

Latest achievements of the Grid Application Support Centre at MTA SZTAKI

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GASuC

Grid Application Support Centre

- **Applications**
 - Recently completed
 - Currently ongoing
- **Lowering barriers for grid application developers**
 - Further development of porting tools
 - Infrastructure test
- **1st P-GRADE Portal User Community Workshop**

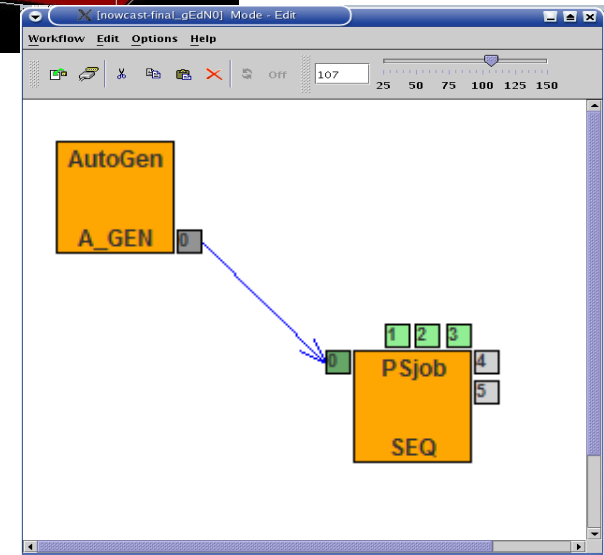
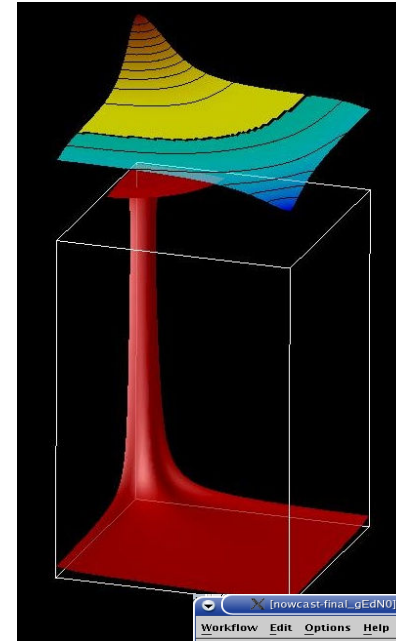
Recently completed

- Earth science
 - Numerical Modeling of Mantle Convection
Geodetic and Geophysical Research Institute, Hungary
 - Fault Plain Solution
 - Earthquake Location Finding
Bogazici University, Turkey
- Distributed systems simulation
 - OMNET++ framework
OMNET community, international

Current

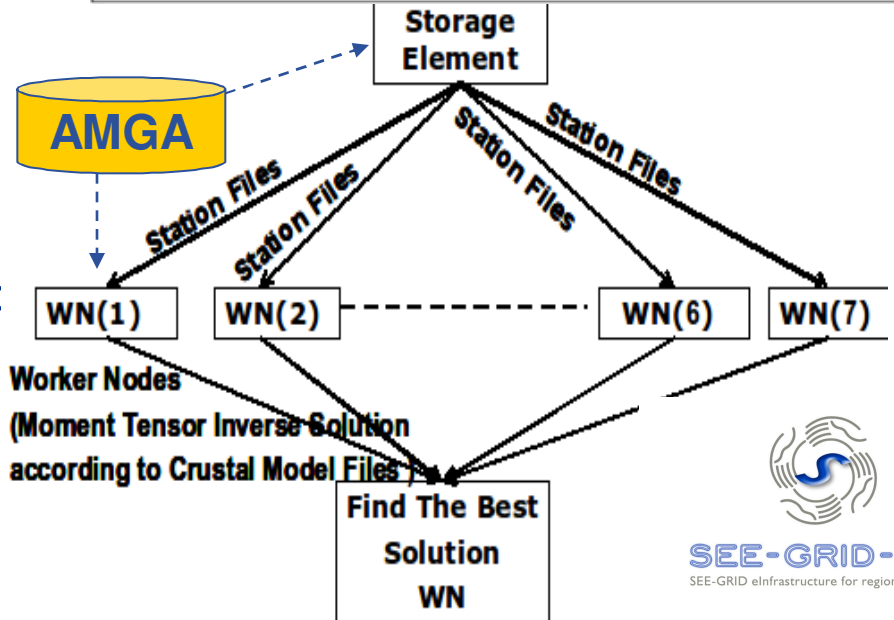
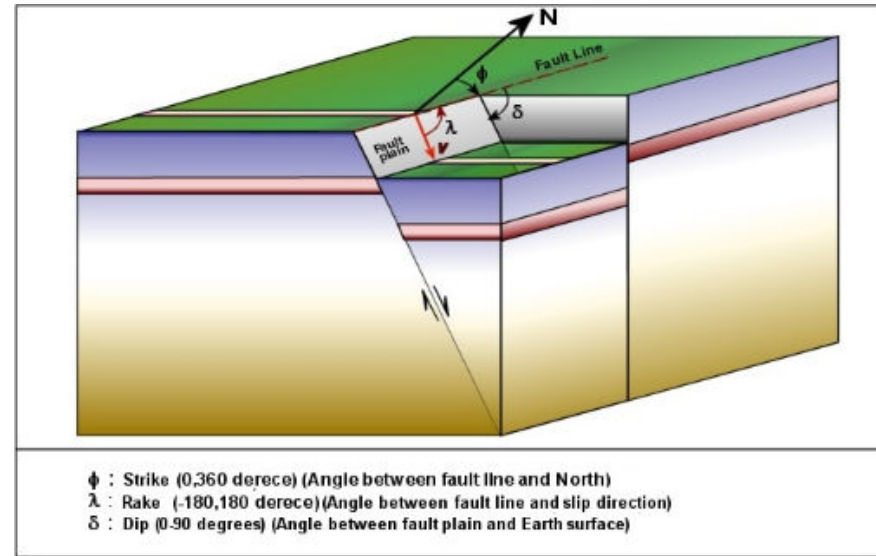
- Life sciences
 - TINKER Conformer Generator
Biological Research Center, Hungary
 - Proteomics analysis for biomarker discovery
University of Groningen, Netherlands

