EFDA

EUROPEAN FUSION DEVELOPMENT AGREEMENT

Task Force
INTEGRATED TOKAMAK MODELLING

US-Japan Workshop on Integrated Simulation of Fusion Plasmas

Plans and status of the European Task Force Integrated Tokamak Modelling Activities

Presented by: Pär Strand

TF Leader : P. Strand,
Deputies: L-G. Eriksson, M. Romanelli

EFDA CSU Contact Person: K. Thomsen

Scope

EFDA(03)-21/4.9.2 (June 24th, 2003) Executive summary:

The aim of the task force is to co-ordinate the development of a coherent set of validated simulation tools for the purpose of benchmarking on existing tokamak experiments, with the ultimate aim of providing a comprehensive simulation package for ITER plasmas.

The remit of the Task Force would extend to the development of the necessary standardized software tools for interfacing code modules and for accessing experimental data.

In the medium term, this task force's work would support the development of ITER-relevant scenarios in current experiments, while in the long term it would aim to provide a validated set of European modelling tools for ITER exploitation

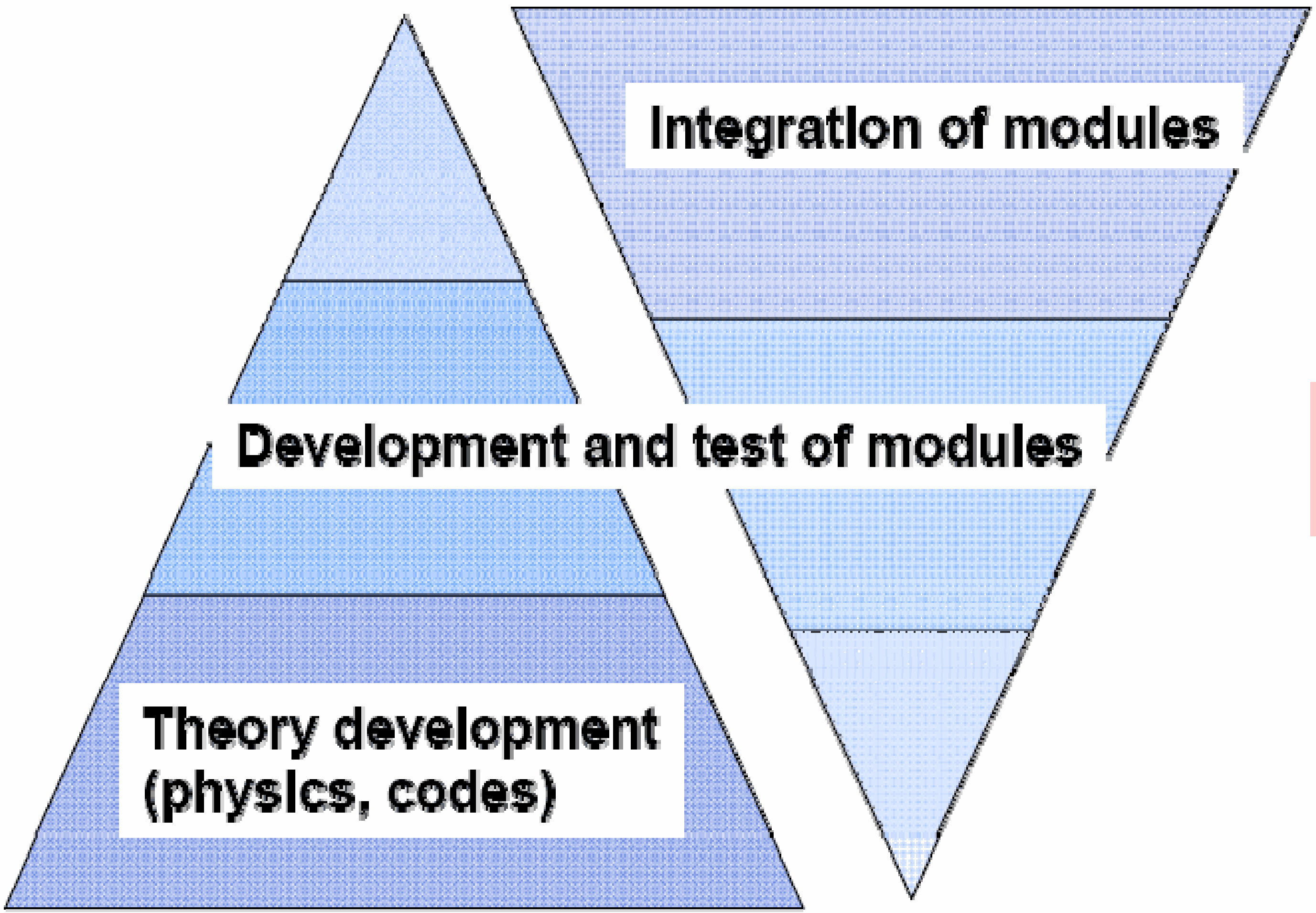
These guidelines remains in effect but may be revised by the findings and recommendations of J. Connors AHG which is discussing the future of EFDA.

General Approach

Robust, flexible and extensible Infrastructure

- Technology developments: (ISIP)
  - Coherent data structures and code interfaces as a basis for modularity and extensibility
  - Code platform and Data access (UAL)
  - "Gateway" essential to pull activities together
    - Storage for simulation and experimental data
    - Development platform for framework tools
    - V&V and QA support structure
    - User access point! Gateway to computing resources.
- Physics development (IMPs)
  - Focused through Integrated Modelling Projects
  - Solid foundation for future computational/modelling capability
    - Strong activity on V&V and QA absolute requirement!
  - Modular establishment of state of the art capacity for key components
    - Advancing/developing existing and new tools towards predictive capability for ITER and beyond
  - Whole device Modelling main objective
    - To be achieved through a set of increasingly integrated physics packages developed over time and employed and tested towards existing devices.
    - Ab initio or first principles modelling capacities directly in the TF toolbox only in the longer timeframe

Role of task force/EFDA



Role of associations

Project Leadership 2005-

Project	Project Leader	Deputy Project Leader
IMP1	G. Huysmans (CEA)	L. Appel (UKAEA)
IMP2	F. Porcelli (Politecnico di Torino)	S. Sharapov (UKAEA)
IMP3	D. Coster (IPP)	V. Basiuk (CEA) D. Kalupin (FZJ) V. Parail (UKAEA) G. Pereverzev (IPP)
IMP4	B. Scott (IPP)	M. Ottaviani (CEA)
IMP5	T. Hellsten (VR)	Y. Peysson (CEA) F. Zonca (ENEA)
CPP	B. Guillerminet (CEA)	M. Stanojevic (DPL, Slovenian Research Agency)
DCP	G. Manduchi (ENEA) (P. Strand)	F. Iannone (ENEA)

IMP#1, DCP and CPP were started as two year Pilot projects ending March 07:

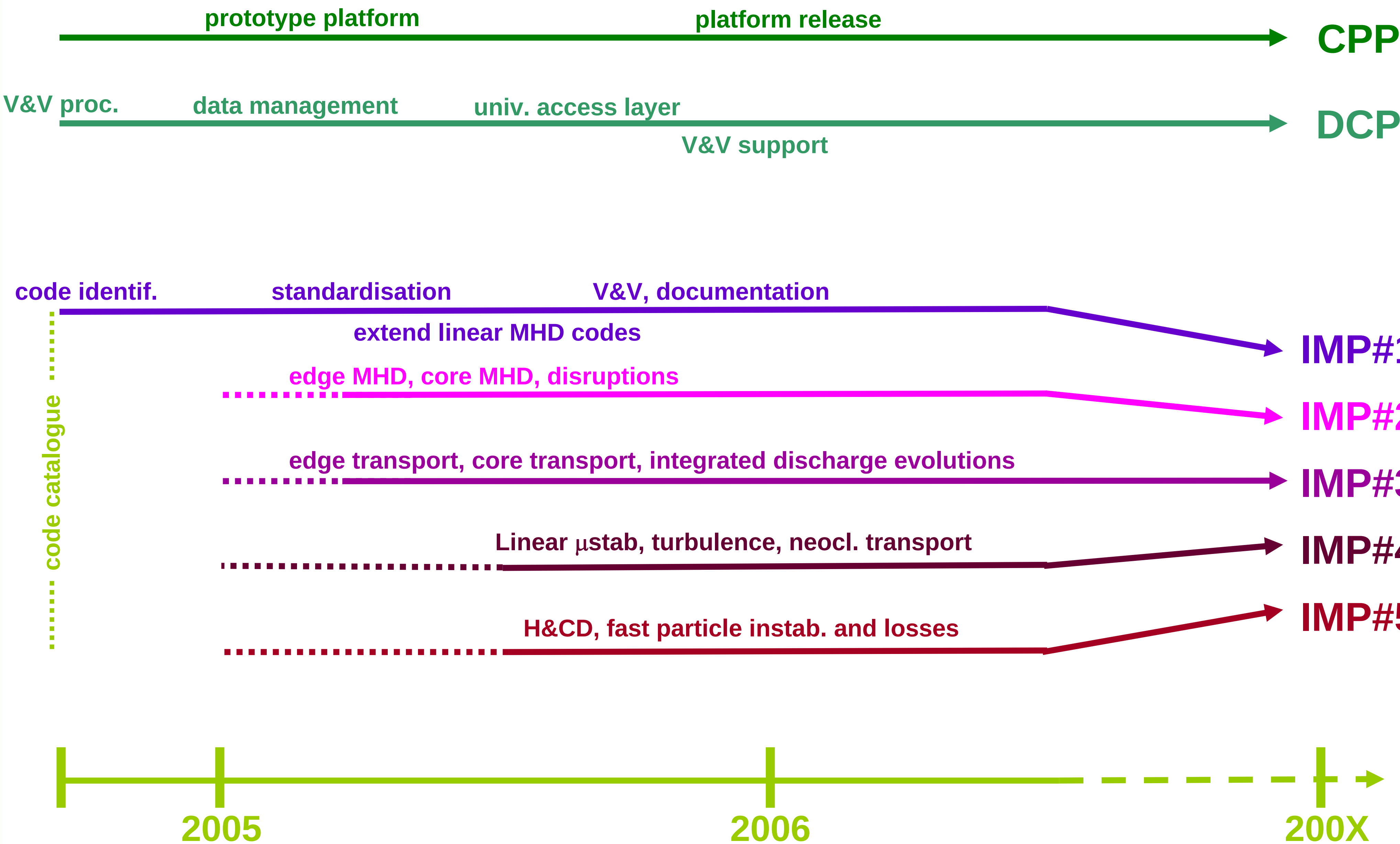
CPP+DCP – Infrastructure and Software Integration Project
IMP#1 – Continuing
IMP#2 – New Project leader
IMP#3 – New task on Whole device modelling

} Calls by January -February

Remaining projects will be renewed by end of 2007.
Hardware: Gateway - Access portal: 128-256 nodes, 30Tb, access to tools 2007(?)

NB: All tasks remain open for participation!

