# Fusion, EFDA, ITM and EUFORIA

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Grids and e-Science 2009:

Advanced Workshop on the future and sustainability of production Grids

2009-06

Santander



## Outline

### Fusion

- Background
- EFDA (European Fusion Development Agreement)
  - Organization of fusion within Europe
- ITM

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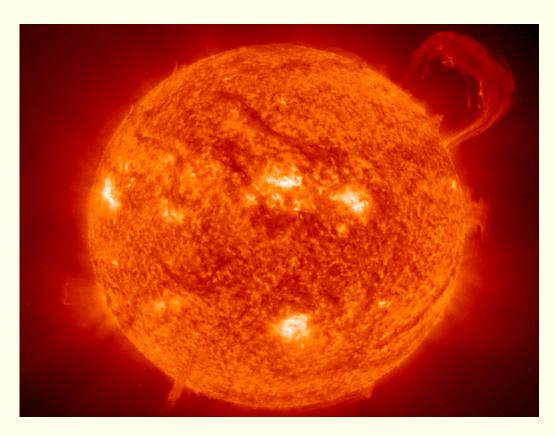
- EFDA Task Force on Integrated Tokamak Modelling
- EUFORIA
  - EU for Iter Applications

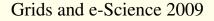
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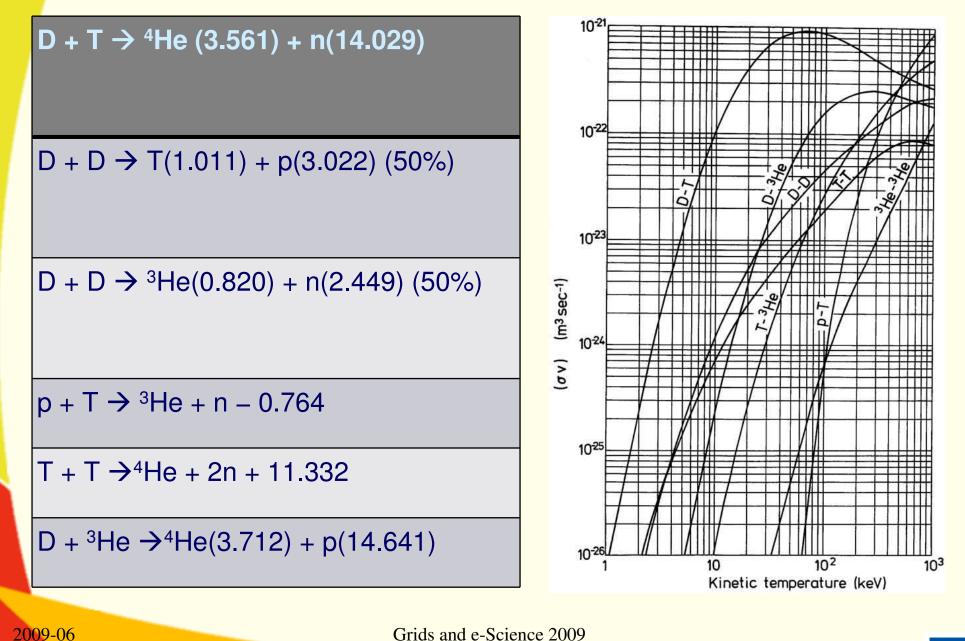
- Energy source for the sun and other stars
- Provides a potential source of base load energy production
- Been working on this for more than 50 years
- Has turned out to be a very difficult problem

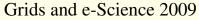
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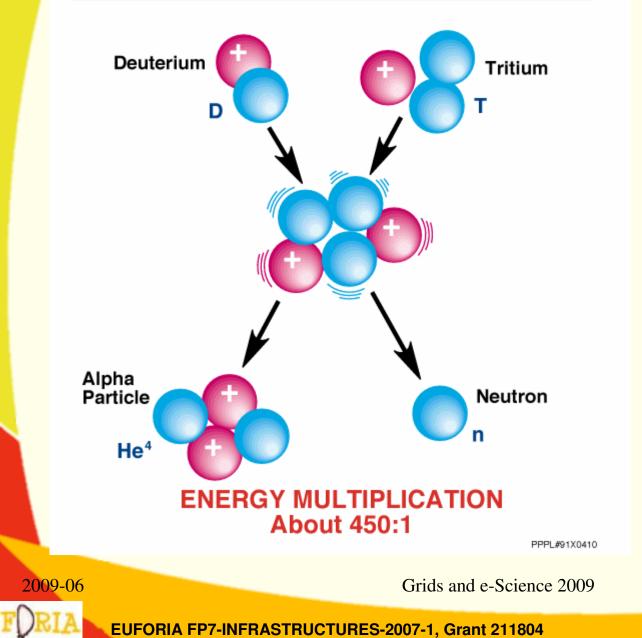


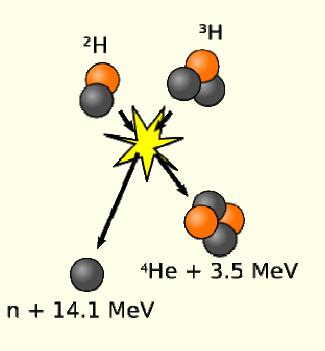






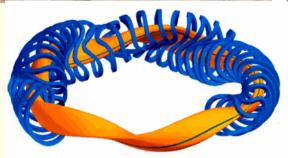
#### **Deuterium–Tritium Fusion Reaction**

