# Scientific Workflows in Fusion

## EUFORIA & EFDA-TF-ITM

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Contributors to EUFORIA

Contributors to EFDA-TF-ITM

International Conference on Parallel Computing
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École Normale Supérieure de Lyon, Lyon, France



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# ParCo2009

- Why should this be of interest/relevance to the ParCo2009 audience?
  - Some of the separate pieces are “grand challenge” levels in their own right
    - Already using significant amounts of CPU resources
    - Will need even more as we scale to future devices
    - Also looking for better algorithms …
  - Community is looking at integrating the pieces together
    - Ontology defined
    - Starting to build infrastructure to launch HPC, GRID pieces from a Scientific Workflow Manager



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# Connections to DEISA

- EUFORIA HPC partners are part of DEISA
- EUFORIA has benefited from the DEISA communities CPU awards
- Already had some joint training activities
  - More in the future?
- Potential overlap with the code porting activities also carried out by DEISA
  - And from now on by the HLST of the HPC-FF



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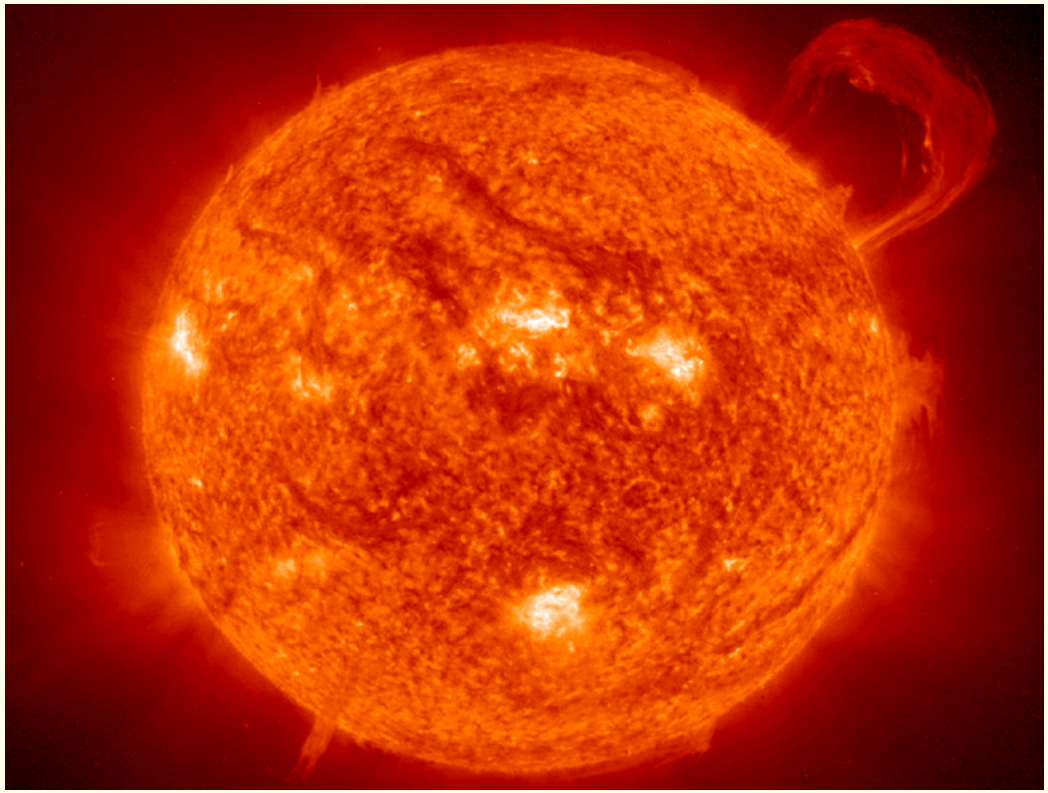
# Fusion

- Energy source for the sun and other stars
- Provides a potential source of base load energy production
- Been working on this for more than 50 years
- Has turned out to be a very difficult problem