Work programme schedule



ISIP I: Data Coordination Project

New Leader: G. Manduchi
Deputy: F. Iannone
Previous Interim leader: P. Strand

Short term storage system solution (F. Iannone)

- ~ 1.5Tb of storage is available through MDS+ server hosted by ENEA http://fusfis.frascati.ena.it/FusionCell
- Equilibrium data under phase 3 data structure from JET, TS and ITER are stored on the ITM MDS+ server (not public, still under test)
- Physics project storage needs are estimated for (4-)12Tb mid of 2007; Some provisional resources made available at EFDA-CSU Garching

Data structures: (J. Lister -> F. Imbeaux – phase 4 proposal)

- Abstract description (XML schemas) of the data model for the Equilibrium reconstruction project (IMP#1), prototyping the TF wide data model, is its final stage of definition (document on ITM TF web site)

Universal Access Layer (UAL)

- The UAL should transfer data in an unambiguous way between codes and databases implementing the standard description of the data structure but hiding complexity from end user (document on ITM TF web site)

Database exploration tools - user access:

Start up work defining needs for

- Logbook browser – finding and characterizing TF database entries
- Relational search capabilities and graphical/plotting engines

Object oriented data structures

- Full description of a tokamak : physics quantities + subsystems characteristics + diagnostics measurements

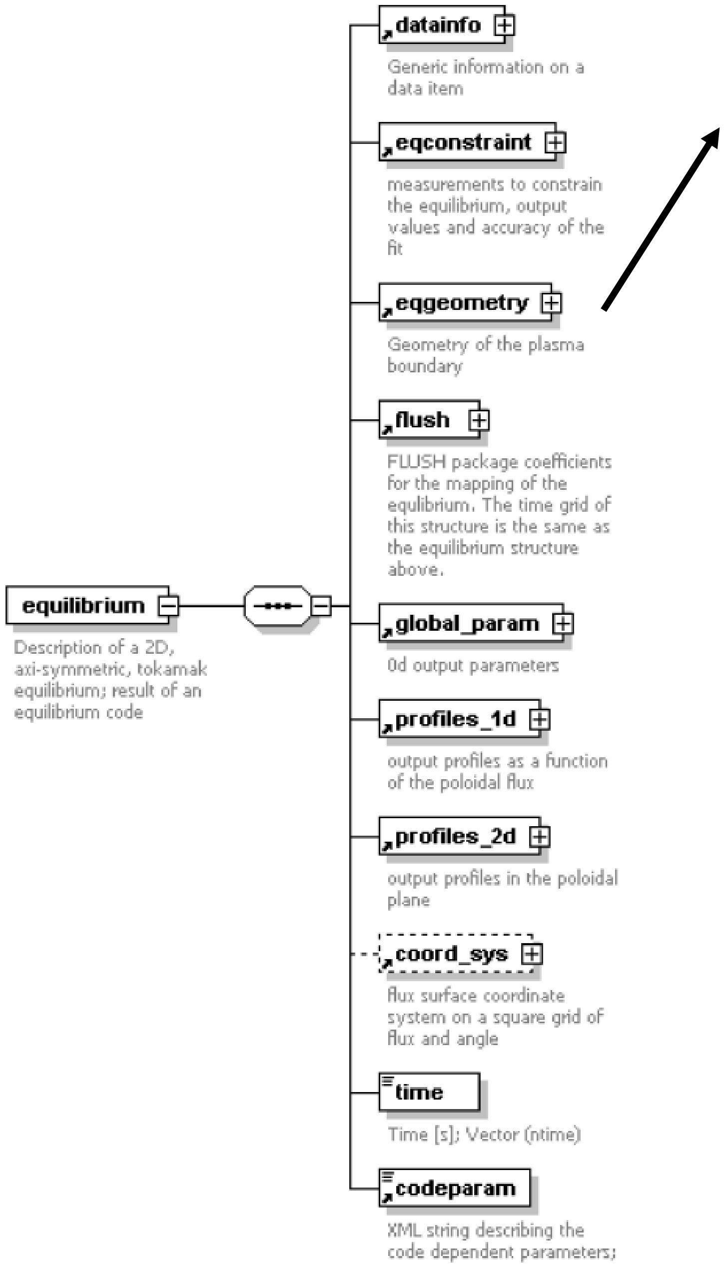
  → "Object based" data structure :

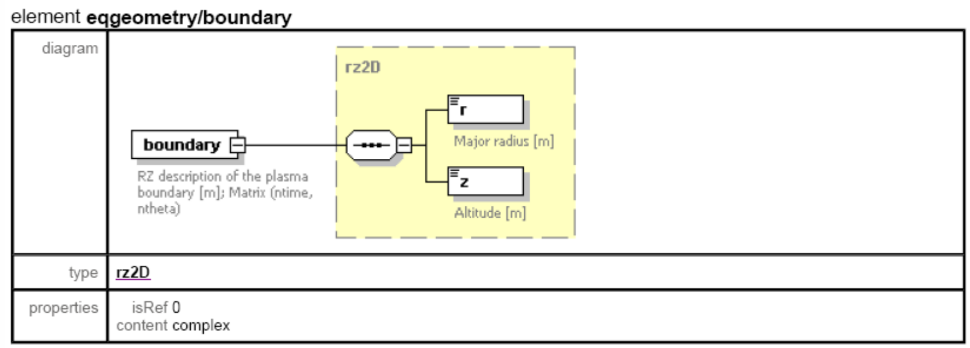
  - High degree of organisation : several subtrees corresponding to « Consistent Physical Objects » (avoid flat structures with long list of parameter names).
    - Subsystem : (e.g. a heating system, or a diagnostic) : will contain structured information on the hardware setup and the measured data by / related to this object.
    - Code results (e.g. a given plasma equilibrium, or the various source terms and fast particle distribution function from an RF code) : will contain structured information on the code parameters and the physics results.

- Code i/o interface uses directly the data structure

- Programming Language flexibility : use of recent software technologies : database structure is defined using XML schemas

Example from phase 4 data structure





<?xml version="1.0" encoding="UTF-8" ?>
<!-- Sample XML file generated by XMLSpy v2006 rel. 3 U (http://www.altova.com) -->
- <top xmlns:xsi="**http://www.w3.org/2001/XMLSchema-instance**" xsi:noNamespaceSchemaLocation="**D:\Mes documents\Travail\ITM-TF\DCP_Phase4\Phase4TOP.xsd**">
- <topinfo>
<dataprovider>**String**</dataprovider>
<description>**String**</description>
<firstputdate>**date**</firstputdate>
<lastupdate>**date**</lastupdate>
<source>**String**</source>
<comment>**String**</comment>
<dataversion>**String**</dataversion>
<shot>**-0**</shot>
……..

Data Access methods

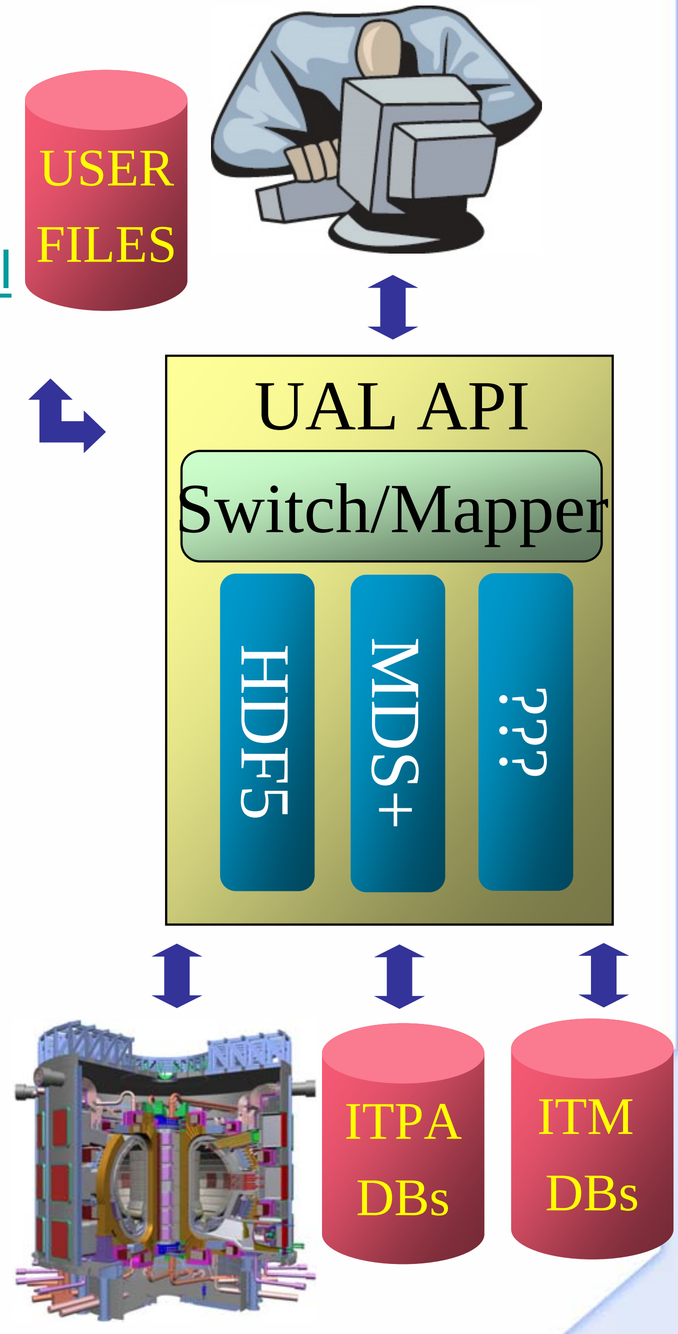
Interim data access system: (W. Suttrop)

- Simple C library with fortran bindings.
  http://www.ipp.mpg.de/~Wolfgang.Suttrop/mdsplus/libitdb
- Further prototyping (IMP#1 efforts):
  - Improved memory handling (G. Huysmans)
  - Tighter connectivity w datastructures (L. Appel)

Universal Access layer:

“Device independent” access to data

- Extensible through plug-in technology
  - MDS+, HDF5, …
  - Single interface to many data sources
- Detailed specification released
- Working Prototype by mid 2007



Example from UAL prototype document

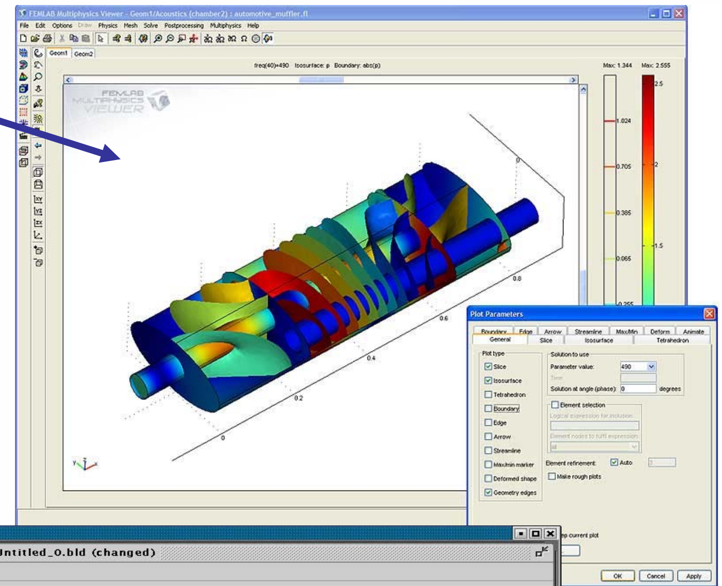
- euitm_open(name,shot,run)
  - Open data base “name”, for a shot number and a run number.
- euitm_get(path, output_structure)
  - Read CPO from an open data base; the location of the CPO is specified by the string argument “path”; output_structure is language dependent and will hold the output data.
- euitm_put(path, input_structure)
  - Write CPO in an open data base; the location of the CPO is specified by the string argument “path”; input_structure is language dependent and will hold the input data.

