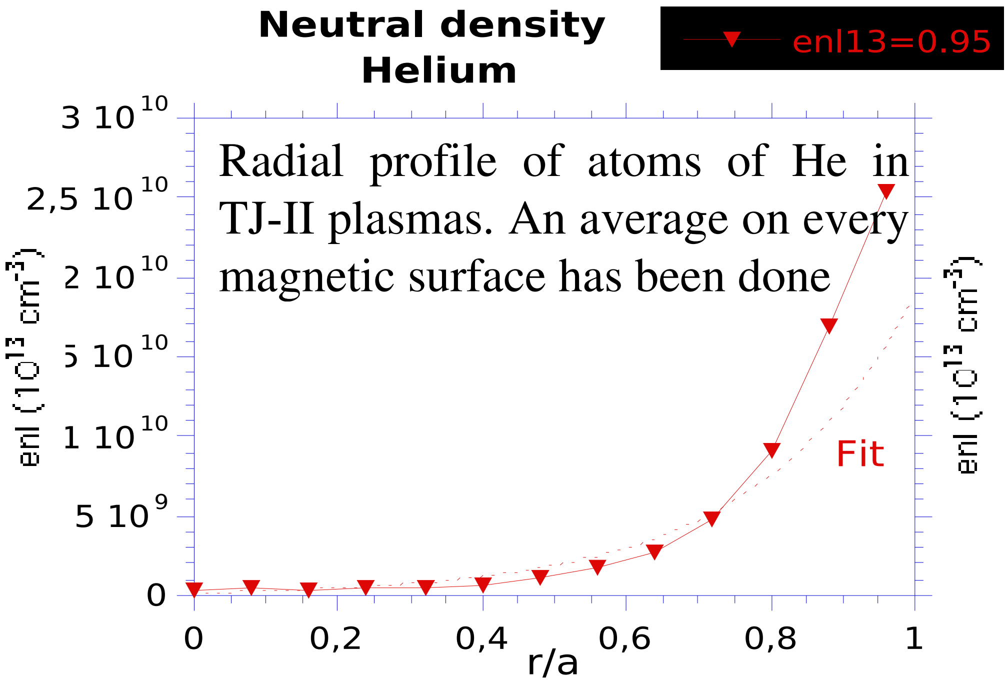
EIRENE Code

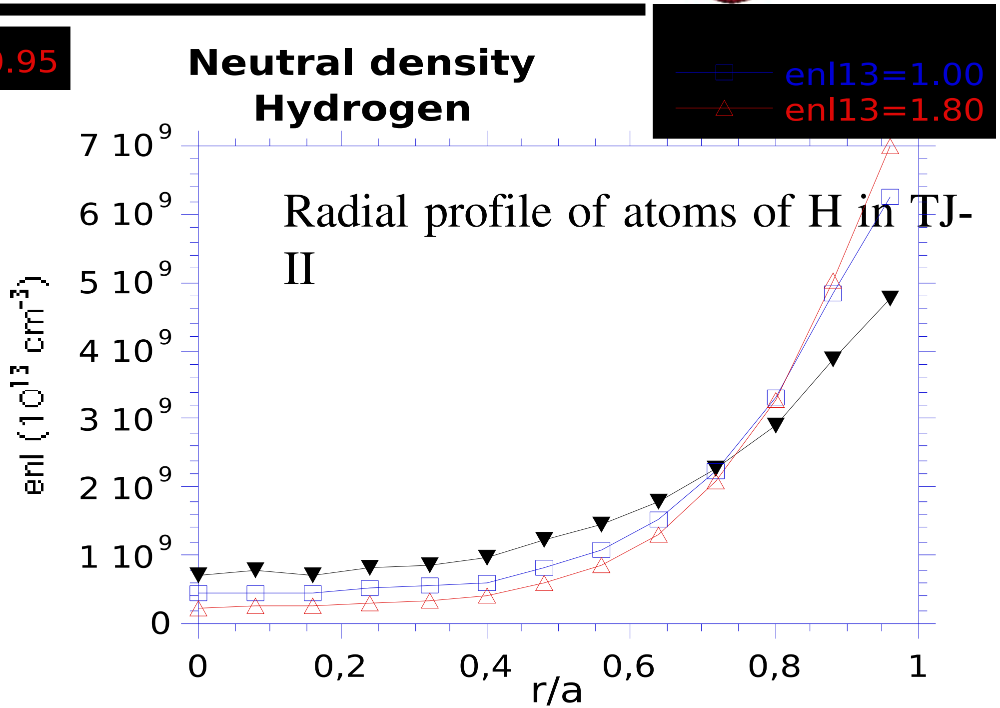


Trayectory of a He atom in TJ-II. Vertical and horizontal proyections. It starts in the green point and is absorbed in the plasma by an ionization process.

