EFDA
EUROPEAN FUSION DEVELOPMENT AGREEMENT
Task Force
INTEGRATED TOKAMAK MODELLING

RUSA,
Uppsala, 5 May, 2009

Integrated Tokamak Modelling TF

Presented by: Pär Strand

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

EFDA CSU Contact Person: D. Kalupin

With commentary on EUFORIA

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.*
- *Fully embedded in the EFDA Mission structure – providing a predictive capabability for burning plasmas (Mission 5).*

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

ITM-TF overview

What is the ITM-TF?

- A collection of
  - Joint hardware & software tools,
  - Coupling technologies,
  - Physics modules & codes,
  - Methodologies and procedures
  - Integreation research
- Resources → People and their knowledge →Collaborative infrastructure

A completely new paradigm for modelling in Europe!!!

Purpose

- To facilitate a European wide standard for collaborative efforts on ITER & DEMO modelling and code development, with impact on current devices
- To provide Core services for future modelling exploitation for ITER and DEMO

Long term vision

- Have a leading role in European modelling efforts in the ITER & DEMO era
- Provide a focal point for model based physics exploration towards a truly predictive capability (Input to facilities review from EFDA - Mission 5)
- Pilot fusion modelling as an European Research Area (ERA) in its own right

ITM-TF Framework

A pan-European simulation environment:

- A new scalable, open ended, flexible and extensible simulation framework
  - (ISIP: Workflow, Code Platform, Schemas, UAL and code interfaces)
- Device independent State of the art physics modules
  - Broad application basis – Broad user base
- Multi device databases (ISIP – EDRG)
  - "Closer" to experiments – improved V&V
  - Assisting Experimental campaigns with new modelling capabilities
  - Allowing for synthetic diagnostics in ITM framework
  - New level of data access (ITPA like processed data not sufficient)
- **Proper V&V basis to secure quality and applicability – close collaboration with experiments to mutual benefits – focus area**

Machine Descriptions
Data mappings
Expertise

EFDA based - Community owned

- A jointly owned and operated infrastructure
- A jointly developed physics capability
  - Organic growth towards improved state of the art tools
  - "Darwinian" selection and development of models
- An integral part of the "new" EFDA

Why a new software structure?

Fusion has (rightly) been accused of being a closed community with little interaction with other communities – the world has changed on us!

New languages have to be supported: C, C++, Java, Python is already being used in fusion applications

- Need to be supported in parallel to Fortran dialects
- Mixed language settings

Expected life time of the code(s) are ~20-30 years

Libraries and other tools

- Proprietary tools increasingly expensive. Offset by a strong move towards Open Source tools. New hardware architecture posing portability and scalability concerns. Longevity

New advanced computing paradigms

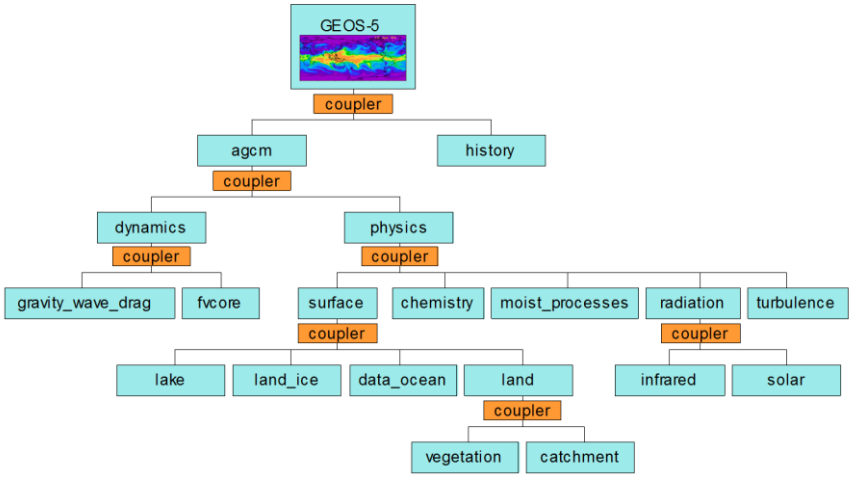
- Efficient use of Grid and HPC resources need to be secured and made available

Modern, framework based, software development paradigms are demonstrated efficient also in scientific environments (climate, weather, combustion, relativity, ...)

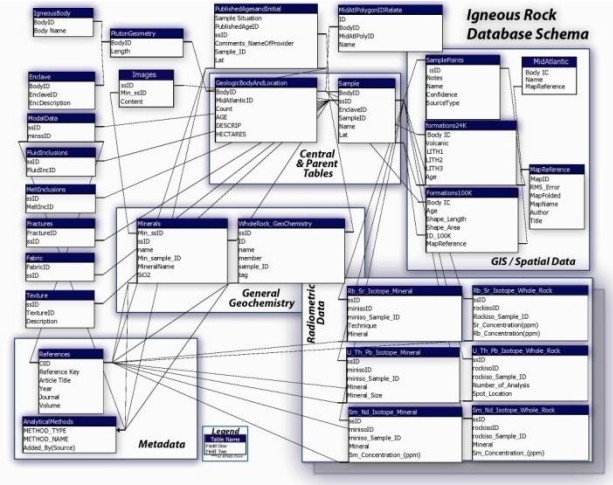
- Should be promoted for efficient use of slim manpower resources in fusion.

Framework tools

Earth Science Climate Modelling Framework

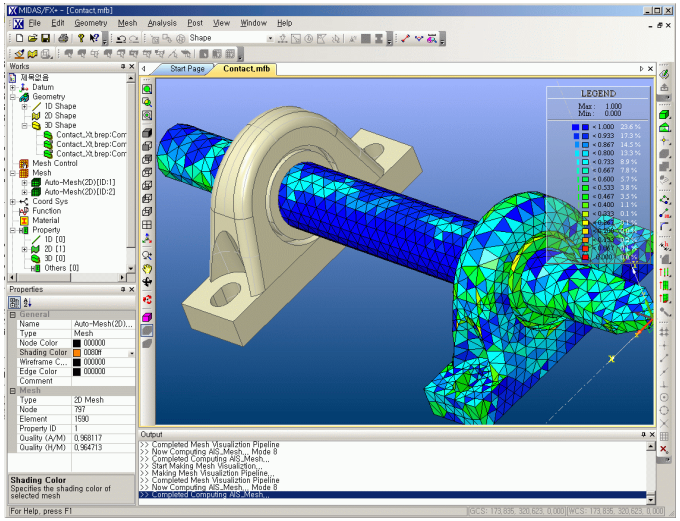


Geon (Geoscience, Kepler):



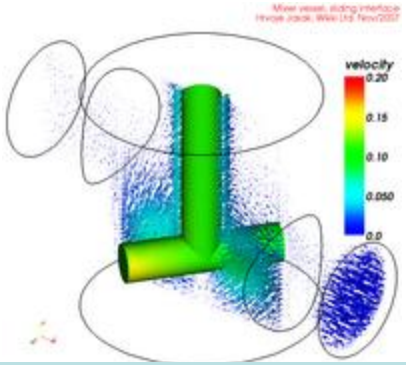
www.CactusCode.org

Salome(Open Cascade) General Purpose



OPENFoam CFD TOolbox

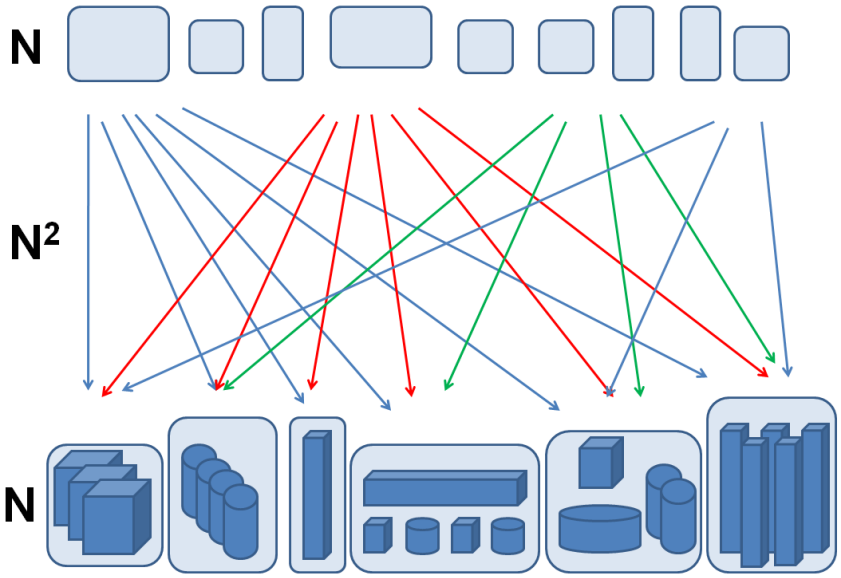
PYRE



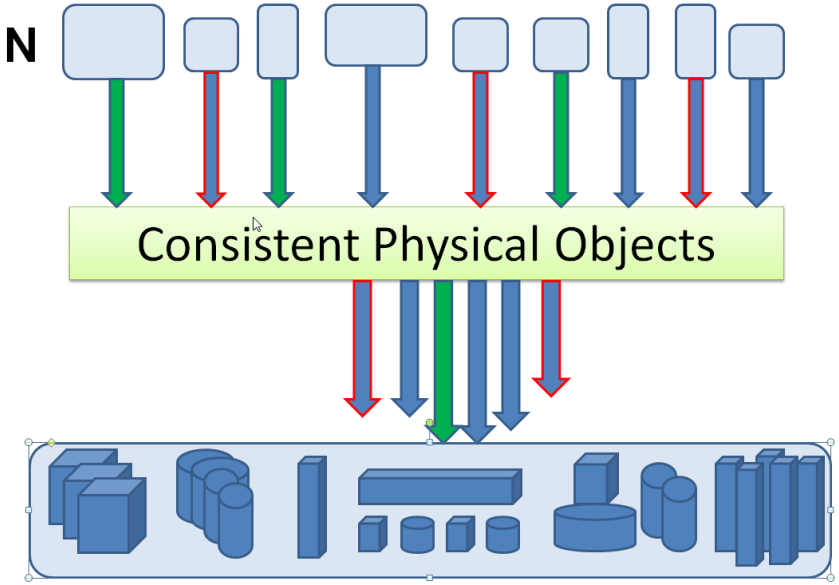
ITM-TF – requirements capture + 2 years pilot activities →Kepler with our own extensions

