HPC-Grid workflows in fusion: The EUFORIA approach

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on behalf of EUFORIA team

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GOBIERNO DE ESPAÑA | MINISTERIO DE CIENCIA E INNOVACIÓN

Ciemat
Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

e-infrastructure

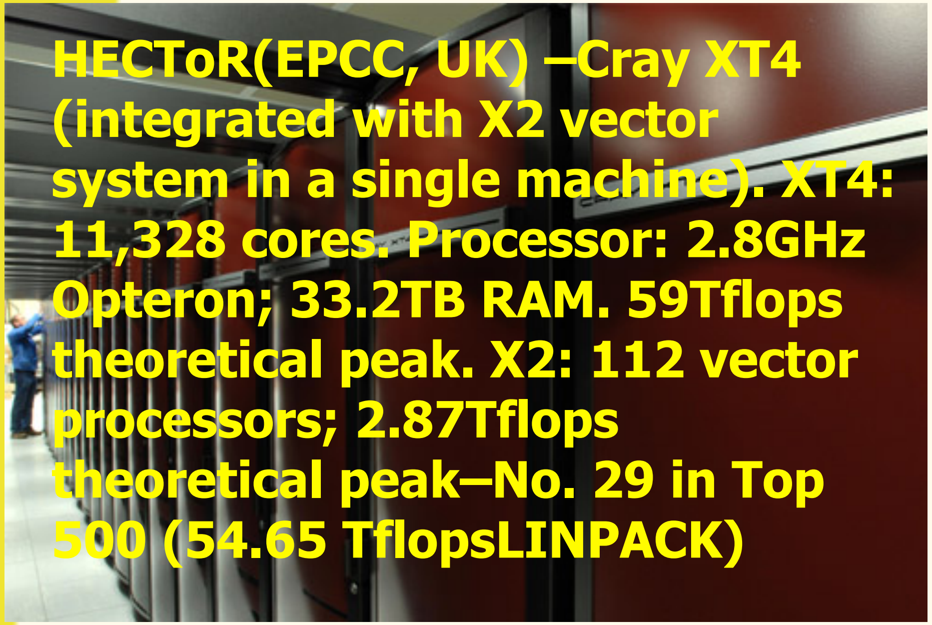
EUFORIA

14 member Institutes
3.65M€ over 36 months

522pms covering

- **Management**
- **Training**
- **Dissemination**
- **Grid and HPC infra-structure & support**
- **Code adaptation & optimization**
- **Workflows**
- **Visualization**

IFRASTRUCTURES: SA1 (GRID) + SA2 (HPCs)



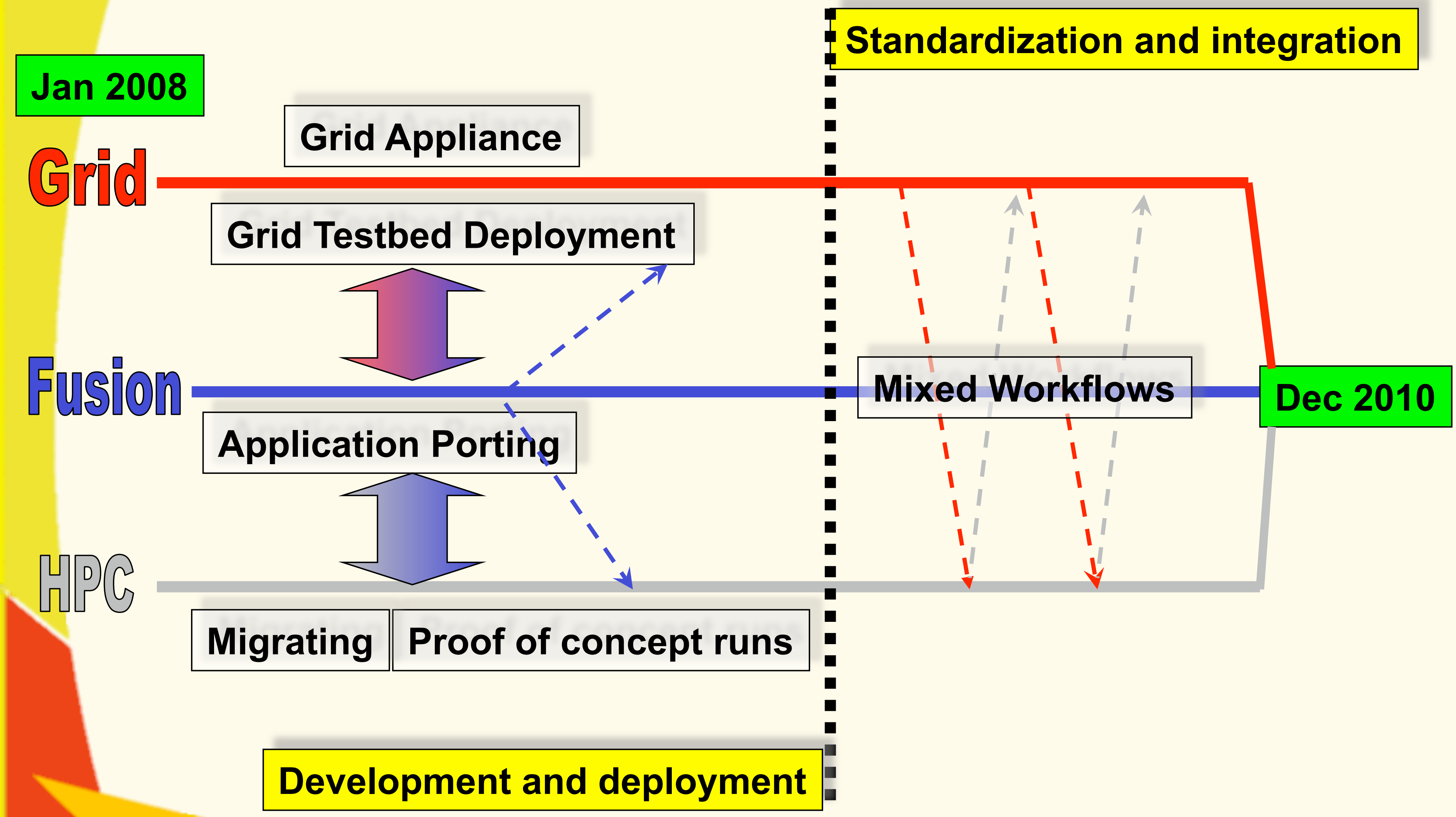
HECToR(EPCC, UK) –Cray XT4 (integrated with X2 vector system in a single machine). XT4: 11,328 cores. Processor: 2.8GHz Opteron; 33.2TB RAM. 59Tflops theoretical peak. X2: 112 vector processors; 2.87Tflops theoretical peak–No. 29 in Top 500 (54.65 TflopsLINPACK)