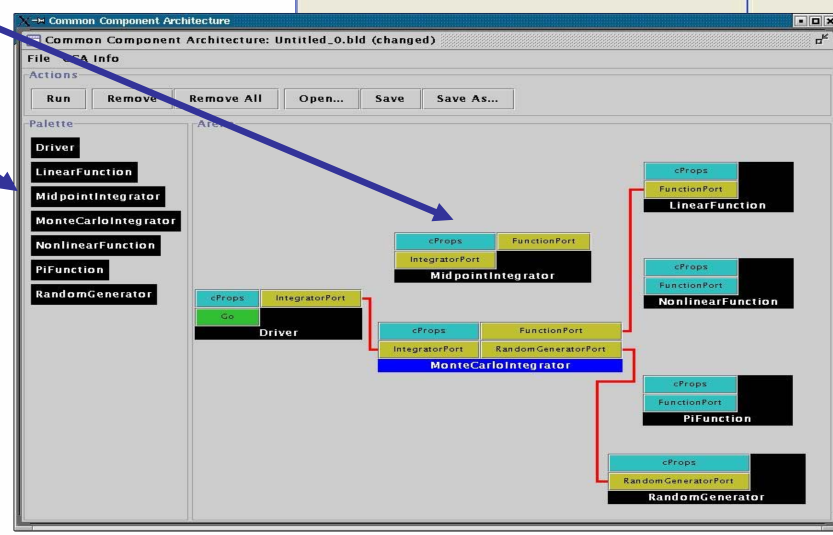
Etc …..

ISIP II:Code Platform Project

Leader: B. Guillerminet
Deputy: M. Stanojevic

- **Requirements:** *version (December 2005)*
  - **End User**
    - *Tools to define the simulation*
    - *Tools to run & monitor the simulation*
    - *Tools for post-processing*
  - **Developer**
    - *Integrate the codes*
    - *Component based*
    - *Debug & test*
  - **Administrator**
    - *Deploy the simulator*
    - *Monitor it*
    - *Manage the archive*
  - **Additional constraints**





CPP: Existing frameworks

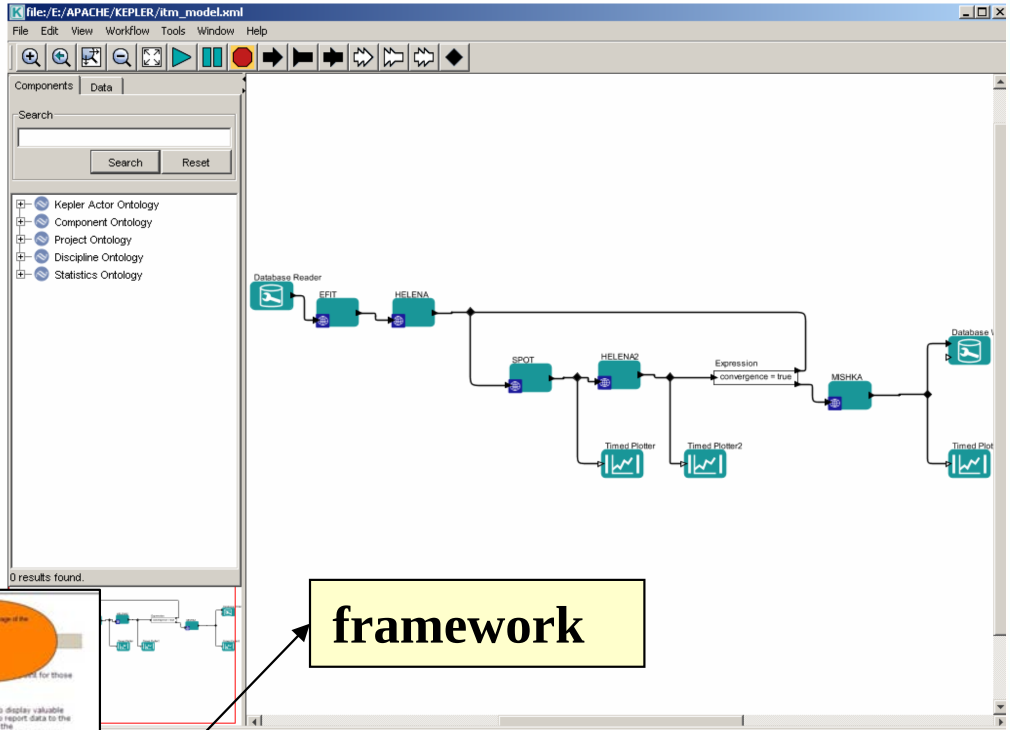
Name	comments	pros	cons
Cactus http://www.cactuscode.org/	Complete framework	Investigating CCA	No component model, no PIC
Pyre http://www.cacr.caltech.edu/projects/pyre	Simple framework	Investigating CCA, WS-RF	No component model
Salome http://www.salome-platform.org	Complete framework	Corba	
Kepler		CCA	
MpCCI	Code coupling	Meshing	No component model, not open source
Xcat3	Java & C++ frameworks	Both CCA & WS-RF models	

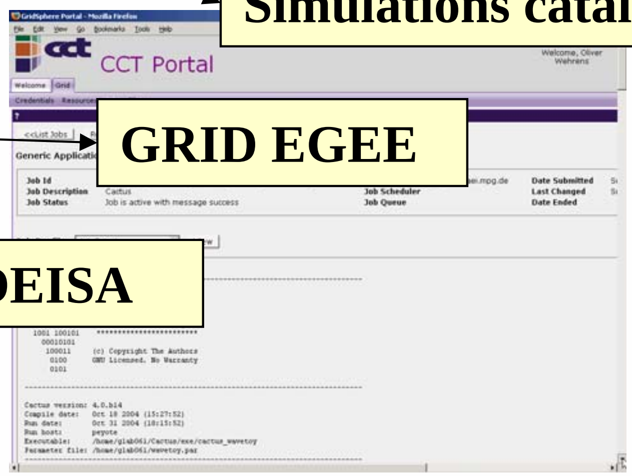
Comprehensive evaluation of different workflow orchestration tools is being finished By end 2006. **Kepler** found to be most suitable (but development work needed)

Grid enabled Portal "vision"

Simplify users access:

- *single sign on authentication (login, passwd, use the VO certificates)*
- *launch our applications (platform simulation, monitoring, …)*
- *Manage the catalogs (codes, experimental and simulation data, …)*
- *acess GRID resources*
- *encryption & security*





User

single sign-on

framework

Codes catalog

Simulations catalog

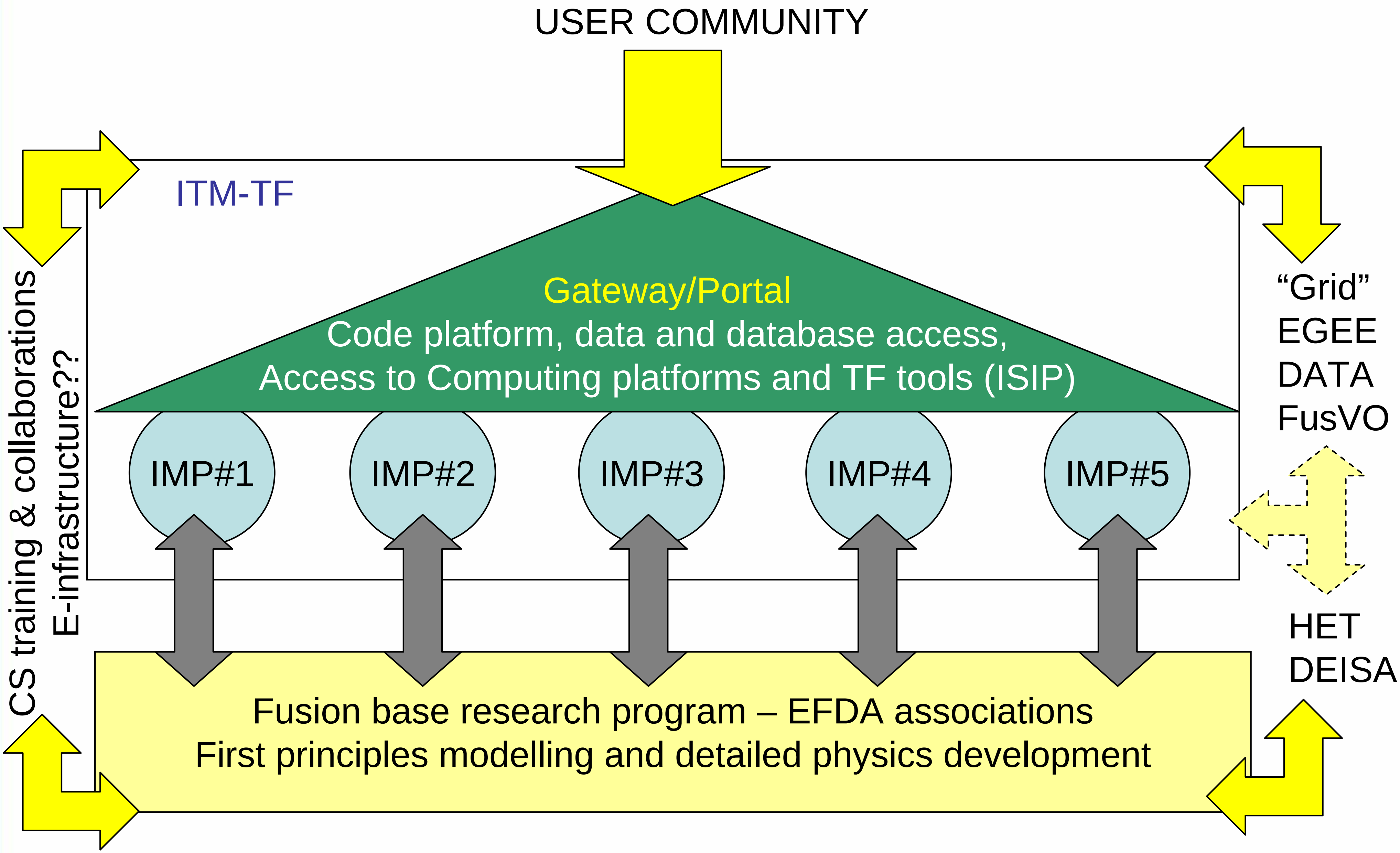
GRID EGEE

GRID DEISA

User database:
•Properties, …

Local Resources

Schematics


USER COMMUNITY
ITM-TF
Gateway/Portal
Code platform, data and database access,
Access to Computing platforms and TF tools (ISIP)
IMP#1
IMP#2
IMP#3
IMP#4
IMP#5
Fusion base research program – EFDA associations
First principles modelling and detailed physics development
CS training & collaborations
E-infrastructure??
"Grid"
EGEE
DATA
FusVO
HET
DEISA