Coupling codes and applications

N modules integrated in N different applications



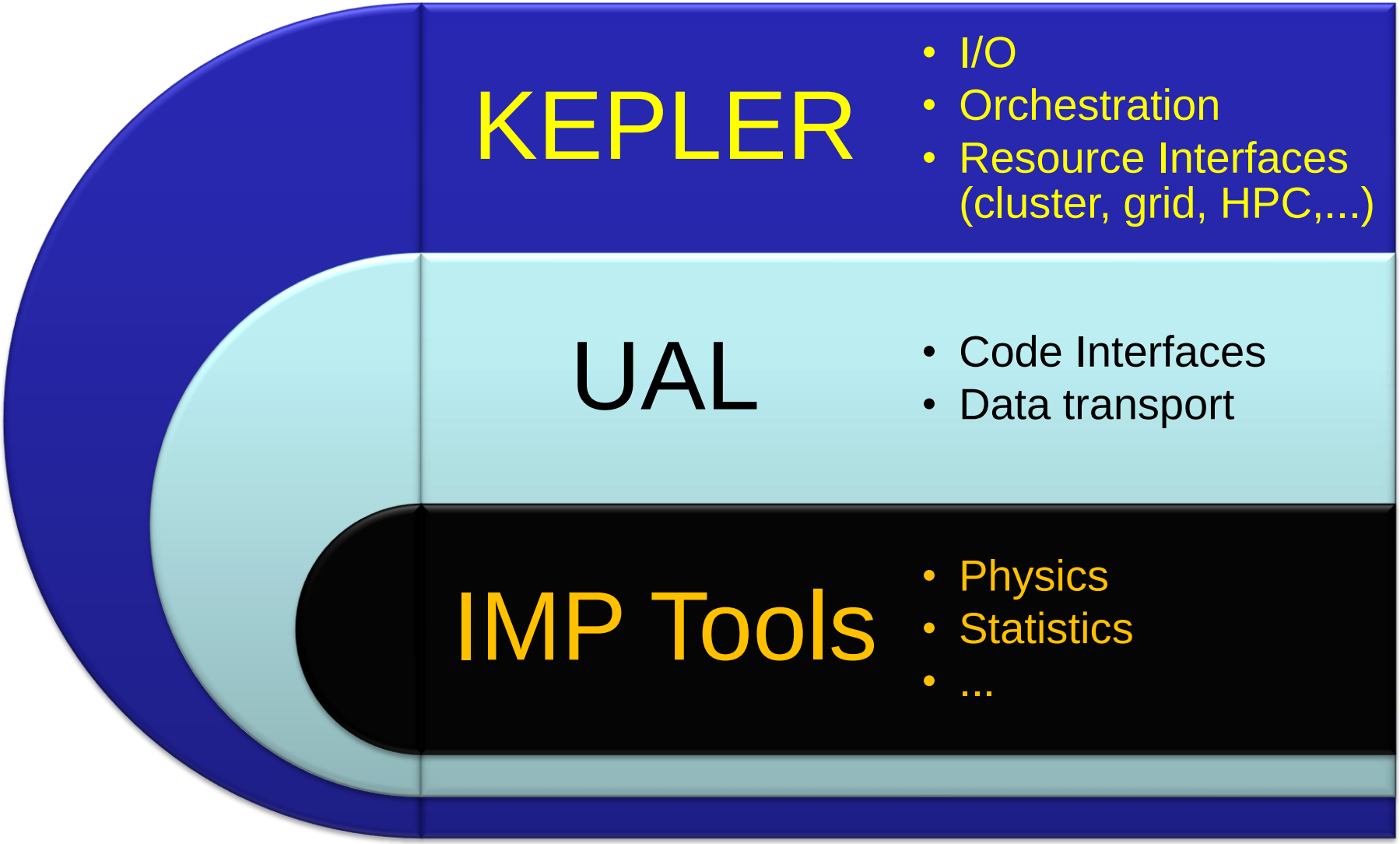
N modules coupled into a dynamic application framework



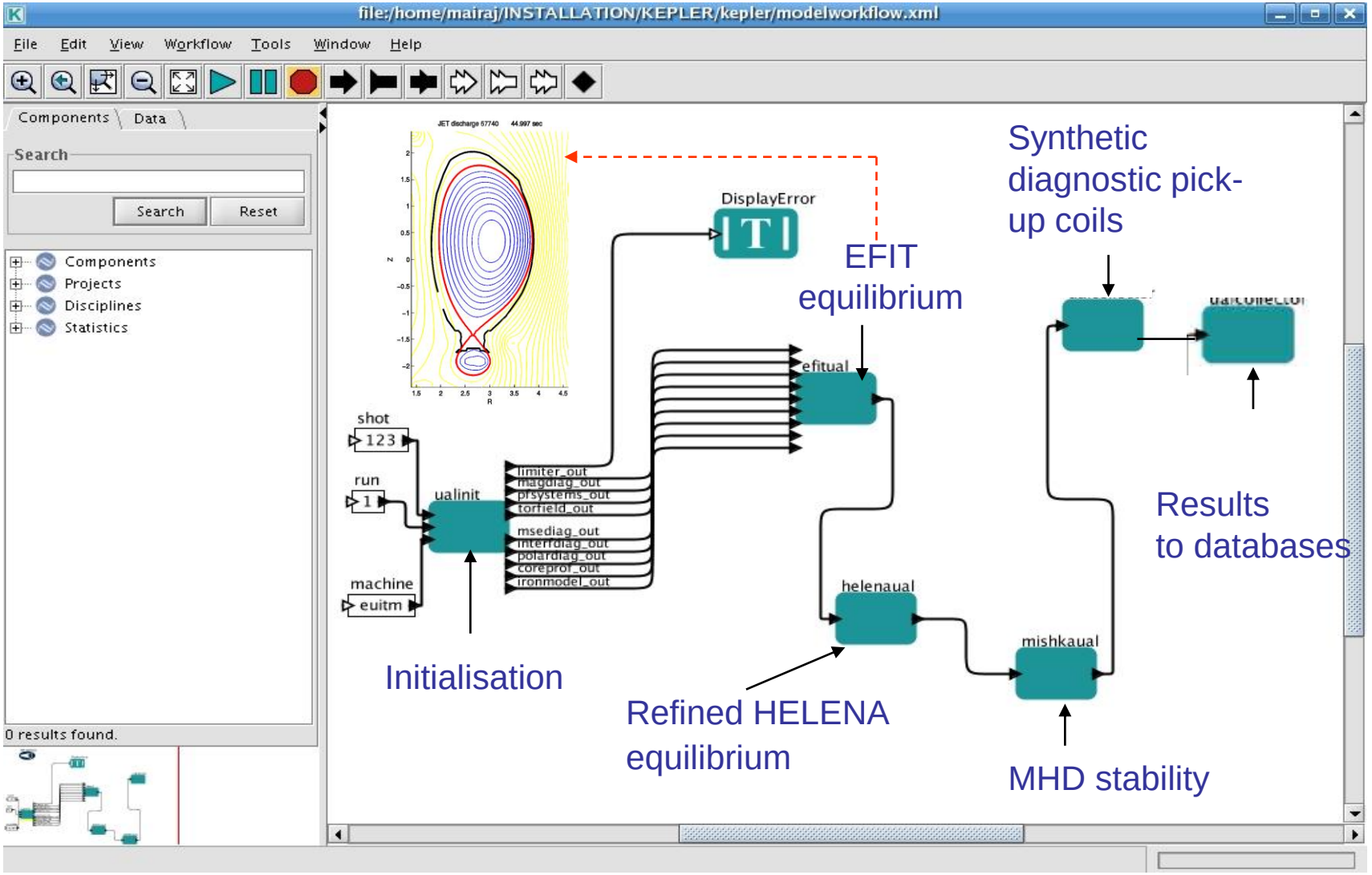
Work balance is different – indications (weather, climate, combustion, relativity, ASCI,..) is that payoff in efficiency, usability, manpower cost and increased collaborations is large once framework is operational

Bastardised from David De Roure

ITM-TF Application Structure



Coupling technology: Kepler Workflow



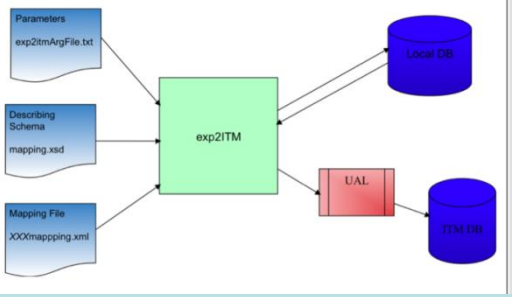
Rapid deployment and testing: Standardized interfaces
E.g., swap Helena with CHEASE – single click effort