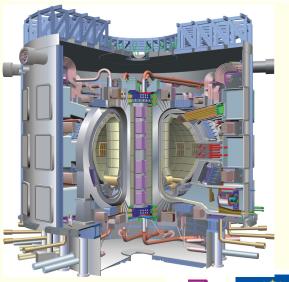




e-infrastructure









- 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

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## NIF at LLNL

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78% B



W7X

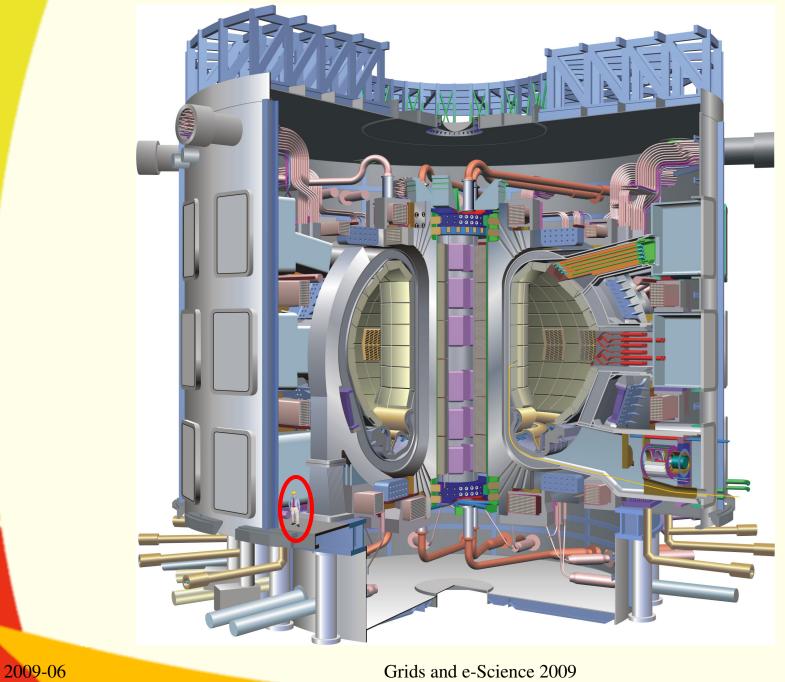




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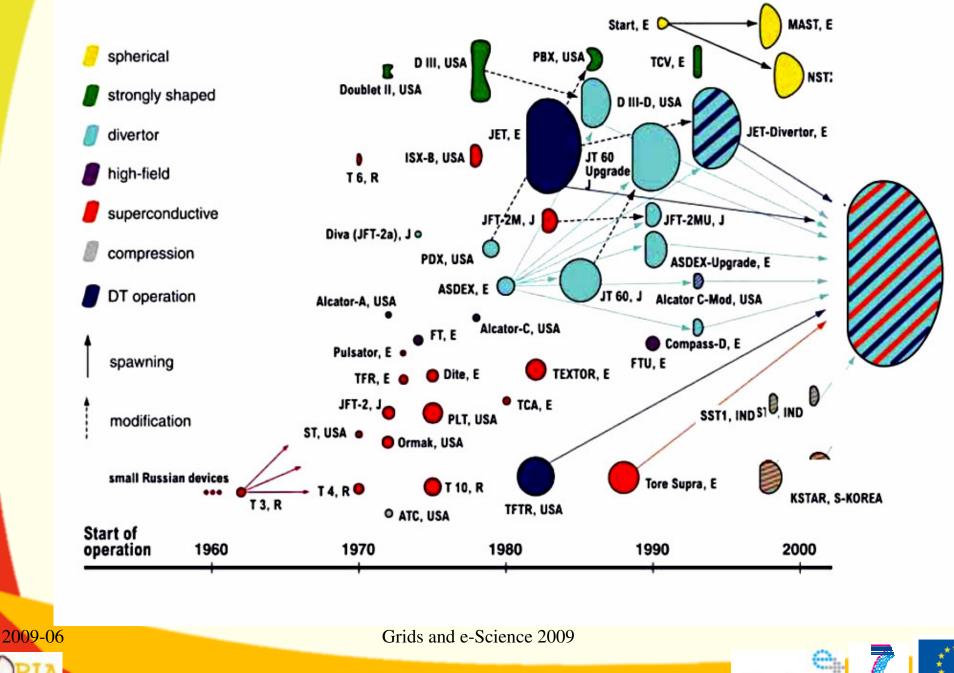




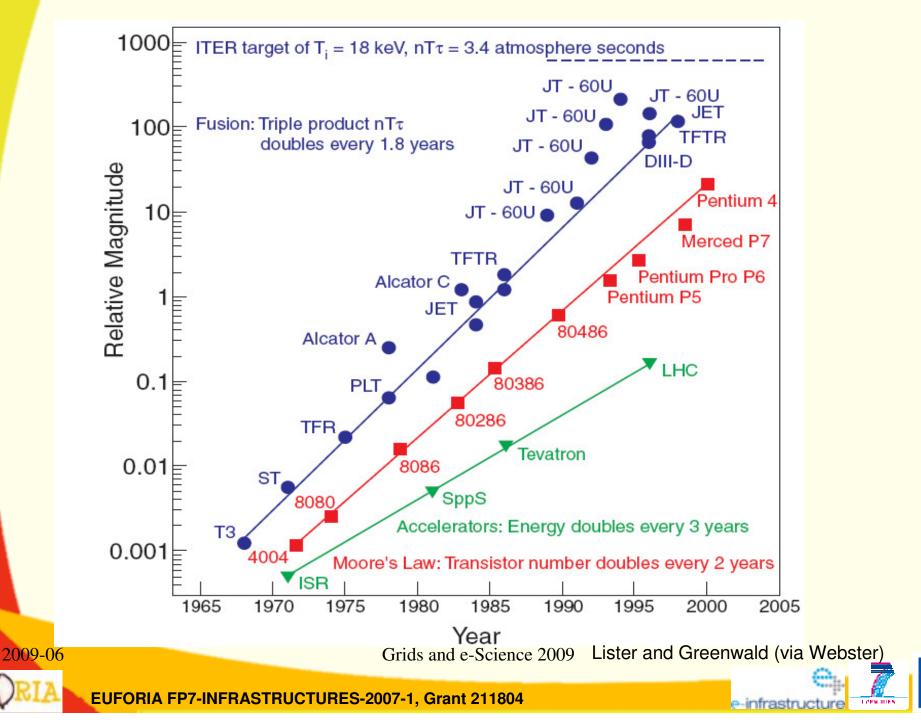


e-infrastructure

COPIE DE



### Fusion developing faster than Moore's Law



### 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





ITER



			Units
	Plasma Major Radius	6.2	m
	Plasma Minor Radius	2.0	m
	Plasma Volume	840	m3
	Plasma Current	15.0	MA
	Toroidal Field on Axis	5.3	Т
	Fusion Power	500	MW
	Burn Flat Top	>400	S
	Power Amplification	>10	
2009-06       Grids and e-Science 2009         FORIA       EUFORIA FP7-INFRASTRUCTURES-2007-1, Grant 211804	e-infra	etructure	