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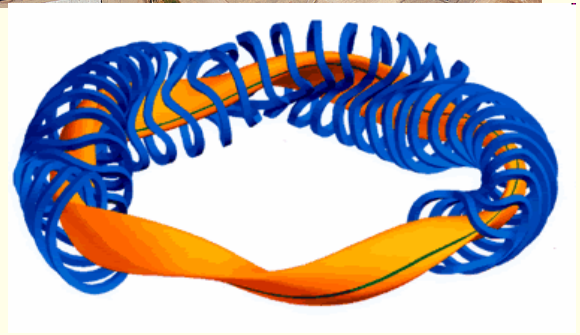
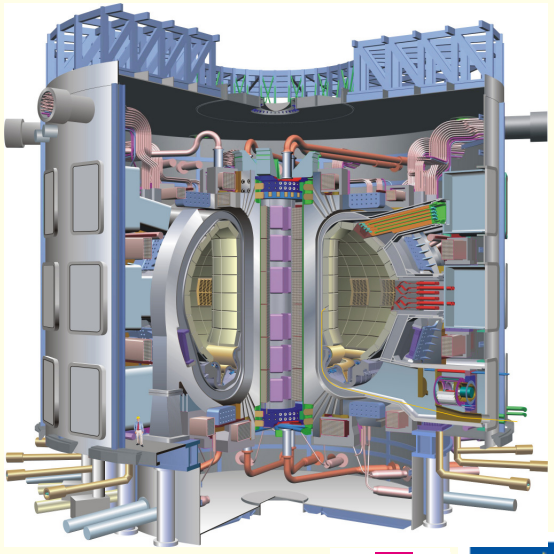
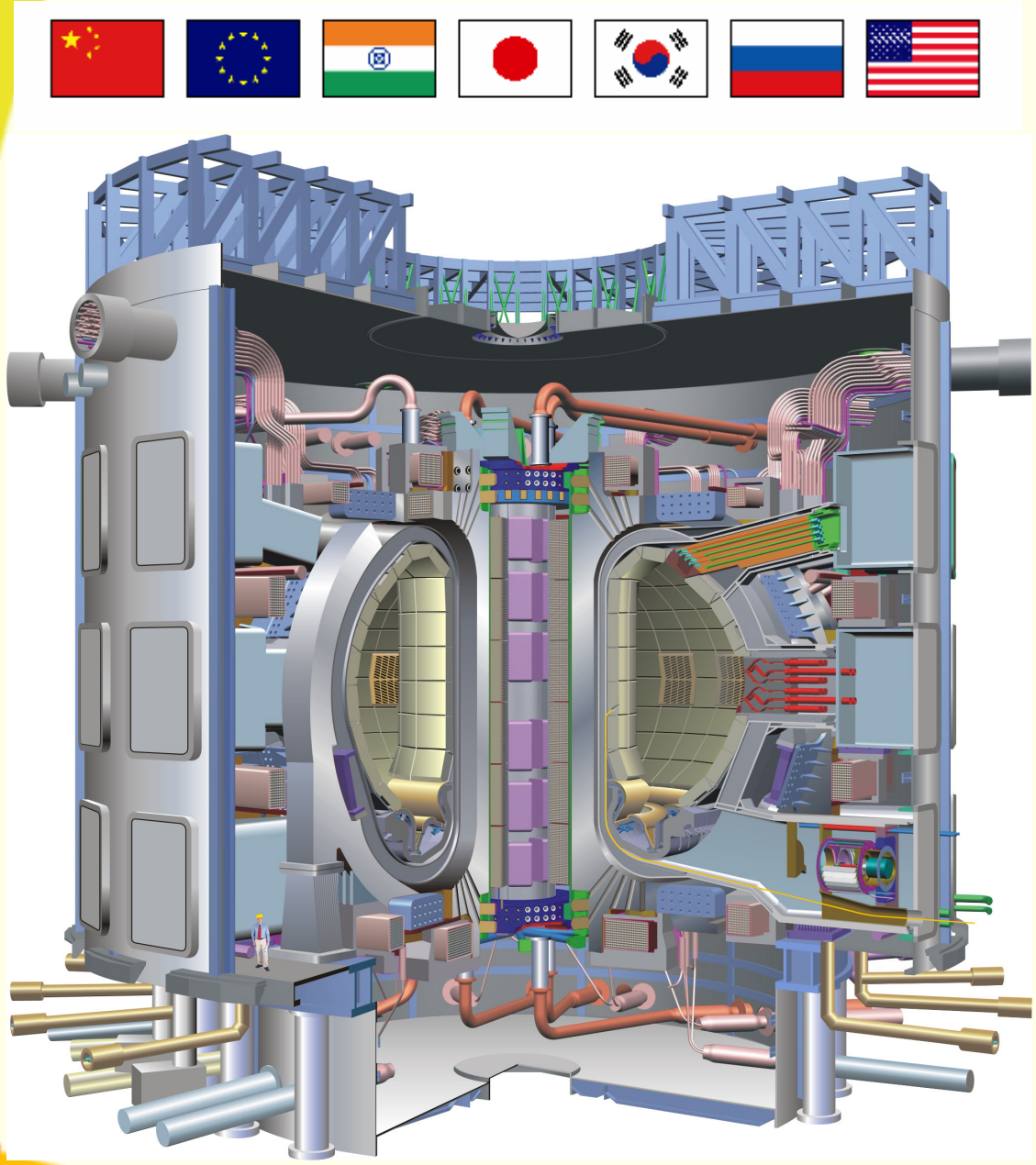
# Fusion

- Two main lines of research
  - Inertial confinement
    - Implosion of small pellets
    - NIF at LLNL
  - Magnetic confinement
    - Two main lines of research at the moment
      - Stellarator – W7X
        - Currently under construction in Greifswald in Germany
      - Tokamak – ITER
        - To be constructed in Cadarache in France





# ITER



| |
|---|
| Involves 7 partners representing more than 50% world population |
| Costs > 10 G$ |
| Under construction in Cadarache, France |
| Key element on the path to fusion energy production |
| |



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# DEISA awarded 2000k cpu hours to EUFORIA

| | EMC3-Eirene | GENE | BIT1 | GEM |
|---|---|---|---|---|
| Cpu hrs req | 300k | 600k | 200k | 1000k |
| Site req | RZG | RZG pref | Both | RZG pref |
| Countries | DE | DE,CH | AT | DE,AT,PT |
| Lead Assoc | Juelich | IPP-Garching | OAEW | IPP-Garching |
| Lead person | H. Frerichs | F. Jenko | D. Tskhakaya | B. Scott |
| Recommend | | | | |
| RZG | 300k(100k) | 600k(200k) | D. Tskhakaya | 100k(33k) |
| BSC | | | 200k(250k) | 800k(1000k) |
| | **Small cases ported to GRID freeing up HPC resources** | | **Moved from running on a single cpu to running on ~ 1024** | |



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# 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

# 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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# Promoted Codes

**BIT1** (s+p) [Kinetic 1D3V (1D in usual and 3D in velocity space) code for simulation of the plasma edge. Code includes nonlinear model for Coulomb and charged-neutral particle collisions, and simplified linear model of plasma-surface interactions.]

**CENTORI** (p) [The CENTORI code is a fully toroidal (arbitrary aspect ratio, arbitrary beta) two-fluid, electromagnetic turbulence simulation code. It builds on the well-documented CUTIE code by allowing the computation of turbulence in realistic tokamak geometries and at high beta.]