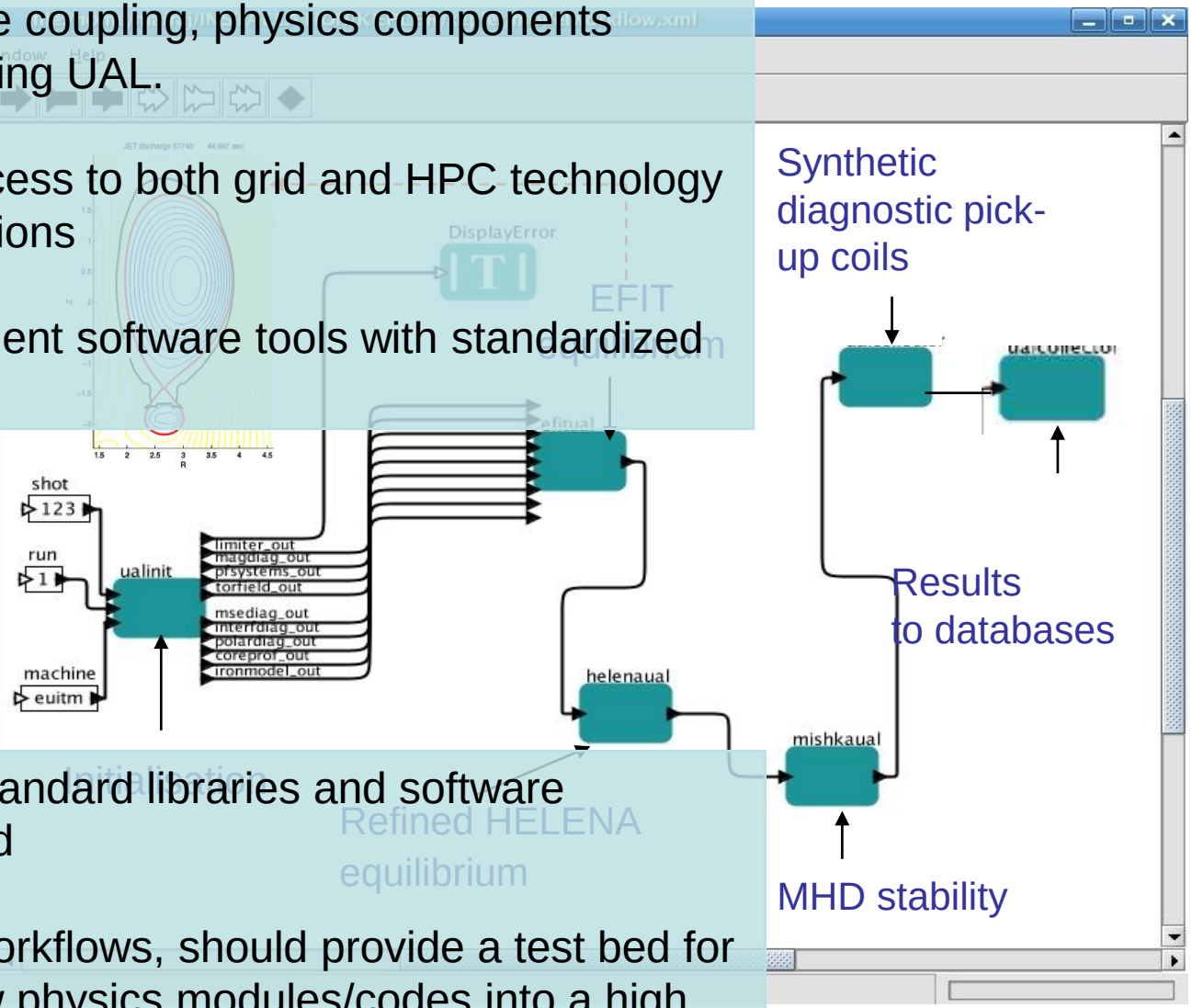
Coupling technology: Kepler Workflow

Allows for Mixed language coupling, physics components automatically wrapped using UAL.

Allows for transparent access to both grid and HPC technology through EUFORIA extensions

Provides device independent software tools with standardized Code interfaces





Provides a platform for standard libraries and software Practices to be developed

In addition to validated workflows, should provide a test bed for Promote and Embed new physics modules/codes into a high Level framework

Physics modules

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

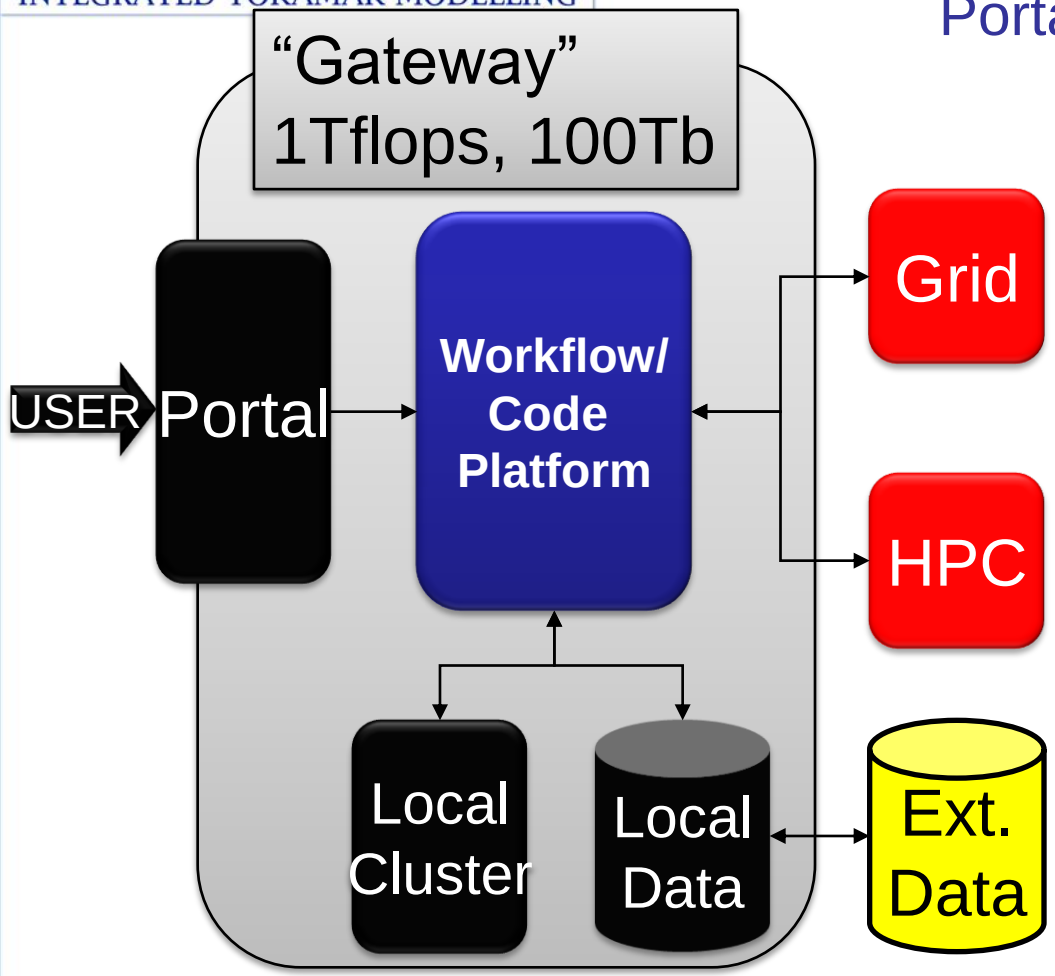
Calls UAL to PUT the CPOout

Plasma state

Contains the state of all CPOs at all time slices

ITM Three Tiered Approach

Portal + Platform + Resources



Portal more important in defining access to resources (certificates)

Data access & application scheduling &

Resource allocation through platform

Visualization, monitoring & steering through platform

ITM tools: standardized data structures, data access, interface definitions, Gateway, Workflow (Kepler)

