# Complex Workflows between HPC and Grid applications

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e-infrastructure

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# Collaborators

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# What we want to show

- The feasibility of mixed HPC-Grid scientific workflows.
- Building blocks for complex fusion modeling workflows. To be used by EFDA -European Fusion Development Agreement-, the European fusion community.
- Developments essential for fusion community that could be reused by other communities. The developments will be accessible for EFDA Associates.
- Results of a pilot project among EGEE-DEISA-EUFORIA.
  - Develop heterogeneous workflows for fusion community.
  - Put workflows in production using real computing infrastructures.
  - Workflows between grid-grid, grid-HPC and HPC-HPC applications.

# Why?

- **To help fusion scientists by enhancing the modeling capabilities for ITER sized plasmas.**
- **To promote innovative aspects:**
  - Dynamic coupling of codes and applications on a set of heterogeneous platforms into a single framework through a workflow engine.
- **To foster a collaboration environment between EUFORIA, DEISA and EGEE: Building Community.**
- **DEMO activities funded by EGEE.**

# Demo

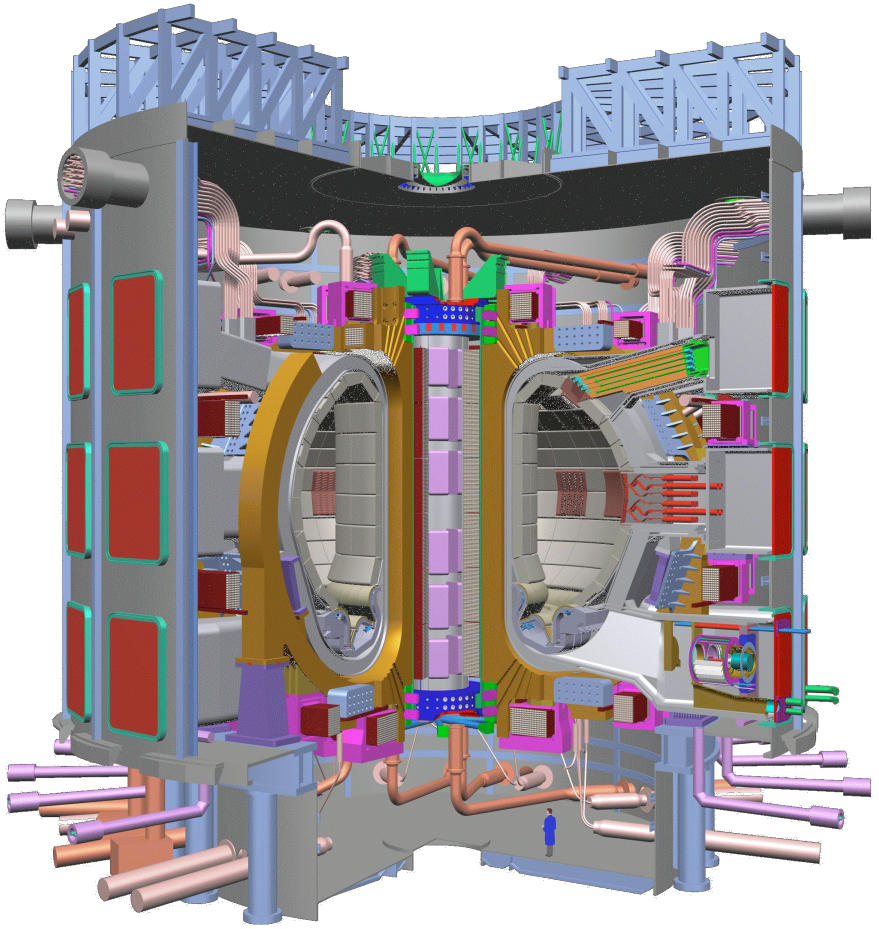
Scientific Gateways

Building Workflows

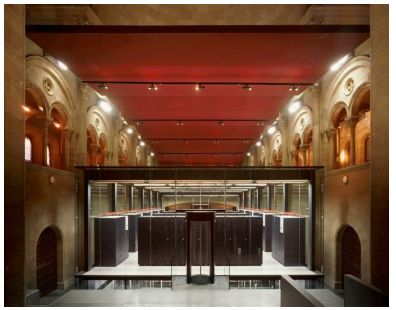
ITER

# TARGET: Fusion community

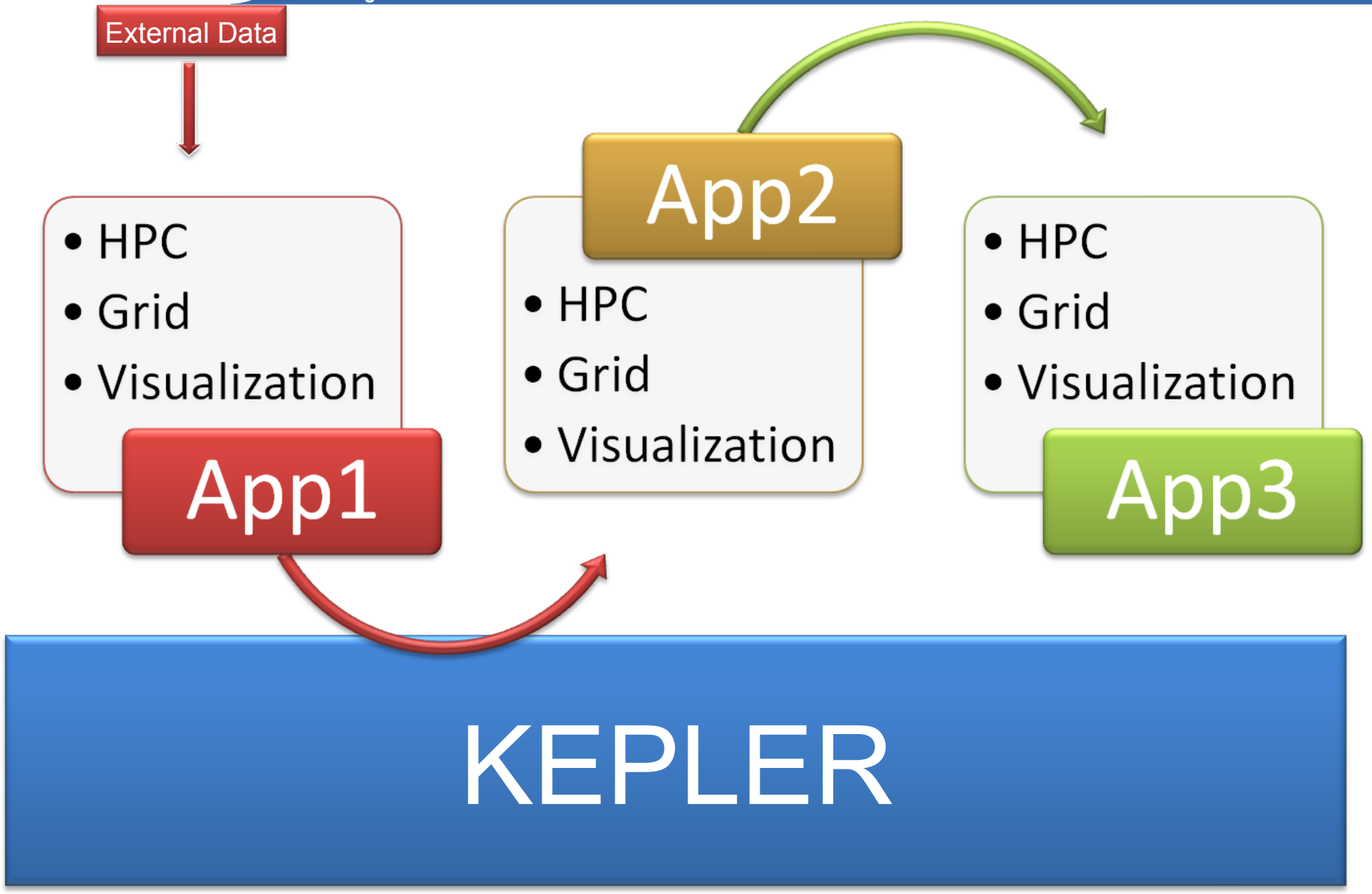
- **Next generation of energy production: social and environmentally acceptable**
- **It still has many open issues: plasma confinement & material science.**
- **It becomes not only a scientific problem but also a large scale computational problem where distributed infrastructures and HPC are required:**
  - Experimental data processing.
  - Experimental scenario development.
  - Theory.