The Gateway - general layout

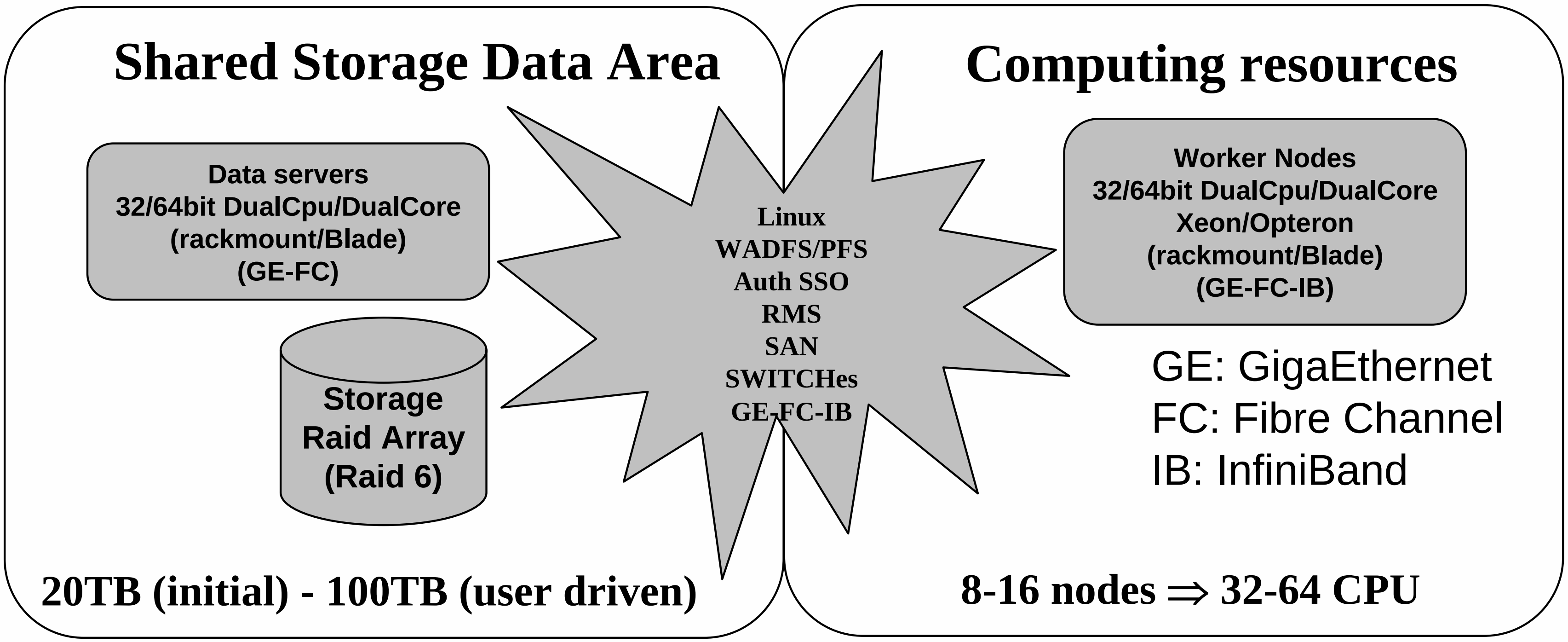
User entry point

Shared Storage Data Area: resources to store large amounts of data generated by simulation codes and originating from experimental data of various fusion devices

Servers and infrastructure: Master node, code platform server, fileserver, etc

Computing resources: a farm of worker nodes to provide gateway elements. The software include operating environment (sys.op. distribute filesystem, resource management system, authentication system, backup)

Technologies layout (schematic)



Integrated Modelling Project 1

Leader: G. Huysmans
Deputy: L. Appel

- Objective:
  - To provide an integrated suite of self-consistent codes (modules) for equilibrium reconstruction and linear MHD stability analysis

- Topic 1A : Experimental Equilibrium reconstruction
  - *CEDRES, CLISTE, **EFIT**, EQUINOX*

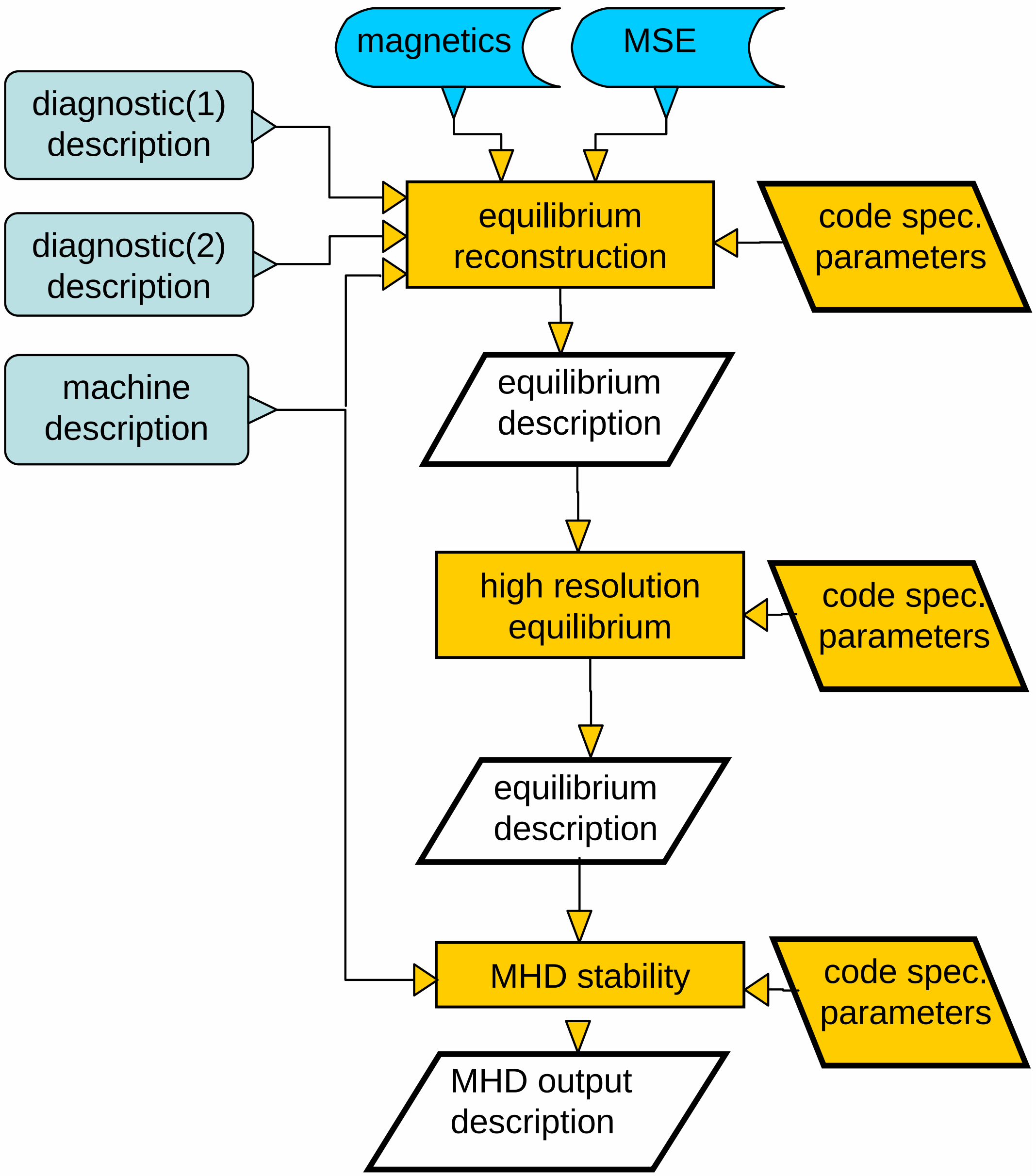
- Topic 1B : Equilibrium codes and linear MHD stability
  - Equilibrium : **CAXE**, **CHEASE**, DIVA, **HELENA**, VMEC, *DINA*
  - Mapping : **COTRANS**, JMC
  - MHD Stability : CAS3D, **CASTOR**, **KINX**, **MISHKA**, TERPSICHORE

- Also:
  - Equilibrium toolbox : **FLUSH**

equilibrium and MHD Stability

- **Standardise contributed codes to become independent of machine /diagnostic data.**
  - Use only external geometry data (from database)
  - Definition of interfaces between codes and machine and diagnostics

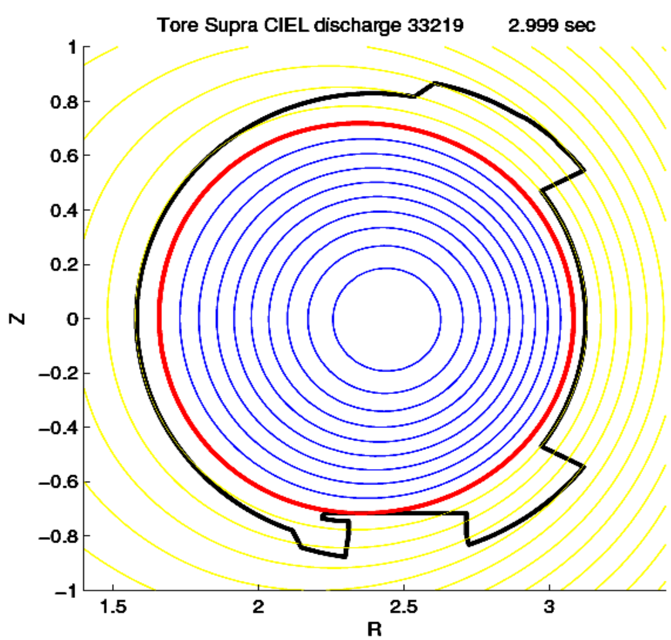
- **Validation and Verification**
  - compare equilibrium and MHD stability codes on benchmark case
  - Apply codes to a relevant experimental problem/data
    - MHD Stability limits in plasmas with an internal transport barrier.

