

JRA1

Grid Codes

Brussels

30 March 2011

JRA1

Partners

- Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain.
- Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany.
- Centro Superior de Investigaciones Científicas (CSIC), Santander, Spain. Keep in touch JRA1-SA1 activity.

JRA1

Scope

- Port codes to the **grid**.
- Contribute to establish complex scientific **workflows** among codes that run on heterogeneous infrastructures.
- 4 codes ported, although 3 were mandatory (According to the DoW). Additional codes were also ported needed for Workflows.

Connection to other Euforia work packages

- **JRA1**

- NA3: dissemination of results
- SA1: Grid Infrastructure
- JRA2: porting of codes to HPC environments
- JRA3: workflows between JRA1 and JRA2 codes
- JRA4: Visualization of the results based on VisIt

JRA1

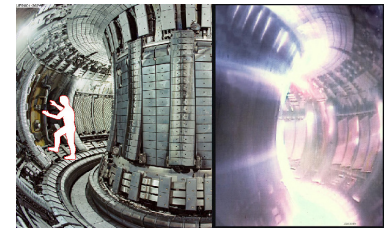
The grid codes

- Strategy:
 - Choose codes with different structures that need different strategies to be ported to the grid.
 - Select codes that act on different plasma zones or theories so that it is easier to establish complex workflows with those codes.

JRA1

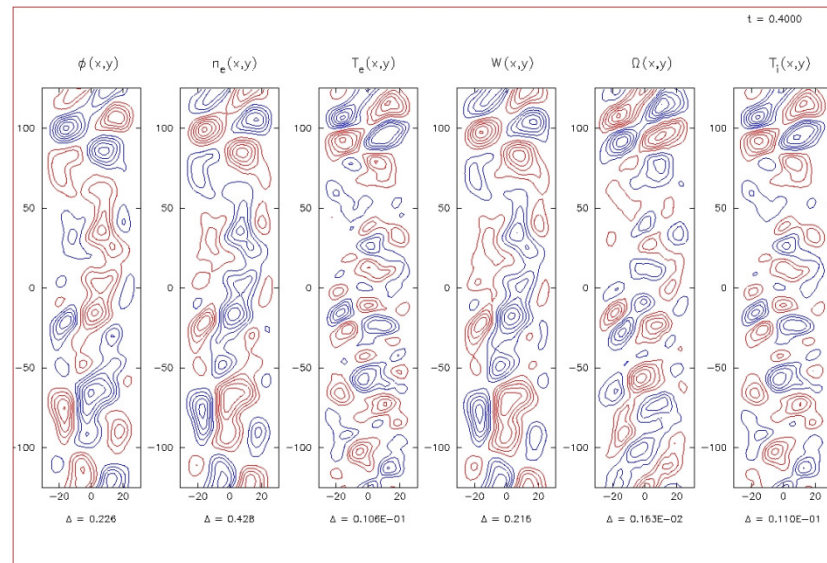
The grid codes

- **GEM**: Linear & non linear Turbulence. Gyrofluid code (Core Transport). **MPI**.
- **BIT1**: Divertor code (SOL Transport). **Parameter Scan**.
- **EMC3-EIRENE**: Neutral transport for tokamaks & stellarators (Neutral Transport). **MC Code**.
- **DAB** (Distributed Asynchronous Bees): Tool for the optimization of any concept in fusion devices. **Asynchronous Algorithm**.
- Plus the previously gridified codes (taken from EGEE code platform): Suitable for workflows.
 - **ISDEP** (MC-Transport)
 - **Ilsa & Helena** (Equilibrium and MHD stability)
 - **VMEC** (3D-Equilibrium suitable for tokamaks and stellarators)



From GEM to gGEM

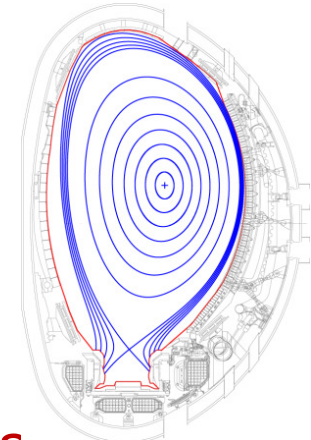
- GEM. **Gyrofluid Turbulence Code: Instabilities behaviour.**
- Versions: **Serial** (small cases) and **MPI** (High scalability, to hundreds of processors).
- Gaining experience in porting MPI codes.
- Uses GridWay and DRMAA.