Recently completed applications

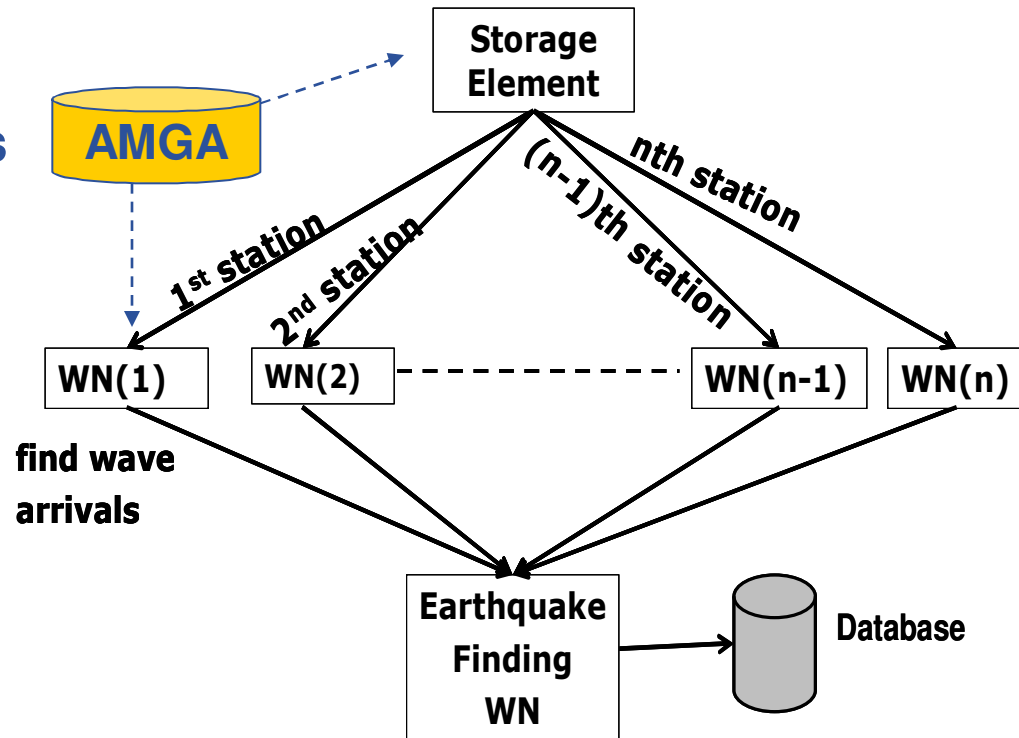


- **Simulating downwellings and upwellings of the outer part of the Earth**
- **Systematic investigation of the parameters that influence mantle convection in 3D**
- **Parameterized workflow:**
 - Generator stage generates input parameters and saves them in grid files
 - Processor stage starts many jobs, each simulates mantels with different parameter sets
- **Implementation:**
 - Workflow in P-GRADE Portal
 - Running on Seismology VO
 - Application specific portlet

- Computes parameters that influence earthquakes
- **Moment Tensor Inversion (MTI) method is used to compute a regional solution**
 - Moment Tensor INVerse Code (TDMT_INVC)
 - Seismic Analysis Code (SAC) library
 - Seismic Data Server Application Service (SDSAS) library
- **Workflow defined with JDL**
 - JDL generated from users' command line inputs
 - Custom scripts to stage files, monitor jobs
 - Jobs submitted to Seismology VO
- **Application specific portal**
 - Under development with P-GRADE

