JRA3

Brussels

30 March 2011

Scope

- JRA3 Activity:

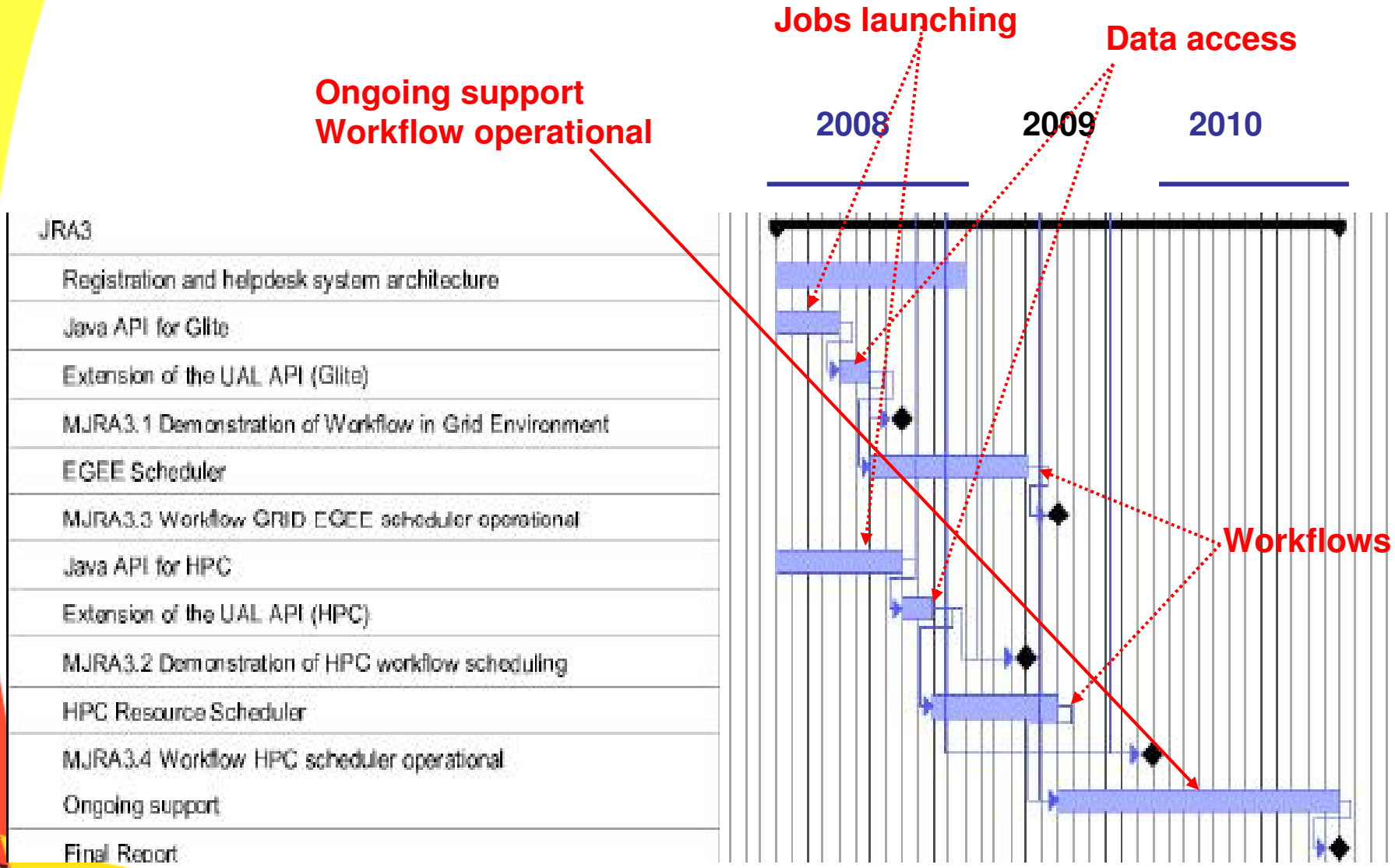
  “Workflow orchestration”

- Partners
  - PSNC, Poznan Supercomputing & Networking Centre, Poland, 24 pm
  - CEA, France, 16 pm
  - EPCC, University of Edinburg, United Kingdom, 8 pm
  - IPP, Germany, 8 pm
  - UDS, France, 8 pm
  - Chalmers, Sweden, 4 pm