**COREDIV** (s+p) [Transport of energy, main ions and impurity ions in the core and the scrape of layer regions]

**EIRENE** (s+p) [EIRENE is a kinetic neutral particle and line radiation transport code.]

**ELMFIRE** (p) [Gyro-kinetic full-f particle code, with mostly global emphasis.]

**ERO** (s+p) [gyro-kinetic for impurity transport in plasma + following of molecular and atomic processes (providing 3D simulation of densities and plasma light emission) + plasma-surface interaction part including simulation of surface contents]

**ESEL** (p) [Turbulence and profile evolution at the outboard midplane in the SOL using a fluid (ESEL) and gyrofluid (GESEL) approach]

**GEM** (p) [gyrofluid (GEM is local, GEMX is nonlocal, 6 moment variable equations for each species, plus field equations for 2 potentials (electric, parallel magnetic); up to three ion species have been run; turbulence and profiles solved together, flow and magnetic current equilibrium are necessarily part of this

**GENE** (p) [GENE is a nonlinear gyrokinetic code to investigate plasma turbulence]

**ISDEP** (p) [Kinetic theory of transport based on Langevin Equations; Ion-ion and ion-electron collisions included; New stochastic terms (heating and turbulence) are envisaged]

**SOLPS** (s+p) [B2-Eirene consists of two codes tightly coupled together: B2 (multi-fluid solving continuity, momentum and energy equations for the plasma component on a cell cetntered grid; EIRENE (Monte-Carlo neutrals code providing sources for B2 based on a plasma background provided by B2)]

**TECXY** (p) [The code simulates 2D multifluid plasma and impurity transport in the tokamak edge including drifts, currents and self-consistent electric field Solves a set of fluid equations (Braginskij equations) describing the edge plasma on a 2D grid including SOL and transition layer

**TYR** (p) [Drift Alfven plasma fluid turbulence and transport in flux-tube geometry.]

# EFDA

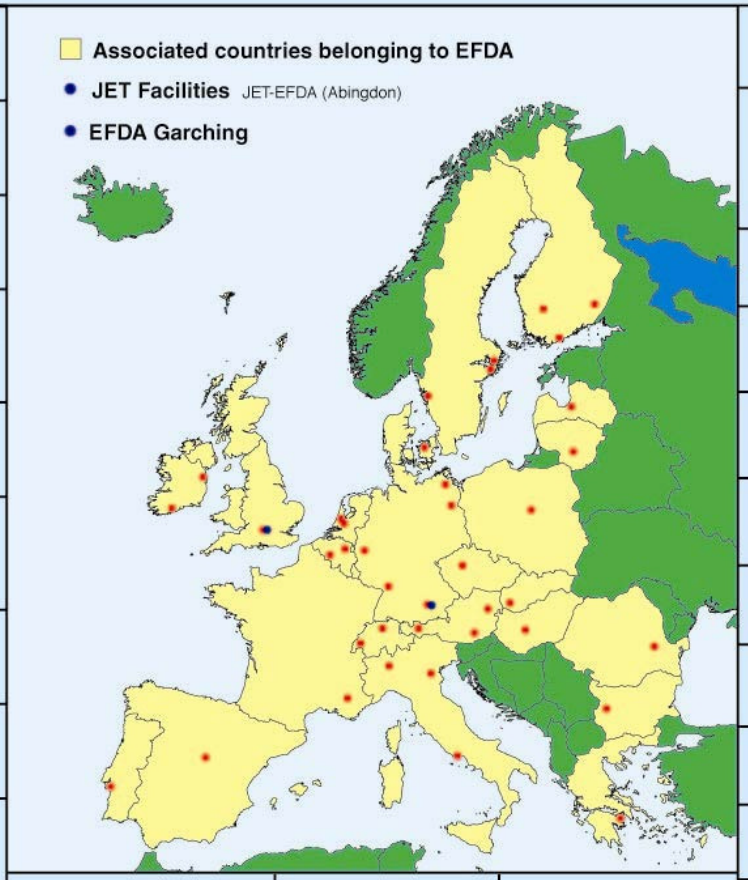
## European Fusion Development Agreement

**All EU Laboratories / Institutions working on Fusion are parties to EFDA**

**Defined under EURATOM under "Contract of Associations"**

**EURATOM : KEY ACTION FUSION Associated Laboratories, parties to EFDA**

- **Euratom - Belgian State** (Brussels) - (Mol)
- **Euratom - CEA** TORE SUPRA (Cadarache)
- **Euratom - CIEMAT** TJ-II (Madrid)
- **Euratom - Conf. Suisse** TCV - SULTAN (Lausanne) - (Villigen)
- **Euratom - DCU** (Dublin) - (Cork)
- **Euratom - ENEA** FTU - RFX (Frascati) - (Milan) - (Padua)
- **Euratom - FOM** (Petten) - (Nieuwegein)
- **Euratom - FZJ** TEXTOR (Julich)
- **Euratom - FZK** TOSKA (Karlsruhe)
- **Euratom - Greece** (Athens) - (Heraklion) - (Ioannina)




- **Euratom - INRNE** (Sofia)
- **Euratom - LEI** (Kaunas)
- **Euratom - CU** TOSKA (Bratislava)
- **Euratom - HAS** (Budapest)
- **Euratom - IPP** Asdex Upgrade - Wendelstein 7-AS Wendelstein 7-X (Garching) - (Greifswald) - (Berlin)
- **Euratom - IPP.CR** CASTOR (Prague)
- **Euratom - IST** ISTTOK (Lisbon)
- **Euratom - Latvia** (Riga)
- **Euratom - MEC** (Bucharest)
- **Euratom - ÖAW** (Vienna) - (Graz) - (Innsbruck)
- **Euratom - RISØ** (Roskilde)
- **Euratom - TEKES** (Helsinki) - (Tampere) - (Lappeenranta)
- **Euratom - UKAEA** MAST - JET (Culham)
- **Euratom - VR** EXTRAP T2R (Stockholm) - (Lund) (Gothenburg) - (Studsvik) - (Uppsala)

JG03.241-6c



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TF Leader : P. Strand,
Deputies: L-G. Eriksson, R. Coelho