Louhi(CSC, Finland)–Cray XT4. 4,048 cores. 4.5TB RAM. 37.68Tflops peak.–No. 70 in Top 500 (26.80 TflopsLINPACK)

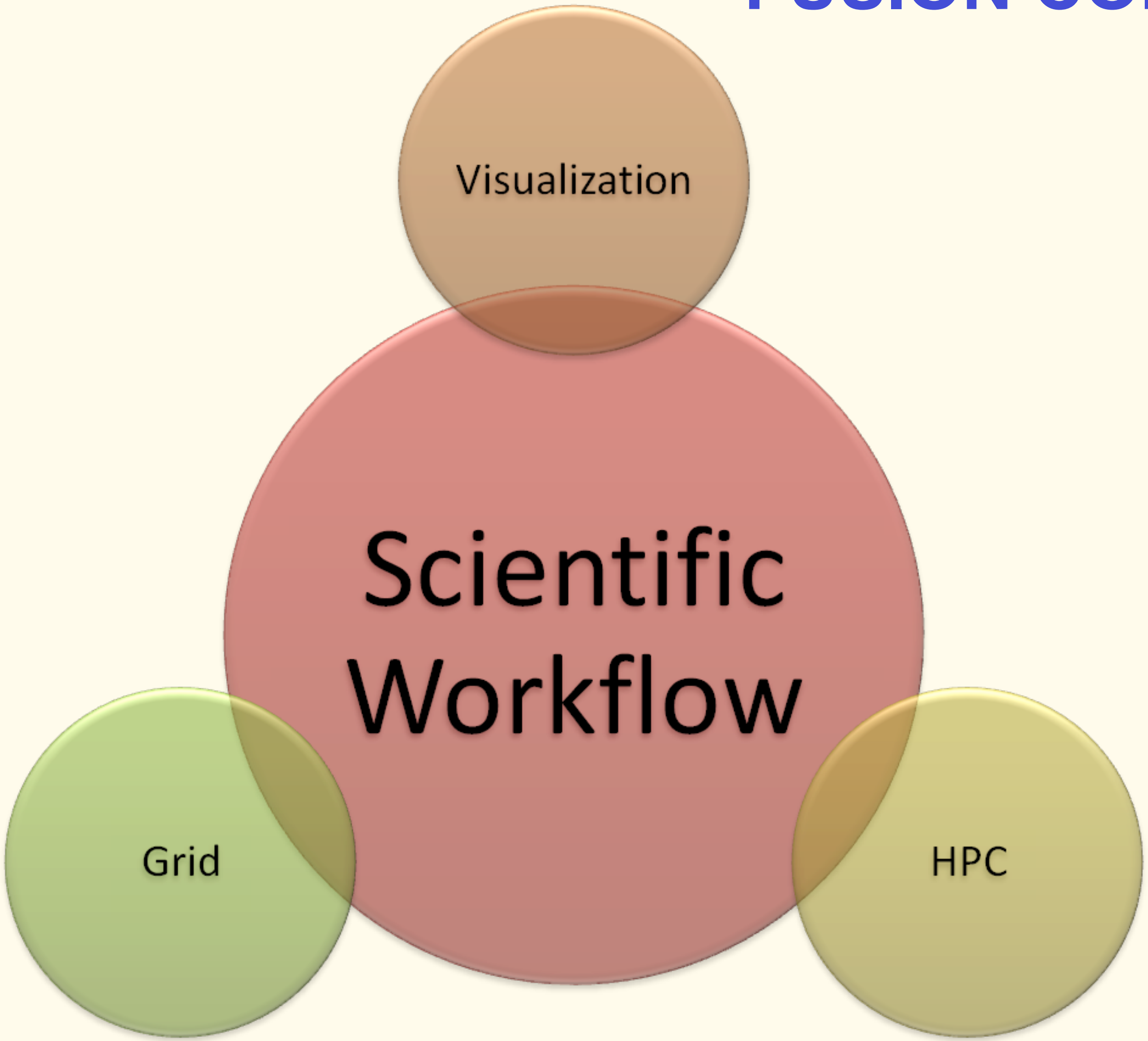
MareNostrum(BSC, Spain)
–IBM Cluster. 10240 cores. Processor: 2.3GHz PPC 970; 20TB. 94.21Tflops peak.
–No.26 in Top 500 (63.83 TflopsLINPACK)