Close contact with the code owner

BIT1

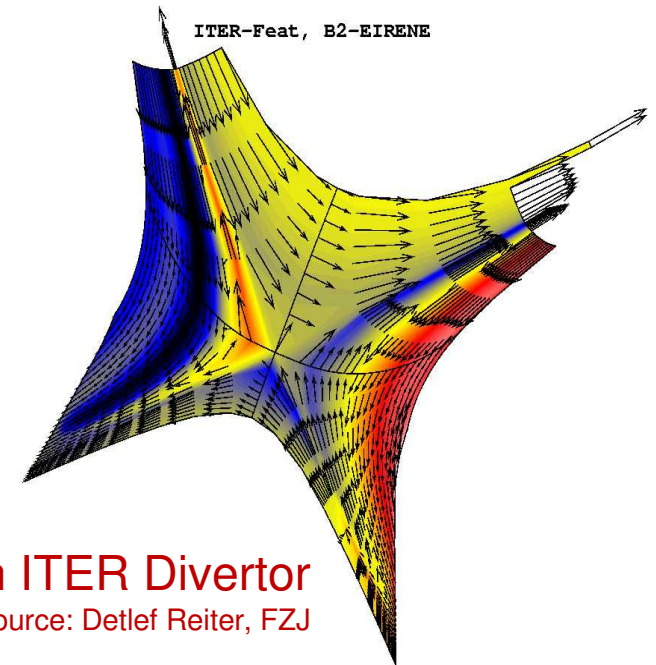
- BIT1: PIC + MC code for **plasma edge simulations**. 1D for plasma model and 2D for neutrals impurities.
3D in velocity space
- Strong need of communication between nodes.
- A wide range of parameters must be scanned → **Parameter scan problem**. A Python script developed to send the jobs. Also adapted to TAPAS4GRID. Kepler actor for TAPAS.
- Present problem: 8 Scrape-off-Layer widths x 8 impurity concentrations x Two types of bulk ions. Average CPU time per job: 7 days.



SEE THE DEMO

EMC3-EIRENE

- **Monte-Carlo** code to simulate **neutral particle transport** in plasmas (plasma-wall interactions).
- Requires several inputs.
- A formatted input file including simulation parameters:
 - Modelling data
 - Plasma background
 - Geometry descriptions
 - Mesh data
- EMC3-EIRENE run using TAPAS4GRID.



Plasma flow field in ITER Divertor

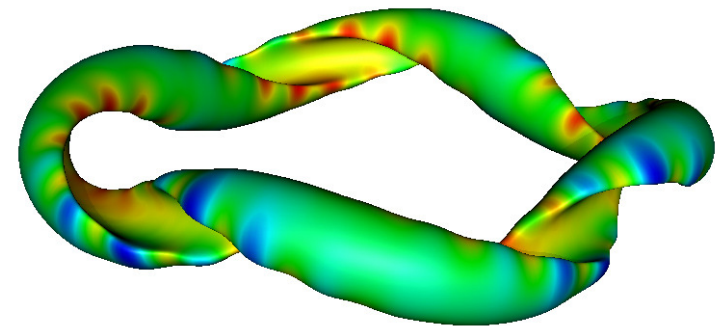
Image source: Detlef Reiter, FZJ

Distributed Asynchronous Bees (DAB)

- Metaheuristics: **Improvement of magnetic configurations.**
- **VMEC** (3D Equilibrium code) ported to the grid: Capable of modelling 3D-tokamaks and stellarators.
- A configuration, given by Fourier representation of magnetic field and pressure profile, estimated on a single node.
- Target functions to optimise

(estimated by grid codes):

1. Equilibrium itself (must exist).
2. NC Transport (**on the grid**).
3. Mercier criterion stability.
4. Ballooning criterion (**COBRA code aslo ported to the grid**).

