egee

Enabling Grids for E-sciencE

# Status report on Application porting at SZTAKI

Author: Gergely Sipos, Ákos Balaskó

MTA-SZTAKI

sipos@sztaki.hu, balasko@sztaki.hu

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www.eu-egee.org

Information Society
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eGee
Enabling Grids for E-sciencE

- **ABC** and **RWavePR** (from University of Perugia, Italy)

  - Computational Chemistry cluster

  - Storage I/O files registered in LFC

  - Parametric job

  - Workflow in P-GRADE

- **EMMIL** (from International Business School, Hungary)

  - Large number of jobs – clustering to minimize Grid submission overhead

  - Custom Web portal interface in Gridsphere

  - Grid execution engine from P-GRADE

- See more at www.lpds.sztaki.hu/gasuc

- Type of program:
    - Sequential Fortran code, multiple data
- Used VO:
    - COMPCHEM
- Used existing tools:
    - P-GRADE Portal 2.7
        - Autogenerating mechanism to generate set of input files by adding variables, and values' interval.
        - Workflows
        - Remote File Management
- Type of solution for porting:
    - Parameter Study
- Difficulties under development:
    - No program developed to collect data.
- Solution:
    - Develop a script to do this.
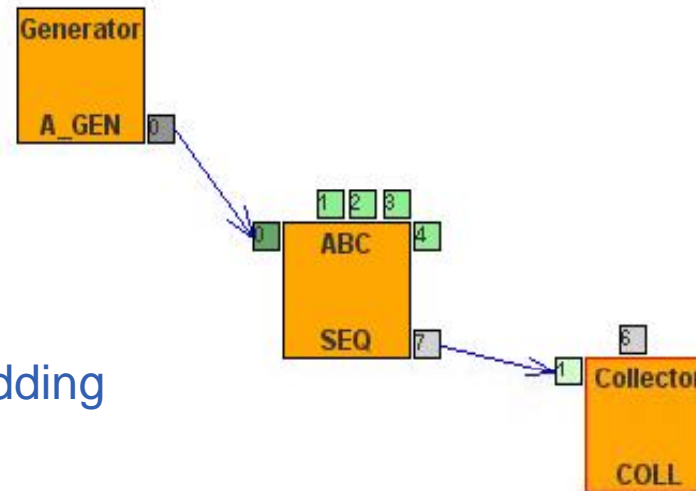
Workflow Manager

Refresh | Back

PS workflow details

PS Workflow	Status	[Output]	[Logs]	[Action]		
ABC_PS_COMPCHEM_AGEN	submitted	N/A	-	Abort	Attach	Delete

Jobs in generator phase

Job	Status	Type	Gridname	Hostname	[Logs]
Generator	finished	auto-generator	compchem_LCG_2_BROKER	Portal Server	Out - -

eWorkflow list

Statistics

Total	Init	Submitted	Rescue	Error	Finished
9	0	9	0	0	0

Workflow	Status	[Output]	[View]	[Action]	
ABC_PS_COMPCHEM_AGEN.1	submitted	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.2	running	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.3	submitted	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.4	submitted	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.5	running	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.6	running	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.7	submitted	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.8	running	N/A	Details	Suspend	Abort
ABC_PS_COMPCHEM_AGEN.9	running	N/A	Details	Suspend	Abort

Jobs in collector phase

Job	Status	Type	Gridname	Hostname	[Logs]
Collector	init	collector	compchem_LCG_2_BROKER	unknown	- - -

June 5, 2008

- Type of program:
    - Sequential Fortran code, multiple data
- Used VO:
    - COMPCHEM
- Used tools:
    - P-GRADE Portal 2.7
        - Autogenerating mechanism to generate set of input files by adding variables, and values interval.
        - PS-Workflow management
        - Remote File Management (LFC Catalog)
        - LCG-2 Brokering
- Type of solution for porting:
    - Parameter Study
- Difficulties under development:
    - No program developed to collect data.
- Solution:
    - Develop a script to do this.