Enabling Grids for E-sciencE

Work plan outline



DEVELOPING A NEW PARADIGM FOR FUSION COMPUTING

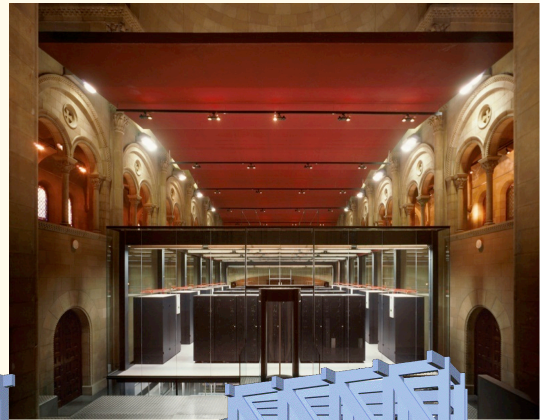


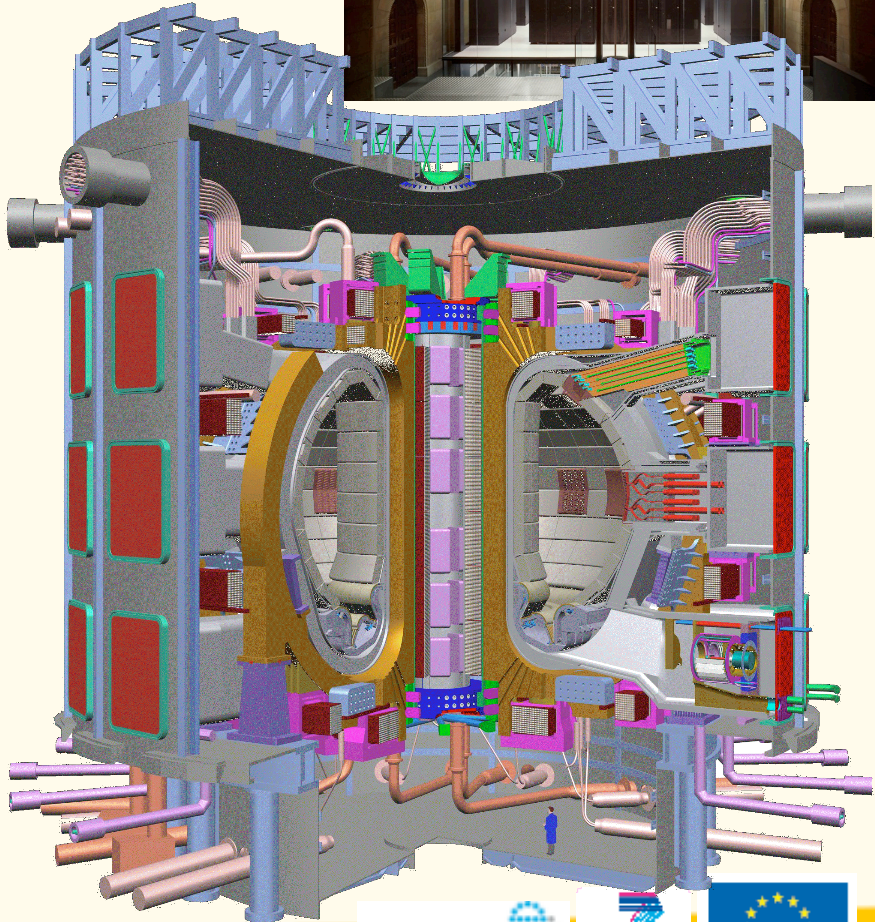
What we have shown

- 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.
- 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.