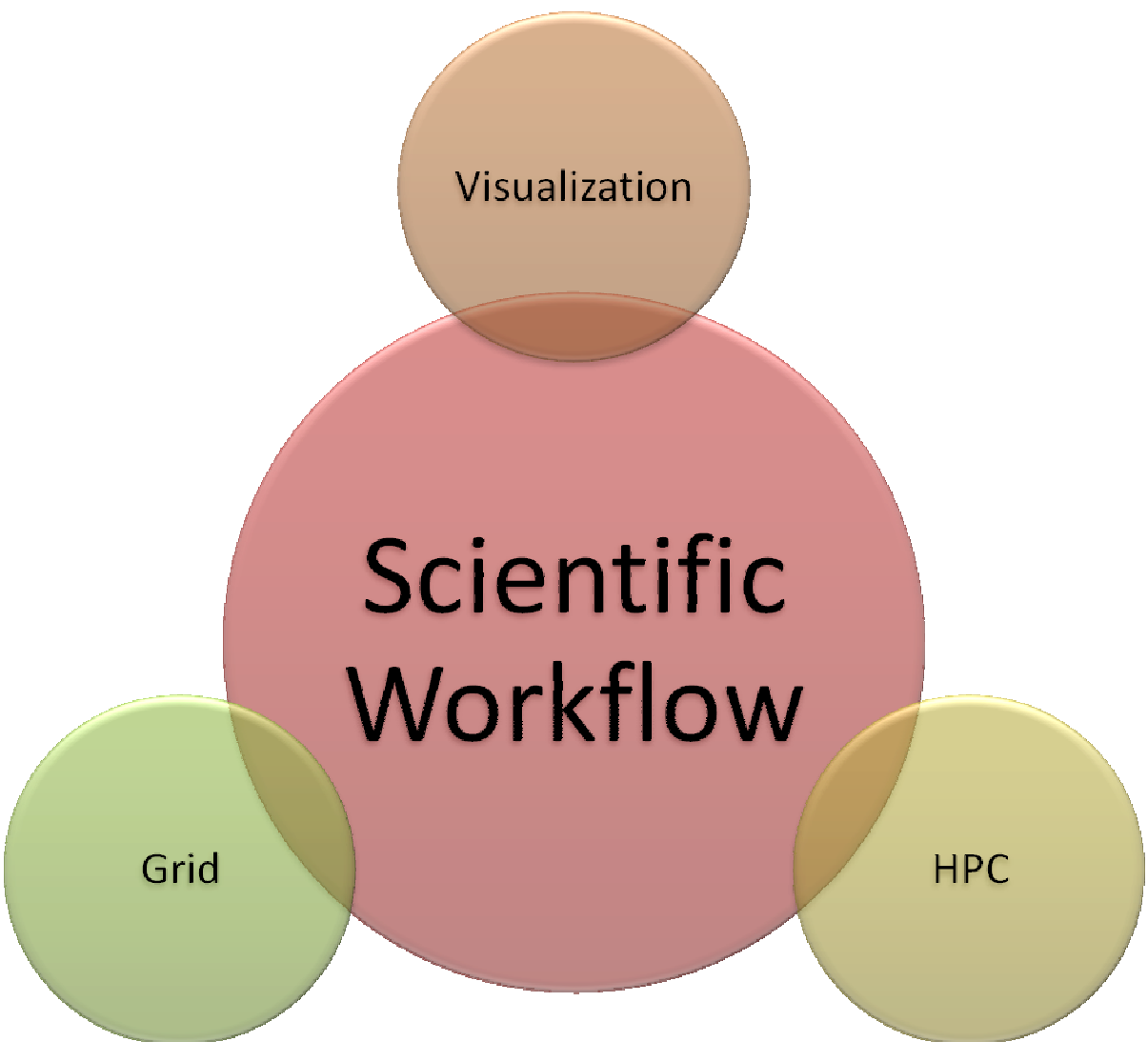


WFs Grid, HPC, and Visualization

- A wide variety of possible WFs (see deliverable).
- Proposals: beyond the demonstration of capability, produce **relevant physical results**.
- **“Pilot-Project”**: Example of WF running on EUFORIA-EGEE-DEISA Infrastructure.
- **Kepler** as the main tool.

WFs: Grid, HPC, and Visualization

- Achieved WFs during the project:
 - Pilot Project: ASTRA (ETS) + Heating (TRUBA, FAFNER,...)
 - TAPAS4GRID + EMC3-EIRENE
 - TAPAS + BIT1 + Visualization
 - Helena + Ilsa
 - VMEC + COBRA + Visualization
 - VMEC + Visualization.