EFDA CSU Contact Person: D. Kalupin

EFDA
EUROPEAN FUSION DEVELOPMENT AGREEMENT

Task Force
INTEGRATED TOKAMAK MODELLING

## ITM-TF charge

- *Co-ordinate the development of a coherent set of validated simulation tools for ITER exploitation*
- *Benchmark these tools on existing tokamak experiments*
- *Provide a comprehensive simulation package for ITER and DEMO plasmas.*
- *Coordinate the European Software developments with the aim to increase quality and reduce parallel efforts. (Streamline the code base)*

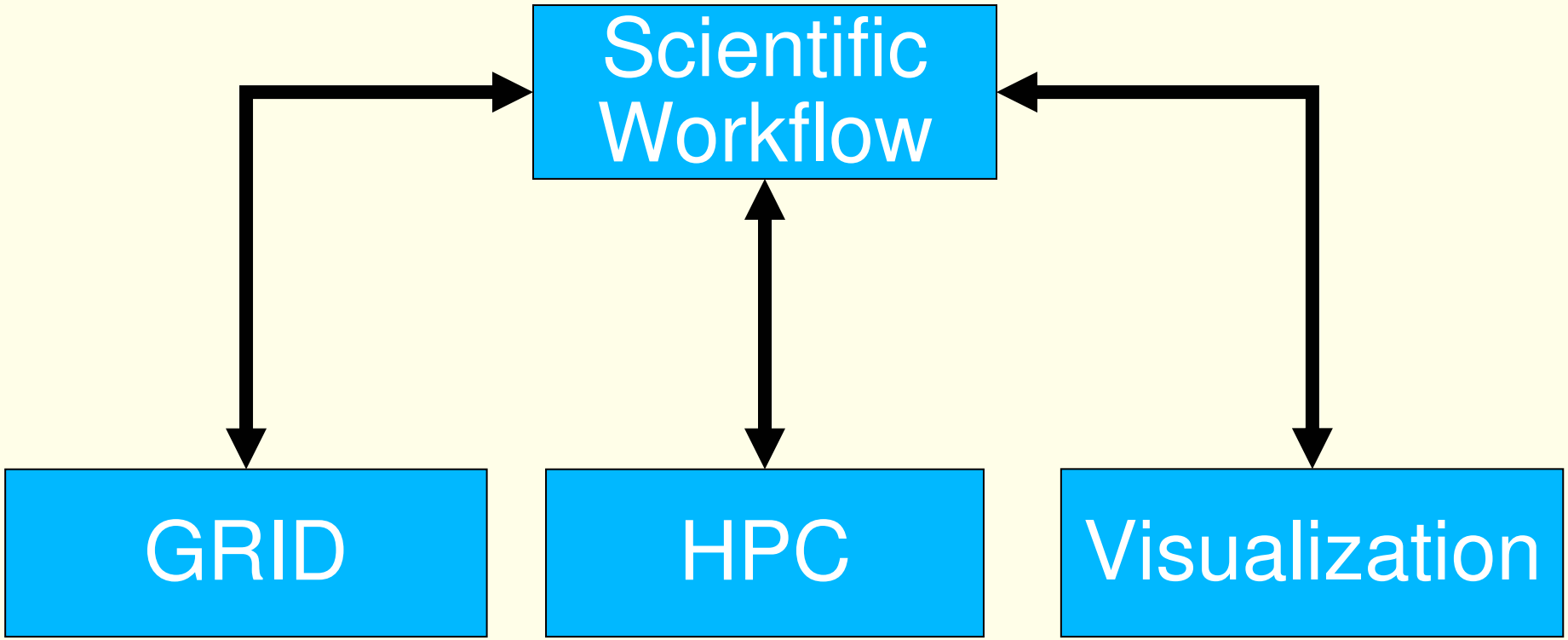
## ITM-TF Remit

- *Development of the necessary standardized software tools for*
  - *interfacing code modules and*
  - *accessing experimental data.*

## Medium term activities

- *Support the development of ITER-relevant scenarios in current experiments.*

# Developing a new paradigm for fusion computing



# Batch, GRID and HPC

| | Batch | GRID | HPC |
|---|---|---|---|
| Current usage within the fusion community | Extensive<br>• JET (339 cpus)<br>• Most associations (IPP-TOK 400 cpus)<br>• Gateway (128 cpus) | • Only at CIEMAT<br>• Starting to see some usage at Juelich<br>• Plans for usage at IPP | • Extensive use of national facilities<br>• Extra-national usage via DEISA |
| Main issue preventing more usage | • Lack of more local cpus | • Lack of knowledge<br>• Difficulties getting certificates | • Difficult for Associations without strong national facilities |
| Currently being addressed by | | EUFORIA<br>• has provided training<br>• also developing facilities to launch jobs from the Gateway | EUFORIA<br>• has provided training<br>• has worked on codes<br>HPC-FF starting August 1st<br>• HLST |
| Longer term | | ? | IFERC computer (2012) |