Generator
A_GEN

RWaveP...
SEQ

Collector
COLL

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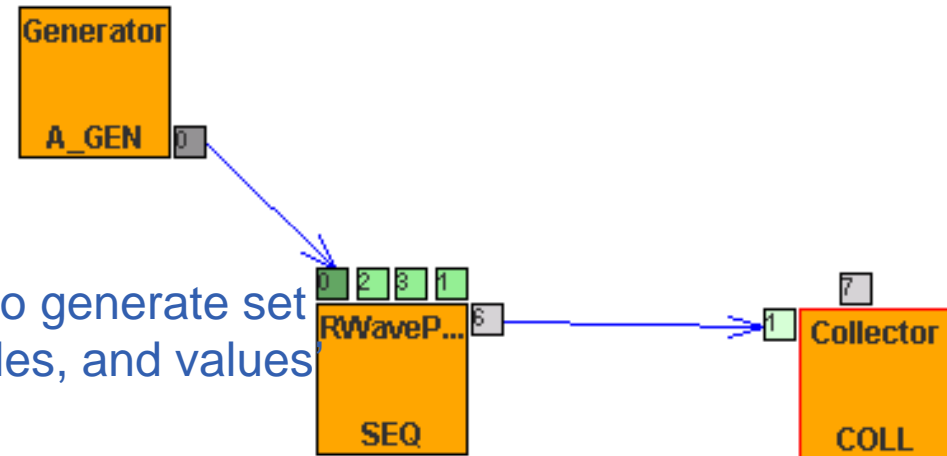
- Type of program:
  - 3 Sequential C program (as Generator, e-Workflow, and Collector)
- Used VO:
  - SEE-GRID
- Used tools:
  - P-GRADE Portal 2.7
  - PS-Workflow management
  - Remote File Management (LFC Catalog)
  - LCG-2 Brokering
- Type of solution for porting:
  - Workflow with Parameter Study
- Difficulties under development:
  - Developing a new portlet as user interface, where users can add inputs, and can see results.
  - Developing script to do workflow generalization, and submission automatically.
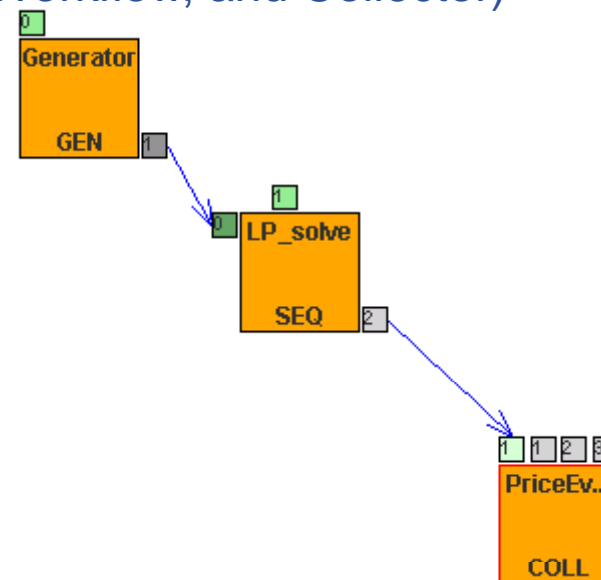
EMMIL P-Grade Procurement Portal

Welcome | EMMIL | Help

Profile | Available Auctions

E.M.M.I.L.