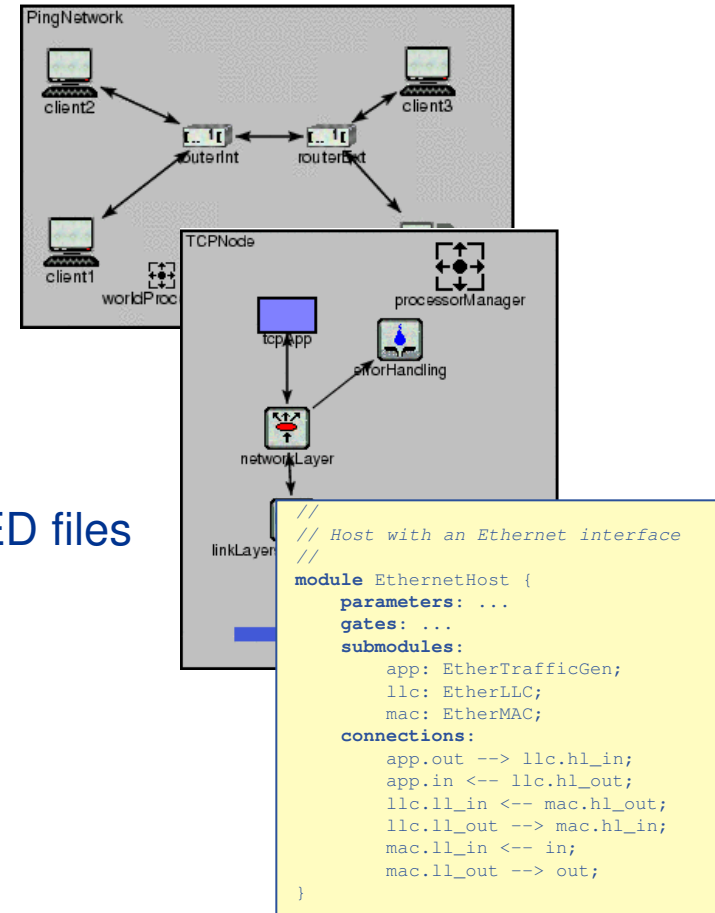


- Finds the hypocenter of an earthquake
- Uses seismic waveform data generated by seismic stations
- Calculation uses HYP071 application
- Workflow defined with JDL
 - JDL generated from users' command line inputs
 - Custom scripts to stage files, monitor jobs
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A generic simulation framework:

- For the simulation of **complex distributed systems**: distributed hardware and software architectures, communication networks, queuing networks, ...
 - An **open** environment
- **Dual licensing**:
 - Academic Public License
 - Commercial License
- **Vivid academic and commercial community**
 - www.omnetpp.org
- **OMNET developers**
 - define new modules (network endpoints) in NED files
 - define simulation parameters in INI file




OMNET user portal

- Automated account cration. Account exists for 1 week
- Only INET and Queuing modules can be used in the topology
 - No binary comes from end user
 - Portal performs grid operations with a robot certificate
- In production:
<https://pgrade-omnet.sztaki.hu>

OMNET developer portal

- Permanent user accounts
- Any distributed system can be simulated
 - Binaries come from end users
 - Grid operations with the users' personal certificates
- To open soon