Present resources

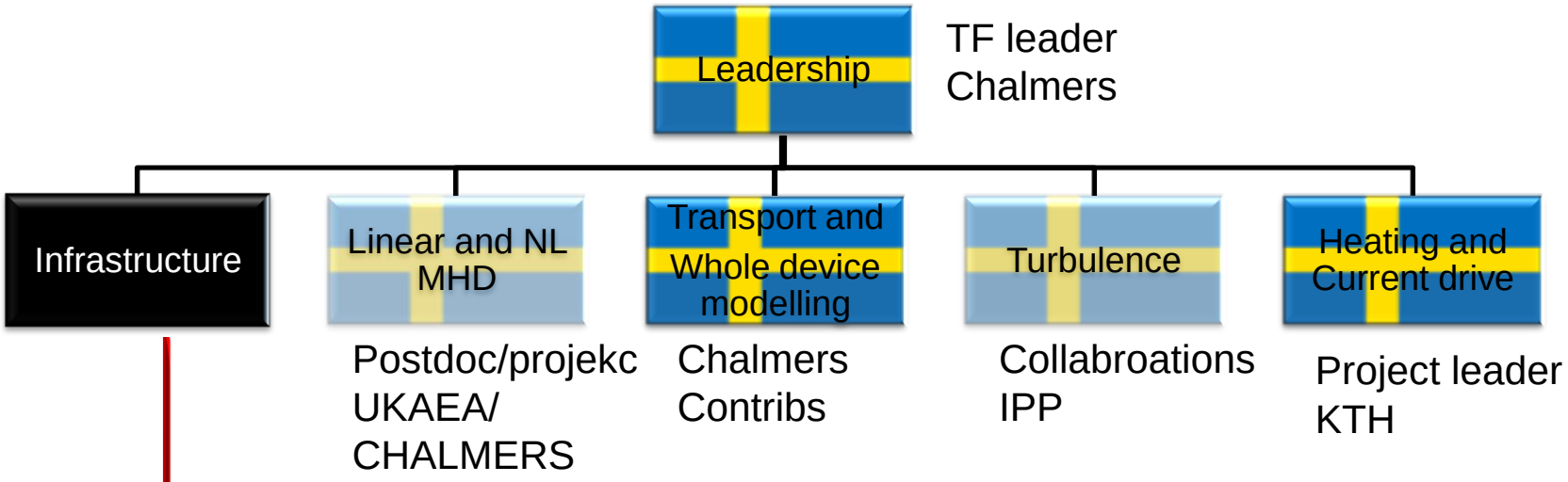
- ITM Gateway located at the Cresco centre in Portici near Naples

- The main purpose of the Gateway is:
  - Provide a development environment for ITM codes
  - Access to and storage of experimental data (especially for validation purposes).
  - Provide access high performance computing resources

ITM project structure

Project	Name	Leadership 2009
ISIP	Infrastructure and Software Integration Project	**F. Imbeaux (CEA)** **G. Manduchi (RFX)** **S. Balme (CEA)**
IMP#1	Equilibrium Reconstruction and Linear MHD Stability	**G. Huysmans (CEA)** **C. Konz (IPP)**
IMP#2	Non-linear MHD and Disruptions	**M. Ottaviani (CEA)** **S. Sharapov (UKAEA)**
IMP#3	Transport Code and Discharge evolution	**D. Coster (IPP)** **V. Basiuk (CEA)** **G. Pereverzev**
IMP#4	Transport Processes and Micro Stability	**B. Scott (IPP)** **G. Falchetto (CEA)**
IMP#5	Heating and Fast particles	**T. Hellsten (VR)** **G. Vlad (ENEA)** **Y Peysson (CEA)**
Tasks Under TF leadership	ITER Scenario Modelling (ISM) Atomic, Molecular, Nuclear and Surface Physics (AMNS) Experimentalists and Diagnosticians Resource Group (EDRG) Integration Team (ITT)	

Swedish Participation ~ 3ppy



Tasks under TF leader:
- ITER Scenario Modelling Group (ISM)
- Experimentalists and Diagnosticians Resource Group (EDRG)
- Atomic, Molecular, Nuclear and Surface Physics Data (AMNS)

Grid, HPC access, visualisation: (Chalmers)

EUFORIA

ITM-TF Milestones

2008

- **Start of the Gateway for IM and deployment of code platform (Real start of ITM collaborative activities)**
  - Implies a complete set of data structures and associated tools
  - A fully operational portal/workflow configuration
  - Major code releases from all of Integrated Modelling Projects

Unexpected manpower losses and other delays: deliverables→ 2009

2009

- **Extended set of platform tools forming a predictive core physics capacity for ITER**
  - Production activities – local clusters and grid, HPC-FF

2011

- **Whole device modelling capability including comprehensive core-edge coupling and first principles elements**
  - Aiming towards Broader Approach IFERC level computations
  - HPC-FF & Prace

	ISIP	IMP#1	IMP#2	IMP#3	IMP#4	IMP#5	TFL Tasks
2008	**CPD** **UAL** **ISE** **KEPLER** PORTAL EUFORIA Integration	**EFIT_ITM** **HELENA** **ILSA** **FLUSH** **CHEASE** --- **CAXE** **KINX** **EFIT_ITM** (predictive) (FBEC)	SAWTOOTH NTM RWM (2D Wall) (ELM) Modules (VDE)	**EUROPEAN TRANSPORT SOLVER** (Prototype) Fixed boundary Modules imported from IMP's or from existing codes	**Neoclassical** **Linear/ quasi-linear** **Turbulence code(s)** ← Transport modules	**C3PO/LUKE** **HMGC (circ)** **EVE** **FPSIM** NBI deposition module(s). Orbit module(s)	
	INTEGRATION TEAM ACTIVITIES (2008/09) **Data structures & Code Interfaces**						
2009	**CPD++** EUFORIA Integration	**EQUINOX** **CLISTE** **CREATE-NL** **FBEC**	RWM (3D Wall) ERR FIELDS VDE ~~3D NL MHD code(s)~~	**ETS** (full version) free boundary (Edge-core integration) EUFORIA Integration	EUFORIA Integration	**HMGC**(non.circular) Orbit following Monte Carlo code (FPGEN)	Synthetic: -3D reflect AMNS toolbox
Bench mark codes				**SOLPS** **ASTRA**			(JETTO) **ASTRA** (CRONOS) DINA

BOLD: Actual name of code or activity, **RED: Priority Support activity**

NON-BOLD: Generic name – indicating multiple codes, merged or new non-named developments

The table lists only major codes or larger activities, in addition a range of important supporting tasks exists

Progress

First framework ready for launch

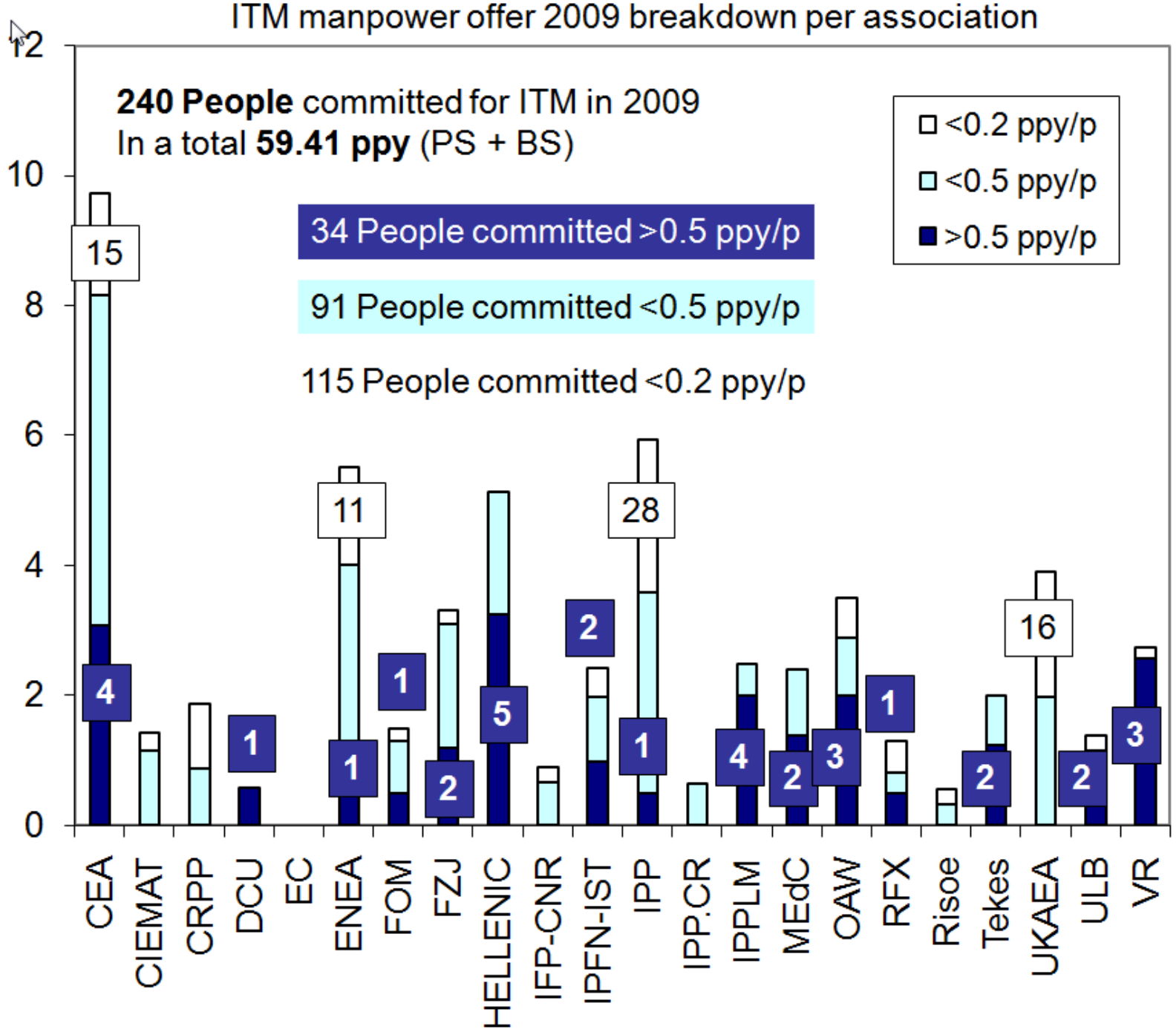
- Gateway (Installed)
- Workflow orchestration tools (v1.0 available now)
- Ontology (data structures) (mature subset in place – finalization 2009)
- Local Data access (Universal Access Layer)
- Databases (simulation and experimental) (to be filled –collaborative effort with experiments)

First range of Applications becoming available

- IMP physics tools & modules ported (continuous development but a first batch of tools are becoming available –IMP1 leading the wat)
- V&V procedures (in place, to be tested in real life)
- Transparent access to full range of computing platforms: local cluster , grid applications, HPC access (→EUFORIA)

Building a broadened user community

- Increased level of collaboration required (experiments & end users)
- Need broader CS involvement for some of our tasks
- Collaborative IT infrastructure needs to become an everyday tool
- Need to develop more efficient communication within the ITM-TF and with other pan European activities as work matures and become more integrated.