Download finished Auction's results

Available Auctions for Suppliers

Index	Buyer	Date/Time	Remaining Time	Supplier's Time (hours)	Products	Numb. of Supp.Bids	Select
1	Acheron Disuressios (details)	Wed Apr 09 17:35:14 CEST 2008	0 days, 2 hours, 57minutes	3.0	(details)	0	Select
2	Acheron Disuressios (details)	Wed Apr 09 17:33:29 CEST 2008	0 days, 9 hours, 55minutes	10.0	(details)	0	Select
3	Acheron Disuressios (details)	Wed Apr 09 17:32:56 CEST 2008	0 days, 9 hours, 54minutes	10.0	(details)	0	Select
4	Acheron Disuressios (details)	Wed Apr 09 17:30:48 CEST 2008	0 days, 4 hours, 52minutes	5.0	(details)	0	Select

Place a new Bid for the Selected Auction

Index	Required Quantity	Start Price (€)	Product Name	Product Description	Price (€)
1	1250	60.0	SCS838C	#8-32 x 3/8 Socket Head Cap Screws Qty (1000)	47.3
2	1400	7000.0	ICAS200D	Industrial Castors 200mm Diameter	6800
3	560	432.0	2MM9108WICRDUL	Fafnir Bearing	400
4	40	12300.0	SRMS101CP188	#10-24 X 1 Stainless Steel Round Machine Srews, Pack of 100	12000

Place Bid

Wed Apr 09 17:38:05 CEST 2008

Place a new Bid for the Selected Auction

Index	Supplier Name	Fix Price (€)	Variable Price (€)
1	Lukacs Kovacs (details)	430	1300
2	Vladislav Sikurevic (details)	650	2300
3	Ibrahim Malerrika (details)	450	3000
4	Nandor Dombovari (details)	130	2500

Place Bid

Direction Help
From: Sofia To: Athen
Get Directions!
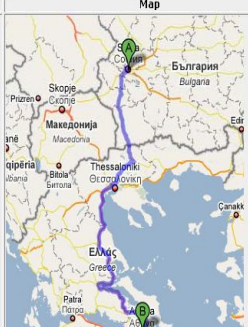
Formatted Directions	Map

Sofia, София-град Bulgaria

804 km (about 10 hours 39 mins)

1. Head **west** — 7.2 km
2. Turn **left** at 18 — 9.2 km
3. Turn **right** at 1/6/E79/ E871 (signs for **Kulata/ Кулата/1/E79**) — 14.1 km
4. Take the exit toward **Kulata/Кулата/Dupnitsa/ Дупница** — 0.3 km
5. Merge onto **1/E79** Entering Greece — 156 km
6. Continue on **E79** — 38.2 km
7. Turn **right** at 12/E79 Continue to follow 12 — 64.9 km
8. Take the ramp to — 0.8 km

Current applications:

- **SIMRI 3D** (from Sorina Camarasu, CNRS CREATIS-LRMN, France)

- **MPI-FD_FDTD** (from Fumie Costen, University of Manchester, United Kingdom)

- **Cortial networks** (from John M. Beggs, Indiana University)

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- Sorina Camarasu (Life sciences)
- Type of program:
    - Sequential C with MPI
    - Needs high-level user friendly interface
    - MPI code might be replaced with other code in the future
- Used VO:
    - BIOMED
- Difficulties of porting:
    - Supporting MPI on many sites
        - Using modified (argument parser) wrapper scripts and tar-ball downloadable from EGEE MPI webpage
    - Extend P-GRADE with custom GUI vs. Extend similar portal with Grid execution engine?
        - We work on option 1, owner works on option 2

- Existing Problem:

  - Only very few sites in Biomed are available for MPI (21%), because only PBS and LSF managers supports MPI