Scope

- **Define a sustainable architecture for jobs launching and scheduling on GRID and HPC infrastructures**
- **Build a unified access to GRID and HPC for**
  - Job launching
  - data access
  - Job orchestration
- **Demonstrate workflows mixing both architectures**
- **Registration and Helpdesk system** (reported by A. Jackson in SA3)
- We have done more:
  - **Training & dissemination**
  - **Reliable/Robust infrastructure**
  - **Ease of use**
  - **Ready for the future:**
    - **Distributed workflows**
    - **Parametric jobs**
    - **Cloud computing**

2008-2010 work plan

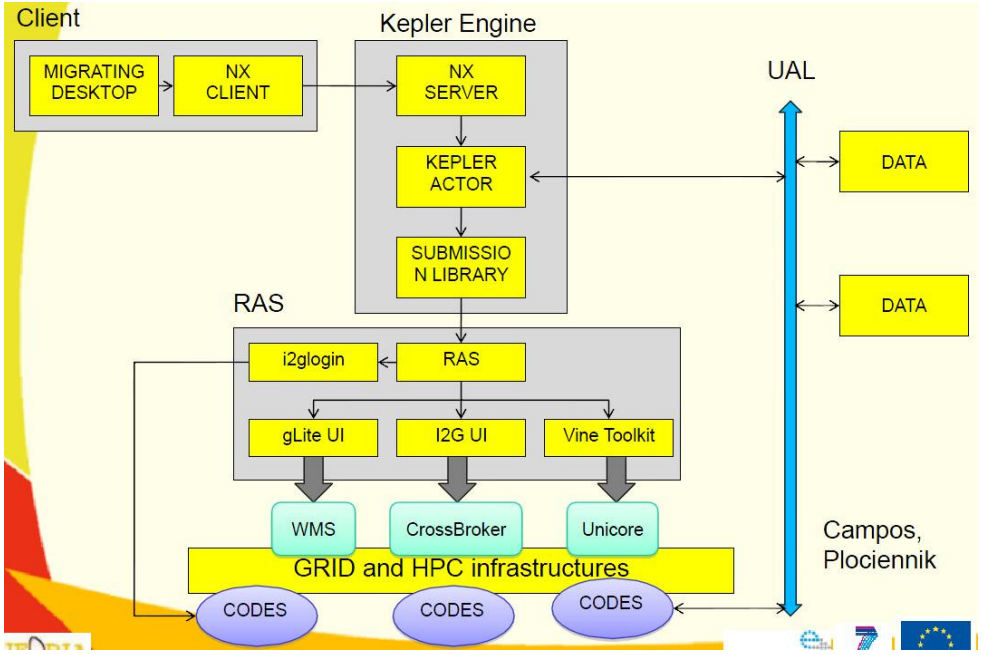


Implementation

- Unified access to GRID and HPC infrastructures
- Reliable/Robust infrastructure
- Ease of use
- Integration and global activities
- Ready for the future:
  - Distributed workflows
  - Parametric jobs
  - Cloud computing

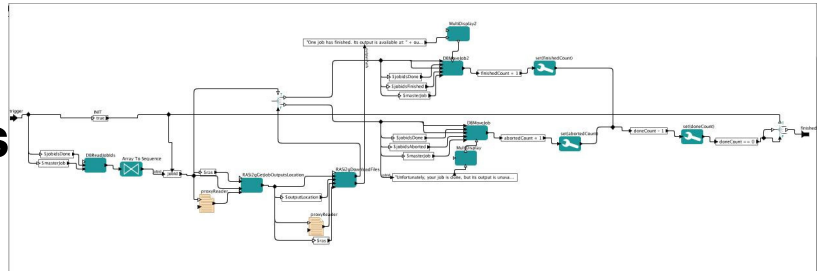
Implementation

- **Unified access to GRID and HPC infrastructures**:
  - **Authorization/Security**
    - *Based on GRID certificates and extended to HPC DEISA*
  - **Execution**
    - *Based on Roaming Access Server*
  - **Data access**
    - *Based on UAL*