ITM manpower offer 2009 breakdown per association
240 People committed for ITM in 2009
In a total 59.41 ppy (PS + BS)
34 People committed >0.5 ppy/p
91 People committed <0.5 ppy/p
115 People committed <0.2 ppy/p
<0.2 ppy/p
<0.5 ppy/p
>0.5 ppy/p
0
2
4
6
8
10
12
CEA
CIEMAT
CRPP
DCU
EC
ENEA
FOM
FZJ
HELLENIC
IFP-CNR
IPFN-IST
IPP
IPP.CR
IPPLM
MEdC
OAW
RFX
Risoe
Tekes
UKAEA
ULB
VR

Coordinating structures within EFDA

ITER→New, more project oriented structure

- **European Task Forces (top-down)**
  - **Integrated Tokamak Modelling (P. Strand)**, Plasma Wall Interaction (E. Tsitrone)
- **Goal Oriented Training Programmes (horizontal)**
  - **GOTiT (D. Coster), …**
- European Topical Groups (bottom-up)
  - H&CD (A.Becoulet), Transport(C. Hidalgo), MHD(P. Martin), Materials(S. Dudarev) and Diagnostics (T. Donne)

- **No real activities to support computational science, applied math or infrastructure development (grid, HPC) →EUFORIA**
  - **New development: High Performance Computing for Fusion in Europe (HPC-FF)**
    - **Bridging the gap on HPC-FF access – coming online after summer**
    - **Implementing agreement explicitly states taking into account EUFORIA developments**

Moving to a distributed computing environment

- Current Thinking:
  - ITER will not have a large centralized analysis and simulation computing facility
  - Will need to use distributed resources
    - Similar to that which CERN is using
    - But with HPC(s) added
    - Centralized databases
  - Will still want to ensure confidence in results, traceability, etc.

EUFORIA - EU Fusion for ITER Applications

14 member Institutes
522pms covering
3.65M€ over three years

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

Started January 2008
Funded under FP7
"Capacities" Programme

Annual review just done
- 945k€, 145 ppm, 48 ppl

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 & parallelisation, CS*
FRANCE:	***CEA*** *- Commissariat à l'énergie atomique – Cadarache*	*Workflow, Fusion, CS*
	Université Louis Pasteur - ***ULP***	*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 ***- PSNC***	Grid, Migrating Desktop, CS
SPAIN:	*Barcelona Supercomputing Center – Centro Nacional de Supercomputación -* ***BSC***	*HPC, Code optimization & parallelisation*
	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 & parallelisation, NA, User support, (GRID)*

Supporting fusion users

- Providing infrastructure
  - Grid (parallel and serial) and HPC infrastructures and support
    - EUFORIA Grid infrastructure (2700Cpus, 40Tb)
    - HPC infrastructure available for application development and proof of principle runs.
    - Production run access: DEISA -2MCpuHrs(2008, 09), EPCC - 1MCpuHrs n(2009), HPC-FF as a target platform!?
- Provide Application porting for select codes to both Grid and HPC
  - EFDA decision: Focus on Edge and Core Turbulence and Transport
- Provide Training
  - Use of and adaptation for grid and HPC technologies
  - Direct Code adaptation for select codes and tools
  - Help to “self-help”
- Provide extended toolkits for existing infrastructure
  - Visualization
  - Workflow extensions (with ITM-TF)
  - Middleware developments

Resources of the Euforia Grid

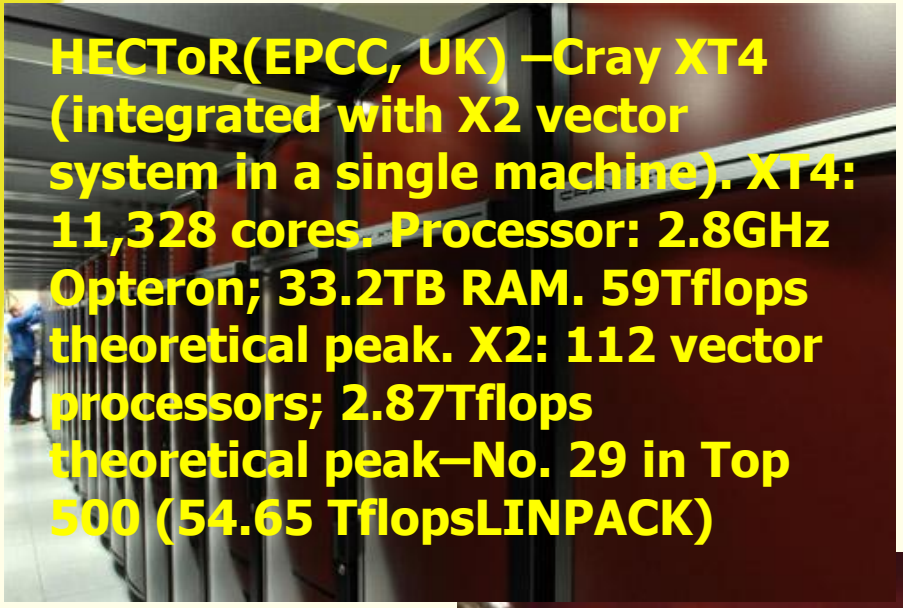
- **Grid Infrastructure supporting the Euforia VO**
  - Centers with infrastructure in Euforia (all in NGI/EGI – next steps? New role for VR SNIC?)
    - IFCA in Santander, Spain
    - FZK in Karlsruhe, Germany
    - Chalmers University, Sweden
    - Ciemat in Trujillo, Spain
- **From the Grid Information System (order 2700 CPUs, 40 TB online)**

```
#CPU|Free|Total|Jobs|Run|Waiting|ComputingElement
-----------------------------------------------------------------------
1488   702    0     0     0     0  i2gce01.ifca.es:2119/jobmanager-lcgpbs-euforia
452    324    0     0     0     0  iwrce2.fzk.de:2119/jobmanager-lcgpbs-i2gpar
640    113    0     0     0     0  svea-gl2.c3se.chalmers.se:2119/jobmanager-lcgpbs-euforia
56     56     0     0     0     0  ce-euforia.ceta-ciemat.es:2119/jobmanager-lcgpbs-euforia
```

Avail Space(Kb)	Used Space(Kb)	Type	SEs
38 TB	6TB	n.a	storm.ifca.es
1.8 TB	129931	n.a	iwrse2.fzk.de
142 GB	--	n.a.	svea-gl3.c3se.chalmers.se

Activity SA2 Objectives

O1) Provide HPC infrastructure support for the code optimization effort within JRA2.



Promoted Codes

Almost All ported onto HPC infrastructure

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.] Grid+HPC adaptation + DEISA, EPCC allocations

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.] CP redevelop

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.] GRID adaptation, EMC3-EIRENE (DEISA)

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

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] Pending

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

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. GRID, DEISA, EPCC time

GENE (p) [GENE is a nonlinear gyrokinetic code to investigate plasma turbulence] DEISA, EPCC time

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] GRID

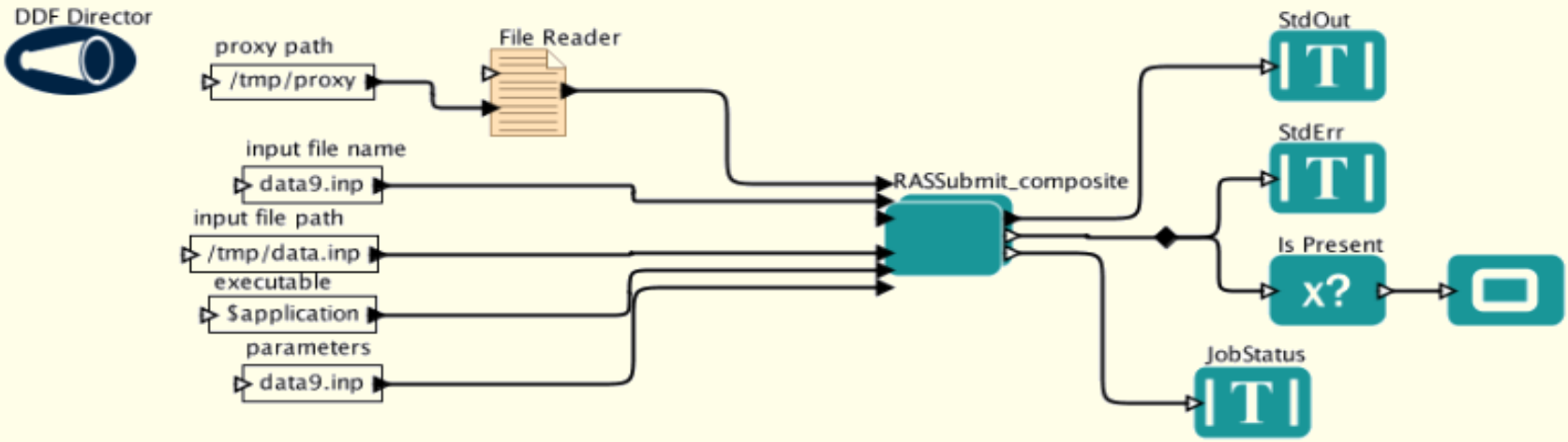
SOLPS (s+p) [B2-Eirene consists of two codes tightly coupled together: B2 (multi-fluid solving continuity, momentum and energy equations for the plasma component on a cell cetntered grid; EIRENE (Monte-Carlo neutrals code providing sources for B2 based on a plasma background provided by B2)] Pending

