Polish Infrastructure
for Supporting Computational Science
in the European Research Space

GridSpace

Experiments in GridSpace Virtual Laboratory – Principles and Examples


ACC Cyfronet AGH
Outline

- GridSpace Motivation and Objectives
- Use Case Story
- Use Case – GridSpace Principles and Solution
- Use Case – Demo
Motivation and Objectives

- Enable scientist to **create, manage, run, share and publish programs** (we call *Experiments*) composed of steps (*Snippets*) written in various programming languages that conduct **entire research method** from raw input data through preprocessing, simulation, analysis, postprocessing to visualization and results study.

- Facilitate employing Computer Centre's resources by (e-)scientists in conducting their research
  - Computing infrastructure (huge power already there)
  - Software packages (already there or to be provided on demand)
  - Legal assets (licenses)

- Improve researcher and research team productivity
  - Release users from doing things that can be automated without any tradeoff
  - Make things that do need user's supervision more interactive
  - Enable once written code to be shared, reusable, published, and protected

- Offer a **generic solution** targeted to a vast range of scientists/domains

- Make it widespread and easily accessible through **single entry point of a web portal**
  - **Experiment Workbench**
Mottos

- Make scientific applications as easily accessible as web sites, ...

- make running scientific application as simple as using web sites, ...

- make writing scientific application as simple as creating web sites, ...

- ...no matter the complex underlying high-performance e-infrastructure.
Use Case Story

- Research team of chemists from Jagiellonian University
- Want to apply a robust method they found published in a top nanochemistry journal
- Method is described textually, no implementation attached
- Hundreds of SEM images to process:
  - Identify pores in nanomaterial
  - Reject irrelevant data
  - Measure the regularity of pore structure
  - Store various metrics of regularity
  - Visualize the metrics in charts and diagrams
  - Choose (manually) a subset of interesting results
  - Extract selected data
  - More thorough visualization of selected data
- One desktop PC, no applicable software
- Three researchers, few MSc students
- They Need help!
Use Case - Solution

Choose proper languages/tools for proper purpose (general-purpose vs domain-specific languages) that were already (or were to be) installed in Cyfronet (Zeus):

- Identify pores in nanomaterial - JNano
- Reject irrelevant data – Bash/AWK snippet
- Measure the regularity of pore structure – Mathematica snippet
- Store various metrics of regularity – Mathematica snippet
- Visualize the metrics in charts and diagrams – GnuPlot snippet
- Choose (manually) a subset of interesting results – manual task
- Extract selected data – Bash snippet
- More thorough visualization of selected data – GnuPlot snippet

Enter GridSpace2 Experiment Workbench (web portal) and choose Zeus UI host (called Experiment Host)

- Write, run, refine, re-run... the snippets one by one in exploratory way until they’re robust,
- Save the resulting experiment as an ordinary file and make it available to your team
- Get the url to the experiment and send it to the team

Team members can paste the url in the browser, log in (using their PL-Grid accounts) to the Experiment Workbench and run the experiment
Let's stay together...

◆ Become PL-Grid user (if somehow you haven't yet)
  ♦ https://portal.plgrid.pl
◆ Play with GridSpace2 demo installation open to all PL-Grid users
  ♦ https://gs2.cyfronet.pl
◆ Use GridSpace2 as an official, validated and certified PL-Grid service (available soon - 16.03.2011)
  ♦ https://gs2.plgrid.pl
◆ Further reading about GridSpace technology on its home web site
  ♦ http://dice.cyfronet.pl/gridspace
◆ Read more on our Distributed Computing Environments (DICE) team and our past, ongoing and future research
  ♦ http://dice.cyfronet.pl
◆ Be our guest at the PL-Grid exhibition stand for more information and live demos
  ♦ Table next to the elevator on ground floor
◆ Contact us if you need any assistance in employing GridSpace in your research