Scientific Workflow

Visualization

Grid

HPC

External Data



- HPC
- Grid
- Visualization

App1

- HPC
- Grid
- Visualization

App2

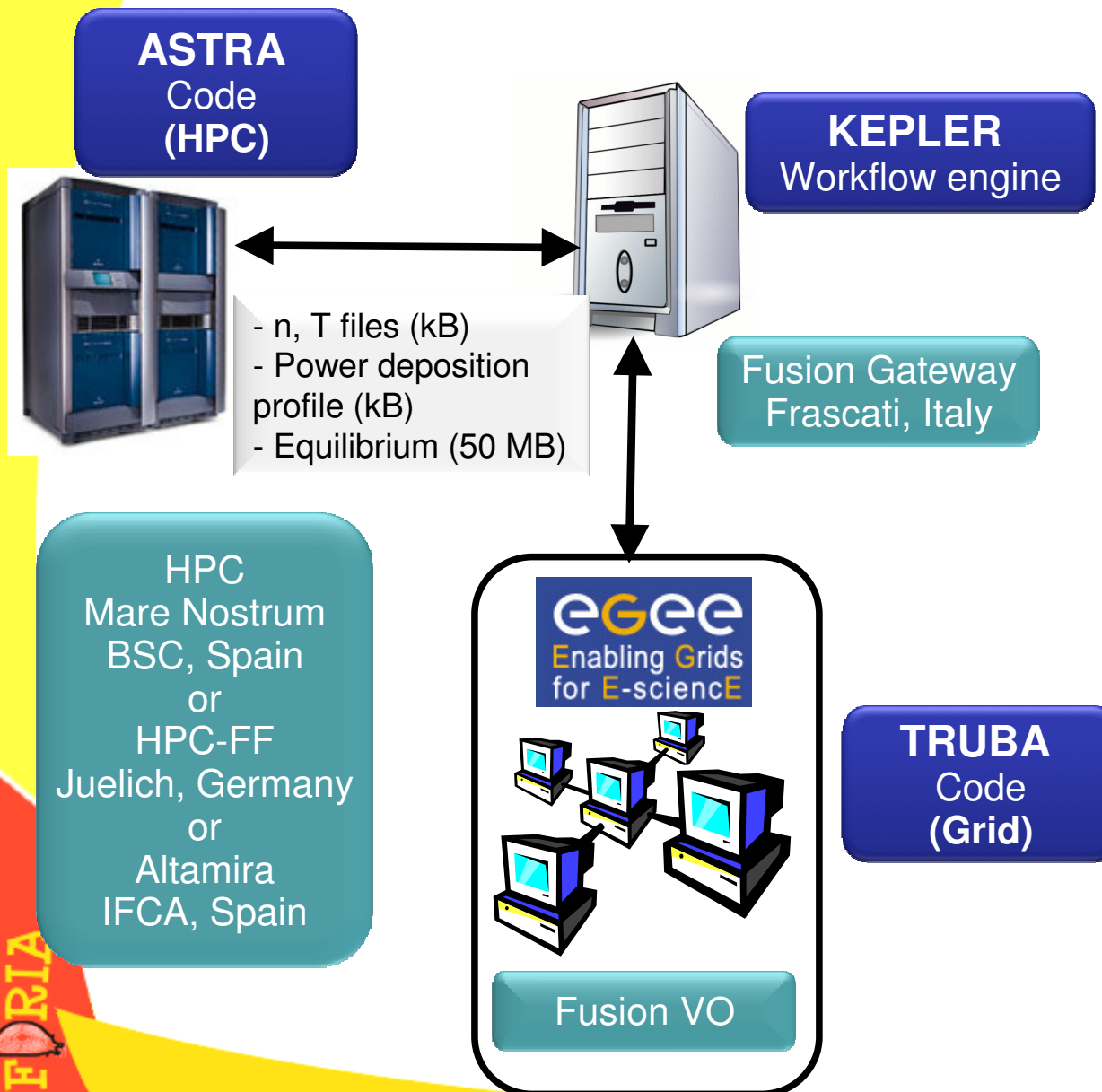
- HPC
- Grid