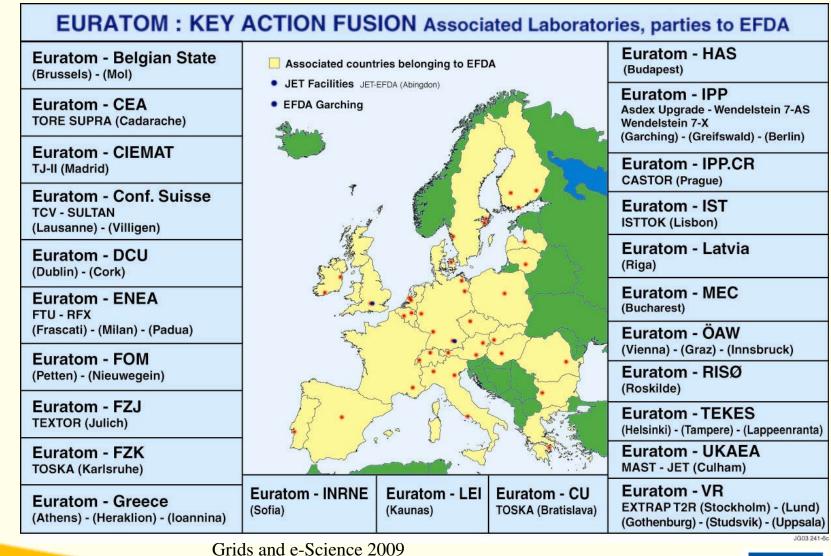
# EFDA

### **European Fusion Development Agreement**

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

Defined under EURATOM under "Contract of Associations"

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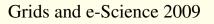


# EFDA

### • EURATOM Budget (for the period 2007-2011)

- Nuclear Security
- Fusion energy research\* €1947 m
  - \*Within the amount foreseen for fusion energy research, at least €900 million will be reserved for activities other than the construction of the fusion energy source ITER.
- Nuclear Fission and radiation protection €287 m
- Nuclear Activities of the Joint Research Centre €517 m





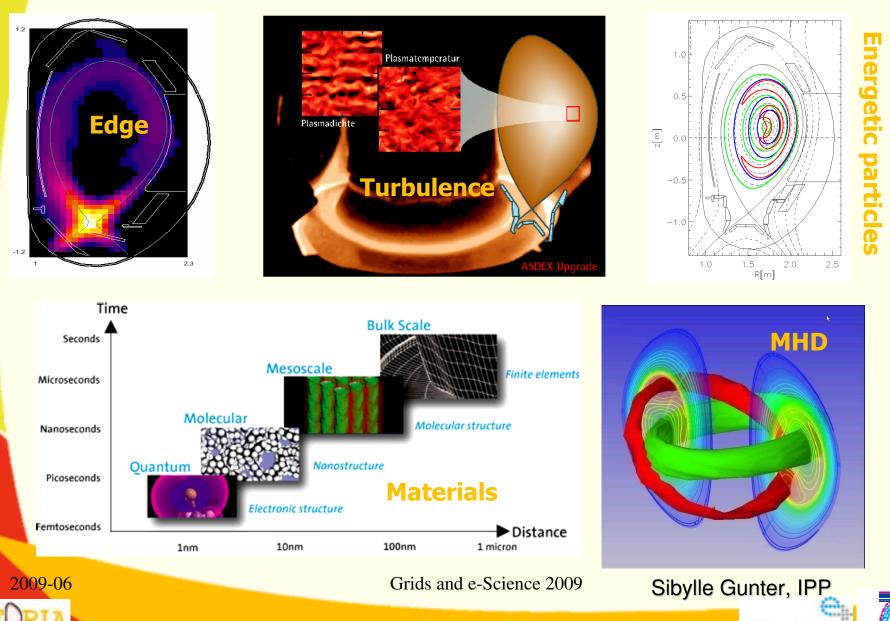


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# Multi-facetted physics

e-infrastructure

0.0950-001



# Large Computation Requirement

### Have requirements for

- Experimental data processing
- Experimental scenario development
- Theory

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- Turbulence
- Large scale MHD
- Materials

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# **Experimental Data**

- JET (per shot)
  - ~ 10 Gb of raw data (JPF)
  - ~ 0.4 Gb of processed data (PPF) from "Chain1"
  - Chain1 takes around 4 minutes to run on 6 processors
  - ~ 0.2 Gb of additional processed data per pulse by "Chain2" and other analysis codes
  - A typical "Chain2" run (they are quite variable as the ICRH and NBI FP codes take most of the time) takes an hour
- AUG

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- ~ 9 GB Raw data
- ~ 0.6 GB Processed data

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# Integrated Data Analysis

- IDA: (ne, Te)
  - 1 time slice for Te and ne: approx. 1 min
  - 10 s shot / 50  $\mu s$  resolution  $\ ->$  140 days on a single CPU
  - (standard is 1 ms resolution only due to limited computation capabilities (power and memory), 50 µs are calculated only for selected shots)
- IDZ: (Zeff)
  - 1 shot with 50 ms resolution approx. 1 hour on a single CPU
- Er

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- more than days
- The plan is to introduce into IDA also the equilibrium solver (equil) and the corresponding magnetic signals. I expect that this will increase computation time considerably.