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.**



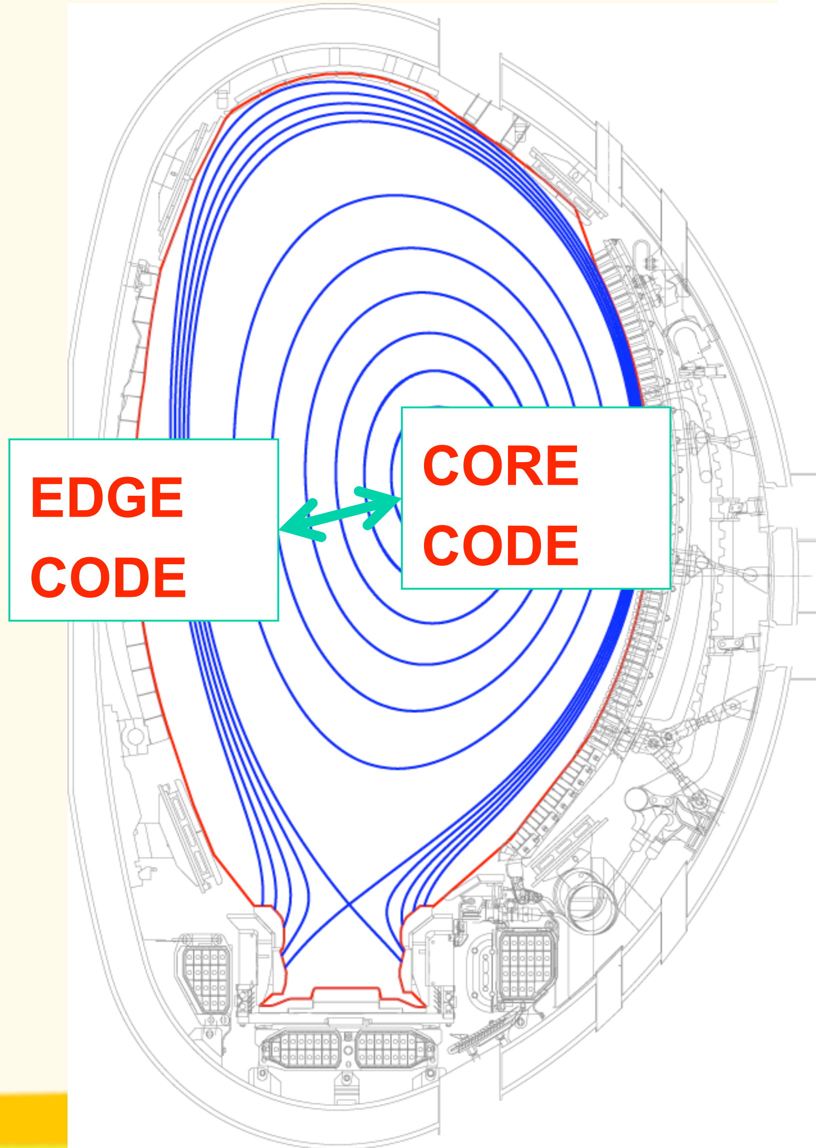


Complex Workflows: Why?

- **Necesity of communicate applications that act on different research fields or time scales.**
- **Problems with very different scales (time and space):**
  - **Time:**

    Cyclotron (Larmor) Frequency ~10^{-10} s → Transport ~ 10 s
  - **Space:**

    Electron Larmor radius ~10^{-3} m → Reactor ~ 10 m
- **They can run on Grid or HPC.**
- **The Workflows can be Binary, Cyclic of more complex (like DAB application).**



Building Workflows

- A universal form to establish a WF in Fusion is using a Transport code (Evolving Plasma Characteristics)

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

$$\frac{3}{2} n^s \frac{dnT^s}{dt} + \nabla q^s = P_{in}^s - P_{loss}^s$$

- **Sources and Losses: Heavy and Complex functions. Calculated on Grid or HPC.**