- Visualization

App3



KEPLER

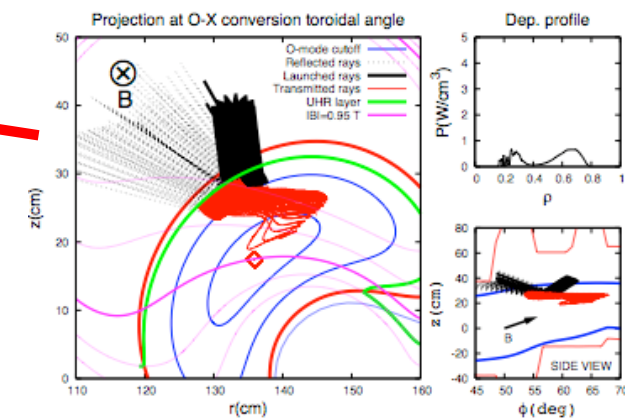
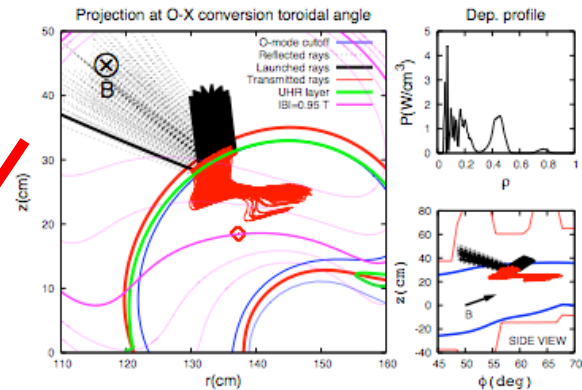
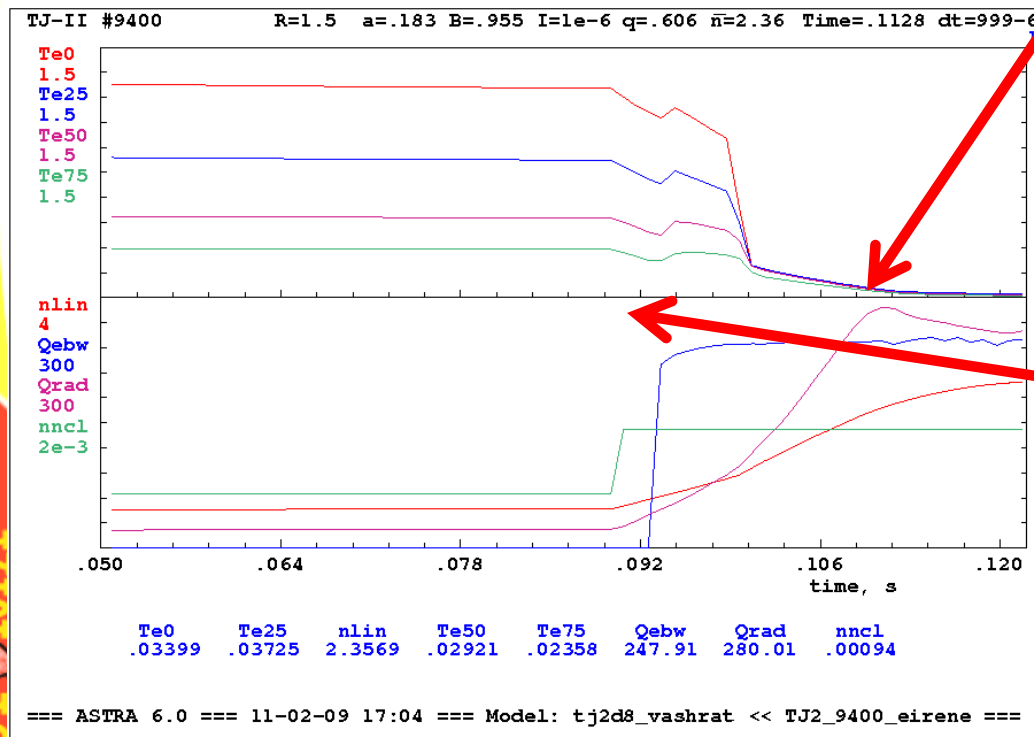
Mixed workflow based on KEPLER: Pilot project