https://n39.hpcc.sztaki.hu:8443/supergrid/autocc - Windows Internet Explorer

https://n39.hpcc.sztaki.hu:8443/supergrid/autocc

OMNeT++ Discrete Event Simulation System

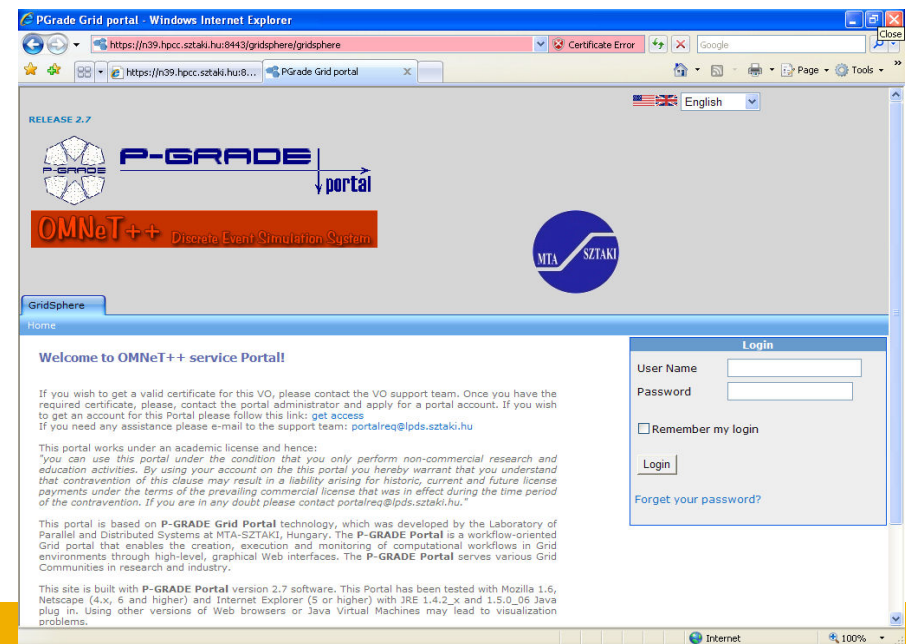
MTA SZTAKI P-GRADE portal

Introduction

This portal provides access to a free on-line service that utilises the power of computing clusters including hundreds of processors to run simulation scenarios defined with the OMNeT++ framework. OMNeT++ is a C++-based discrete event simulation package primarily targeted at simulating computer networks and other distributed systems. With the support of [EGEE Grid Application Support Centre](#) the OMNeT++ framework has been ported to the [EGEE Grid](#) computing platform. The work has exploited the parameter definition services of OMNeT++ and the parameter study support features of [P-GRADE Grid Portal](#). Using these facilities we have created a distributed application that enables the execution of OMNeT++ simulations on the EGEE and [SEE-GRID](#) infrastructures. OMNeT++ users can achieve significant speedup in system simulation with this solution.

Features

The grid-based OMNeT++ environment enables users to upload NED and INI files into the portal environment and to perform simulations based on them using machines of a distributed grid platform. The system takes care about load-balancing, file transfer, brokering and other distributed computing issues automatically. Users do not need to modify their OMNeT++ NED and INI files to perform simulations on the Grid, the same simulations that have been tested and used on your local computer can be performed in the grid now – the only difference that you will



PGrade Grid portal - Windows Internet Explorer

https://n39.hpcc.sztaki.hu:8443/gridsphere/gridsphere

RELEASE 2.7

English

P-GRADE portal

OMNeT++ Discrete Event Simulation System

MTA SZTAKI

GridSphere

Home

Welcome to OMNeT++ service Portal!

If you wish to get a valid certificate for this VO, please contact the VO support team. Once you have the required certificate, please, contact the portal administrator and apply for a portal account. If you wish to get an account for this Portal please follow this link: [get access](#)
If you need any assistance please e-mail to the support team: portalreq@lpds.sztaki.hu

This portal works under an academic license and hence:
"you can use this portal under the condition that you only perform non-commercial research and education activities. By using your account on the this portal you hereby warrant that you understand that contravention of this clause may result in a liability arising for historic, current and future license payments under the terms of the prevailing commercial license that was in effect during the time period of the contravention. If you are in any doubt please contact portalreq@lpds.sztaki.hu."

This portal is based on [P-GRADE Grid Portal](#) technology, which was developed by the Laboratory of Parallel and Distributed Systems at MTA-SZTAKI, Hungary. The [P-GRADE Portal](#) is a workflow-oriented Grid portal that enables the creation, execution and monitoring of computational workflows in Grid environments through high-level, graphical Web interfaces. The [P-GRADE Portal](#) serves various Grid Communities in research and industry.

This site is built with [P-GRADE Portal](#) version 2.7 software. This Portal has been tested with Mozilla 1.6, Netscape (4.x, 6 and higher) and Internet Explorer (5 or higher) with JRE 1.4.2_x and 1.5.0_06 Java plug-in. Using other versions of Web browsers or Java Virtual Machines may lead to visualization problems.