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# Large Range of Scales

#### Time

- 10<sup>-11</sup> << 10<sup>-8</sup> << 10<sup>-4</sup> << 10<sup>-2</sup> << 10<sup>+1</sup>
- (plasma freq; ion cyclotron freq; electron collision time; ion collision time; confinement time)

Space

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- 10<sup>-4</sup> << 10<sup>-3</sup> << 10<sup>+0</sup> << 10<sup>+4</sup>
- (Debye; ion Larmor radius; a; electron mfp)

Eliminate some processes by choosing the physics model

But still need to bridge

- 10<sup>+5</sup> in time
  - (10<sup>+3</sup>)<sup>2</sup> in space

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### Major Theoretical & Algorithmic Speedups

relative to simplest brute force, fully resolved, algorithm, for ITER  $1/\rho_* = a/\rho \sim 700$ 

Massively parallel computers (Moore's law 1982-2007)	x10 <sup>5</sup>
Total combined speedup of all algorithms	x10 <sup>23</sup>
Implicit electrons	x5-50
High-order / spectral algorithms in 5-D, 2 <sup>5</sup> x 2	x64
$L_r \sim a/5 \sim 140 \ \rho \sim 10 \ correlation \ lengths$	x5
$ \begin{aligned} k_\theta \rho_i &= 0, 0.05, 0.1, \ldots, 1.0 \\ n &= 0, 15, 30, \ldots, 300 \end{aligned} \mbox{ (i.e., 1/15 of toroidal direction)} $	x15
Flux-tube / Toroidal annulus wedge, $\downarrow$ simulation volume	
Field-aligned coordinates (nonlinear extension of ballooning coord.) $\Delta_{\parallel}/(\Delta_{\perp} q R/a) \sim a/(q R \rho_*)$	x70
Continuum or $\delta f$ PIC, reduces noise, $(f_0/\delta f)^2 \sim 1/\rho_*^2$	x10 <sup>6</sup>
- average over fast ion gyration, $\Omega_{ci}$ / $\omega_{\star}$ ~ 1/p_{\star}	x10 <sup>3</sup>
- ion polarization eliminates $\rho_e$ & Debye scales $~(\rho_i\!/\rho_e)^3$	x10 <sup>5</sup>
- ion polarization shielding eliminates plasma freq. $\omega_{pe}/\Omega_{ci}$ ~ $m_i\!/m_e$	x10 <sup>3</sup>
Nonlinear gyrokinetic equation	

Hammett, APS DPP, Orlando, 2007

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# **EFDA**

EUROPEAN FUSION DEVELOPMENT AGREEMENT

Task Force INTEGRATED TOKAMAK MODELLING Grids and e-Science 2009 Advanced Workshop on the future and sustainability of production Grids

PALACIO DE LA MAGDALENA,

Santander.

ITM

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

EFDA CSU Contact Person: D. Kalupin



# EFDA ITM-TF

#### 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.

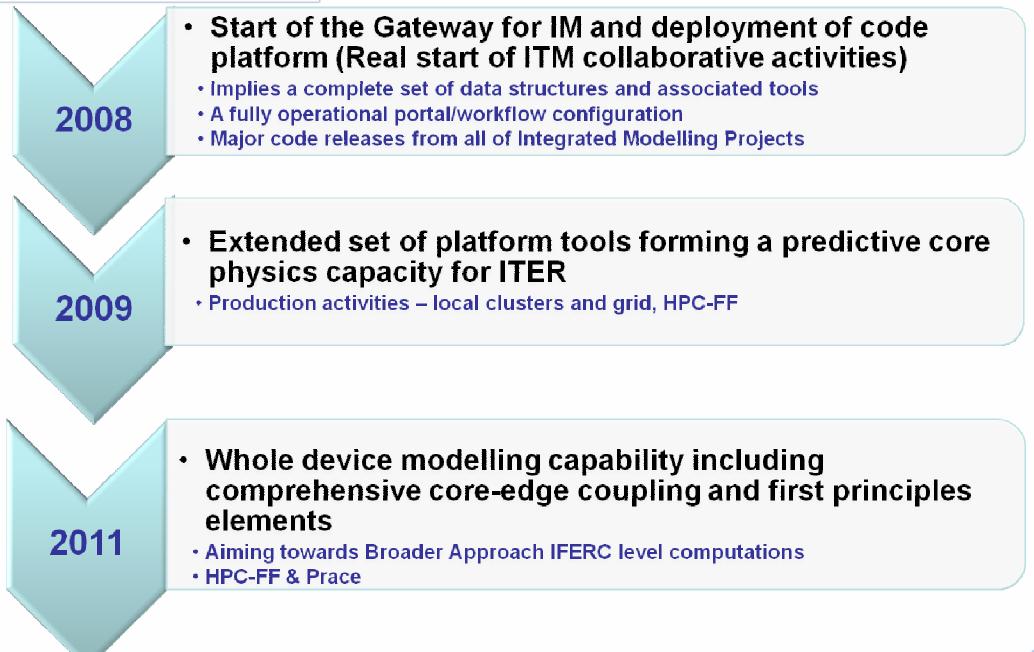
EFDA SC (03)-21/4.9.2 (June 24th, 2003)



# EFDA ITM-TF

- Staffed by people from the associations under "Task Agreements"
- 240 people involved
- 60 ppy (1/3 under "Preferential" or "Priority" support → 40% from Brussels (remaining paid 20% by Brussels))
- ~ 400 people in Europe involved in fusion theory and modelling