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

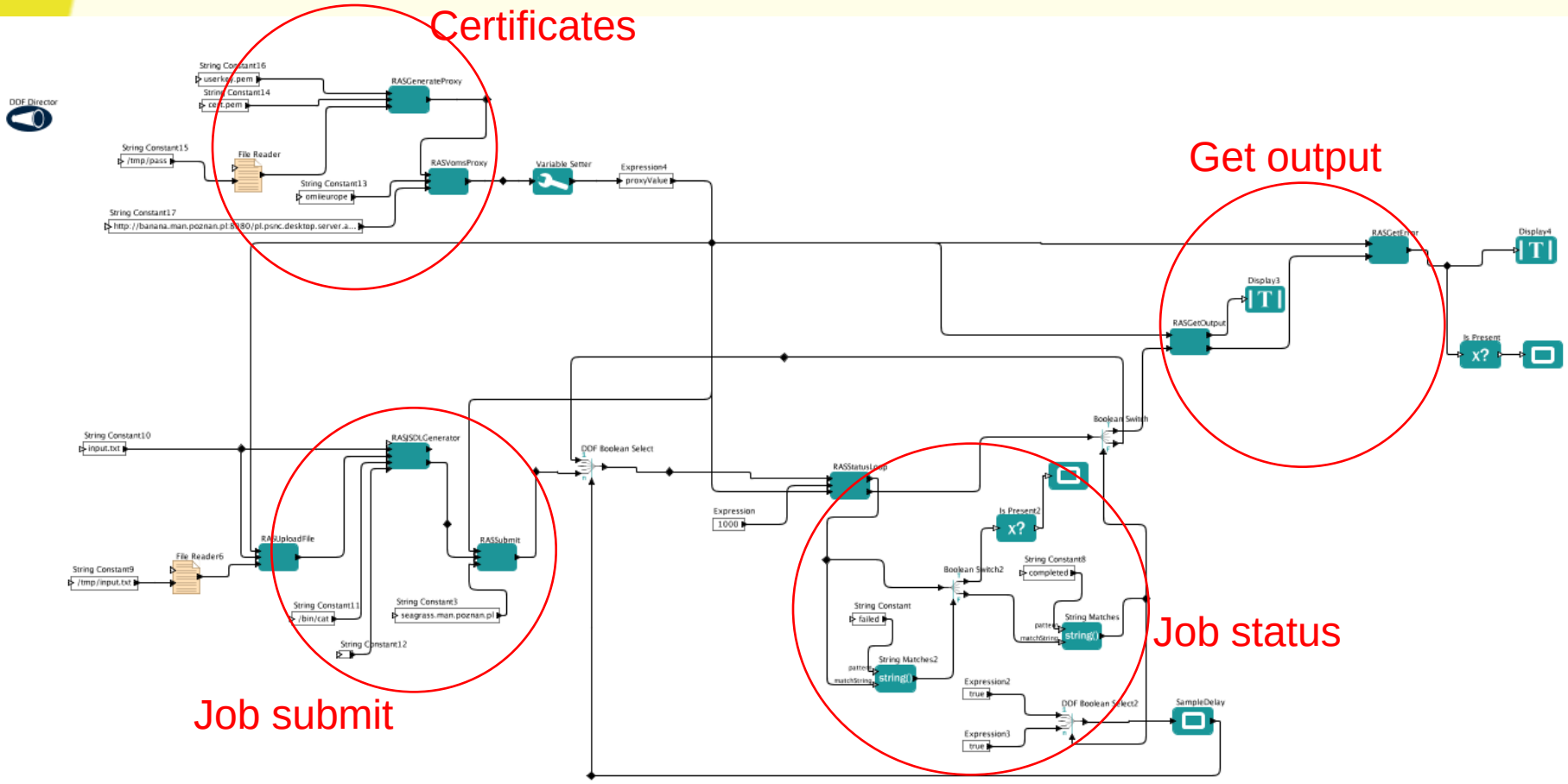
TYR (p) [Drift Alfven plasma fluid turbulence and transport in flux-tube geometry.] HPC, EPCC time

Simple HPC workflow

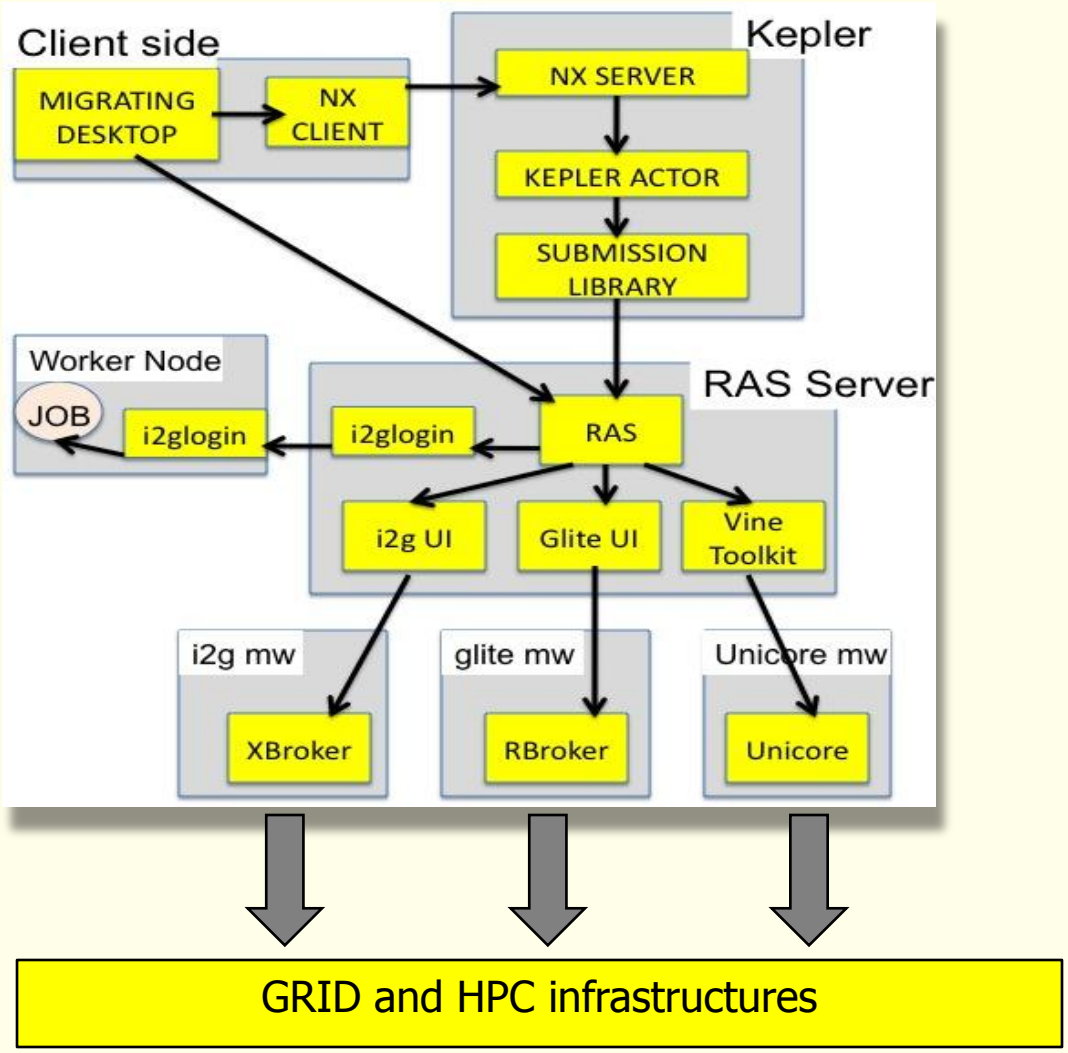
- KEPLER actors for HPC infrastructure – usage of UNICORE 6.1.3
- Presented usage of BIT1, but actors enable to run ported applications (that for example could be run using JSDL)
- Simple composite actors hides the complexity for the user