Login

User Name

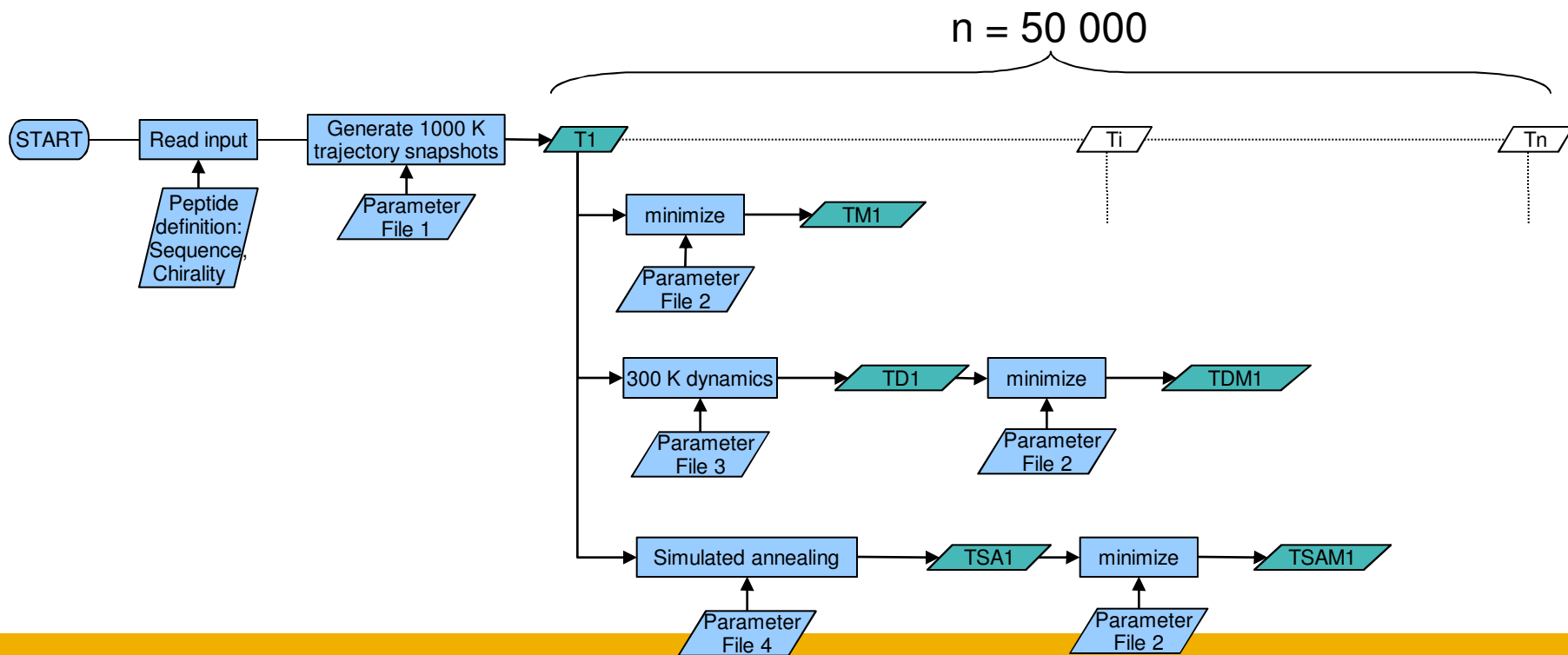
Password

Remember my login

[Forgot your password?](#)

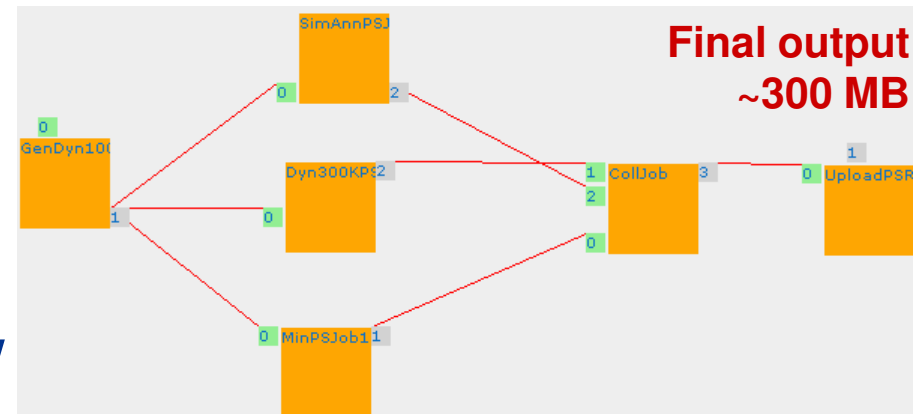
Current applications

- **Complex Fortran package for molecular mechanics, dynamics**
 - Hundreds of use cases
 - Focus on molecular design for drug development: QSAR studies
- **End users are biologists**
 - User friendly interface needed
- **Current model runs for 7 days**
 - 2GHz PC with 1GB memory