- 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 for complex models: MPI from 256 CPUs (can be larger depending on the used modules).
- And the other (TRUBA) on the grid (thousands of jobs).

Mixed workflow based on KEPLER: Pilot project

Input: Plasma (n, T, Equilibrium) →
 Plasma Evolution (ASTRA-HPC) →
 Heating properties (TRUBA-grid) →
 Plasma Evolution (ASTRA-HPC) →
 Heating properties (TRUBA-grid) → ...



Deliverables and Milestones

Issue	Date	Title	Comments
DJRA1.1	M1	Report on the Description of Sequential Code to port to the grid.	Delay due to internal discussions.
DJRA1.2	M12	Report on the Description of Sequential code to be ported to the Grid	In time
DJRA1.3	M12	Report on the first scientific Publications related to JRA1 activities	In time
DJRA1.4	M17	Report on the possible complex workflows using grid codes. these workflows are also suitable for HPC codes	In time
DJRA1.5	M24	Interim report of a complex workflow running on EUFORIA infrastructure	In time
DJRA1.6	M32	Report on the full implementation of mixed workflow codes	1.5 months delay
DJRA1.7	M34	Publication of scientific results	In time
MJRA1.1	M31	Complex workflow between grid and HPC applications. Pilot Project	In time
MJRA1.2	M31	Report on MJRA1.1	In time
MJRA1.3	M29	Second mix workflow	In time

JRA1

Summary

- **Several codes** of different natures successfully ported to the grid, including MPI code.
- **Complex workflows** established among:
 - Grid codes + Visualization
 - HPC-Grid codes + Visualization
 - Contribution to "PILOT-PROJECT"
- **Several tools** used in the work: Kepler, TAPAS, Gridway.

JRA1

Sustainability

- **Grid team** willing to give **support** to fusion users under scientific collaboration basis.
- **Fusion VO** keeps as production infrastructure.
- **Expertise** on using **Kepler** as workflow engine and **VisIt** as graphic tool.

JRA1

End of presentation

Thank you!

Questions?

EUFORIA