- **Fluxes: Transport Coefficients: Again Complex and heavy functions.**

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

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

KEPLER

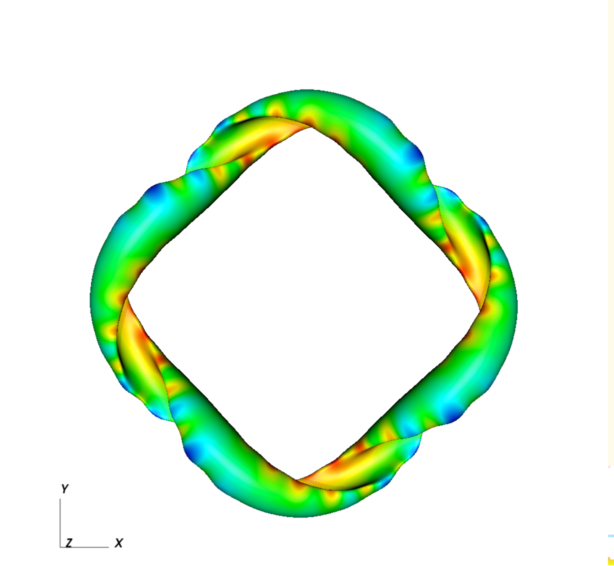
- Flexible workflow engine that comes from ISI in USA. Available for free usage. https://kepler-project.org/
- It enables the communication with UNICORE (UNICORNIO) and gLite.
- It permits establishing complex workflows:

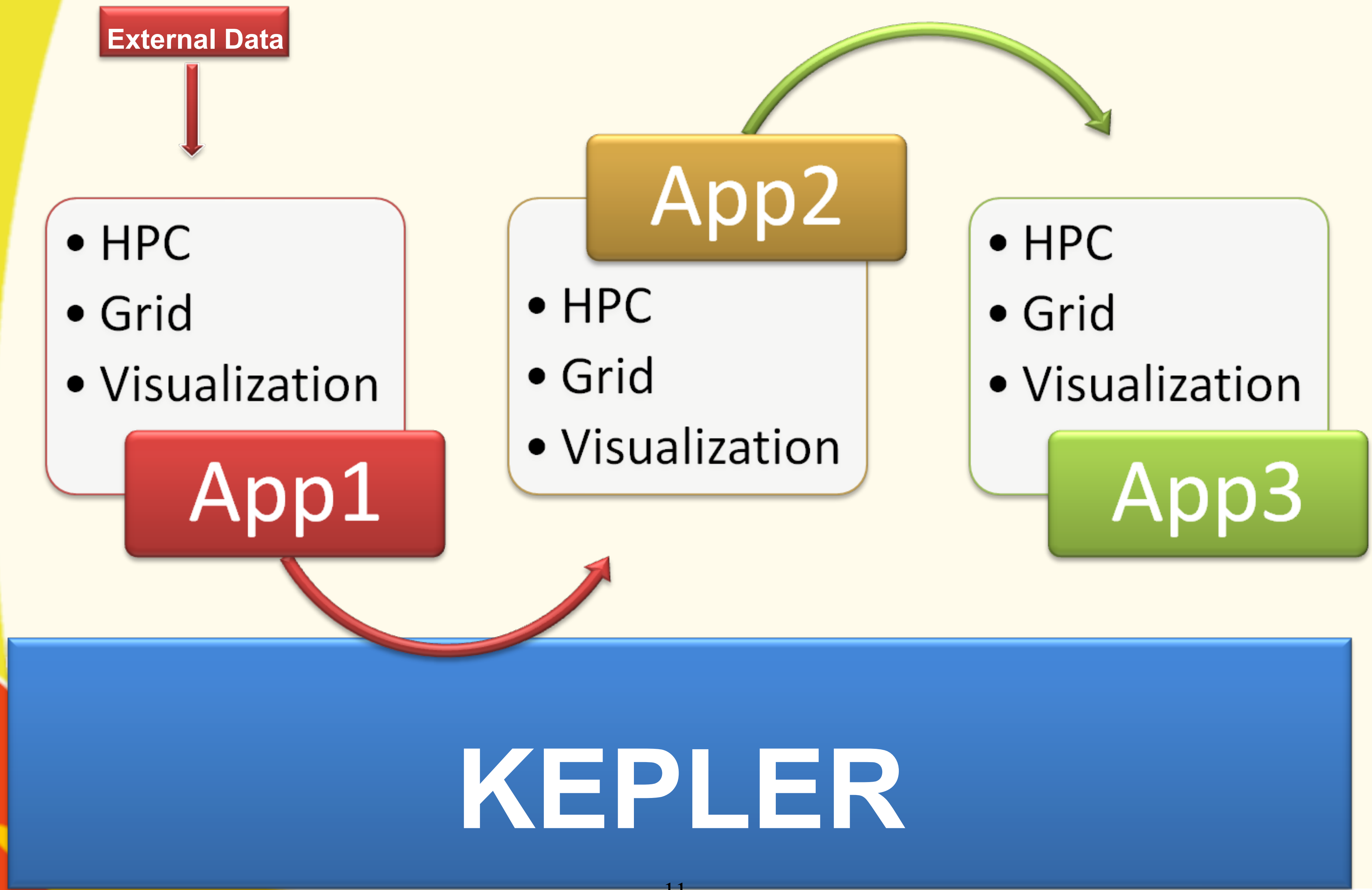
  Grid - Grid

  HPC - HPC

  Grid - HPC
- The applications are actors launched by Kepler.
- Visualization based on Visit

(5D FILES!)