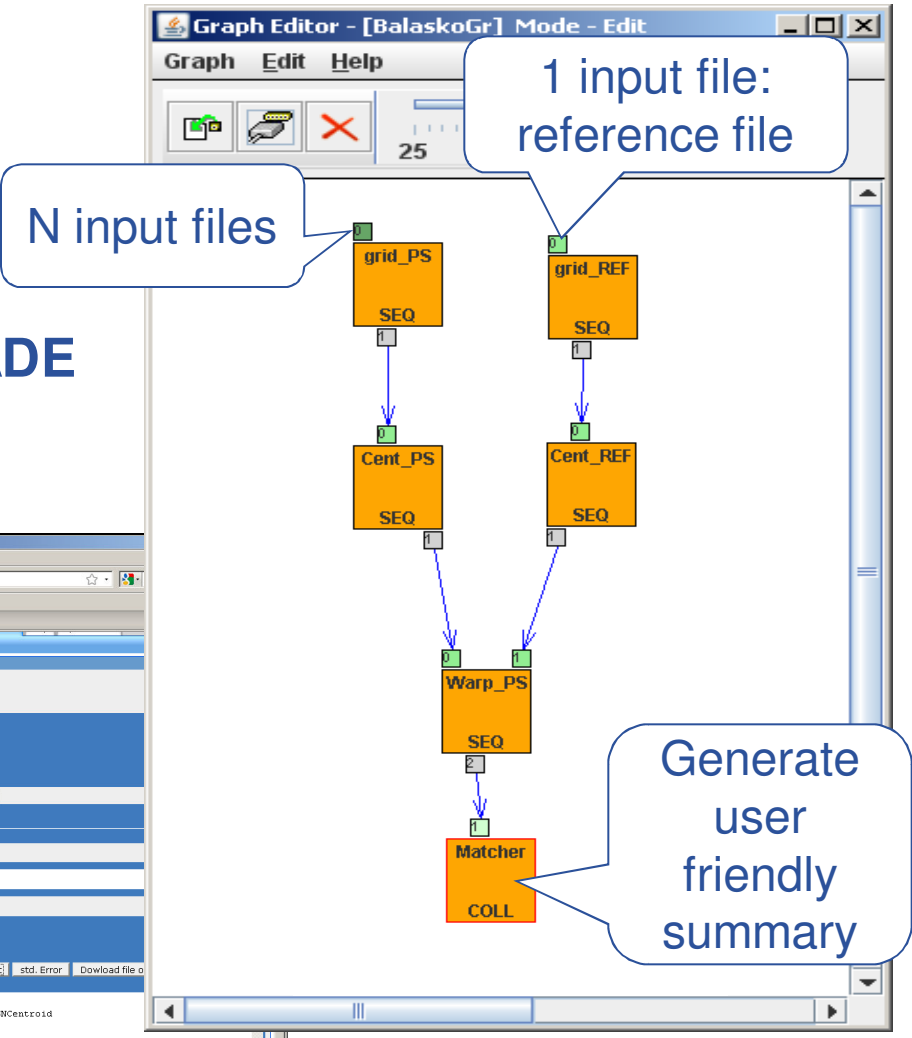


- **Parameter study workflow in WS-PGRADE**
- **50.000 jobs would flood any VO – put 1000 conformer in one job**
 - 3 x 50 jobs, ~10MByte I/O / job
- **Using this method the running time:**
 - VOCE: ~1 day
 - SEEGRID: ~2 days
 - Biomed VO: ~1.5 days
- **Optimization:**
 - Run generation stage of the workflow locally
 - Install TINKER package on CEs
 - Use multiple VOs for different workflow branches
 - Use bigger VOs with more CEs

**Grid execution
3 x 50 jobs**



- Mass spectrometry to identify proteins
- Target users are non-IT persons
 - Graphical portal
 - Fault tolerant execution
- First tests ongoing with WS-PGRADE
 - Dutch Life Science Grid (DLSG)



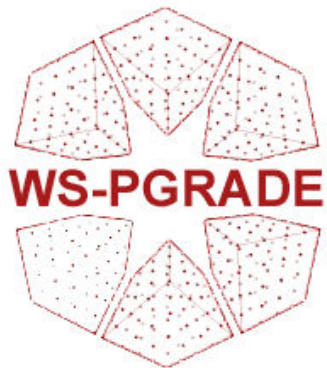
PGrade Grid portal - Mozilla Firefox

Workflows

Workflow name: BalaskoWPS
 Note: 2010-1-28
 Workflow Graph: BalaskoGr

2010-1-28 12:44 finished Details Delete

Job	Status	Instances	Actions
CENT-PS	finished	9	View finished View all content(s)
REF-GEN	finished	1	View finished View all content(s)
Matcher	finished	1	View finished Hide



Lowering barriers for grid application developers

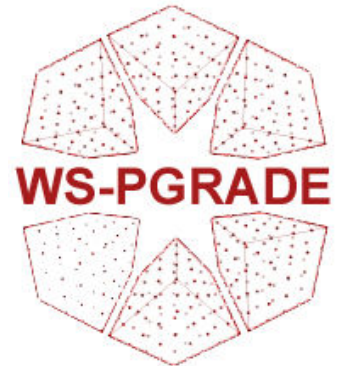
- **P-GRADE Portal**

- Release 2.9.1 (24/Feb/2010)
 - <http://portal.p-grade.hu/?m=releases&s=1>
 - Support for LSF, PBS, ARC, BOINC job submission
 - Workflow repository
 - Using local files for parameter studies
 - Improvements in grid file management, proxy management,
 - Automatic account creator service
 - ...
- Application specific portal development package
 - Control your P-GRADE workflow through any Web interface