# **ITM-TF** Milestones

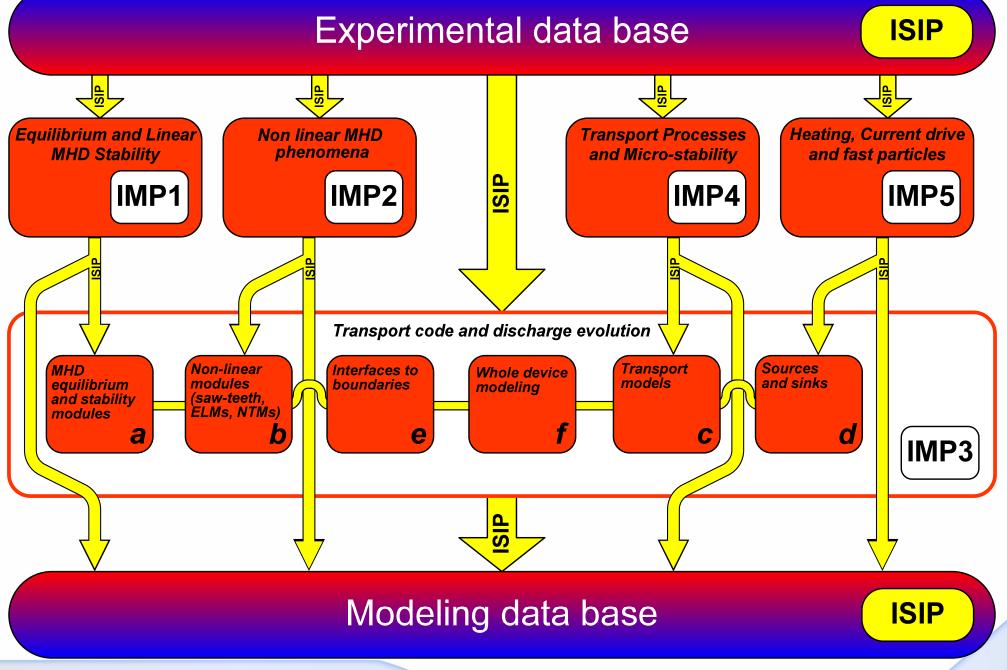


**Task Force** 

RATED TOKAMAK MODELLING

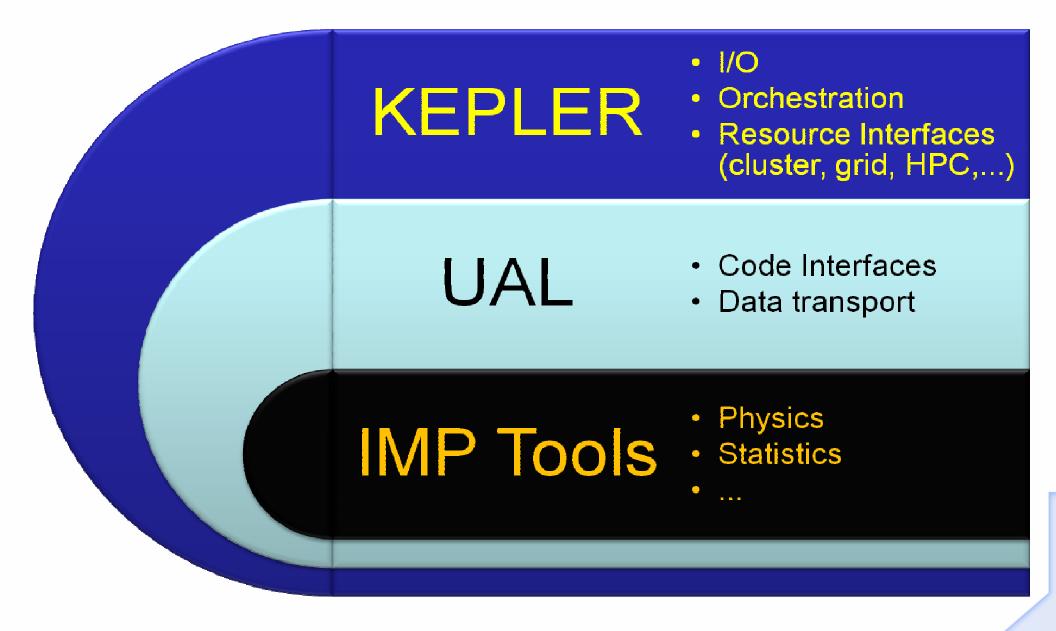


# ITM





### **ITM-TF Application Structure**



### **ITM-TF Application Structure**

#### Framework (Kepler)

Calls the wrapper, specifying the present time of the simulation, orchestrates run.

#### Wrapper (FC2K, WS2K) Calls UAL to GET the CPOin and CPOout at the requested time slices

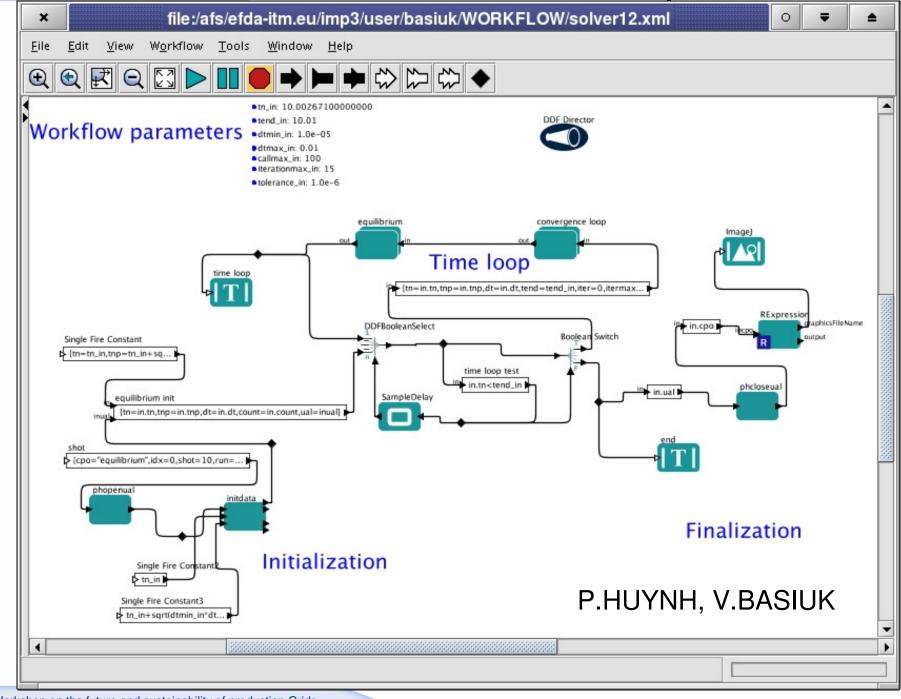
#### Physics code

Receives CPOin, CPOout,

Physics calculations Updates CPOout

Updates data management nodes Calls UAL to PUT the CPOout

### **KEPLER Transport Workflow**



Advanced Workshop on the future and sustainability of production Grids

**Task Force** 

INTEGRATED TOKAMAK MODELLING

# **E**UFORIA

14 member Institutes3.65M€ over 36 months

#### 522pms covering

- Management
- Training
- Dissemination
- Grid and HPC infrastructure & support
- Code adaptation & optimization
  Workflows
  Visualization