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

Example of Workflow

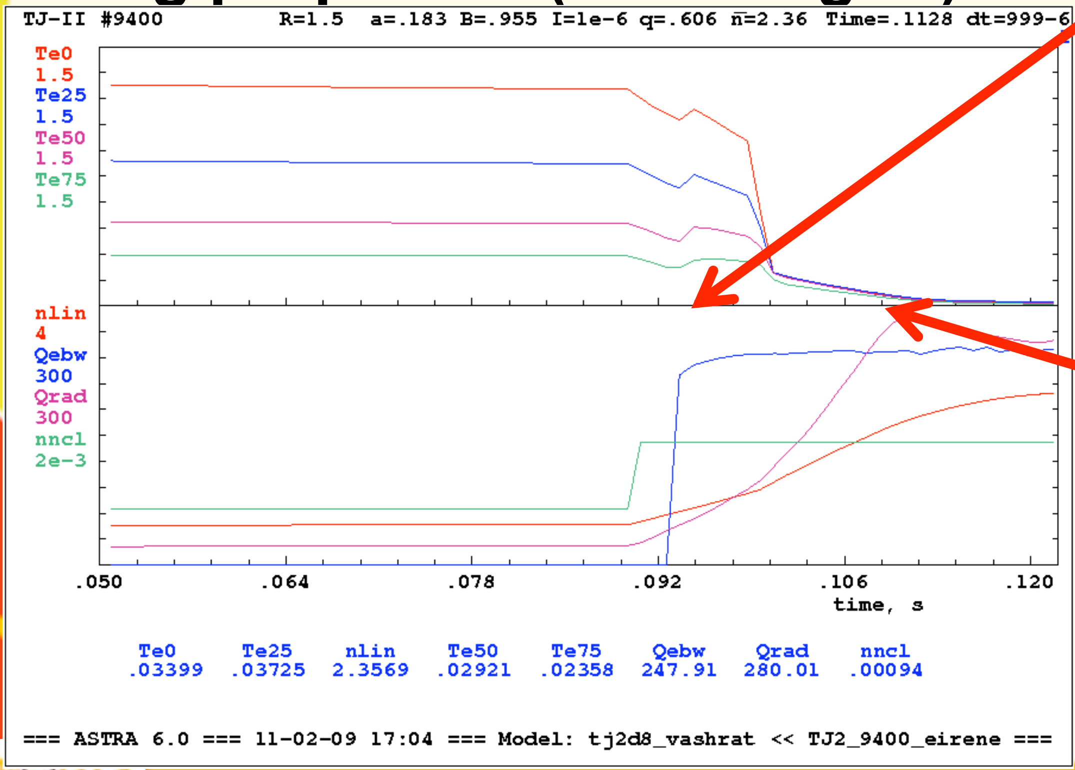
Input: Plasma (n, T, Equilibrium) →

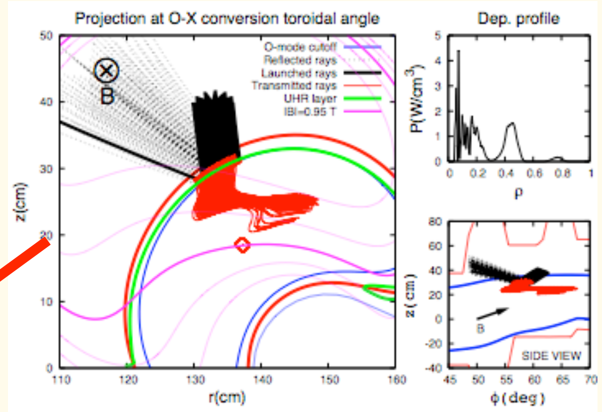
Plasma Evolution (ASTRA-HPC)→

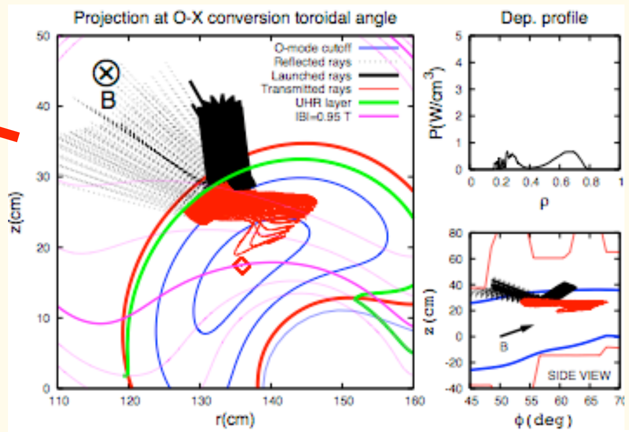
Heating properties (TRUBA-grid)→

Plasma Evolution (ASTRA-HPC)→

Heating properties (TRUBA-grid)→…

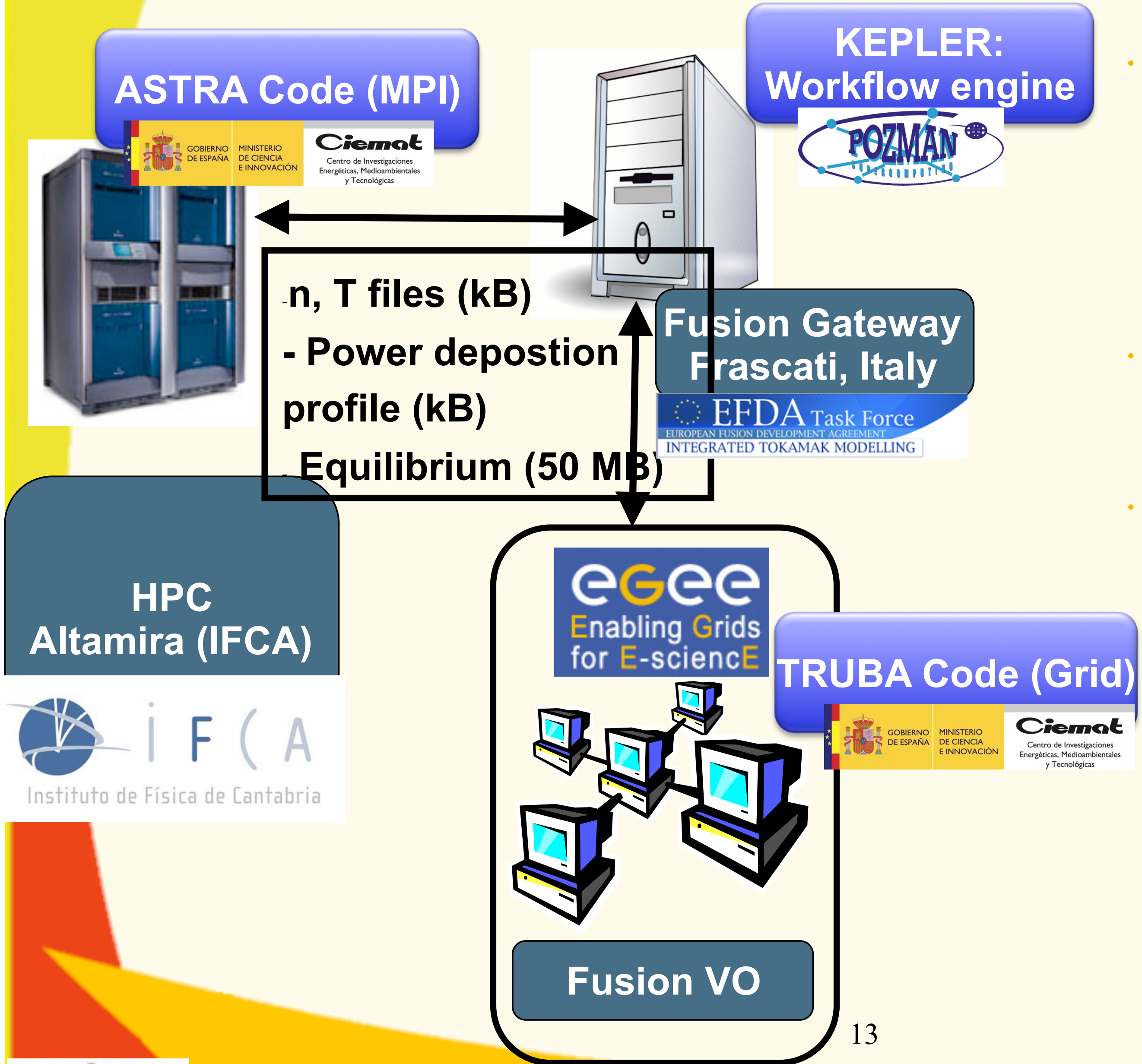