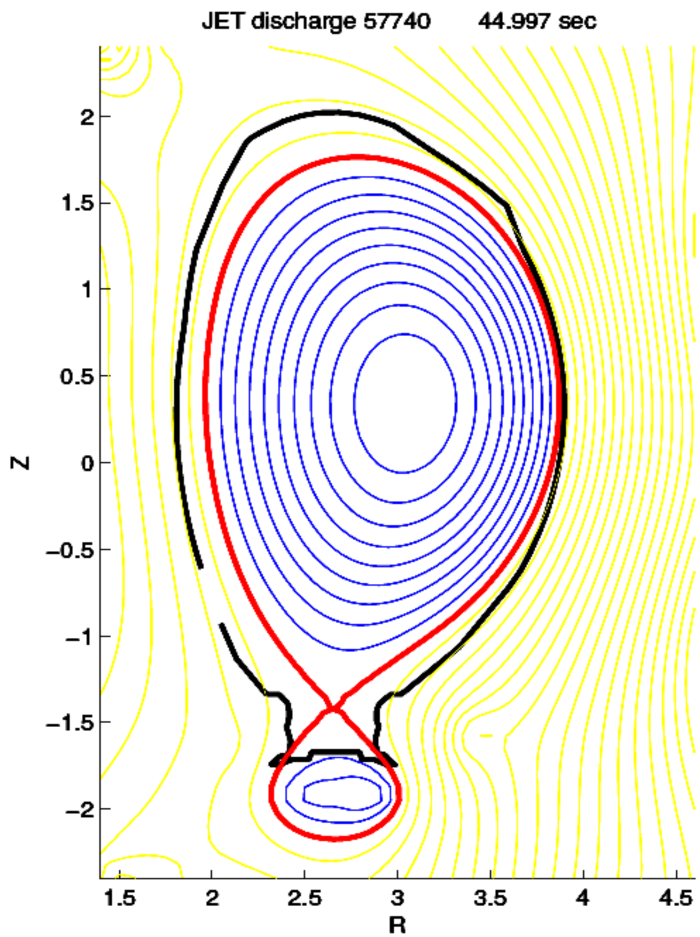


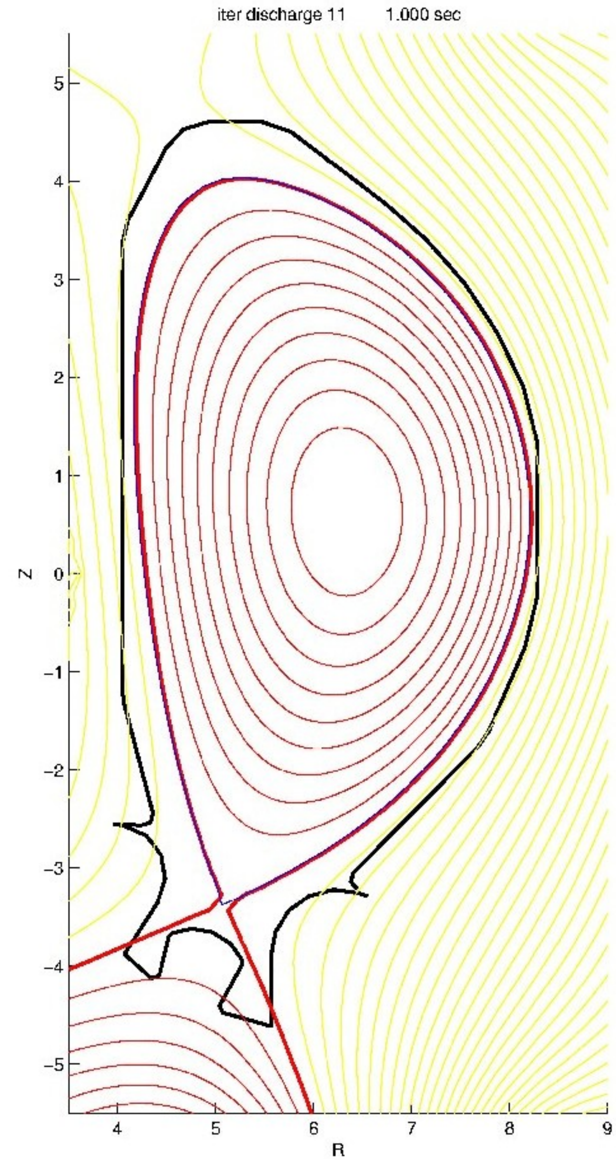
Machine independent EFIT_ITM

- EFIT has been adapted to use the ITM structures and to use external geometry information
  - **A unique version of EFIT can now be used for ITER, Tore Supra, JET, etc**
  - Using only TF tools for
    Data storage,
    access
    and data structures

Validation effort underway







IMP1: the on-going tasks

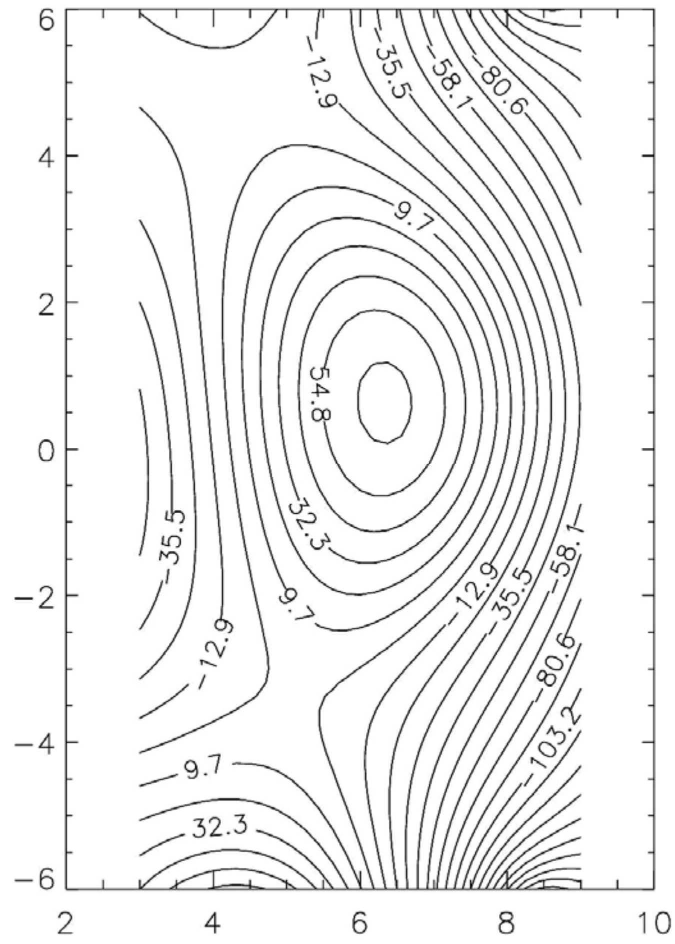
- adaptation of high resolution equilibrium, mapping and linear MHD stability codes to the ITM data structures.
  - Status
    - *High resolution equilibrium codes* CHEASE (H. Lutjens), HELENA (G. Huysmans, C. Konz), and CAXE (S. Medvedev) have been adapted to use ITM data structures.
      - codes have common interface
      - codes verification ongoing
    - *Linear MHD Stability codes* CASTOR (C. Konz), KINX (S. Medvedev), MISHKA (G. Huysmans) have been adapted to use ITM data structures.
      - Verification on synthetic test case and ITER test case
  - To be done
    - Verification on more synthetic benchmarks

Soloviev	KINX(γ=0)	MISHKA-1 (∇.v=0)	CASTOR (γ=0)
CHEASE	-0.2230	-0.1916	
HELENA	-0.2205	-0.1900	-0.2230
CAXE	-0.2252		

ITER scenario #2	KINX	MISHKA-1
CHEASE		-2.57e-4
HELENA	-3.5e-4	-2.52e-4
CAXE	-2.5e-4	

IMP1: the on-going tasks

- **Create a unique version of the CASTOR and MISHKA MHD stability codes (combining the existing versions into one framework)**
  - Status:
    - CASTOR, MISHKA-1 and MISHKA-D have been combined into new framework ILSA (C. Konz, E. Strumberger, EPS2006)
      - Verified on synthetic benchmarks
      - Full adaptation to ITM data structures
- Provide a toolbox for the equilibrium operations
  - Status
    - FLUSH (JET) library being adapted to ITM requirements (H. Leggate)
    - First application to ITER test case



Integrated Modelling Project 2

Leader: F. Porcelli
Deputy: S. Sharapov

- **Objective**: Non linear MHD phenomena
- **Initial work on RWMs, sawteeth and ELMs has started.**

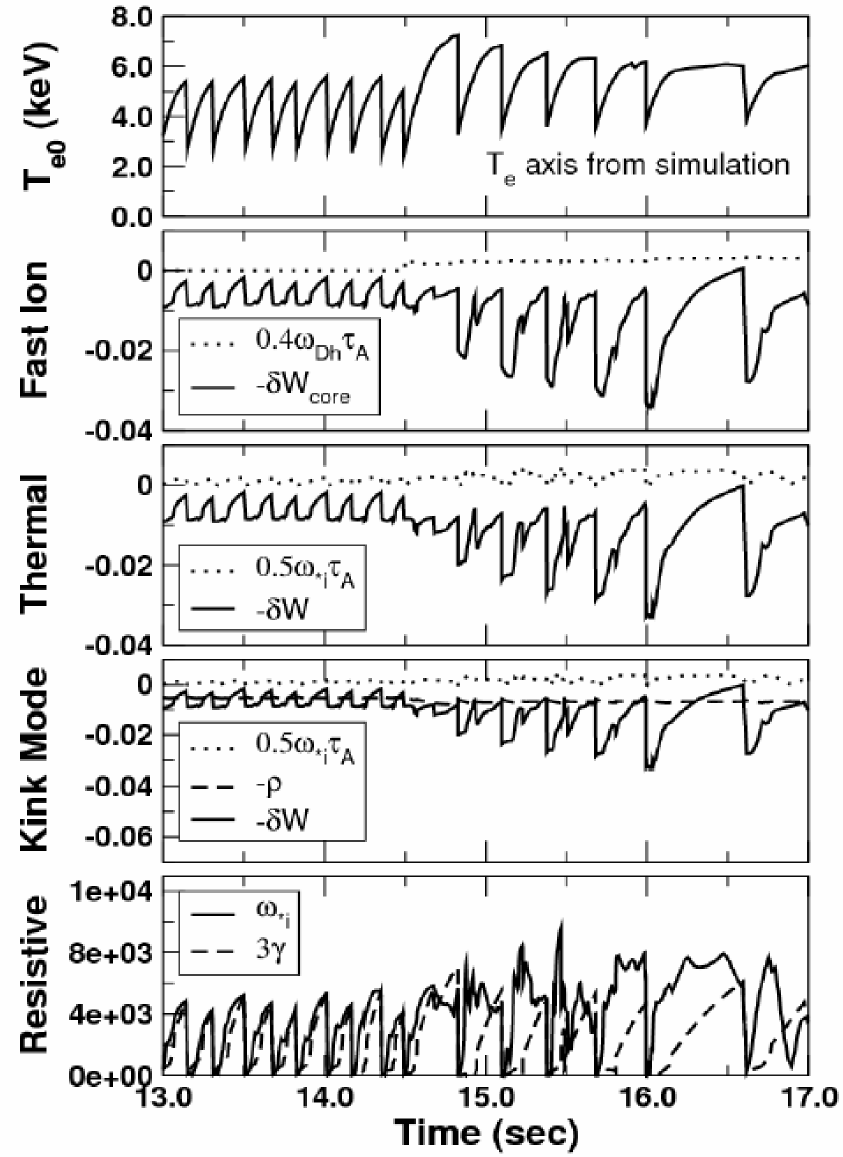
- **RWMs meeting held at JET**, **Nov 24-25,2005**. List of open issues has been compiled. Initial work on the assessment of plasma kinetic damping and of nonlinear coupling between mode amplitude and plasma rotation.

- **ELMs meeting held @ JET Feb 13-14.** Stability boundaries and width of plasma displacement as a function of equilibrium parameters. Influence of X-point on linear MHD stability. Nonlinear evolution of edge-ballooning modes. Nonlinear simulation of full ELM cycle.

Integrated Modelling Project 2

Sawteeth meeting held @ JET Feb 16-17. Work on integrating a model for the prediction of the sawtooth period and amplitude in the JETTO, ASTRA, TRANSP, BALDUR transport codes, together with fast particle behavior from the PION code, and prescriptions for fast particle losses and redistributions during sawtooth crashes, fishbones and TAE (tornado) modes. Initial work on the prediction of the sawtooth crash time, comparison with recent JET data.

F. Porcelli et al., FEC 2006, Chengdu



Integrated Modelling Project 3

Leader: D. Coster

Deputy: V. Basiuk, D. Kalupin, V. Parail , G. Pereverzev

Objective:

–To provide the computational basis for a modular transport code, taking account of the core, the pedestal and the scrape-off layer. Ultimately, to enable the simulation of complete tokamak scenarios, e.g. for ITER.