# Fusion community



- Using top computational environments.
- Wide range of applications: serial, MPI, shared-memory, …
- Complex experiments: Necessity of connecting different models (applications) → WORKFLOWS
- Several applications running and exchanging data in different infrastructures.
- Necessity for an easy and widely known environment.
- EGEEIII: Grid used by fusion community. Distributed applications suitable for the grid. Relevant scientific output.


External Data
• HPC
• Grid
• Visualization
App1
App2
• HPC
• Grid
• Visualization
• HPC
• Grid
• Visualization
App3
KEPLER

# KEPLER

- Flexible workflow engine that comes from ISI at USA. Available for free usage. https://kepler-project.org/

- It enables the communication with UNICORE and gLite.

EGEE and EUFORIA funded the development work to interface Kepler to gLite

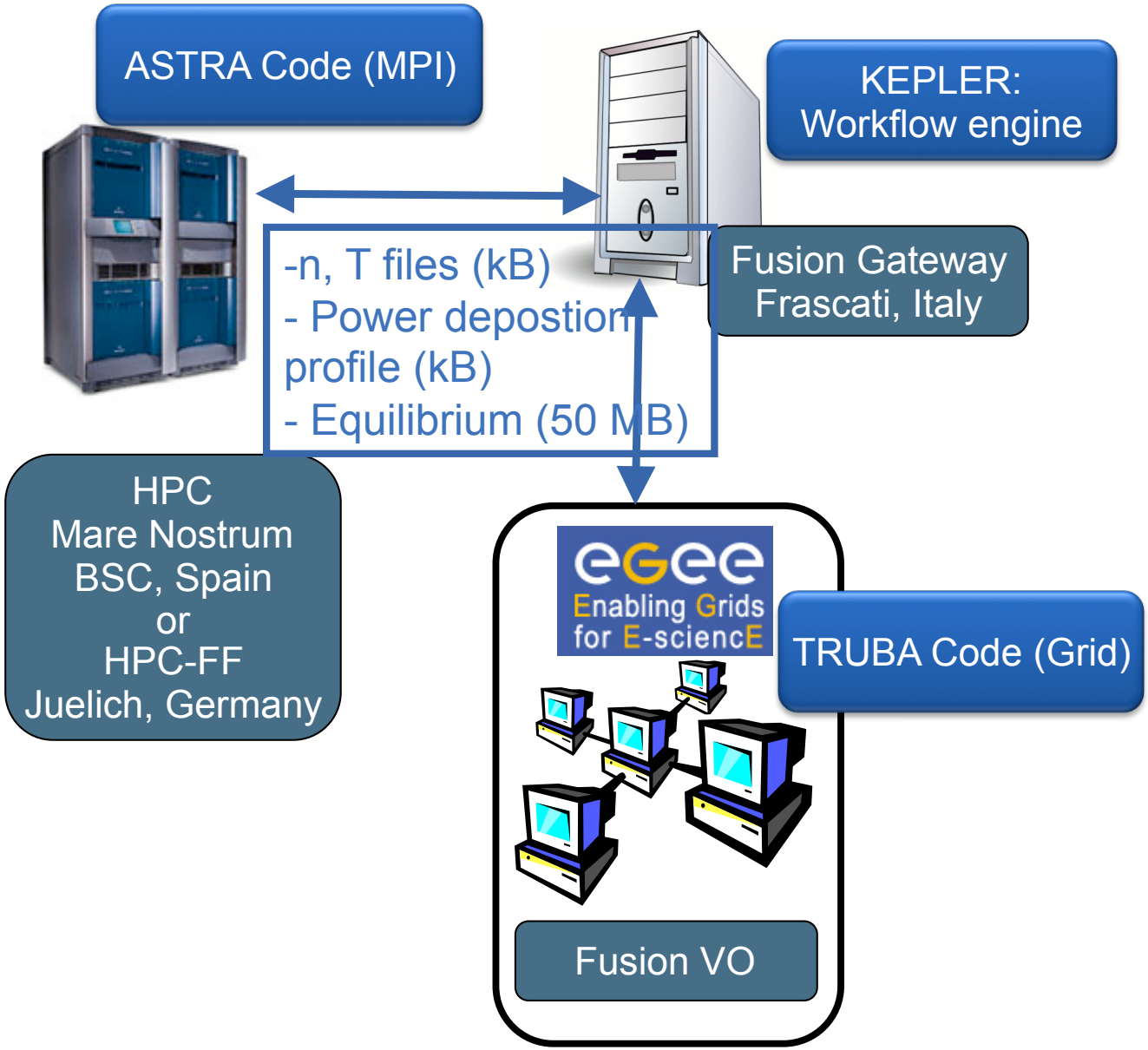
- It permits establishing complex workflows:
  - Grid- Grid
  - HPC-HPC
  - Grid-HPC

- The applications are actors launched by Kepler.