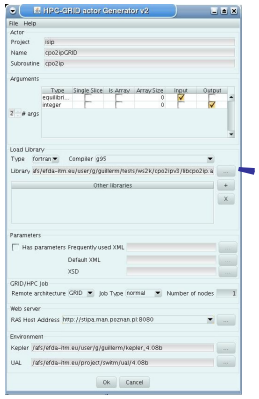


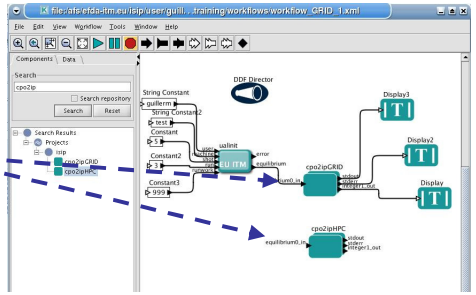
Implementation

- **Reliable/Robust infrastructure**
  - **Handling of the infrastructure errors**
    - *Based on new internal workflows*
  - **Using standard middleware on HPC**
    - *Based on new RAS actors and RAS Unicore server*
  - **Integration of new UAL releases**
    - *Based on automatic generation of the remote data access library*

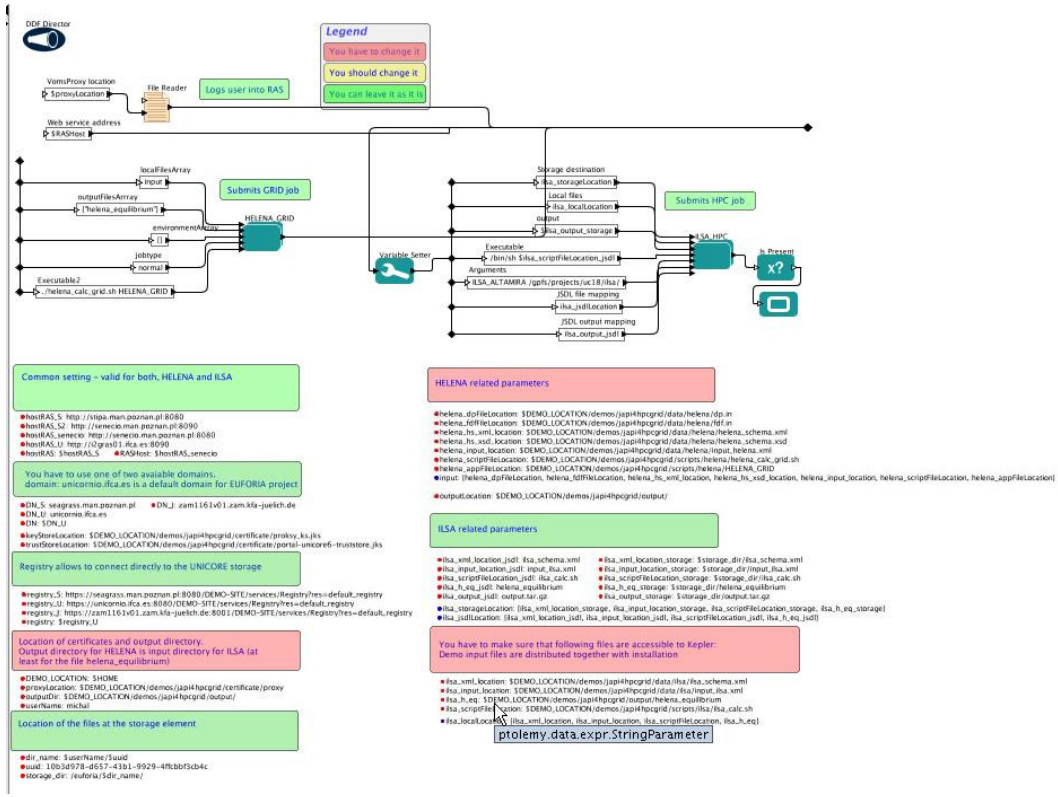


- **Ease of use**
  - **Tools for C++ or Fortran codes**





- **Integration and "Global" activities**
  - **Workflows mixing GRID & HPC**

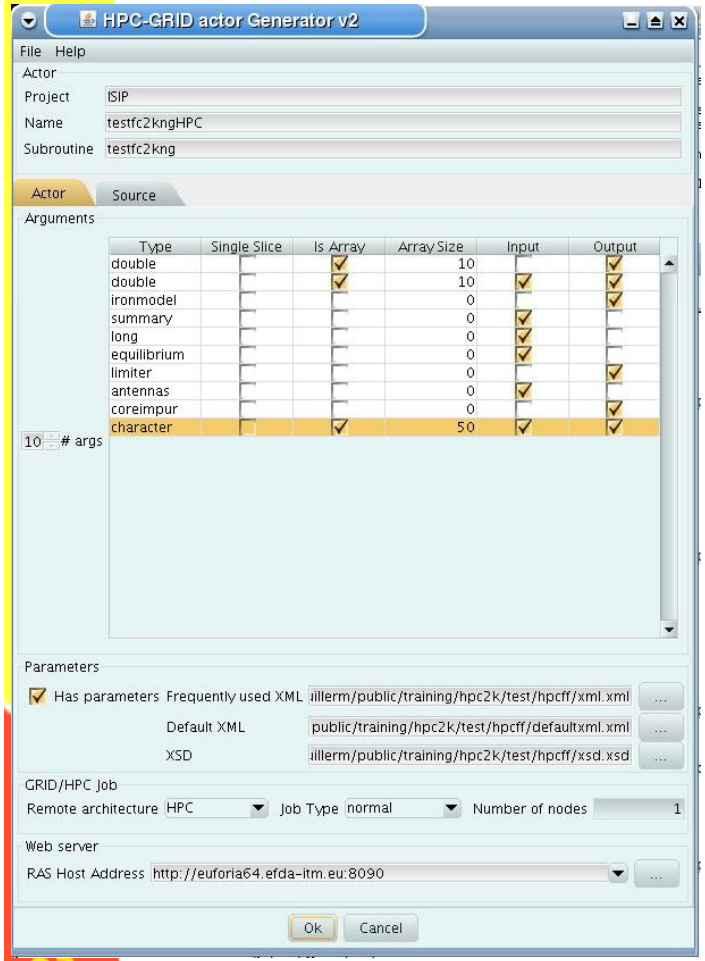


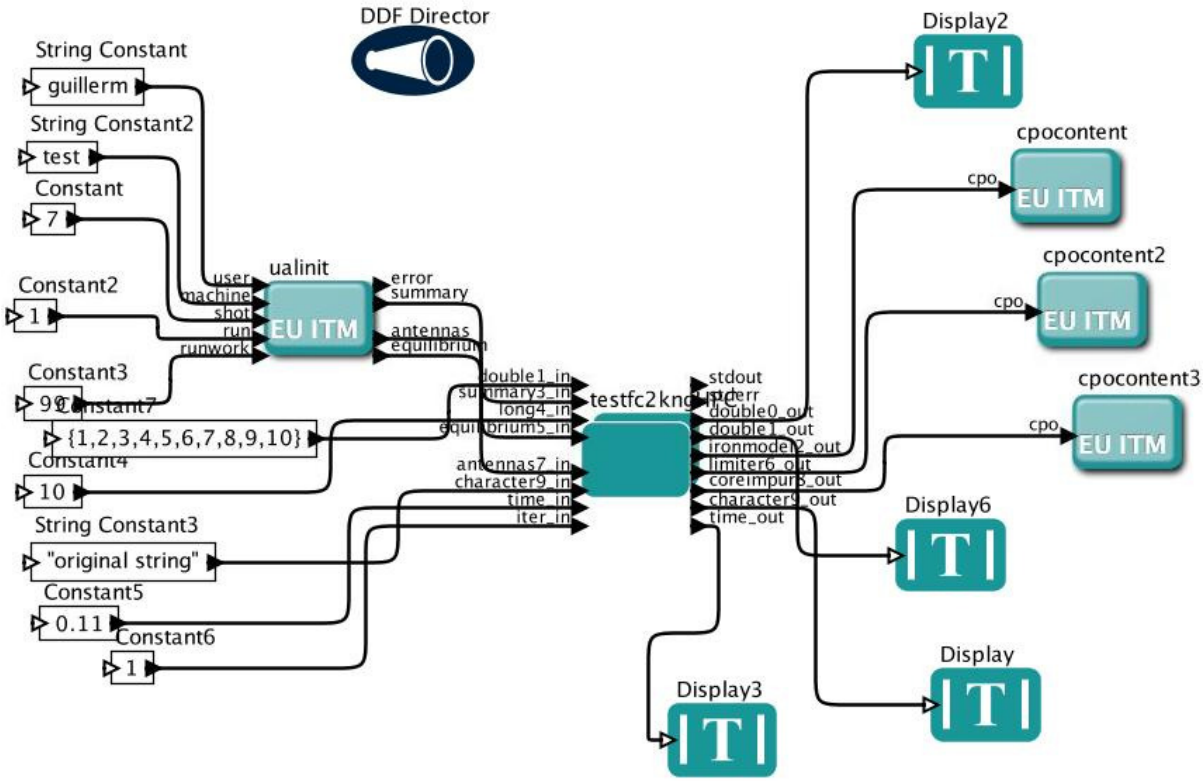
  - **Pilot project**: EUFORIA-EGEE-DEISA
    - Applied to Fusion Simulation Codes