EUFORIA FP7-INFRASTRUCTURES-2007-1, Grant 211804

System Architecture



- Kepler launches the different actors and organizes the workflow.
- Kepler runs on the fusion Gateway.
- 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)

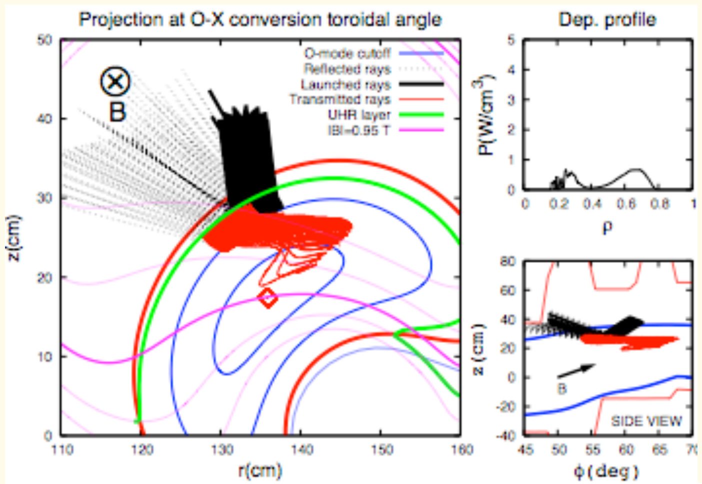
- TRUBA-grid. Serial. Thousands of independent jobs (10 min CPU per job): One job per ray.