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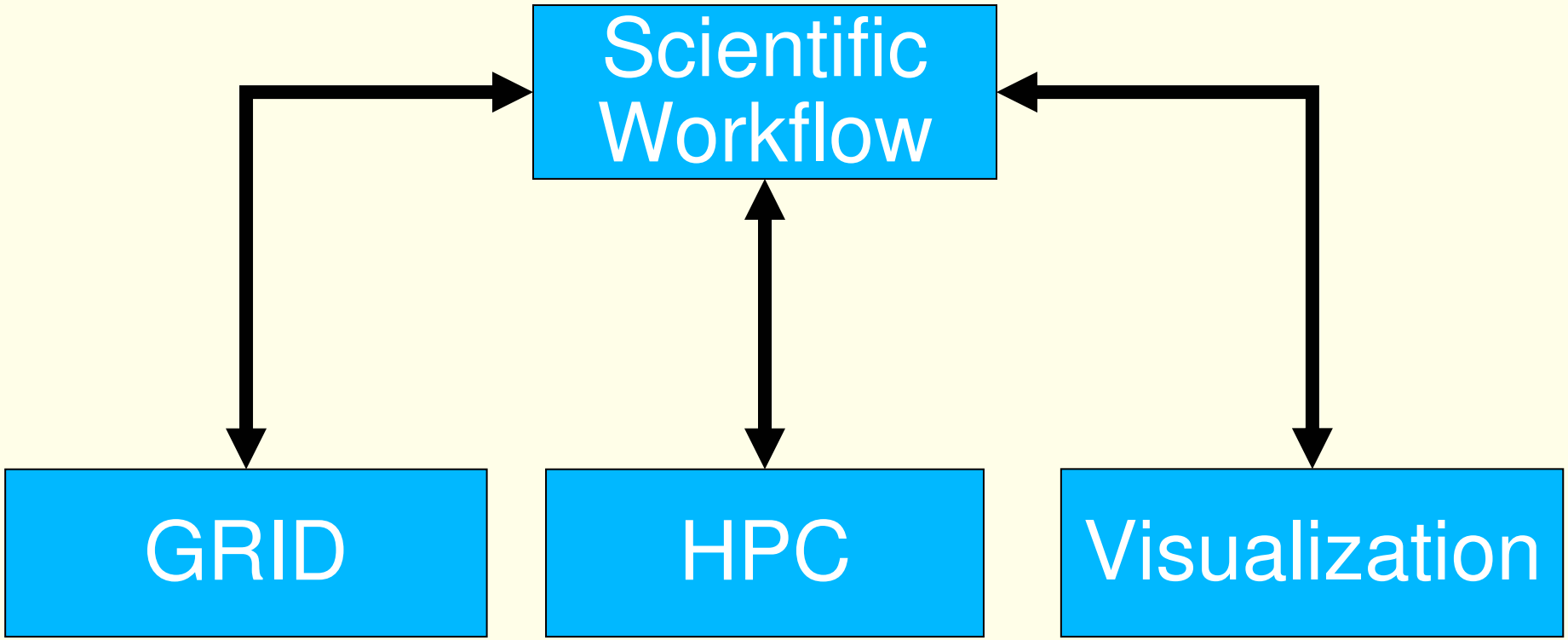
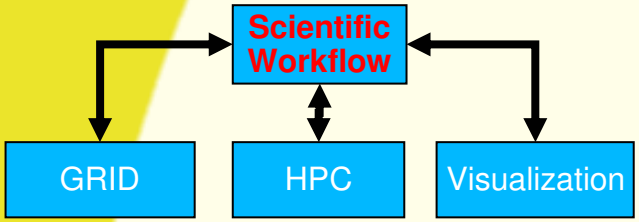
# Developing a new paradigm for fusion computing






# Scientific Workflows

- Need to make a convincing case that scientific workflows will
  - Enhance productivity
  - Allow for new approaches problems to be solved
  - Allow for traceability, reproducibility, …
  - Allow for a better use of resources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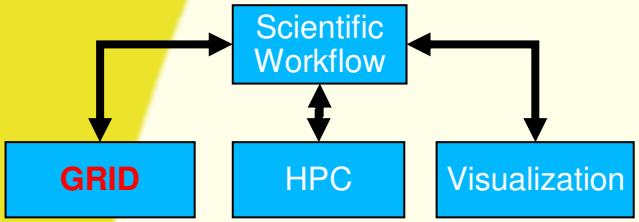
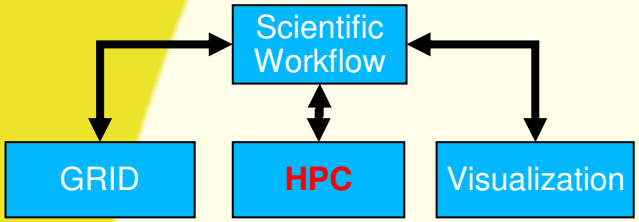



# Grid Computing

- Grid computing needs
  - To be transparently coupled into the scientific workflows
  - Needs to be reliable (every launched job should run)
  - Needs to improve performance (if resources are available, a launched job should start rapidly)
  - To inter-operate with the other levels at the data access level




# HPC

- Need to be transparently coupled into the workflows
- HPC facilities will need to deal with jobs coming from workflows
  - Negotiations about resource availability and expected response times
  - Deal with communications between the different parts of a workflow
  - Better integrate inter-operability of data between HPC and the other levels



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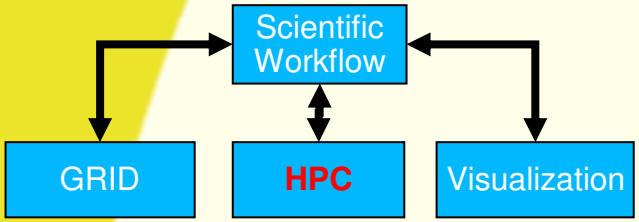
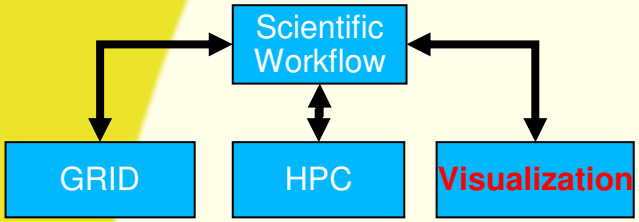



# HPC, II

- Need to better prepare jobs to scale from the present 1k – 10k cpus to 100k – 1M cpus
  - This means at the development stage
    - Having machines exposing large numbers of cores to code developers interactively or almost interactively (< 5 minute turn around)
    - Helping the code developers with algorithms, …
    - Helping the code developers with better IO strategies
  - At the production stage
    - Having the resources available