Pilot project

EUFORIA-DEISA		
Milestone		*Comments and status*
ED1*: Demonstrate the technical feasibility of launching jobs from Kepler to a DEISA HPC*		*Done. Use gnuplot. Tutorial and film of a sample run on DEISA machines will be on the website*
ED2*: Demonstrate a real scientific application launched from Kepler to a DEISA facility*		*Done. Execute ELMFIRE on HPC resources.*
ED3*: Demonstrate production capability*		*Done*
ED4*: Demonstrate the possibility of 2-way communication with the scientific workflow during the run of the job on HPC resources*		*Do not have realistic possibility to do it.*
EUFORIA-EGEE		
EE1*: Demonstrate the feasibility by deploying a test case*		*Done. Use gnuplot*
EE2*: Demonstrate a real scientific application*		*Done. Execute VMEC*
EE3*: Demonstrate the possibility of 2-way communication with the scientific workflow during the run of the job on grid resources*		*Done. Use the UAL (Fusion data access) implementation on grid resources*
EUFORIA-DEISA-EGEE		
EDE1*: Demonstrate the technical feasibility of launching jobs from Kepler to a Mixed DEISA and EGEE environment*		*Done. Run simple Fibonacci numbers calculators on HPC and grid in parallel.*
EDE2*: Demonstrate a real scientific application launched from Kepler to a Mixed DEISA and EGEE environment*		*Done. Run sequentially two fusion codes (MHD equilibrium) on both GRID and HPC*
EDE3*: Demonstrate production capability*		*Done.*

