

POZNAŃ SUPERCOMPUTING AND NETWORKING CENTER



Support of the workflow orchestration system for fusion
modelling. PSNC ITM-TF 2012 activities

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PSNC

- Implements innovative technologies for scientific community
- Affiliated to the Institute of Bioorganic Chemistry of the PAS
- Research and development center for new generation computer networks, modern applications, portals, parallel and distributed computing
- Integrator of scientific research results via development of services for public administration, healthcare, education and the social area
- Provider of the HPC infrastructure: over 300 TFLOPS (HPC, PC Cluster, GPGPU)
- Operator of Polish National Research and Education Network PIONIER, connected to the GEANT2
- EU projects partner – 95 (coordinator of 6 EU projects, and projects like EUFORIA, ITM-TF)
- 290 employees

HPC Center

- HPC infrastructure
 - PC clusters
 - GPGPU clusters
 - Prototypes on future promising technologies
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- Hierarchical data infrastructure
 - Fast external source of data (computing)
 - Part of National Data Storage
 - Part of European Data Infrastructure



PSNC activities in 2012

- **EFDA ITM-TF Core Programming Team (2 ppy)**
 - User support, documentation (First line support)
 - Maintenance and Upgrade of existing tools
 - Development of new tools / features for the ITM-TF platform
- **EFDA High Level Support Team HLST (0.5 ppy)**
 - ITM-HPC-Workflow: implements the infrastructure used by one of the leading USA group (IPS framework) on the HPC-FF (and/or IFERC) and evaluates it
- **2012 EFDA ITM-TF work programme (0.32 ppy)**
 - WP12-ITM-ISIP-ACT1-T2 (Prepares and provides Tutorials)
 - WP12-ITM-ISIP-ACT3-T1 (**Deploys strategies for HPC and GRID execution of components and workflows, evolution of HPC2K**)
- In co-operation with IPP (Garching) and CEA (Caradache)

EFDA ITM-TF Core Programming Team

- The Core Programming Team can be seen as an important resource for ITM ISIP, with guaranteed availability and significant critical mass, which is required for some of the ISIP tasks
- It consisted 4 computer scientists team (working half time for the CPT) : M.Plociennik, M.Owsiak, T. Zok , B. Palak
- 3 main group of activities
 - User support, documentation (First line support)
 - Maintenance and upgrade of existing tools
 - Development of new tools / features for the ITM-TF platform
- CPT work has been appreciated by ITM-TF leaders

EFDA ITM-TF CPT new developments

- New improved release procedures, parallel versioning of the data structure and UAL engine
- Testing framework for the main services and for automatic validation of the UAL releases.
- Developed easy CPO copy tool from one data version to the other
- Extending existing UAL functionality with complex numbers
- Concept and prototype of a central installation of Kepler on the Gateway
- Execution of
 - Kepler sessions from Multi Instance Composite
 - multiple Kepler sessions on one PC cluster
 - JNI based application via shared libraries from running Java application
- Providing procedures for patching Kepler (ITM version)

EFDA ITM-TF CPT Support Actions

- First line support on daily basis (each working day)
 - over 90 trouble tickets have been solved
 - 200 users
 - responding to users questions via direct mailing exchange
 - large number of smaller problems has been solved during five code camps (not being reported via tracker)
- At least one member of the Core Programming Team was present to any major 2 weeks ITM-TF Code Camp
- CPT members update the documentation in the ITM portal, in the TWiki and developer comments/notes in the involved projects
- Taking part in remote progress review meetings once a month with the ISIP leadership, plus additional meetings on specific technical aspects

EFDA ITM-TF CPT Maintenance

- Maintenance and upgrade of existing tools
 - Releasing of ITM platform
 - Installing monitoring services (Nagios)
 - Work on bugs and fixes:
 - UAL related (memcache, dependencies, wrappers, compilers, MPI, etc.)
 - Memory problems
 - Bugs in Kepler actors
 - Installation and upgrade of software in switm (Doxygen, visit, poco, eclipse, Python, BLAS, LAPACK, MUMPS, etc)
 - Tests of new releases:
 - 4.09a, 4.09b, 4.10a, 4.10a.1
 - gfortran 4.7
 - remote UAL
 - Increasing stability of Remote UAL

EFDA HLST – PSNC Activities

- **Network bandwidth issue with helios computer**
 - investigated the network bandwidth issue that has arisen when the IFERC CSC computer in Japan
- **ITM-HPC-Workflow: implements the infrastructure used by one of the leading USA groups (IPS framework) on the HPC-FF and evaluates it**
 - The Integrated Plasma Simulator (IPS) is a framework for coupled multiphysics simulation of fusion plasmas, in the context of many-task computing.
 - Continuation of the IPS evaluating plan, after the “EU-US Workshop on Software Technologies for Integrated Modelling” in 2010.
 - Part of EU-USA international collaboration activities
 - Evaluation of how it could be used within the EU fusion program.