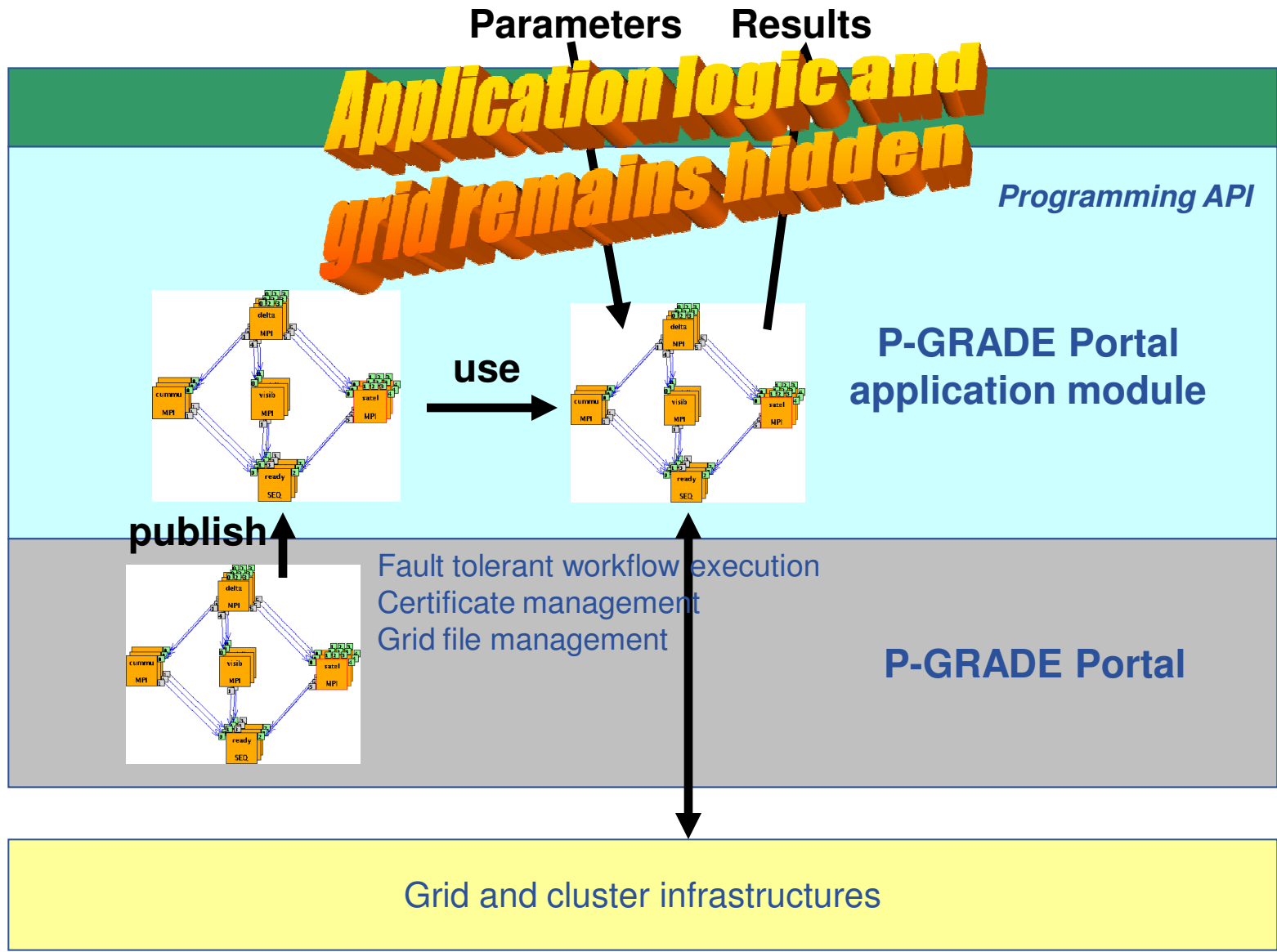


- **WS-PGRADE Portal**

- www.wspgrade.hu
- Advanced workflow patterns
- Database integration
- Service oriented architecture
- ...
- **Presentation on Thursday at 9:40**



Develop an application specific grid portal (Science gateway)