  - MPICH must be installed at least, to be able to run MPI code
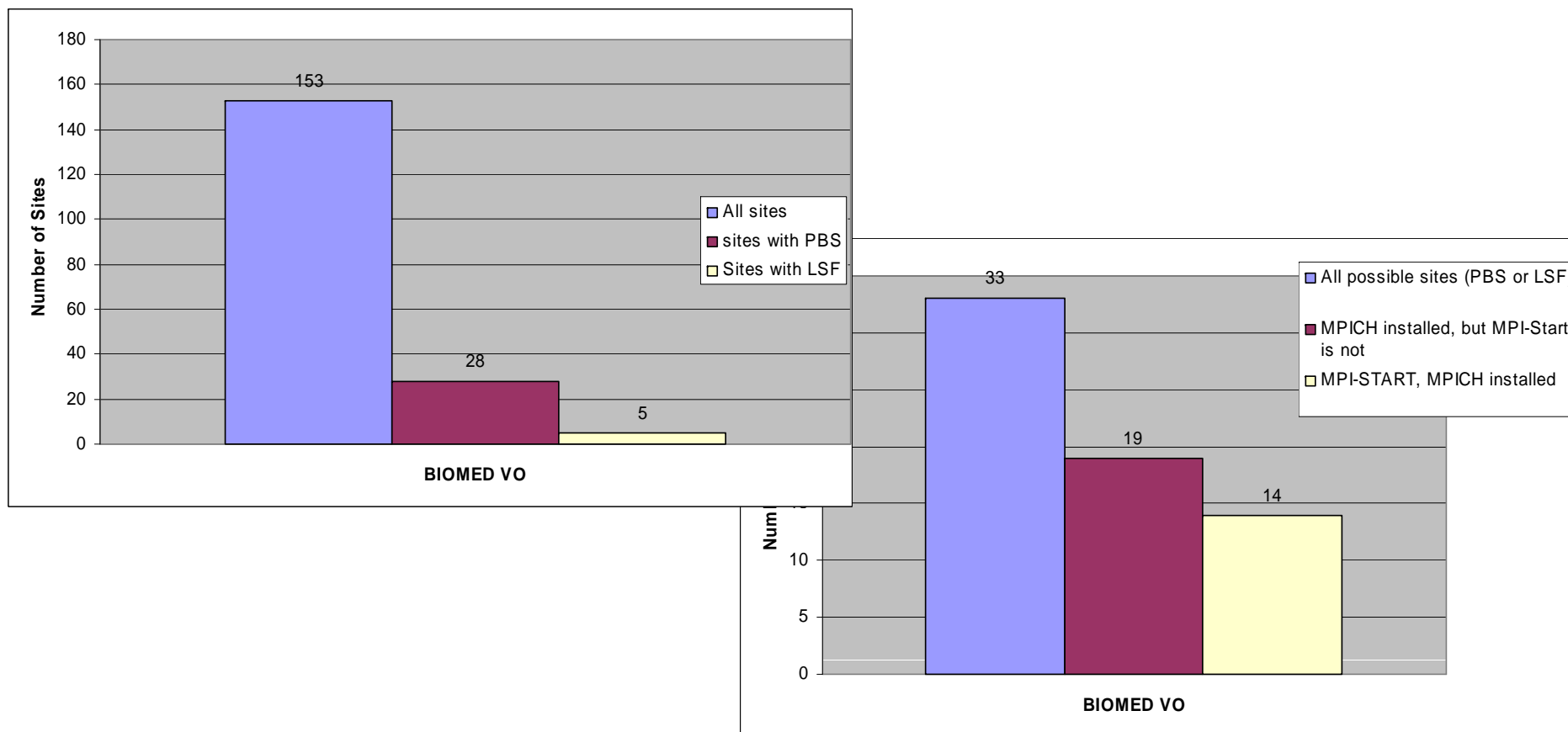
- Fumie Costen (Uni of Manchester)
- Type of program:
  - Fortran with MPI
- Used VO:
  - BIOMED
- Used tools:
  - Command line tools (lcg-*, glite-wms commands) on BIOMED UI
- Difficulties of porting:
  - Same as earlier
  - One execution generates so many small files that WN cannot deal with it
    - Developing a script that copies each output files to an SE separately, saves LFN into a log file, delete local file.
    - Modify source code to use script for file upload
  - .

- John M. Beggs (Indiana University)
- Type of program:
    - C with MPI, MATLAB
- Difficulties of porting:
    - Executing MATLAB code on grid
        - Solved?