Progress within IMP3 has been somewhat more limited than hoped for:

– Depends on the CPP project which is still evaluating candidates for the code platform

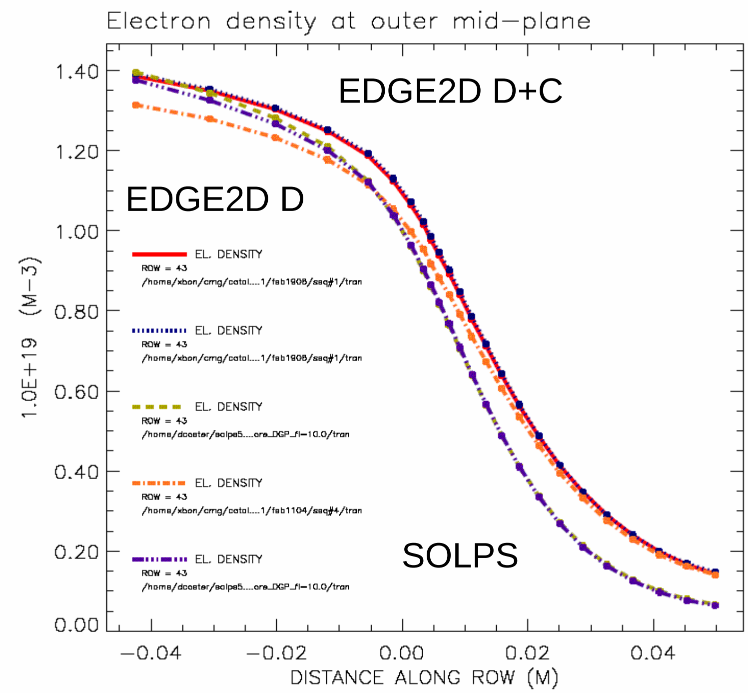
– Reliant on voluntary participation in an area where much of the physics is relatively well known and as such is not that highly valued in terms of publications, prestige etc

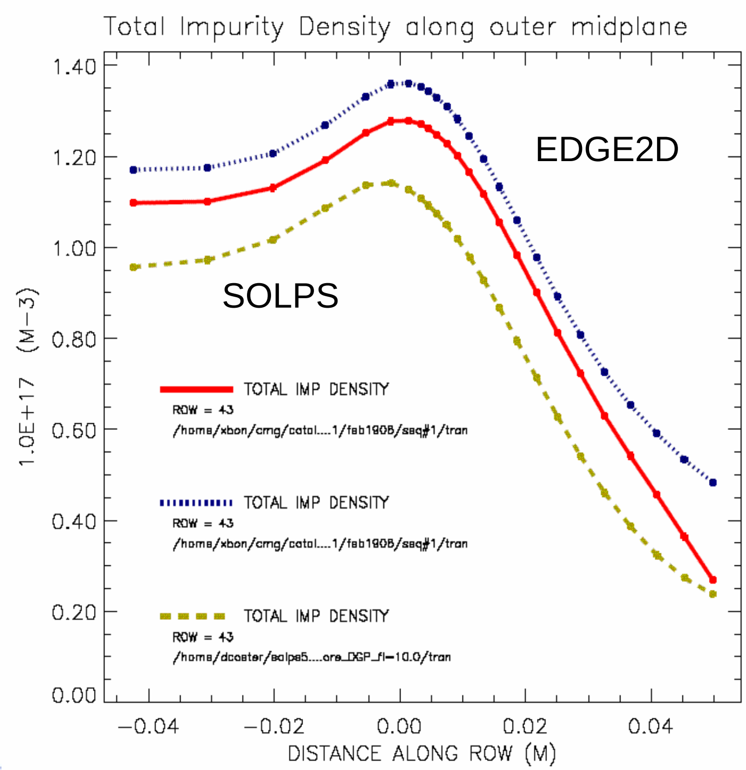
– A significant part of the activity needs to be in V&V of existing codes, modules etc and this is dependent on shared infrastructure and resources.

– Within this context, JET has played, and continues to play, a key role because significant resources are available (infrastructure and orders/secondments)

Edge Code Benchmarking

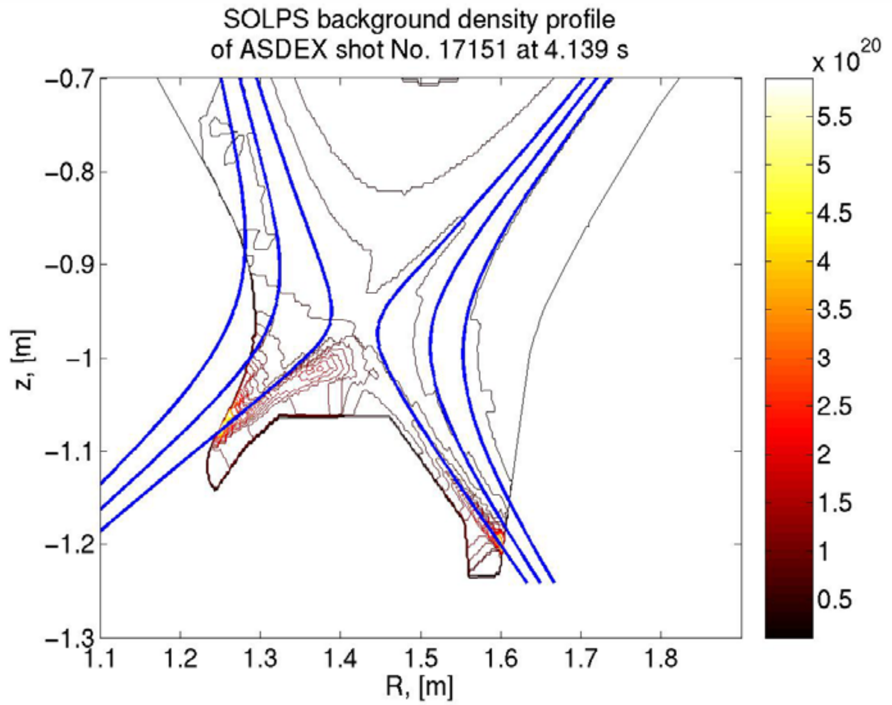
- **ITPA activity:**
  - code-code comparison
    - Phase I: pure D, no drifts
    - Phase II: pure D, drifts
    - Phase III: D+C, no drifts
    - Phase IV: D+C, drifts
  - SOLPS-EDGE2D/NIMBUS →
    - Phase I completed successfully (reported on at PSI 2004)
    - Phases II and III in progress
  - SOLPS-UEDGE
    - Phase I underway
    - Phase II expected to start soon
- **Additional code-experiment**
  - JET: SOLPS-EDGE2D/NIMBUS
  - AUG/D3D: SOLPS-UEDGE

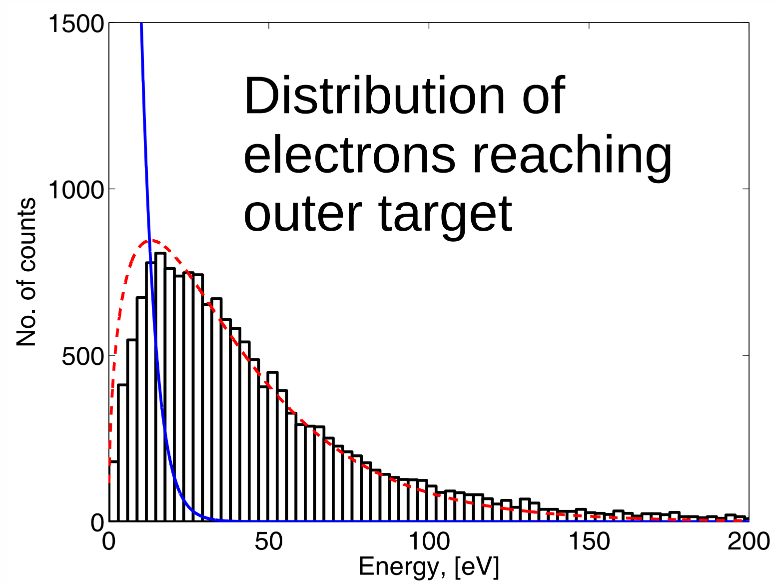




Using MDS+ to connect SOLPS to ASCOT

- ITPA standard pedestal MDS+ tree created based on AUG shot 17151 (provides the equilibrium data)
- 2D background (n_e, T_e, T_i, …) written as MDS+ tree by SOLPS (IPP-Garching)
- → provides input to ASCOT. Due to open field lines, special care must be taken with the Monte Carlo collisions
- Planned: output of ASCOT to be saved to a MDS+ tree





ASCOT: (**A**ccelerated **S**imulation of **C**harged Particle **O**rbits in a **T**okamak)
T. Kurki-Suonio, L. Aho-Mantila, J. Heikkinen, V. Hynönen, T. Kiviniemi, A. Salmi, S. Sipilä, V. Tulkki

Common interface to transport models

developed with JET IM project

CALL ANOMALOUS(MODEL, PROFILES, GEOMETRY,TRANSPORT,[DIAG],ifail)

Derived types:

Standardized Inputs: PROFILES, GEOMETRY defined in generic modules (type definitions and allocations,…)

Standardized Output: TRANSPORT defined in same generic modules (fluxes + eff.diff for transport channels)

Model dependent data: WEILAND; GLF23, RITM, EDWM in specific model dependent module (MMM95 under testing)

[DIAGNOSTIC]: Optional diagnostic output supplied in model dependent formats.

Simple and extensible interface: New models need to supply

1. Default settings for options
2. A mapping to actual model call (by template)
3. Derived types for model specific inputs/outputs (may be empty!)

Integrated Modelling Project 4

Leader: B. Scott
Deputy: M. Ottaviani

Objective:

To develop a suite of unified, validated codes to provide quantitative predictions for the linear properties of a range of instabilities, including: ion-temperature-gradient (ITG) modes, trapped electron modes (TEM), trapped ion modes (TIM), electron-temperature-gradient (ETG) modes, micro-tearing modes, etc.

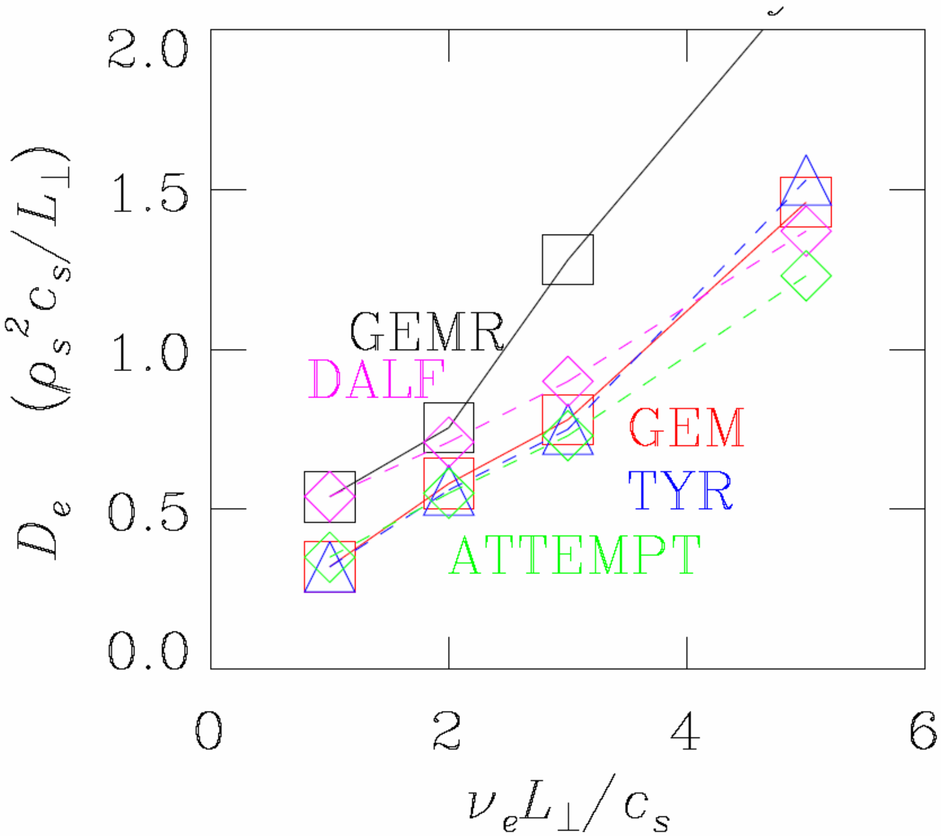
- Three Formalised tasks:
  - Catalogue Codes, standardise documentation
  - Code verification and benchmarking
  - Development and exchange of elements of theoretical basis for model