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## **Consortium Members**

\*\*\*\*

1.09%-01

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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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FOPTA				

# Project objectives

Bringing a comprehensive framework and e-infrastructure to the fusion modelling community oriented to the development of ITER physics needs with particular emphasis on Grid and HPC activities

### Focus area: Edge and core transport and turbulence

Deployment of Grid and HPC infrastructure

Adaptation and Optimization of Fusion Codes

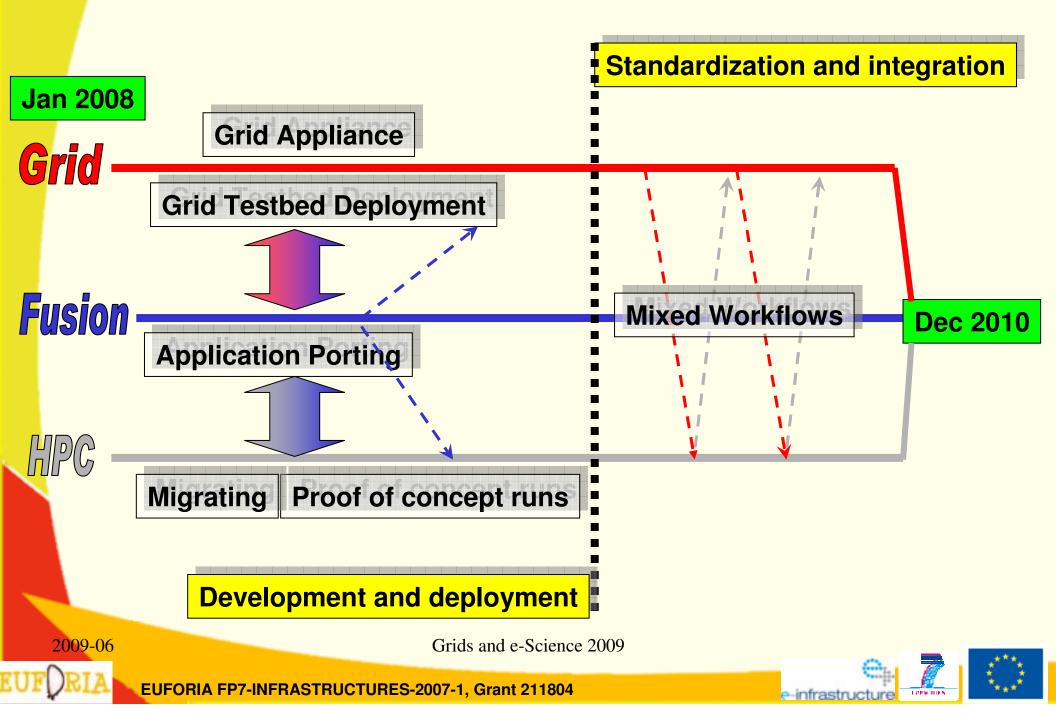
Platform oriented Grid and/or HPC

#### Development of advanced tools for

- Workflow management
- Visualization tools
- Data mining

In addition, there is a number of outreach and dissemination activities planned to introduce the fusion community at large to the developed infrastructure and make contact with other infrastructure and research projects with similar or associated orientations.

# Work plan outline



# Team - Work Package Managers

The EUFORIA programme is organized under three headings: Networking (NA), Service activities (SA) and Joint Research Activities (JRA) and 10 WP's.

		WP #	# of pm's allocated	Work package title	Lead participant short name	WP managers
:	ng	NA1	16	Management	Chalmers	Pär Strand (PSG)
	Networking	NA2	25	User Documentation and Training	UEDIN	Lorna Smith (PSG)
	Net	NA3	24	Dissemination	CIEMAT	Miguel Cardenas
	Service Activities	SA1	1 <b>1</b> 5	Grid Infrastructure Deployment and Operation	CSIC	Isabel Campos (PSG)
	ice Act	SA2	25	HPC Infrastructure	BSC	Jose Maria Cela (PSG)
	Servi	SA3	31	HPC and Grid Support	UEDIN	Lorna Smith
Inint Bacaarch Activitiae	vities	JRA1	72	Adaptation of codes for Grid Infrastructure	CIEMAT	Francisco Castejon
	h Activ	JRA2	110	Adaptation of codes for HPC infrastructure	Åbo	Jan Westerholm (PSG)
	t Researc	JRA3	68	Workflow orchestration - physics integration support	CEA	Bernard Guillerminet (PSG)
	Joint	JRA4	36	Visualization	STRASB	Eric Sonnendrucker

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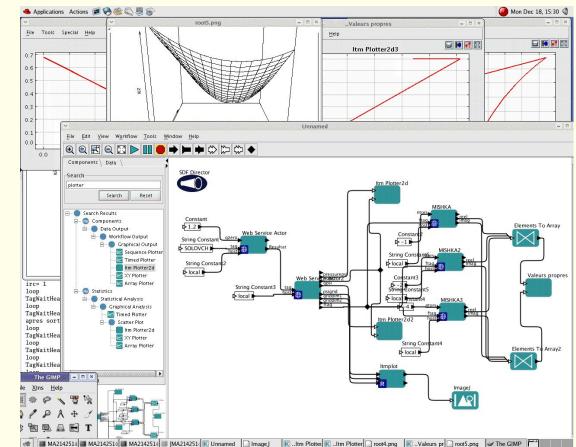
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# Workflows

The objective is to schedule jobs on the GRID and HPC infrastructures together with jobs running on other computing facilities.