The real 3D geometry of TJ-II vacuum chamber is considerd.

EIRENE Code



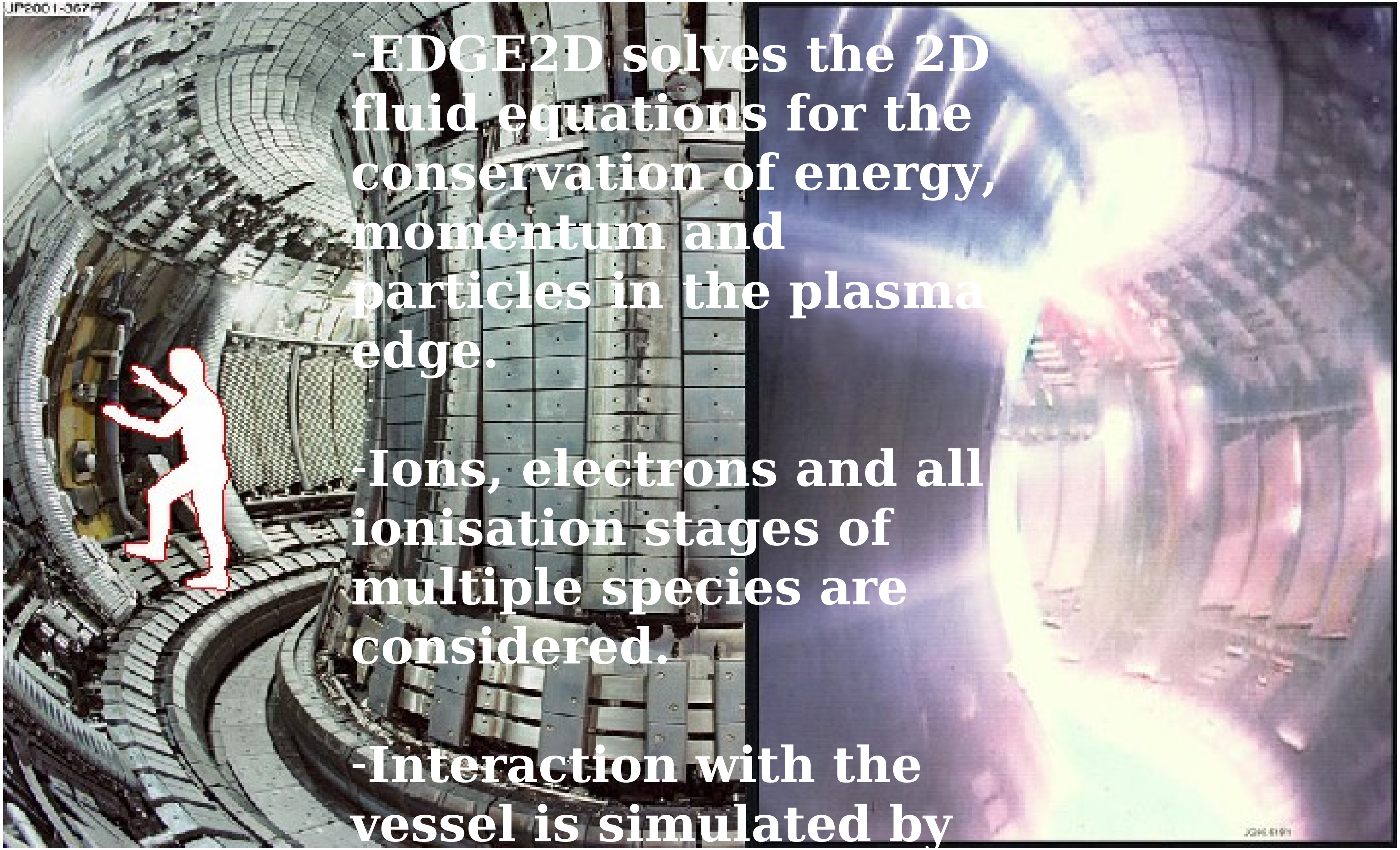


Two parts: 1) Following trajectories (Totally distributed) --> **GRID**

2) Reduction to put all together.

EIRENE Code comes from IPP (Jülich, Germany) and is extensively used by Fusion community.

EDGE2D: Determine plasma shape



-EDGE2D solves the 2D fluid equations for the conservation of energy, momentum and particles in the plasma edge.