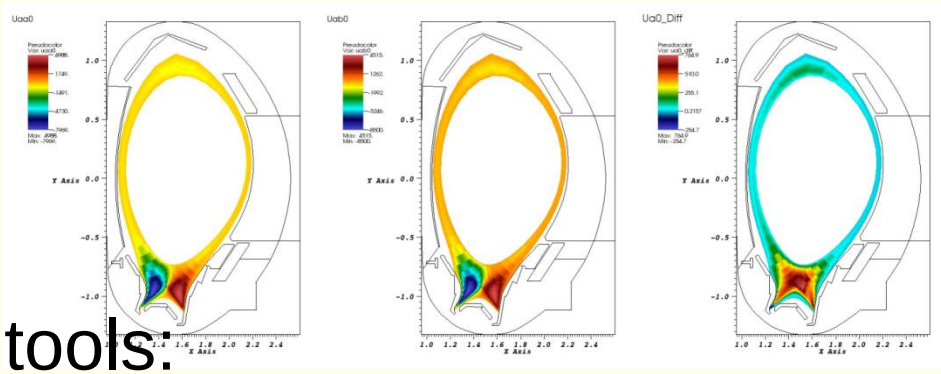
Example of composite actor - details



The EUFORIA Services in the broader view



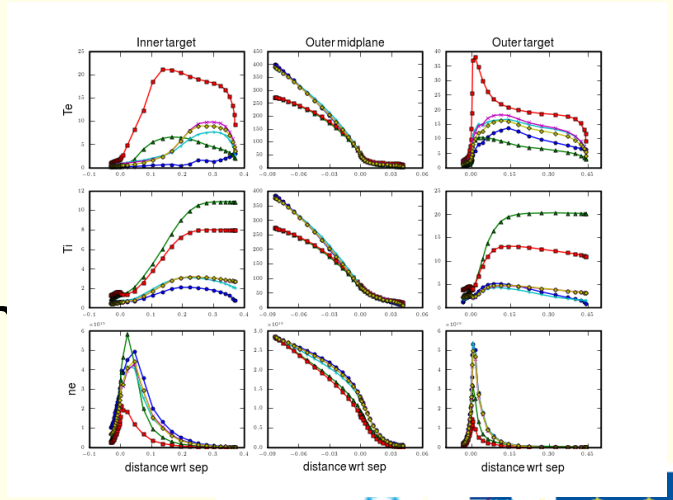
Visualization



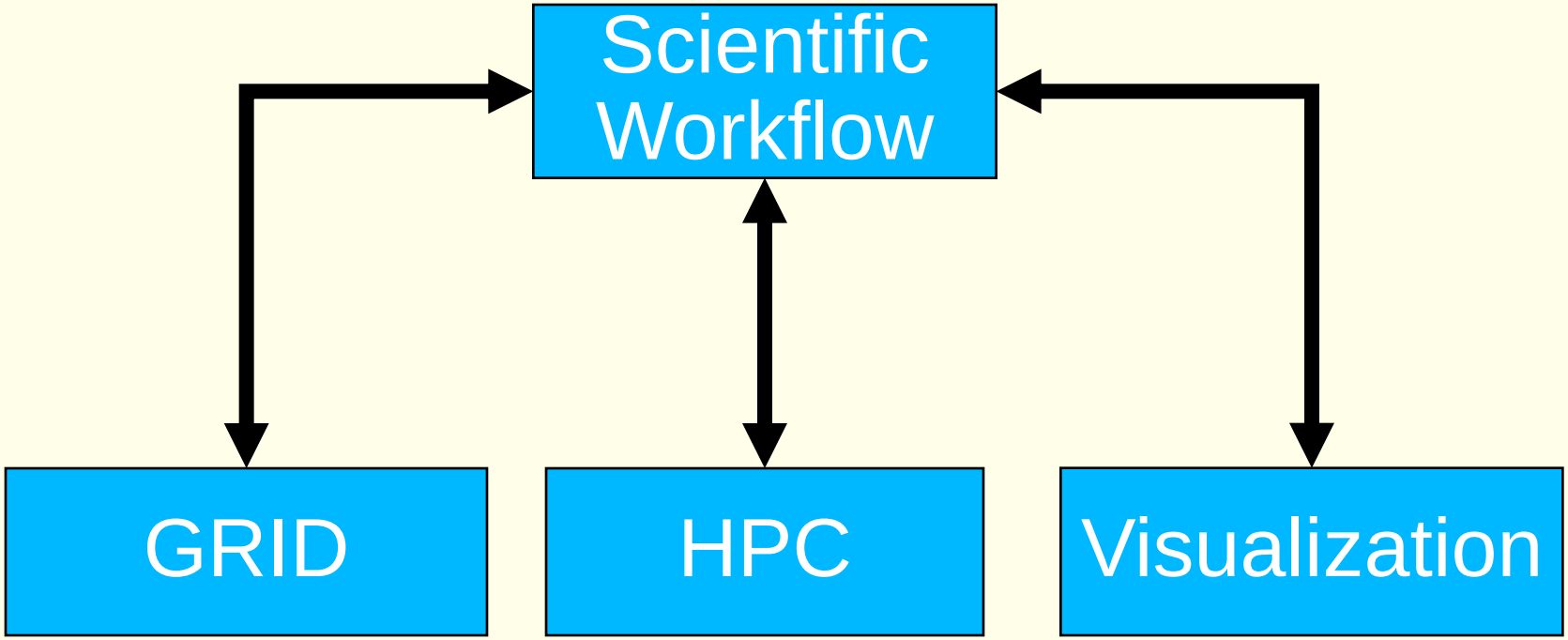
- DJRA4.1 (M12) Defining tools:
  - Choice of existing tools and demonstrate with fusion dataset (numpy, matplotlib,Visit,…)
- DJRA4.2 (M18): Integrate ITM data access (UAL) into Python/VisIt and integrate Python/VisIt into

  ITM workflow manager (Kepler)
- DJRA4.3 (M24):
- Provide compression scheme ar

  visualization for 4D dataset

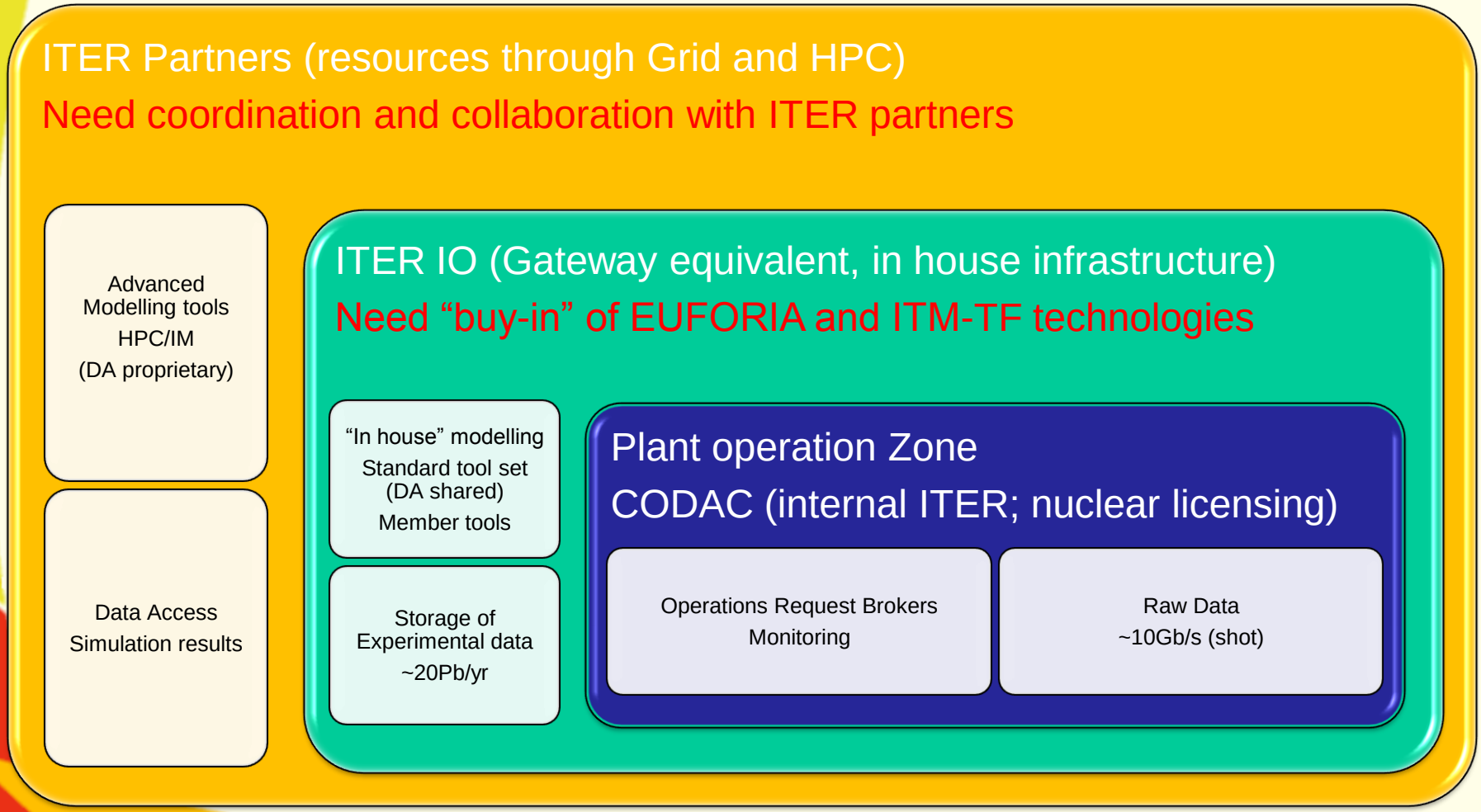


Developing a new paradigm for fusion computing



EUFORIA FP7-INFRASTRUCTURES-2007-1, Grant 211804

Prototyping the ITER Modelling infrastructure



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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 to 512-1024 cores, DEISA time)
  - TYR (128 to 4096 cores)
  - Building a framework for supporting users (support@euforia-project.eu)
- Coordinating and facilitating contacts with other activities
  - EFDA (ITM-TF, HPC-FF), DEISA, EGEE, PRACE,…
  - ITER (semi-informal)

Collaborations

Topical Groups & Task Forces

- Collaboration and increasing exchanges foreseen during WP09
- Continued discussion on collaborative formats/opportunities

Related projects

- GOTiT
- EUFORIA
  - HPC-FF, PRACE, DEISA, EGEE, EGI…

International IM Initiatives

- Formal Bilateral Agreements with US (JP)
  - Kepler, SWIM, CPES and FACETS SciDAC projects
  - BPSI

ITER

- ITPA IMAGE activity to continue under ITER: IMEG
- Format finalizedstarting active work now!