# Visualization

- Challenges in visualization include
  - Visualizing the data flowing around a workflow so that the scientist can monitor/diagnose a running job
  - Deal with very large amounts of data produced in a distributed environment
  - Help provide the scientist with a better understanding of his/her results
  - Help the scientist by producing visualizations with that “Wow!” factor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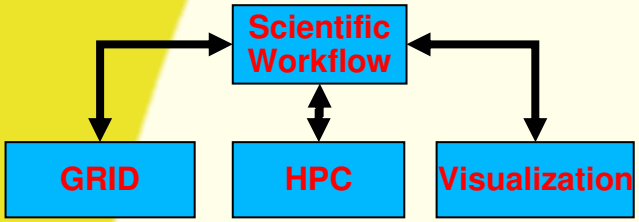


# Over all

- Need to make it simpler to move data between the different parts of a workflow
  - Remote data access
  - High speed data transfers
  - Better integration
- Need to think now about very large data sets
  - What is the “best” relationship between petaflops and petabytes?


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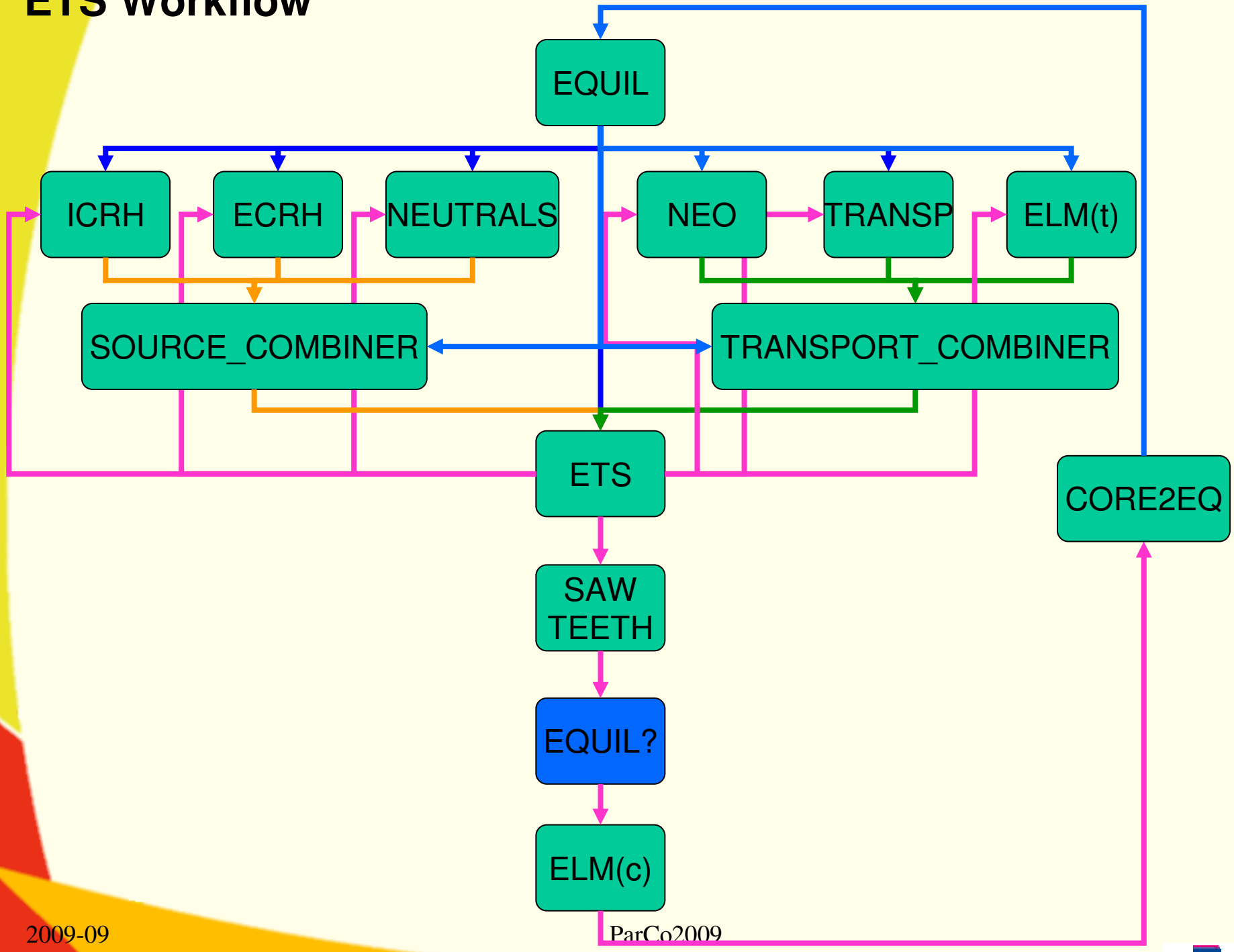
# ETS Workflow