- The workflows are prepared by the users.

- Kepler is a de-facto standard in fusion community.

# System Architecture




- **Kepler launches the different actors and organizes the workflow.**
- **Kepler runs on the fusion Gateway for managing the data.**
- **One actor (ASTRA) running on HPC: MPI from 16 CPUs.**
- **And the other (TRUBA) on the grid (thousands of jobs).**

# Resources needed

- Kepler: can run on a PC but we run it on the Fusion Gateway (A cluster with 128 CPUs with a huge memory capacity and a fast access to data) to manage the data produced by the workflow.

- ASTRA: MPI from 16 CPUs (depending on the transport model)

INPUT: Several small files (100 kB)

Equilibrium (50 MB)

- TRUBA-grid. Serial. Thousands of independent jobs (10 min CPU per job): One job per ray.

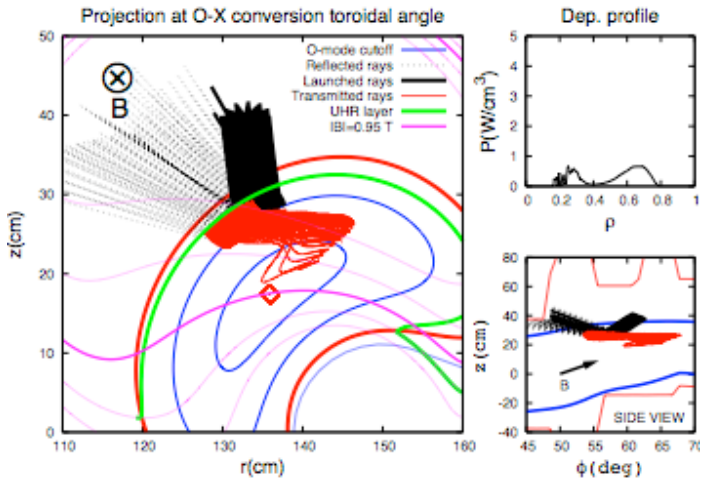
The same INPUT as for ASTRA.

Usage of Data Catalogue.

Wall- clock Time: About 48 hr.

Memory requirements:

Several equilibria kept during the evolution.