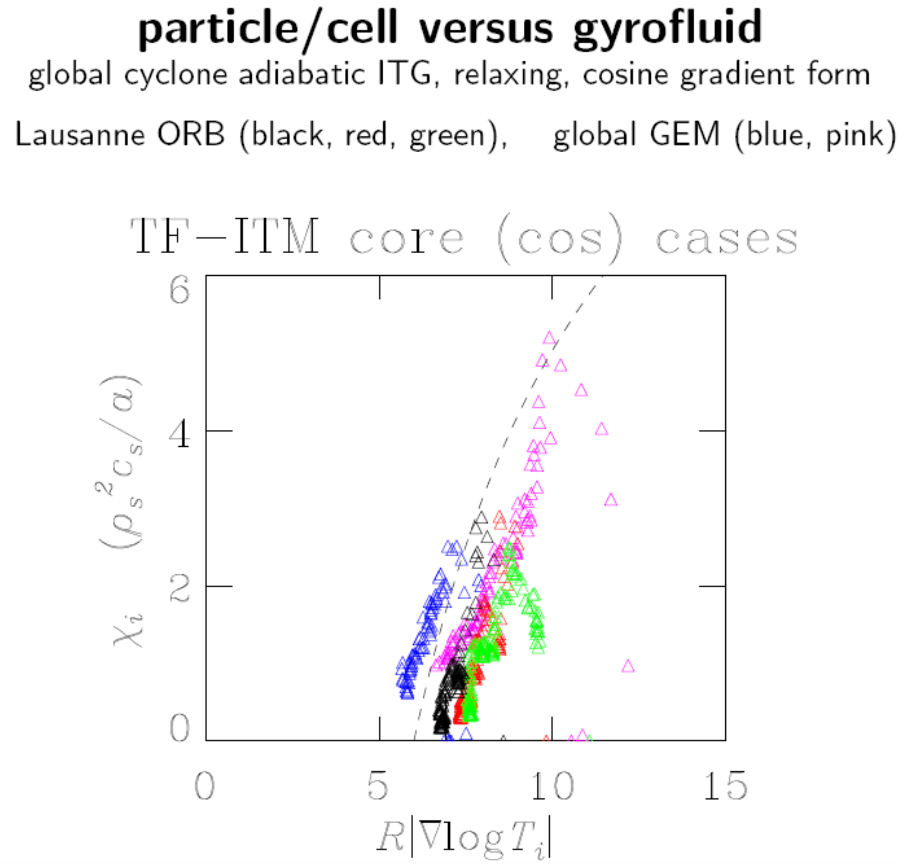
- Benchmarking campaign has started (will run for 2 years)
  - Cyclone like base case and (unique to Europe) edge
  - also comparing neoclassical and turbulence code equilibria

IMP#4: Code Verification & Benchmarking

Core and edge standard cases:

- L-mode edge near 100 eV and 2 x 10^{13} cm^{-3}
- Standard Cyclone base case for core (local and global modes)





First results reported at the EPS meeting in Rome 2006

global GEMR code differs at higher ne because it corrects for gradient relaxation

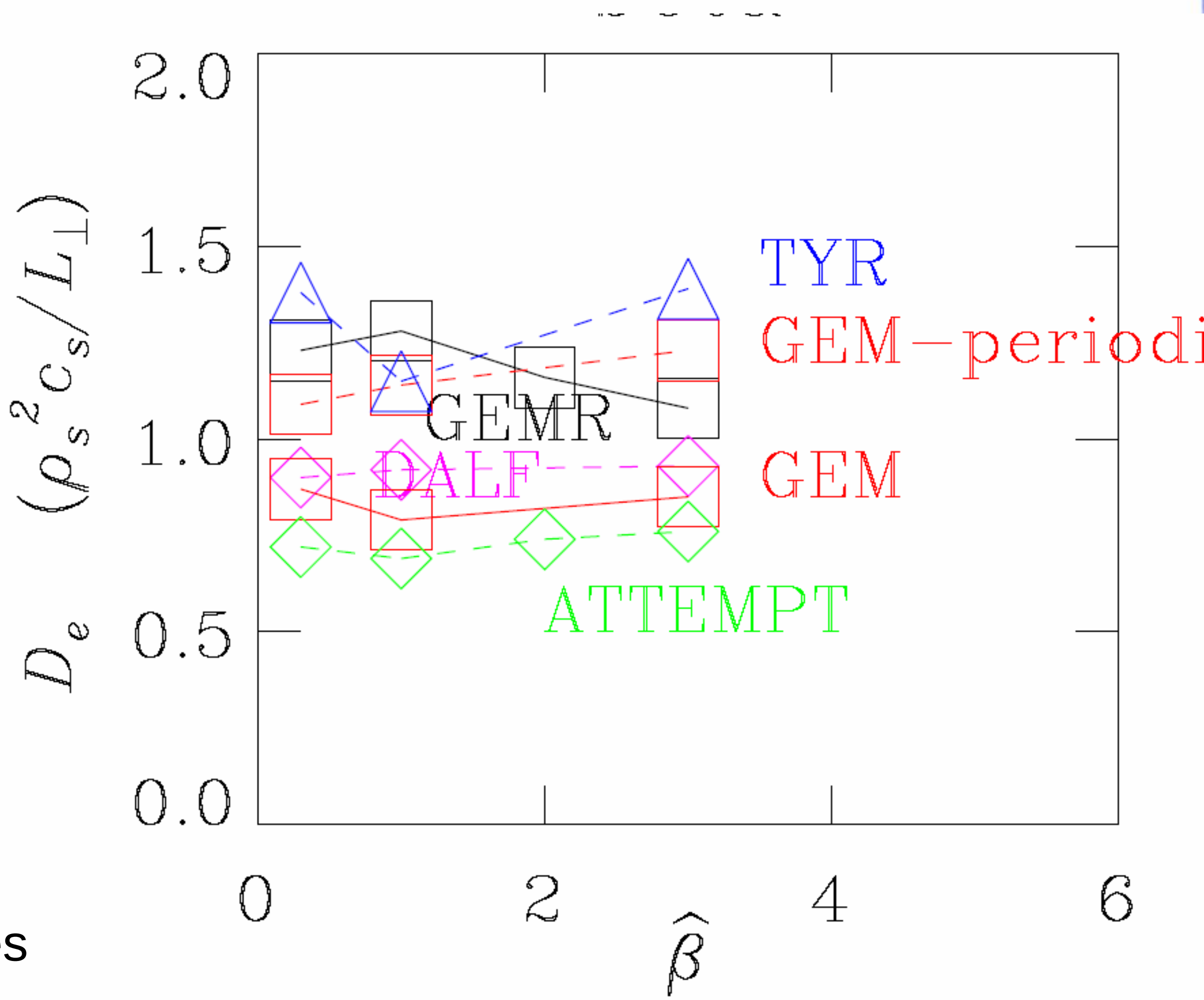
Edge benchmarking

first series:

cold ion four field model in ASDEX-Upgrade L-Mode cases

mainly flux tube codes, one global one in “thin atmosphere" domain

0.915 < r/a< 1.0



beta scan problematic enough to expose differences among the codes

- non-periodic: gradient relaxes, buffer diffusion zones -> dissipation
- periodic: obviously non-viable for global case, admits unphysical radial jet flows

IMP#5, heating current drive and fast particles

Leader: T. Hellsten
Deputy: Y. Peysson, F. Zonca

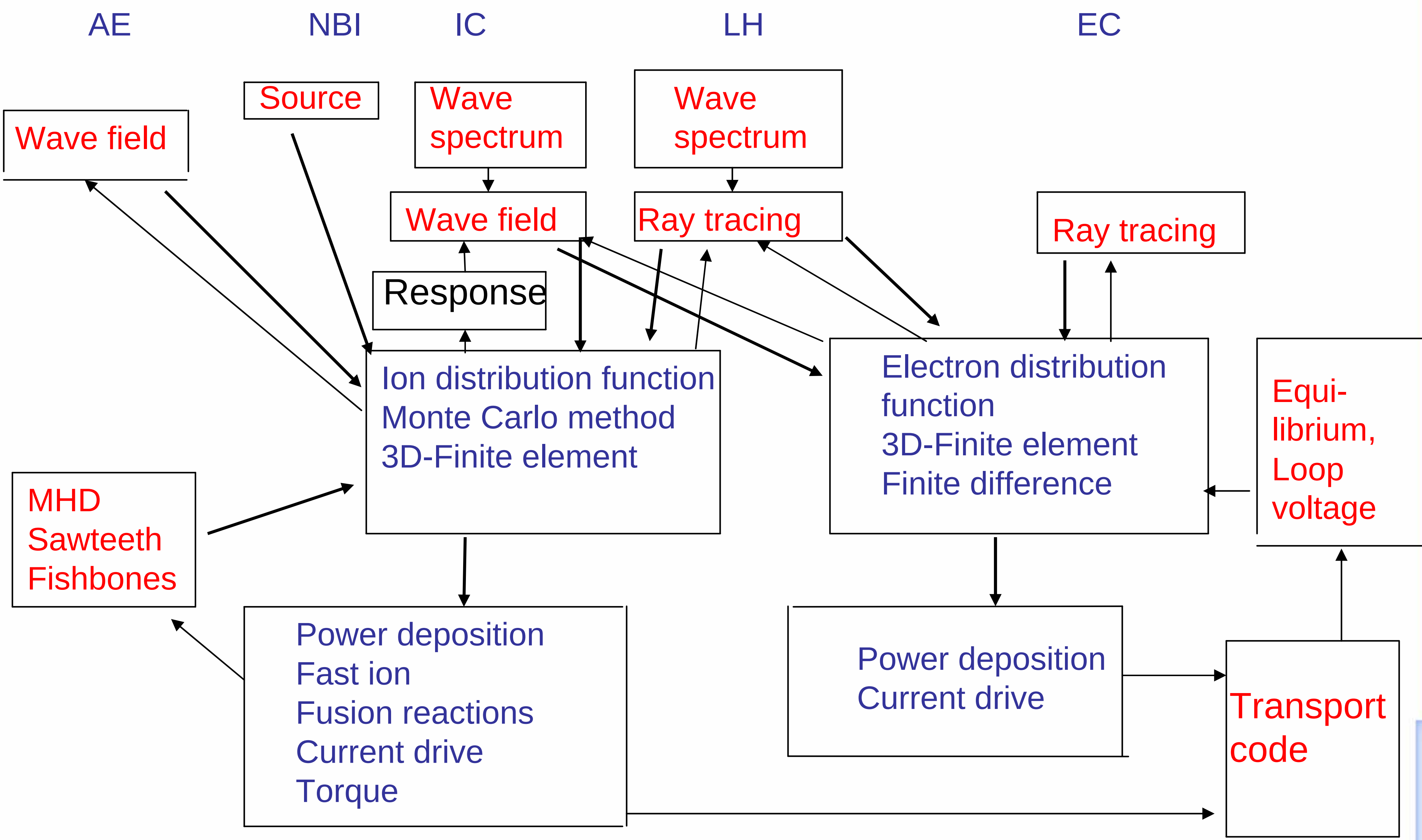
- **Objective**: develop the computational basis for a modular package of codes simulating heating, current drive and fast particle effects

- **Area covered**: ECRH, ICRH, NBI, LH, alpha particle and fast particle interaction with instabilities

- **Goal**: self-consistent calculations validated against experiments

- **Priority**: realistic modelling applicable to ITER standard and advanced scenarios

IMP# 5: global picture



Major complexities if comprehensive modelling is desired.