- launch and control jobs in a transparent manner for the users.
- data communication: data transfers and visualizations are required at run time and to access the experimental and simulated data.
- middleware connectivity for Kepler Workflow (java Library for gLite, HPC)
- scheduler notification tools
- Integration with ITM tools (UAL Universal Access Layer)



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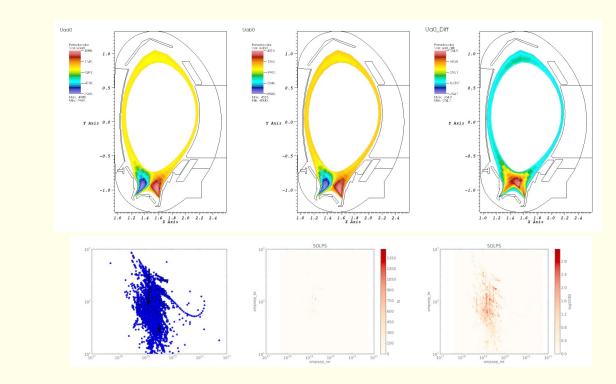


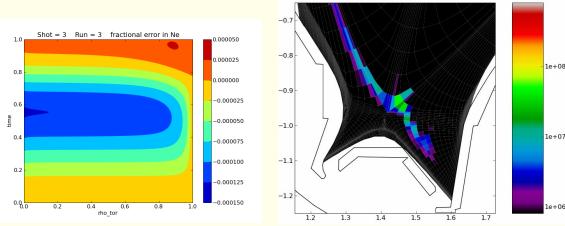
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# Visualization

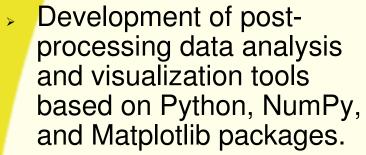
SOLPS # = 24204 T = 1.980010

infrastruc





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- Development of postprocessing data analysis and visualization tools based on Vislt.
- Integration of Python, NumPy, Matplotlib into the Kepler workflow.
- Integration of Vislt or VTK into the Kepler workflow.
- Development of a lossy wavelet based compressed data format.
- Develop visualization techniques for 4D and 5D particle distributions.

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## EU Fusion "Ontology"

- Abstracted data structures
  - Description of a "Complete" set of data for describing plasma operation and simulations
    - Abstracted through XML schemas
    - Unambiguous description with agreed sign and other conventions
    - SI-units (with eV)
    - Consistent Physical Objects (CPO)
      - Groupings of related data basis for code interfaces
    - Machine descriptions
      - Allowing for device independent codes!
  - Serializations

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- Transformations providing
  - Language specific implementations of CPOs (f90, C++,..)
  - Database structures
- Used in workflow tool to connect modules.
  - Automagic creation of Kepler Actors

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## EU Fusion "Ontology" (II)

- Access and Storage
  - Universal Access Layer (UAL) providing invariant API based on CPOs
  - Plug-in API for backend
    - MDS+ implemented implications on data structures
    - HDF5 next step

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- Code Coupling Mechanism
  - Used in workflow tool to connect modules.
- NB: The tools and structures are generic, the EUFORIA toolset is portable to other modelling areas





# EUFORIA in brief

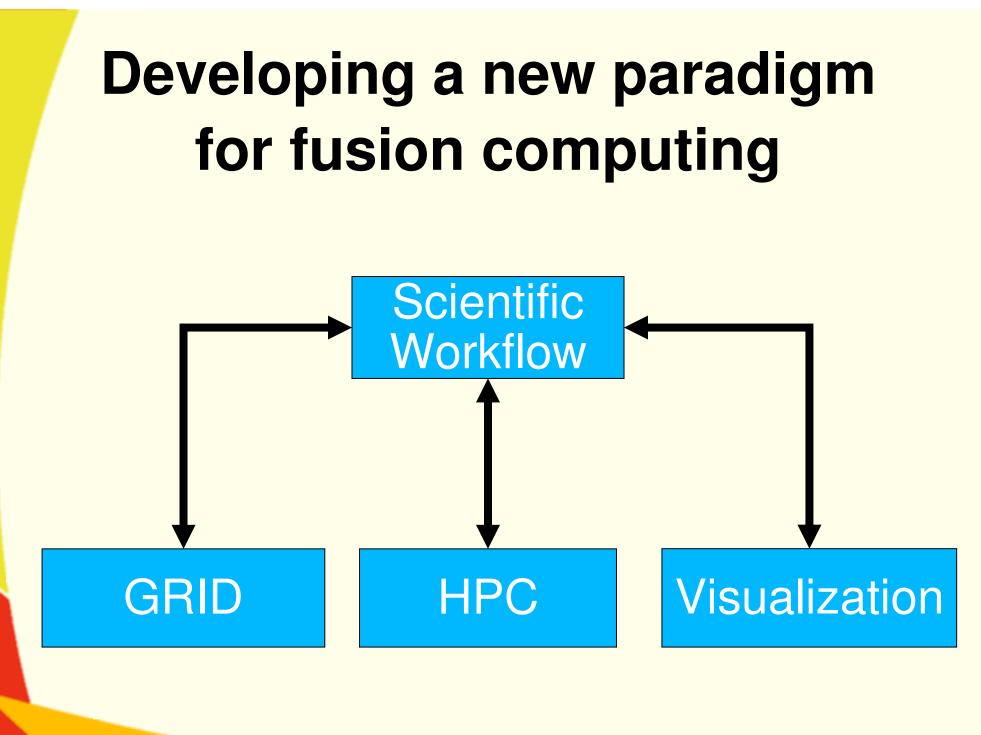
- 3.65M€, 36 months, 522 pm's
- Coordinated by Chalmers (IPP deputy)
  - ITM-TF connectivity to guarantee broad access
  - Intended to boost ITM-TF activities towards HPC and grid computing
- "Edge and core turbulence and transport"
- Deployment of Grid and HPC infrastructure
- Adaptation and Optimization of Fusion Codes
  - Platform oriented Grid and/or HPC
  - > First profiling and priorisation of codes done.
- Development of advanced tools for
  - > Workflow management
  - Visualization tools
  - Data mining