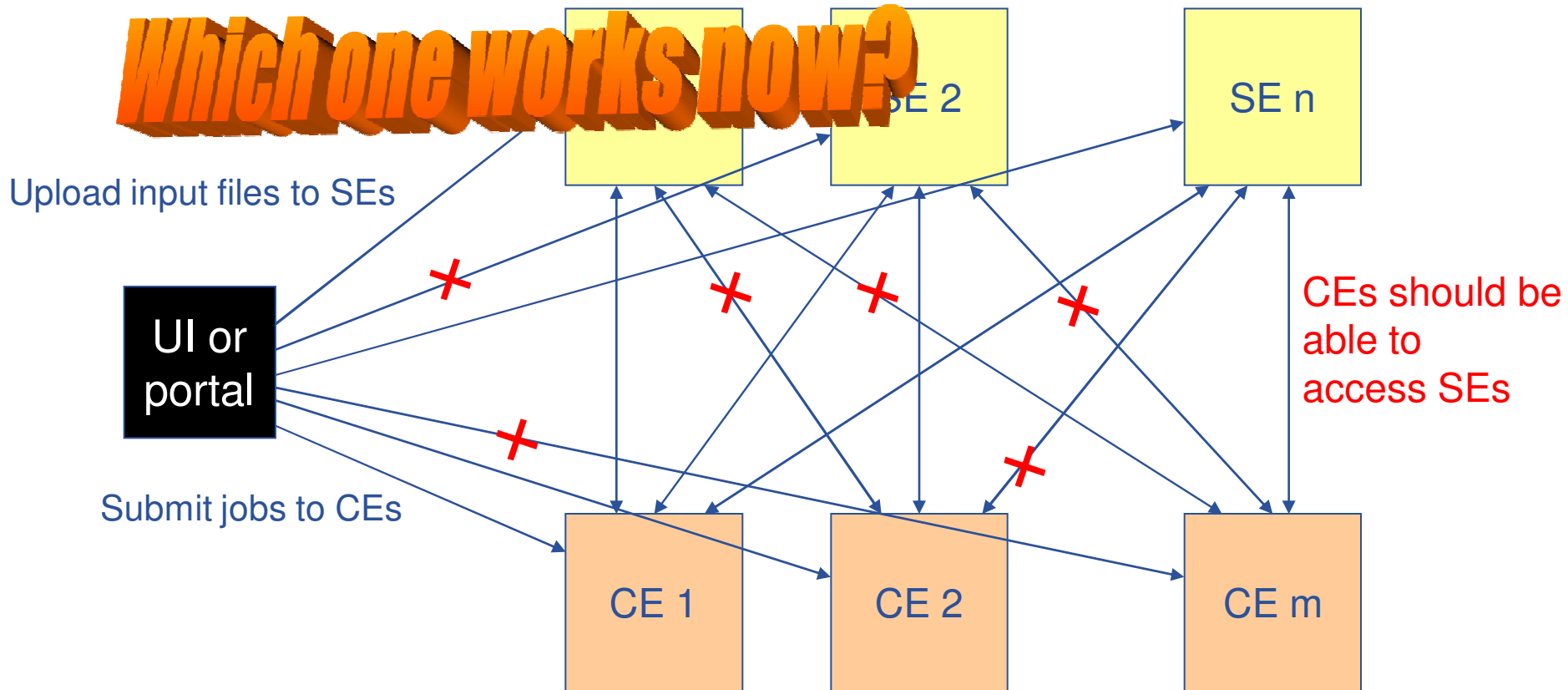


www.portal.p-grade.hu



Some of these links are broken

Which one works now?



- **SZTAKI porting team**
 - ported ~15 applications since the start of EGEE-3
 - is active in the international recognition of grid porting support
 - Is the main developer of successful porting and grid hosting tools
- **Porting services**
 - Provide solution for individual users, for small teams
 - Help large groups establish their own porting expertise
- **Apply for porting assistance at www.lpds.sztaki.hu/gasuc**
 - **SZTAKI will provide international porting support in EGI too**



Free event!
Register now!

- Home
- Program
- Tutorial
- Program committee
- Organizing committee
- Call for presentations
- Important dates
- Contact

Home

In the last two years P-GRADE portal became popular and many Grids and VOs selected it as their science gateway for their user communities (see <http://portal.p-grade.hu/?m=installations&s=0>). Due to the increased interest and number of user communities, the developers would like to provide stronger support and faster response to the requirements of the user communities. In order to achieve this goal we organize the 1st P-GRADE Portal User Community Workshop. The major goal is to share experience of using P-GRADE Portal among the various user communities and portal developers. The program is discussion-oriented. Every presentation will be followed by 15 minutes discussion time in order to give opportunity for the users to express their P-GRADE experience and for the developers to better understand the problems.

The presentations and discussions will be organized in the following sessions:

1. P-GRADE portal installation, administration and maintenance This session is for system admins who manage P-GRADE portal installations. Here we would like to discuss problems they encountered and improvements they recommend.
2. Applications developed by P-GRADE portal This session is for application developers who develop applications using the portal. Here we would like to discuss what they like and what they do not like or miss in the portal.
3. End-user experience with P-GRADE portal Representatives of end-user communities are welcome to share their experience with the portal.
4. Further development of P-GRADE portal Portal developers will present future plans on the further development of the portal. User communities are welcome to give presentation on their additional needs to improve the portal.

A half-day WS-PGRADE portal tutorial will be also part of the program. WS-PGRADE is the second generation of the P-GRADE portal that will be presented and demonstrated during the tutorial. Two application-specific portals developed by the user communities will also be presented: the generic purpose WS-PGRADE portal will also be presented: ProSim portal for protein folding simulation and CancerGrid portal for drug design.

The whole event is free of charge. We would like to share experience with the P-GRADE portal user community in order to improve the portal for their sake and not to make profit from this event.

EGEE Application Porting Support Group

www.lpds.sztaki.hu/gasuc

Questions?