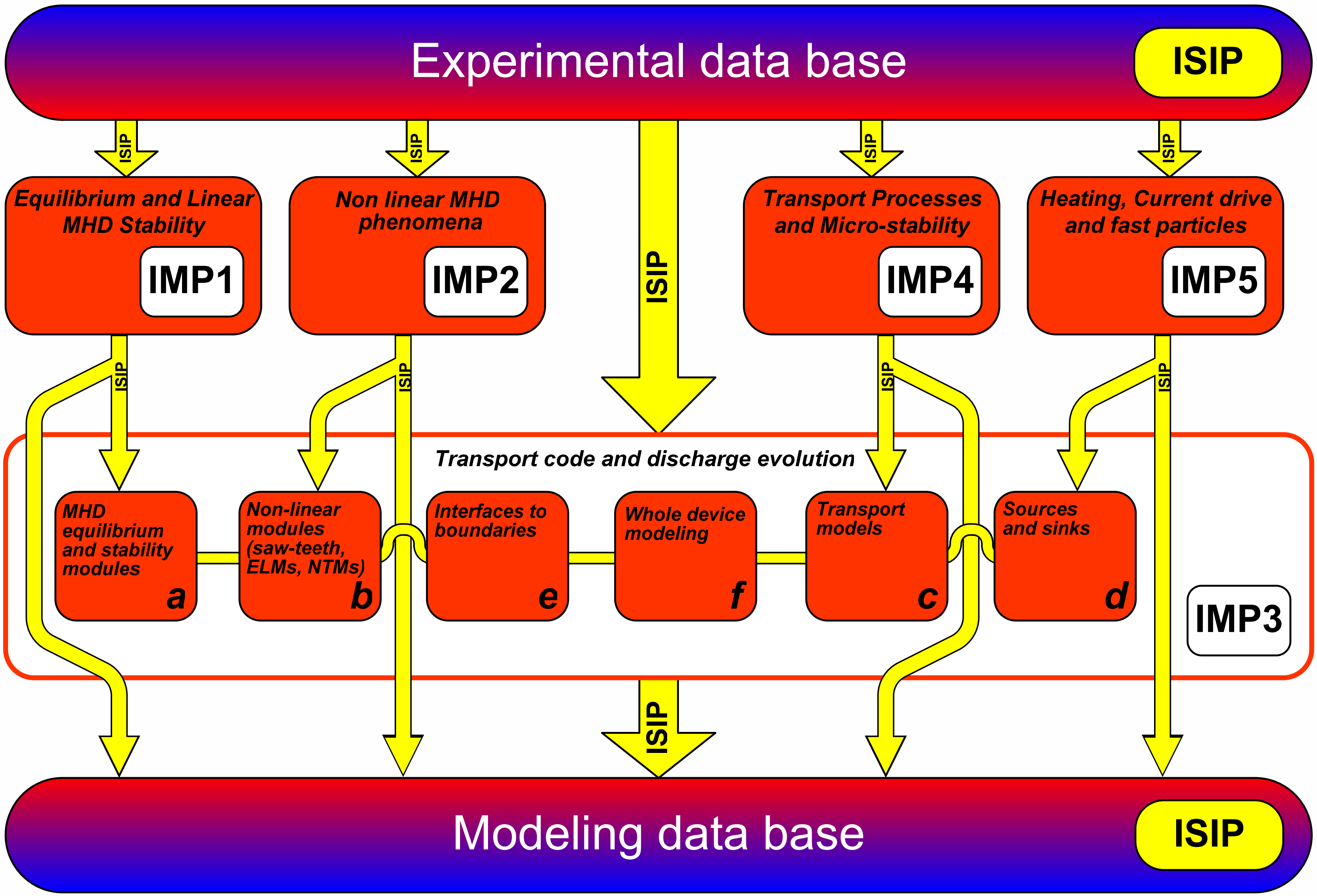
Integrated Modelling Project 5: strategy/outlook

- **Short term** (~6 months):
  - Identify the most effective data structure for linking codes between them on the ITM Platform (ongoing, good progress).
  - Some benchmarking activity (to start soon).
- **Medium term** (~2/3 years):
  - fast code development for basic ITER modelling
    - ICRF, one code available, but some extension needed
    - ECRH/ECCD, In good shape, several codes available.
    - Benchmarking of these codes on ITM-TF platform.
- **Long term** (> 3 years):
  - Development of modular advanced codes for comprehensive modelling and integration in specific problems.
    - Several ICRF full wave codes available.
    - Developments of 3D Fokker-Planck modelling.
    - Improvements in plasma response functions.
    - Description of AE modes etc. in Fokker-Planck treatment.

    …

Project relations

Associations/Expertise



User tools

Near term Focus areas

- ITM will be starting to deliver tools!
- Technology developments essential
  - Code platform and UAL short term focus areas
  - Gateway essential to pull activities together
    - Storage for simulation and experimental data
    - Development platform for framework tools
    - V&V and QA support structure
    - User access point!
  - Ad Hoc sharing of distributed resources Not A very efficient Model
- Public releases to be put under QA procedures
  - V&V on physics models and platform tools short term focus – Increased Interaction with experimental community

V&V and QA in General

- **Level 0** – Ad Hoc approach (mainly at individual code level)
  - Non systematic approach, metrics and reporting left to individuals
  - No monitoring and forced adherence to any standards
- **Level 1** – Consistent V&V (codes or packages)
  - Following predefined procedures
    - Detailed consistent reporting
    - Verified operation
    - Critical assessment of “performance”
    - Critical assessment of experimental applicability
  - Openly reported in standardized formats
- **Level 2** – Consistent QA (@ Organization or TF level)
  - A superset of requirements over level 1 relating to
    - Software Management
    - Software Engineering

  Detailed procedure with checkpoints guaranteeing conformance to quality and reliability goals

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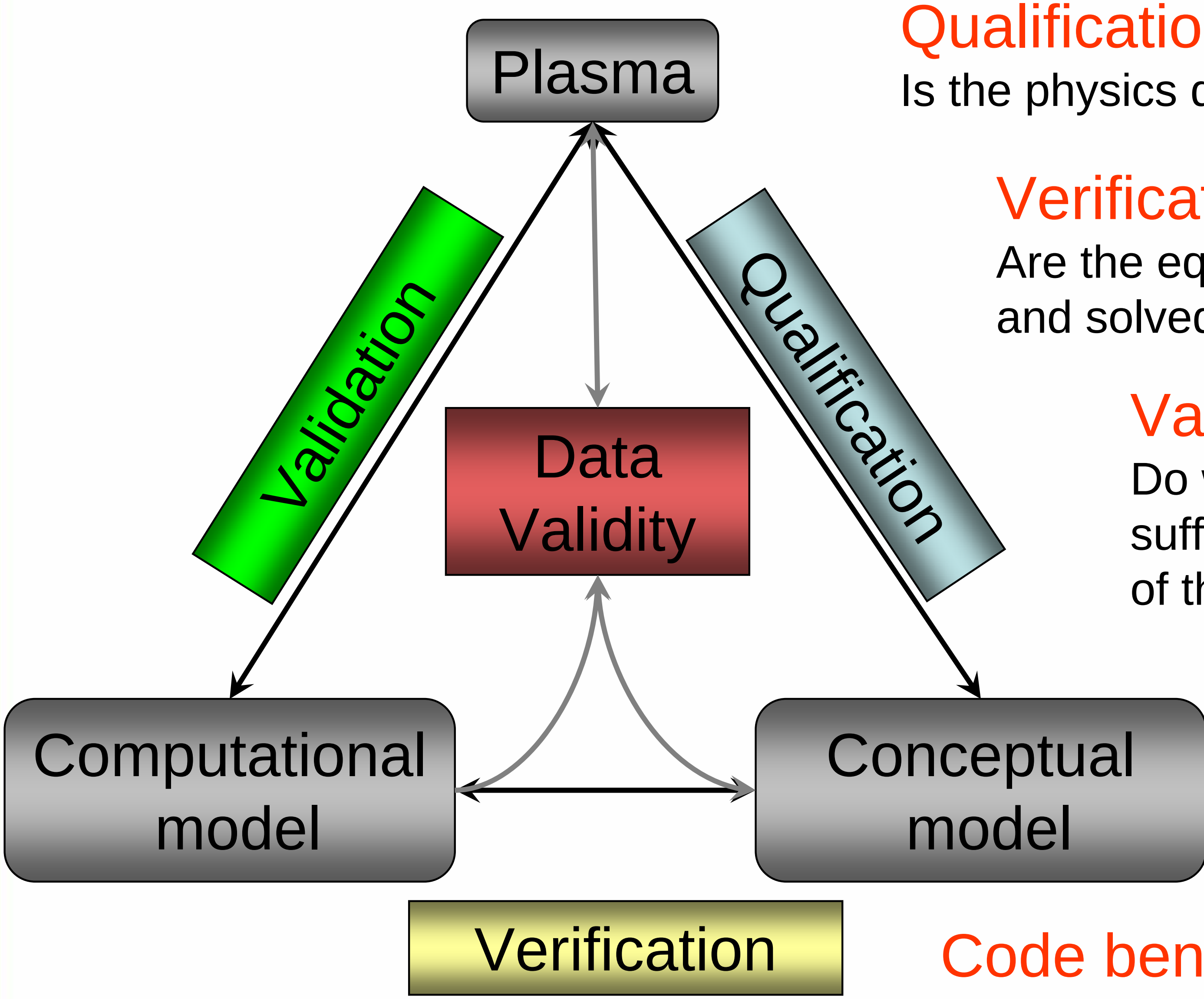
- **Level 3** – QA procedure under nuclear licensing requirements
  - ITER requirement for codes within Plant Operating Zone

Oversimplified view



Qualification:

Is the physics description adequate?

Verification:

Are the equations implemented and solved for correctly?

Validation:

Do we have a reliable and sufficiently accurate description of the plasma?

Data Validity:

Is our measured data a sufficient representation of reality?

Code benchmarking: (C2C)

A tool in both V&V and physics exploration

TF V&V procedures: EFDA-TF-ITM(04)-8

International collaborative activity

- ITPA coordinating committee endorsed in June 2006 the creation of an expert working group under the CDBM group on the technologies of IM.
  - IMAGE: Integrated Modelling – A Global Effort
    - Chair: P. Strand
    - Main collaborators BPSI (JP), FSP (US), ITM-TF (EU), ITER Physics Team and ITPA TG, China and other parties have also expressed an interest.
    - First official gathering in Lausanne, ITPA CDBM spring meeting 2007
  - Standardization of formats and interfaces
  - Machine descriptions
  - Transport Solvers
  - V&V metrics and standardized test cases
  - Software Standards

Conclusions

- The European Integrated Modelling Community is structured and at work
- The foundations in terms of physics and modelling technologies are established, introducing QA in the process.
- The links with other ITER, ITPA and some ITER PTs have been established.
  - Need to expand and expand from this starting point with active collaborations
- The tools are developed for any tokamak (fusion device)
- The weaknesses of the present TF structure have been identified and modifications/needs proposed to EFDA and the Commission (Connor AHG - this afternoon). The main issue is about resources.

- Physics projects (IMPs) are progressing well, Technology support has developed more slowly due to lack of hardware resources and specialist competences (mainly in computational science and data access areas.)
  - Some IMP tasks slowed down or blocked due to lack of integration tool (platform)
  - Rapid deployment of the gateway, code platform and other joint tools are critical for future development of the projects. Priority for 2007!
  - Commitment from EFDA leadership to the development of the TF.