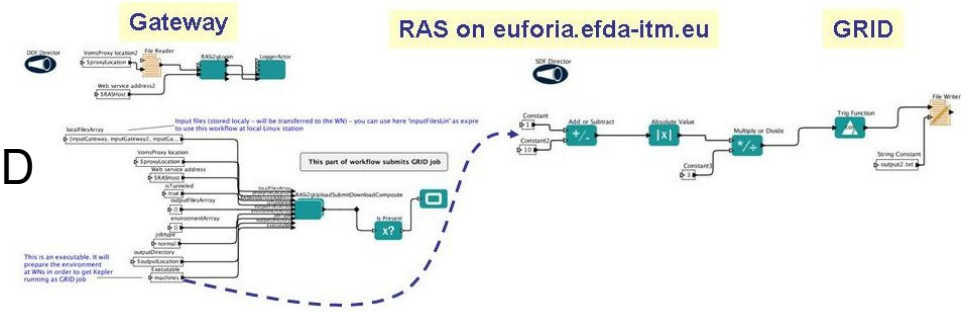
Example of HPC use



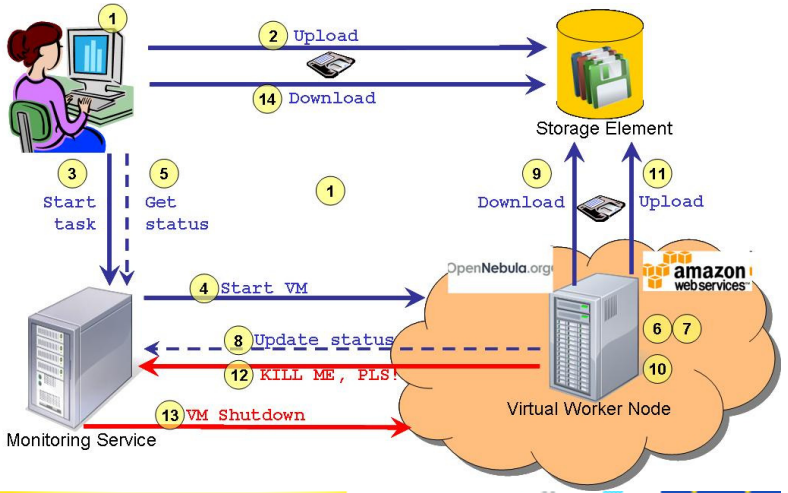


Implementation

- **Ready for the future:**
  - **Distributed workflows**
    - Workflows executed on GRID



  - **Parametric jobs**
    - Parallel Jobs submission => handling of array of job ids
    - TAPAS actor
  - **Cloud computing**
    - Transparent usage of Amazon EC2 and Open Nebula resources



Uses & impacts

- Change in use paradigm:
  - Codes are no longer dedicated to an infrastructure: GRID, HPC, cluster …and Cloud
  - Codes are distributed components
  - Data access is transparent
  - Applications are assembling of distributed components

- Major impacts on several fields/domains:
  - **Super-computer domains**
    - Unifying GRID, HPC and Cloud infrastructures is a major step
    - Used by others projects, (for example EGI_inspire SA3 activity).
  - **Modelling community**
    - RAS actors are implemented in a standard workflow engine (KEPLER: used by the modelling community) => benefit for users from the unified access to GRID, HPC and Cloud computing.

Uses & impacts

- **Fusion simulations**
  - EUFORIA was mainly targeting the fusion community.
  - Close collaboration with ITM-TF: trainings + tools => starting production run.

- **ITER**
  - This huge fusion device will benefit from the development done by EUFORIA for fusion simulations and modelling.

Sustainability path

- **Developments committed back to Open Source repositories (KEPLER)**
  - RAS actors (GRID, HPC & Cloud) => available for other communities and users
- **Developments shared with the Fusion community (ITM-TF):**
  - Revision control using SVN and the ITM Gforge system
  - UAL developments are included in the standard ITM version
  - HPC2K updates have been committed to ITM
  - Demonstrations and examples with Fusion codes are now moving to production run
  - Several JRA3 partners are now working within ITM-TF

Sustainability path

- **Training & dissemination**
  - ITM general meetings: Portici (2008), Karlsruhe (2009)
  - Supercomputing Conferences: SC09 (Portland), SC10 (New Orleans)
  - EGEE meetings: Uppsala
  - GridKa 2009 school
  - ITM & PSNC web sites
  - Public videos: YouTube

- **Further deployment of the tools developed**
  - EGI_Inspire: Fusion, interest from Quantum Chemistry community (under evaluation)
  - PSNC will continue to support new middleware releases (gLite, UNICORE …)
  - ITM-TF is developing a parallel UAL version for HPC-FF

Deliverables & Milestones

Issue	Date	Title	Comments
DJRA3.1	M4	Java API for Glite	Delay due to architecture improvement => M9
DJRA3.2	M6	Extension of the UAL API for GRID	Delay due to unavailability of the data storage & UI (M12) => M16
DJRA3.4	M8	Java API for HPC	On time
DJRA3.5	M10	Extension of the UAL API for HPC	unavailability of the data storage & UI (M12) => M18
DJRA3.7	M12	Registration and Helpdesk System	On time
DJRA3.3	M16	EGEE Scheduler	On time
DJRA3.6	M18	HPC resource scheduler	Safety limitations on HPC => M24
MJRA3.1	M8	Demonstration of workflow in Grid environment	M9
MJRA3.2	M16	Demonstration of HPC workflow scheduling	On time
MJRA3.3	M18	Jobs scheduling within GRID infrastructure	On time
MJRA3.4	M24	Jobs scheduling within the HPC infrastructure	On time

End of Presentation

- Thank you!