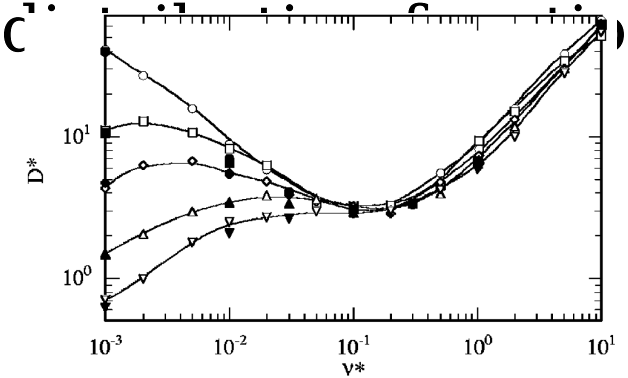
-Ions, electrons and all ionisation stages of multiple species are considered.

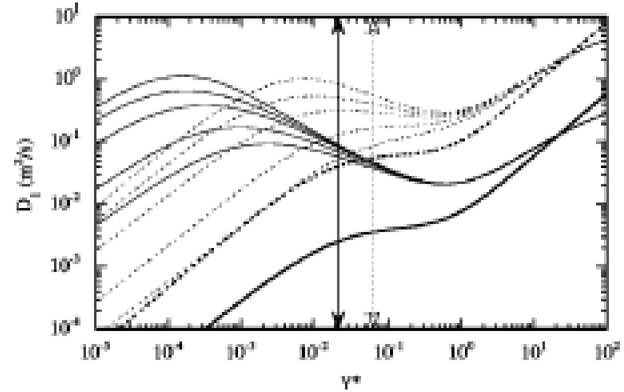
-Interaction with the vessel is simulated by

Variation of Parameters

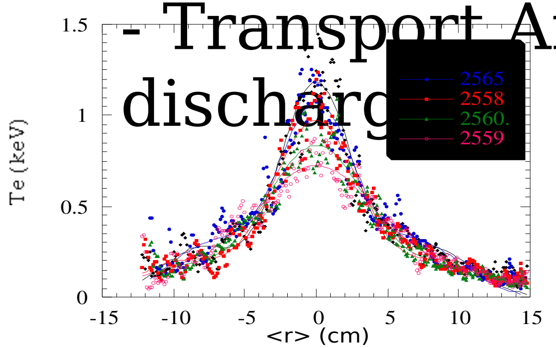
Run the same code with different enter parameters. Examples:

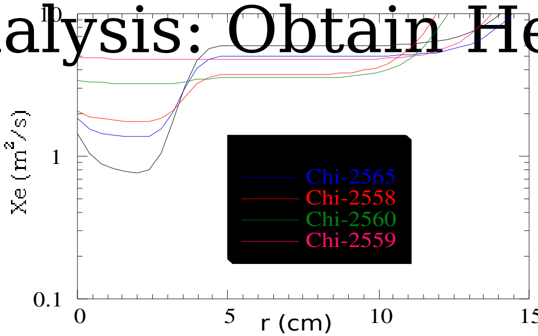
- NEOCLASSICAL TRANSPORT: DKES Code (solve for Monoenergetic coefficient and convolution it with d… …n).

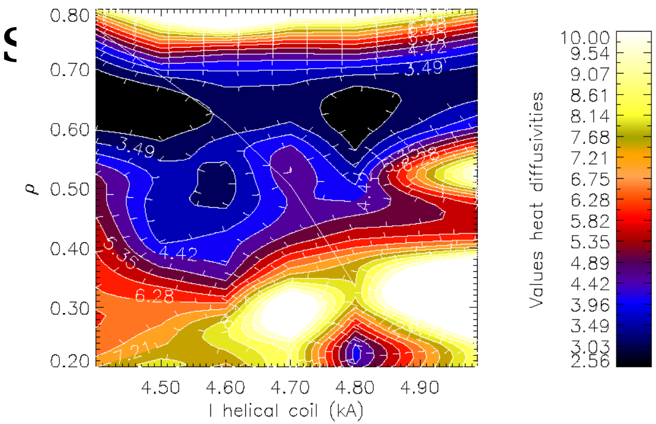




- Transport Analysis: Obtain Heat Diffus… discharg…







EUFORIA: A new project submitted to FP7

Bring Fusion community users to use e-Infrastructures in Europe.