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Range of outreach and training activities

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EUFORIA FP7-INFRASTRUCTURES-2007-1, Grant 211804

e-infrastructure

## How is EUFORIA Working towards this Goal?

Scientific Workflow	• JRA3	В
GRID	<ul> <li>JRA1, SA1</li> <li>EGEE, EGI</li> </ul>	n "(
HPC	<ul><li>JRA2, SA2</li><li>DEISA</li></ul>	tł C
Visualization	• JRA4	•
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But we also eed to sell" this paradigm to he fusion ommunity

NA2, NA3





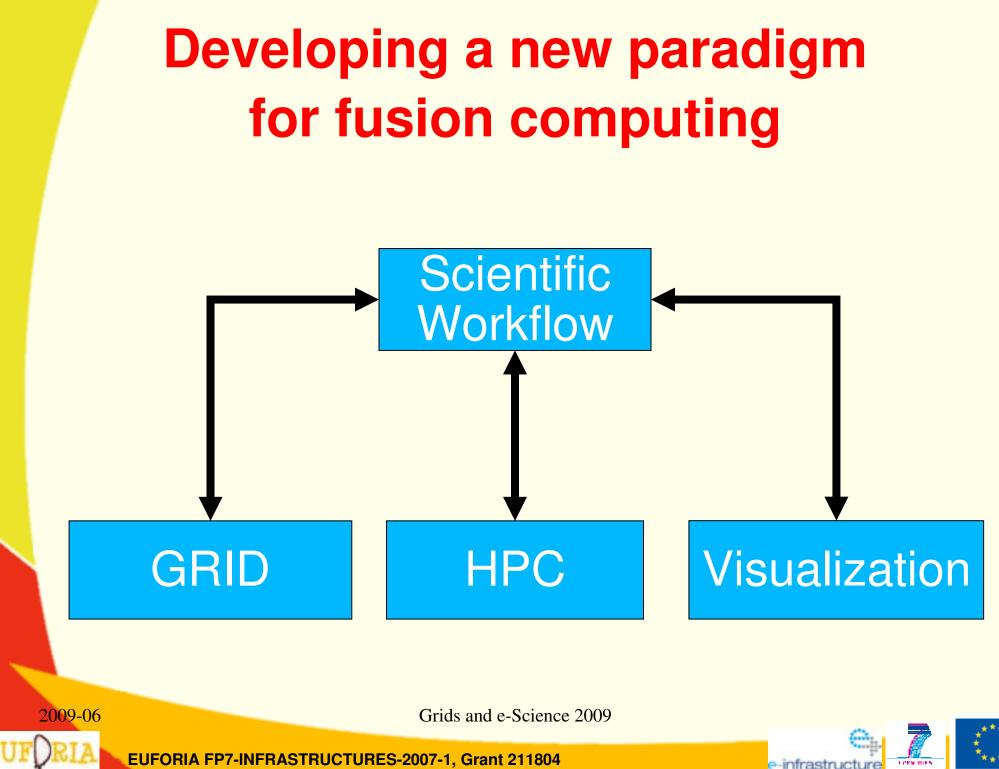
## Batch, GRID and HPC

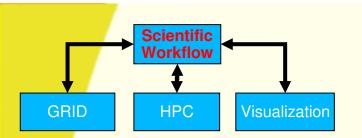
	Batch	GRID	НРС
Current usage within the fusion community	Extensive • JET (339 cpus) • Most associations (IPP-TOK 400 cpus) • Gateway (128 cpus)	<ul> <li>Only at CIEMAT</li> <li>Starting to see some usage at Juelich</li> <li>Plans for usage at IPP</li> </ul>	<ul> <li>Extensive use of national facilities</li> <li>Extra-national usage via DEISA</li> </ul>
Main issue preventing more usage	<ul> <li>Lack of more local cpus</li> </ul>	<ul> <li>Lack of knowledge</li> <li>Difficulties getting certificates</li> </ul>	<ul> <li>Difficult for Associations wothout strong national facilities</li> </ul>
Currently being addressed by		EUFORIA • has provided training • also developing facilities to launch jobs from the Gateway	EUFORIA • has provided training • has worked on codes HPC-FF starting August 1 <sup>st</sup> • HLST
Longer term		?	IFERC computer (2012)



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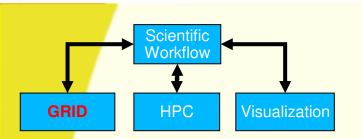
### Scientific Workflows

- 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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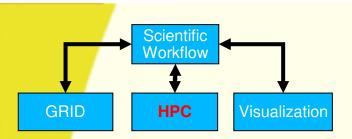


## Grid Computing

- 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





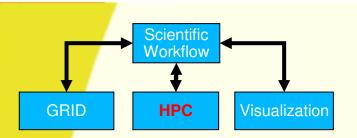


#### HPC

- 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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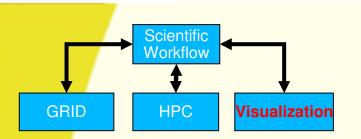


#### HPC, II

- 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





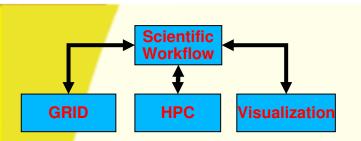


#### Visualization

- 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









- 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?





## What has EUFORIA demonstrated?

- Ability to launch a GRID job from Kepler and then retrieve the results
- Ability to launch a HPC job from Kepler and then retrieve the results
- Ability of a GRID job to write results to the Gateway using the UAL
- Deployment of applications on the EUFORIA GRID
  - EMC3-EIRENE partially shifting to Grid (TEXTOR DED)
- Succesful support/optimization on HPC
  - BIT1 (sequential → 512-1024 cores, DEISA time)
  - TYR (128 → 4096 cores)
  - Building a framework for supporting users
- <u>Coordinating</u> and <u>facilitating</u> contacts with other activities
  - EFDA (ITM-TF, HPC-FF), DEISA, EGEE, PRACE,...
  - ITER (informal)

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