



*Polish Infrastructure  
for Supporting Computational Science  
in the European Research Space*



## **Experiments in GridSpace Virtual Laboratory – Principles and Examples**

**M. Bubak, B. Baliś, T. Bartyński, E. Ciepiela, W.  
Funika, T. Gubała, D. Hareźlak, M. Kasztelnik,  
J. Kocot, M. Malawski,  
J. Meizner, P. Nowakowski, and K. Rycerz**

*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