Take the mos[redacted]
Exploitation [redacted]
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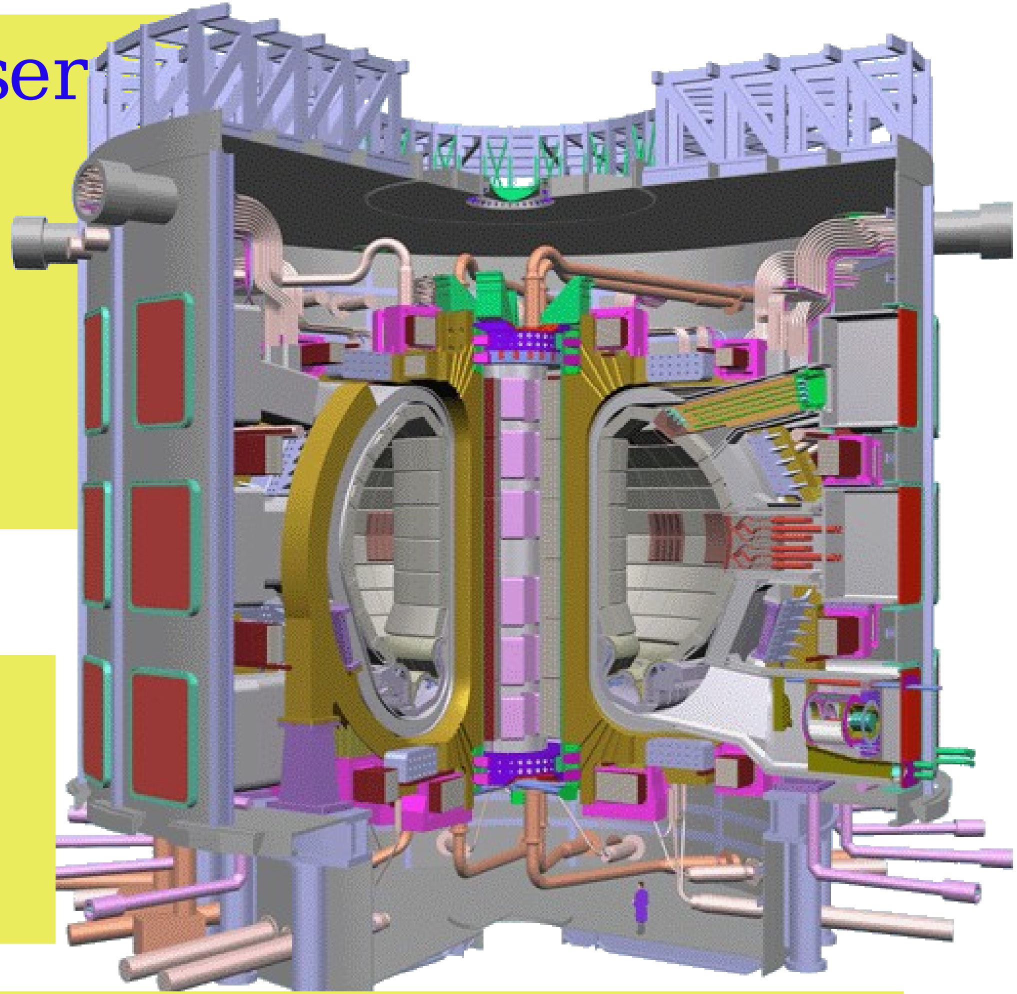

Consortium with people from Fusion, Grid and HPC communities.

¡More applications to the Grid!

Final Remarks

- Computational Plasma Physics is a challenging discipline that can push forwards Physics Frontiers.
- Present generation of Supercomputers (~50 Tflops) are overcome by some open problems. Needed simulations for ITER: e. g. Integrated models towards Numerical Tokamak and Stellarator.
- Grids are powerful tools for distributed calculations (the poor man's supercomputer).
- Fusion VO is working: Several applications are running.
- New applications to be ported to the grid envisaged.
- Possible Workflows that involve both types of computation.
- Slow increasing of grid using by the Fusion Community.
- EUFORIA Project can boost the grid use.

uture of Fusion Plasmas Modelling

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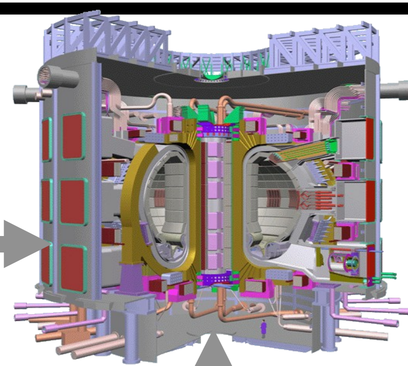
Module Development

- Linear & Non-linear MHD Instabilities
- Fast Particle Driven InstabiInstabilities
- Turbulent Transport
- Plasma- Wall Interaction
- Kinetic Theory and Plasma Heating



Integrati on

Numerical Tokamak

Integration

Numerical Stellarator

DEMO

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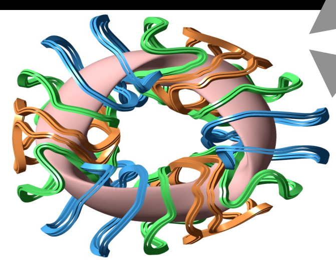

- Equilibrium & Stability
- Global Neoclassical Transport

General Knowledge