# Live DEMO

# Example of Workflow

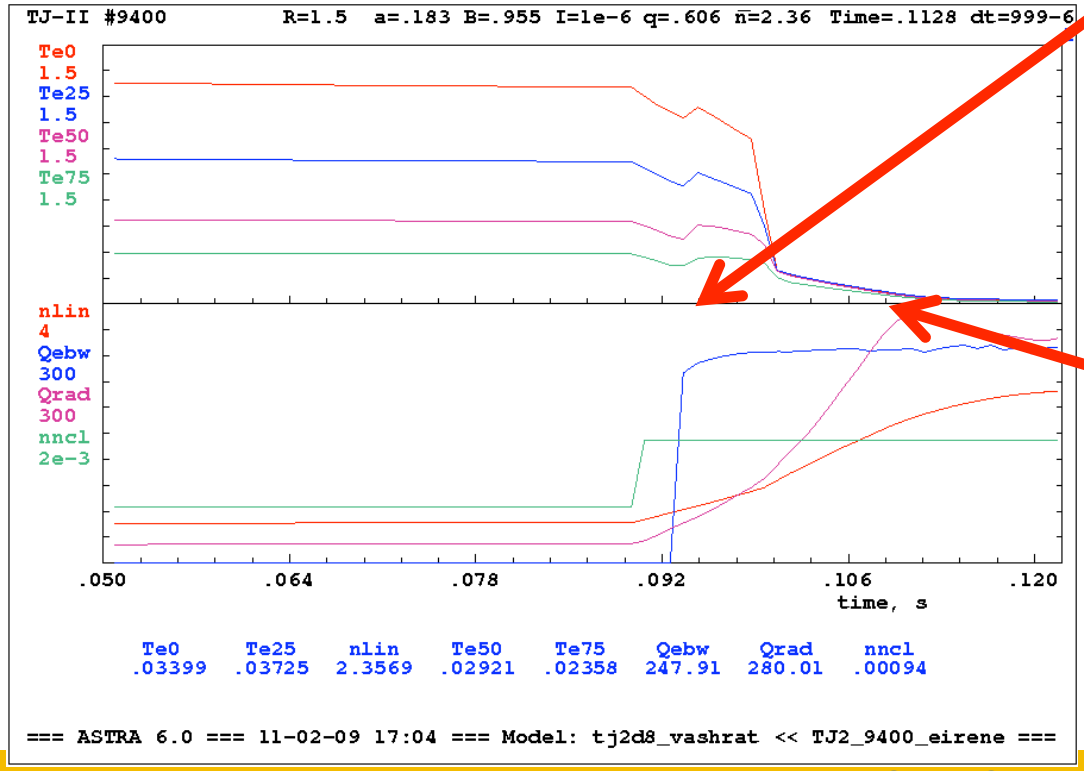
**Input: Plasma (n, T, Equilibrium) →**

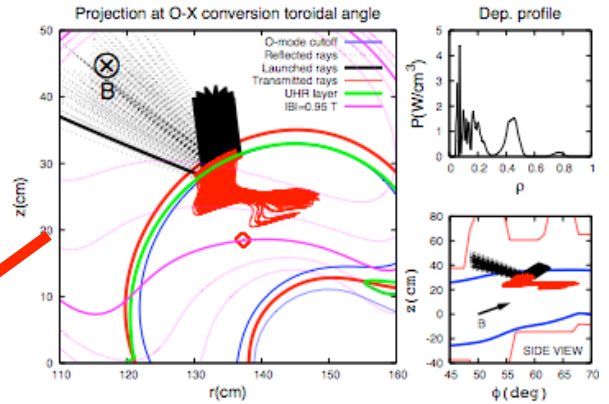
**Plasma Evolution (ASTRA-HPC)→**

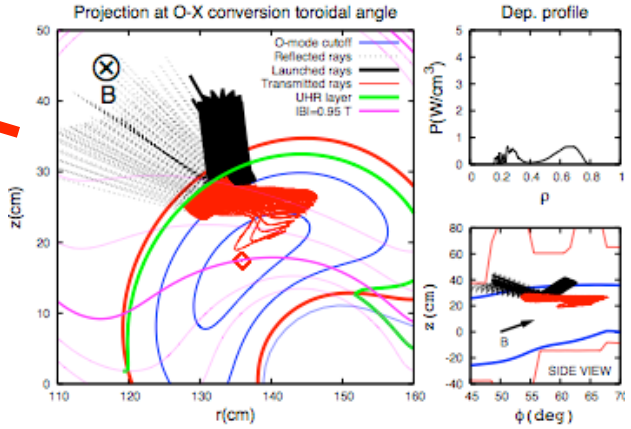
**Heating properties (TRUBA-grid)→**

**Plasma Evolution (ASTRA-HPC)→**

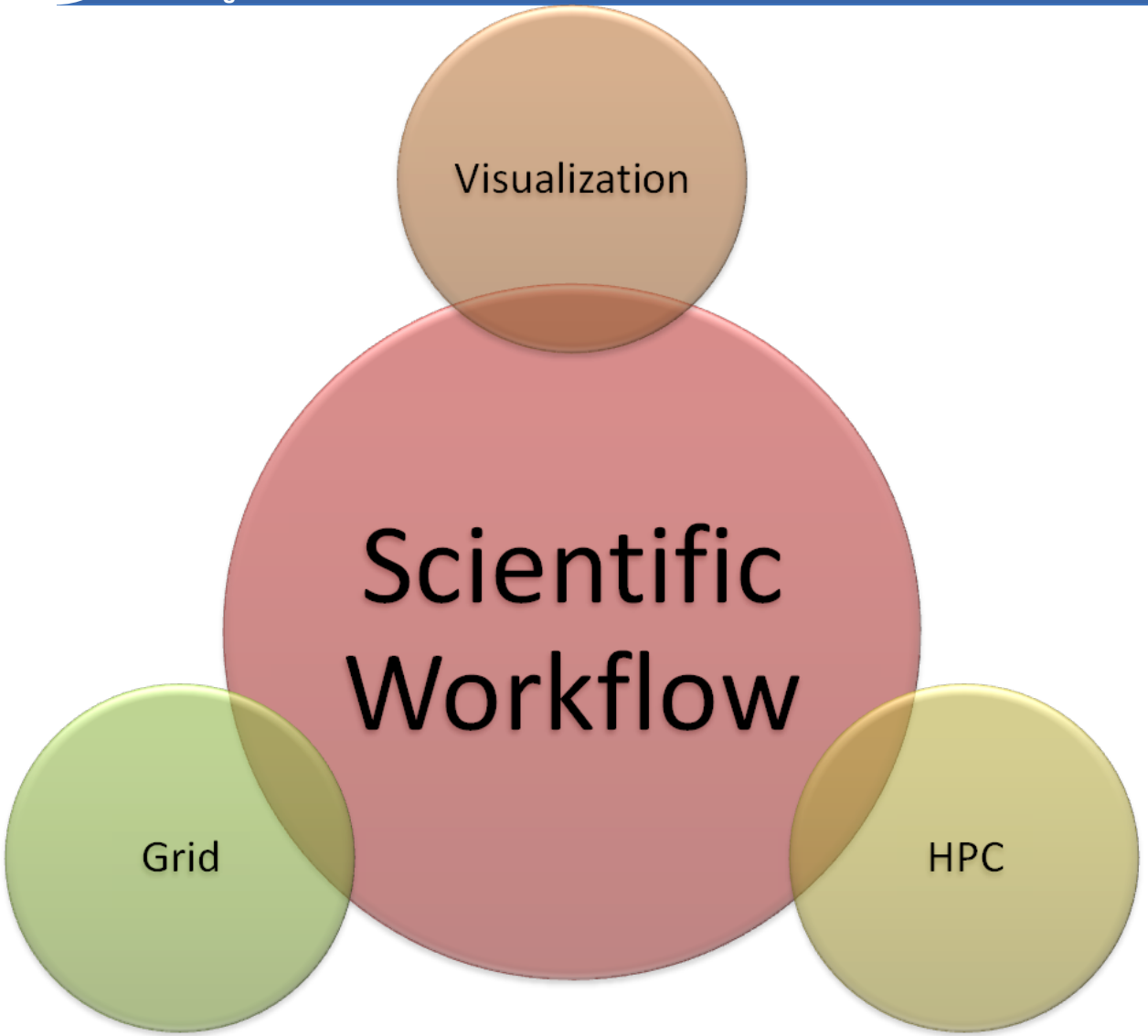
**Heating properties (TRUBA-grid)→…**



# CONCLUSION: A NEW COMPUTING SCHEME READY



# CONCLUSIONS

- **After EGEE Projects, Fusion has become a Heavy User Community of the grid.**
- **More than 10 fusion applications running on the grid:**
  - Covering different fusion research topics.→ IMPORTANT FOR THE DIVERSITY OF WFS.
  - Using several parallelization strategies.
- **New computing paradigm in fusion that establishes workflows of heterogeneous applications running on different architectures.**
- **Relevant scientific results on the grid: 15 fusion papers in peer reviewed journals, including a PhD thesis plus two more in preparation.**

# CONCLUSIONS

- **Fusion Gateway: Access to European Fusion Resources.**
- **Grid-Computing resources: Fusion VO (~45,000 CPUs, Working during EGI).**
- **HPC Resources:**
  - Fusion devoted computer: HPC-FF (100 Tflops).
  - Mare Nostrum: Access Committee.
  - Altamira (CSIC. Spain). Under collaboration.

- **This tool will be used by Fusion community (EFDA, ITM, …) AVAILABLE FOR OTHER COMMUNITIES.**

- **The results of the workflow here presented published in:**

**Á. Cappa, D. López-Bruna, F. Castejón, et al. "Calculated evolution of the Electron Bernstein Wave heating deposition profile under NBI conditions in TJ-II plasmas" Accepted in Contributions to Plasma Physics, 2010.**