EFDA-HLST ITM-HPC-Workflow

- Study of the documentation of the IPS
- Compilation, installation and configuration of the IPS on the HPC-FF, also with the XPLASMA libraries
- Running and evaluating provided IPS examples
- Compilation, preparation of IPS workflows and test run of ITM-TF example codes:
 - HELENA model
 - HELENA and ILSA models
 - JALPHA, HELENA and ILSA
 - Initial work on the tightly-coupled use case including loops over the equilibrium - turbulence - transport workflow
- Preparation of a dedicated server in PSNC for better IPS testing

EFDA-HLST ITM-HPC-Workflow

- Preparation of a numerous benchmarks with different numbers of parallel processes on typical cluster and SMP machine.
- Performance analysis
- Discussion and the comparison with the approach implemented in the ITM during the Innsbruck ITM Code Camp in December
 - The results of evaluation have been sent to the USA partners (including the DoE)
- The work is planned to be continued and extended in the 2013

WP12-ITM-ISIP-ACT3-T1

- Identify missing functionalities in the ITM-TF platform and develop new functionalities:
 - Deploy strategies for HPC and GRID execution of components and workflows
 - The deployment of the procedures and tools prepared in past years for executing components of advanced physics workflows on HPC and GRID facilities
 - Evaluation of the proposed strategies and the design of new ones when needed depending on the Use Case
 - Remote execution of whole Kepler workflows
 - The maintenance of GRID and HPC services on the Gateway
 - The consistent evolution of HPC2K
 - Improvements in order to make the tool more robust
 - New features

ACT3-T1 Remote execution of Kepler workflows.

- Dividing time range (time slices) of given shot/run equally among the running processes.
- The task for Kepler submission as a remote MPI workflow was composed of three objectives:
 - submission of the Kepler workflow at Gateway using Gateway cluster
 - submission of the Kepler workflow at HPC-FF
 - submission of the Kepler workflow at Grid.
- 3 working use-cases were implemented

Publications

- **Publications**

- Y. Frauel, D. Coster, B. Guillerminet, F. Imbeaux, A. Jackson, C. Konz, M. Owsiak, M. Plociennik, B. Scott, P. Strand, the contributors to the EUFORIA project, European Task Force on Integrated Tokamak Modelling Activity, **Easy use of high performance computers for fusion simulations**, Fusion Engineering and Design, Available online 23 April 2012, ISSN 0920-3796, 10.1016/j.fusengdes.2012.04.015. (<http://www.sciencedirect.com/science/article/pii/S0920379612002669>)
- Plociennik, M.; Zok, T.; Owsiak, M.; Palak, B.; Guillerminet, B.; Frauel, Y.; Imbeaux, F.; Scott, B.; , **"High level tools for fusion simulations workflows in distributed computing environment,"** High Performance Computing and Simulation (HPCS), 2012 International Conference on , vol., no., pp.602-608, 2-6 July 2012 doi: 10.1109/HPCSim.2012.6266980

- **Contribution to conferences and workshops**

- M. Plociennik, M.; Zok, T.; Owsiak, M.; Palak, B.; Guillerminet, B.; Frauel, Y.; Imbeaux, F.; Scott, B.; , **"High level tools for fusion simulations workflows in distributed computing environment,"** High Performance Computing and Simulation (HPCS), 2-6 July 2012, Madrid

WP12-ITM-ISIP-ACT1-T2

- The main goal of the activity was to provide ITM members with the tutorial in following areas:
 - Building simple workflows in Kepler
 - Building complex workflows in Kepler (loops, composite actors, integration with Python, visualization using build-in actors)
 - Integration of Kepler and ITM tools (FC2K, ISE)
 - Visualization within Kepler (VisIt, Python, Kepler based actors)
 - Workflow debugging (Kepler actors for debugging, TotalView)
- Performed tasks
 - Delivery of tutorial sessions
 - ITM-TF Code Camp Garching (03.2011)
 - Preparation of on-line materials
 - Exemplary workflows development

Plans for 2013

- **EFDA ITM-TF Core Programming Team (2 ppy)**
 - Support to Users, documentation (First line support)
 - Maintenance and Upgrade of the existing tools
 - Development of new tools / features for the ITM-TF platform
- **EFDA High Level Support Team HLST (0.5 ppy)**
 - ITM-HPC-Workflow: further evaluation of the IPS framework
- **2013 EFDA ITM-TF workprogramme (0.32 ppy)**
 - Prepare and provide Tutorials
 - Deploy strategies for HPC and GRID execution of components and workflows, evolution of HPC2K)
- Co-operation with CEA – **support of the ITER Integrated Modelling Analysis Suite for IO**

Thank you !!

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EFDA HLST activities - overview

- Parallelise and optimise codes, including single node optimisation, Open MP and MPI parallelisation, for massively parallel computers;
- Improve the performance of existing codes already designed for parallel platforms;
- Initiate the transfer of other codes to multiprocessors platforms;
- Include Check-point/Restart functionality in the most CPU time consuming codes;
- Make existing codes into community tools and merge codes if needed;
- Choose algorithms, mathematical library routine to adapt applications to the computer architectures and to specific geometries;
- Provide consultancy to existing HPC specialists at the Associates;
- Identify best suited machines for future generations of HPC systems for Fusion applications;
- Exploit the developments and choices made by the ITM Task Force and progress achieved under the EUFORIA Project, especially in the fields of standards, graphical users interfaces, common data bases and parallel visualisation, for the benefit of the HPC-FF users.