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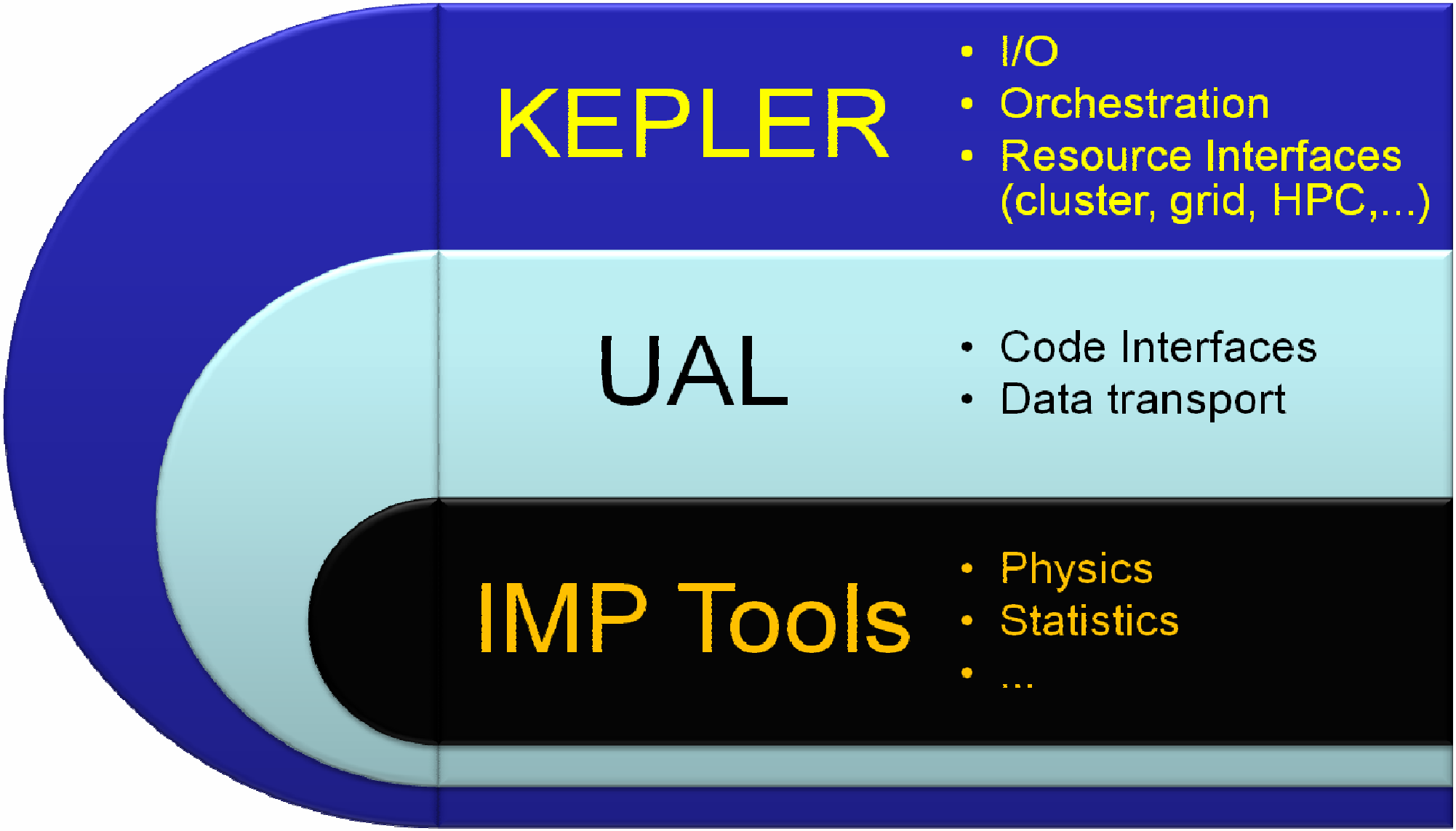
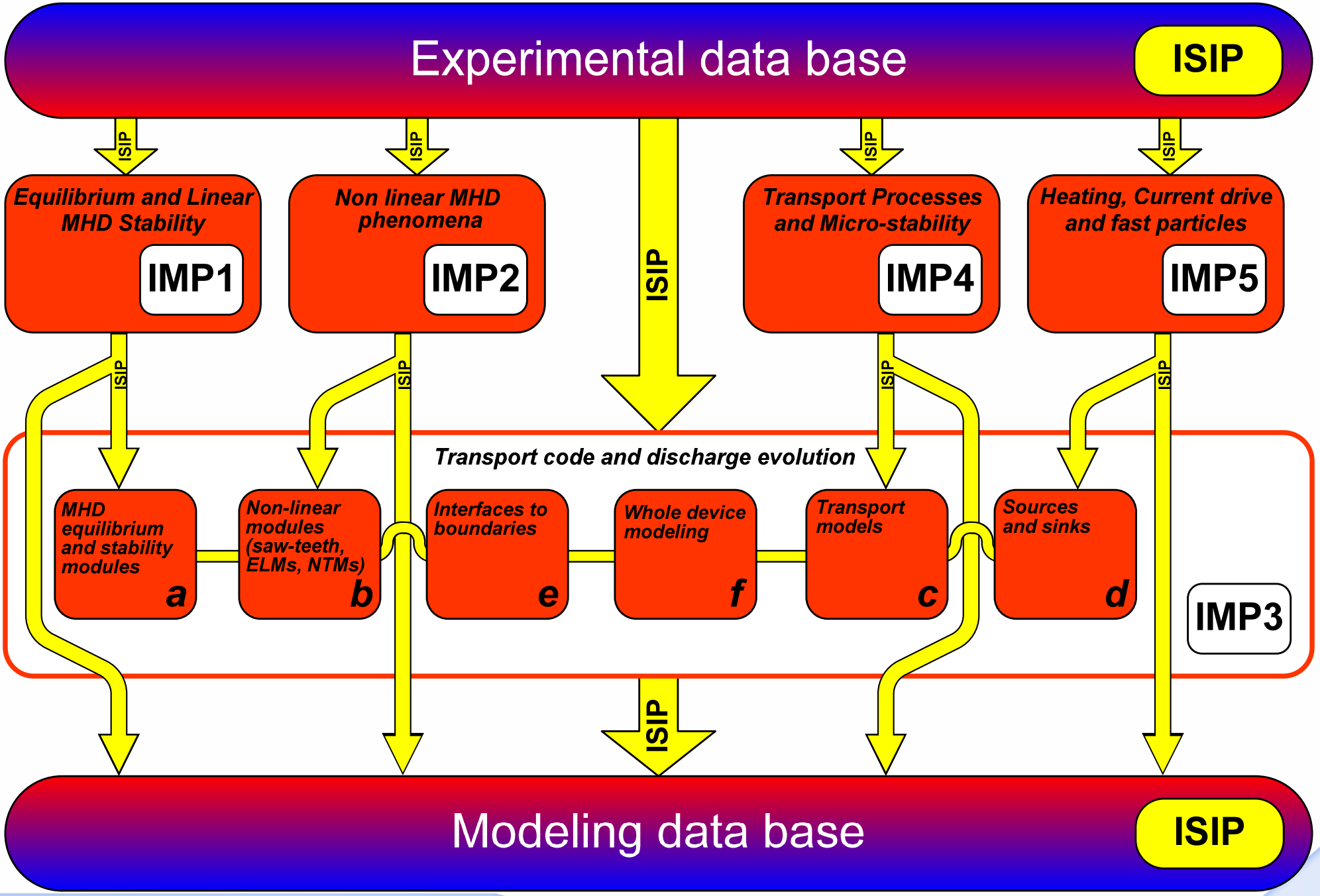
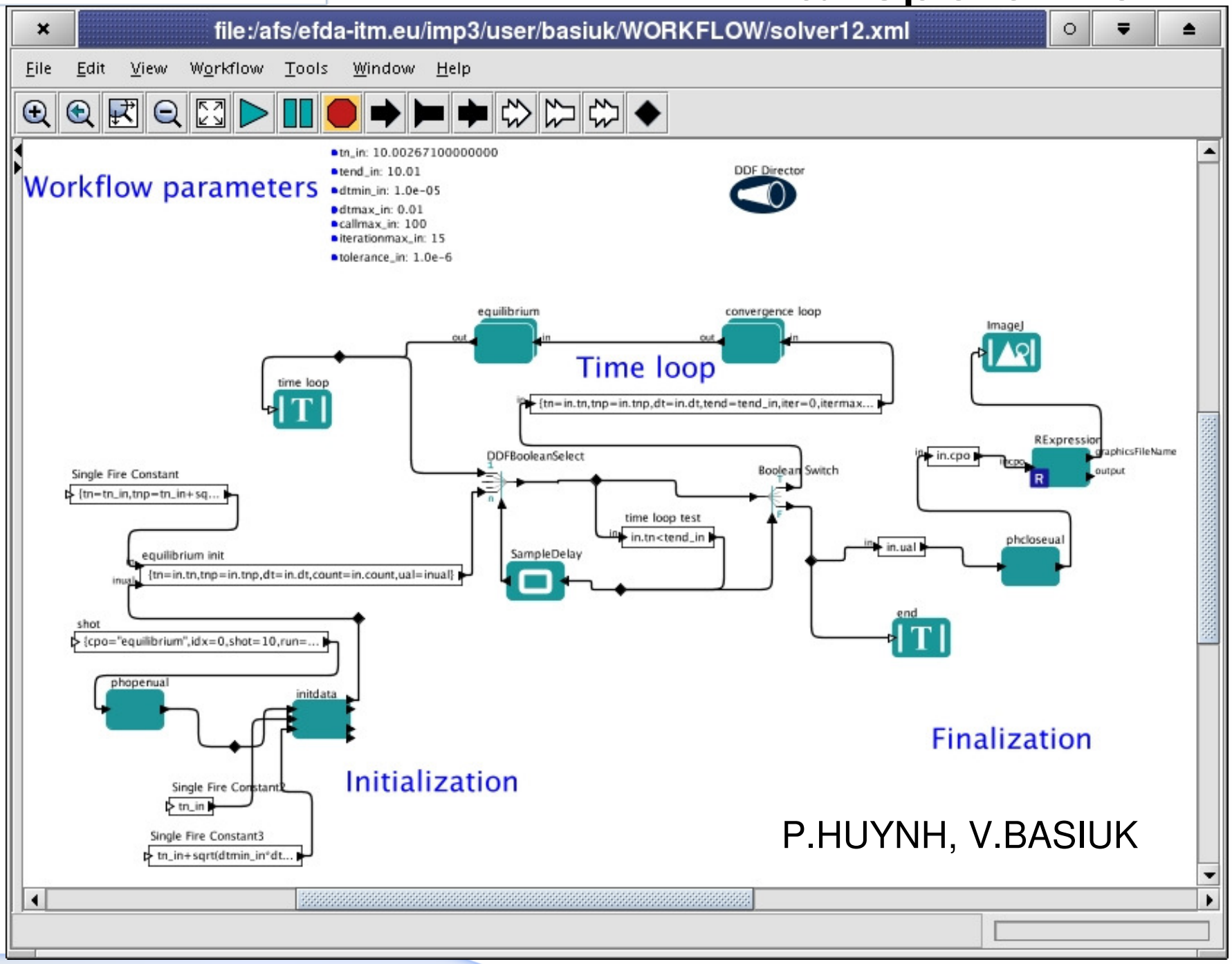
# ITM-TF Application Structure



# ITM


Experimental data base
ISIP
ISIP
ISIP
ISIP
ISIP
Equilibrium and Linear MHD Stability
IMP1
Non linear MHD phenomena
IMP2
Transport Processes and Micro-stability
IMP4
Heating, Current drive and fast particles
IMP5
ISIP
ISIP
ISIP
ISIP
Transport code and discharge evolution
MHD equilibrium and stability modules
a
Non-linear modules (saw-teeth, ELMs, NTMs)
b
Interfaces to boundaries
e
Whole device modeling
f
Transport models
c
Sources and sinks
d
IMP3
ISIP
Modeling data base
ISIP

# KEPLER Transport Workflow



# Summary

- EUFORIA
  - Has ported/optimized a number of codes
    - For the GRID
    - FOR HPC
  - Demonstrated the ability from a central workflow to
    - Launch a job on the GRID
    - Launch a job on HPC
    - Launch a sub-workflow on the GRID
    - Launch a work-flow on HPC
- ITM
  - Has demonstrated KEPLER workflows
  - Code integration using the UAL
- Now need to make this “routine”