The same INPUT as for ASTRA. Usage of Data Catalogue.

Wall- clock Time: About 48 hr.

Memory requirements:

Several equilibria kept during the evolution.



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.
- Tradtional use of HPCs.
- 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: Test Bed: EUFORIA-VO

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.

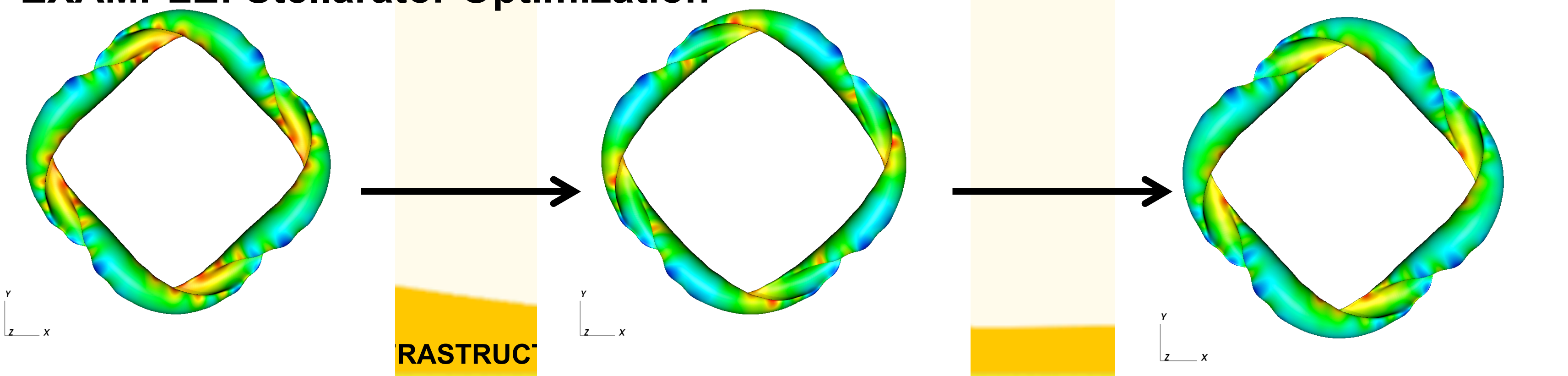
- The results of the workflow here presented published in:

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" Contributions to Plasma Physics, 2010.

Distributed Asynchronous Bees (DAB)

- Metaheuristics: Artificial Bee Colony Algorithm and VMEC (Variational Moment Equilibrium Code)
- 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:
  - 0) Equilibrium itself (must exist).
  - 1) NC Transport.
  - 2) Mercier Criterion Stability. (VMEC 8.46).
  - 3) Ballooning Criterium (COBRA code on the grid).

EXAMPLE: Stellarator Optimization



Consortium Members

Country	Institute	Capabilities
SWEDEN:	*CHALMERS University of Technology (coordinating)*	*Fusion, Grid, (CS)*
FINLAND:	*CSC - Tieteellinen laskenta Oy*	*HPC, (Grid),*
	Åbo Akademi University	*Code Optimization, CS*
FRANCE:	*CEA - Commissariat à l'énergie atomique – Cadarache*	*Workflow, Fusion, CS*
	Université Louis Pasteur	*Visualization, Applied Math*
GERMANY:	*Forschungszentrum Karlsruhe GmbH -FZK*	*Grid, Code parallelisation*
	Max-Planck-Institut für Plasmaphysik - IPP	*Fusion, (HPC, Grid)*
ITALY:	ENEA	Fusion, Grid, HPC, **GATEWAY**
SLOVENIA:	*University of Ljubljana -LECAD*	*Visualization, CS*
POLAND:	Poznan Supercomputing and Networking Centre	Grid, Migrating Desktop, CS
SPAIN:	*Barcelona Supercomputing Center – Centro Nacional de Supercomputación -BSC*	*HPC, Code optimization*
	Centro de Investigaciones Energéticas Medio Ambientales y Tecnológicas -CIEMAT	*Grid, Code parallelization, Fusion, Grid, NA*
	Consejo Superior de Investigaciones Cientificas - CSIC	*Grid, CS, (NA activities)*
UNITED KINGDOM:	*The University of Edinburgh - EPCC*	*HPC, Code Optimization, NA, User support, (GRID)*

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