Experimental Devices

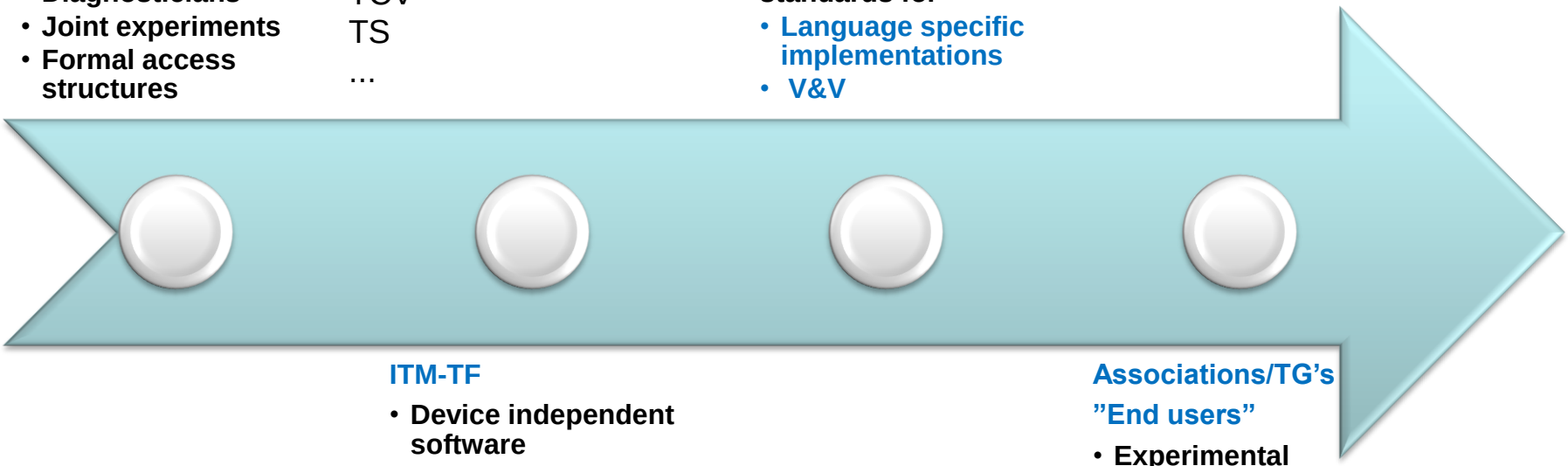
- **Machine Descriptions**
- **Data Mappings**
- **Experimental data and expertise**
- **Diagnosticians**
- **Joint experiments**
- **Formal access structures**

Collaborations/Discussions ongoing:

AUG
JET
MAST
TCV
TS
…

Coordination

- **Exploring Joint software developments (reducing the duplication of work)**
- **Support the development of joint European (?) standards for**
  - **Language specific implementations**
  - **V&V**



ITM-TF

- **Device independent software**
- **Framework**
- **Gateway**
- **Simulation databases**
- **Verification and Validation**

Associations/TG's

"End users"

- **Experimental Validation**
- **Physics Exploitation**
- **Requirements**

Joint in all "levels" -- validation and exploitation

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Work Programme 2009

Responses just in: 60 ppy allocated

Continuation of 2008 Work Programme

- Maintenance of installed software
- Continued development of new physics modules
- Continued activities on Code Platform

Focus areas – Priority Support Areas

- Infrastructure and Software Integration Project
- Integration Team
- Coordination activities towards AMNS, EDRG
- European Transport Solver (ETS)
- Free boundary equilibrium code
- VDE's
- 3d reflectometry modelling

Next step of Integration

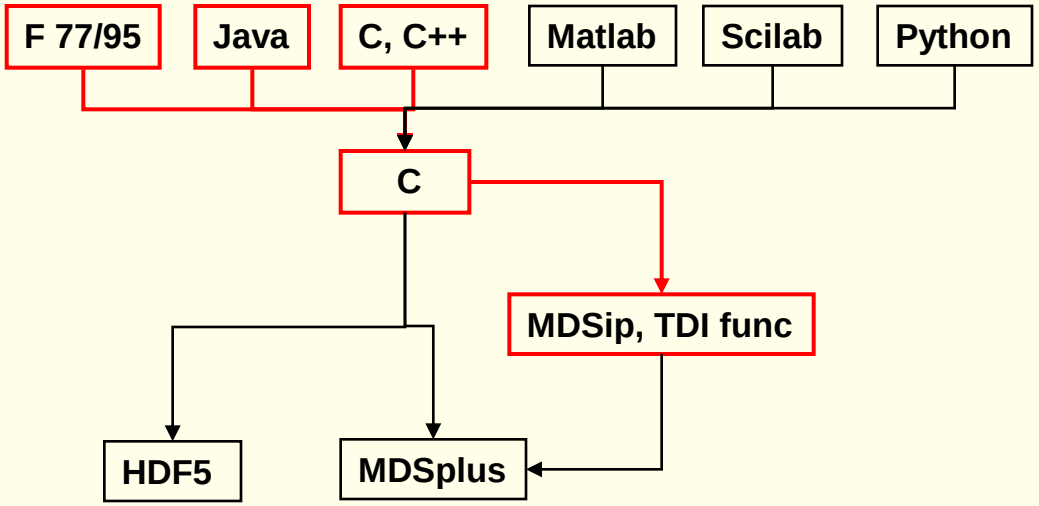
- Providing tools and modules for use at Experiments and in Associates

UAL (Universal Access Layer):

Read/write “gateway” data from grid and HPC

- **High level**
- **Low level**
- **Transport**
- **Storage**

- **Implement only the “red boxes”**
- **Installation on the UI:**
  - **Intel 32bits infrastructure**
  - **Fortran 32bits compiler: g95**
  - **Java SDK 5 or +**
  - **MDS+, Blitz, UAL**



- **libUAL.tar.gz**
- **tdi.tar.gz**

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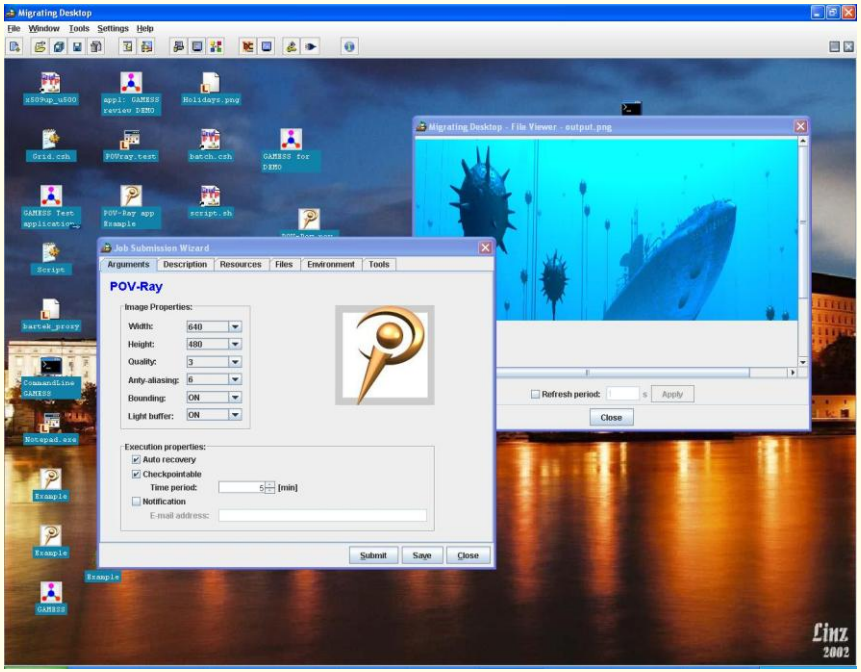
Access Portal - Migrating Desktop

- An advanced graphical user interface that hides the complexity of the grid middleware
  - a flexible personalized working environment
  - independent of the user location,
  - scalable and portable
  - a single sign-on mechanism,
  - support for multiple grid infrastructure
- Used in other project (DORII aimed at exploring the Scientific Workflows)



MD is being adapted for EUFORIA use and will be extended to our HPC environment and visualization tools. Unicore and Vine Toolkit

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2009 Training

- Main event will be a code camp
  - Bringing together code owners with experts
  - Getting codes ported to Grid of HPC (depending on demand)
  - Lectures and hands on sessions
  - Working closely with EUFORIA JRA1 and JRA2 work packages (code porting and optimisation for Grid and HPC)
  - Needs the involvement and enthusiasm of code owners to be worth doing

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Workshops

- FFT workshop (remote) already held this year
- Planned series on
  - Tools and techniques for HPC programmers
    - Build tools (Makefiles, autobuild)
    - Revision tools (i.e. cvs, svn)
    - Design and debugging
  - PGAS Languages
    - Introduction to the new parallel programming languages
    - Lectures on specific languages
  - Grid workshops still to be planned

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