



# Virtual Laboratory in World-Wide Web

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# Outline



- **Science-as-a-Service**
- **e-Science-as-a-Service**
- From computational experiment to **service**
- From computational experiment to **executable scientific publications**
- **GridSpace2** – web-oriented distributed computing platform
- **Collage Authoring Environment** – executable publication framework
- Science made possible by GridSpace2/Collage Authoring Environment: multiscale application in **Mapper** project
- Conclusions and future prospects



# Science-as-a-Service

Applying software-as-a-service principles  
and IT best practices to science

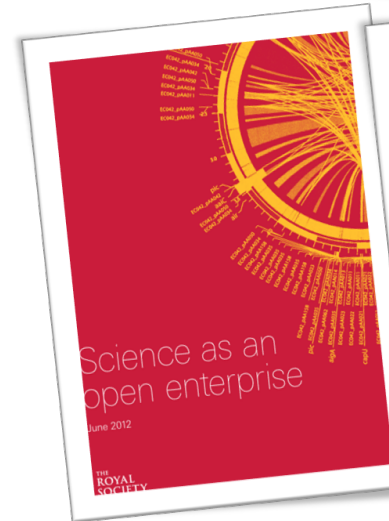
GridSpace2  
all about

## “as-a-service” model

- Proved successful in multiple areas in IT
- Infrastructure-as-a-Service
- Platform-as-a-Service
- Software-as-a-Service

## Software-as-a-service model applied to science

- Core service providers
- Outsourcing
- Service market, competitiveness, ecosystem
- Cost-effectiveness, resource sharing, low entry costs, pay-per-use
- Scientific experiments as a service
- Science as an enterprise
- Crowdsourced science
- Open science



EGI Community Forum 2013, Manchester, 9 April 2013



# e-Science-as-a-Service

Applying software-as-a-service principles  
and IT best practices to e-science

GridSpace2  
all about

...and especially **e-science**

- Data centers as computing power and data storage providers
- Software providers
- IT staff to hire
- Base software platform, tools, problem solving environments
- Computational experiment as a service
- Shared e-infrastructure, reusable and reproducible experiments
- Executable scientific publications



**executable paper  
grand challenge**

knowledge enhancement in the computational sciences



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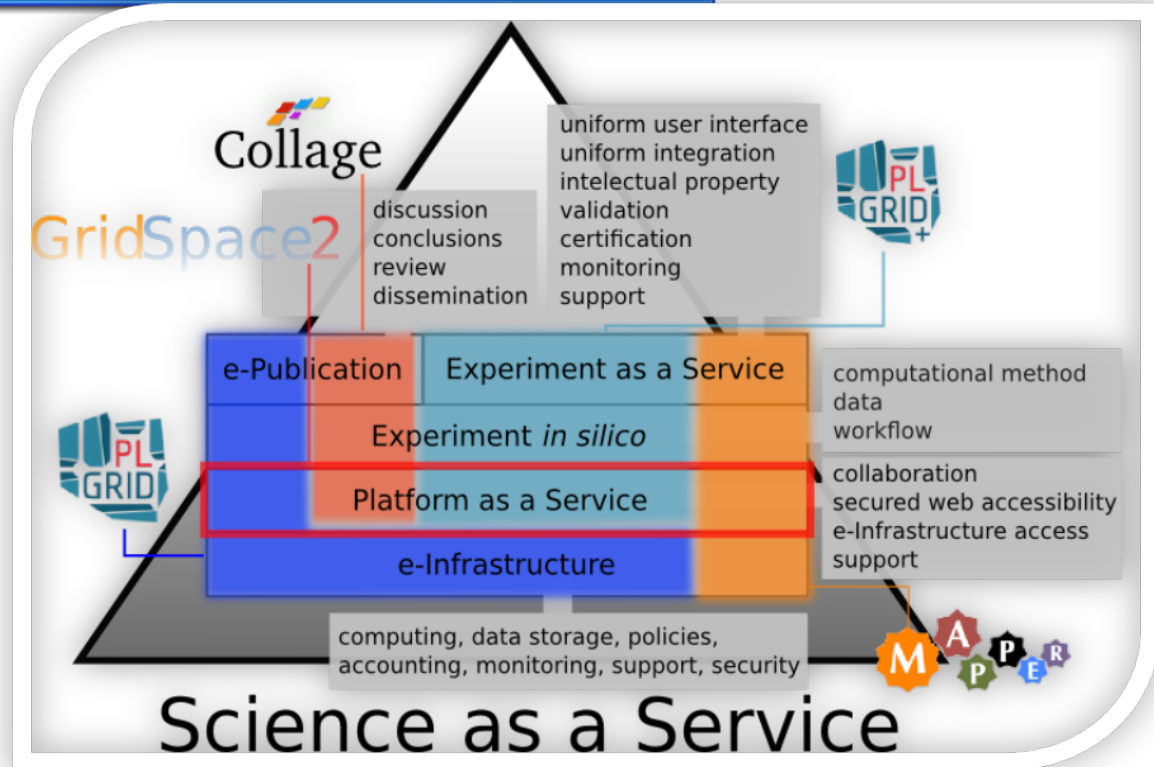
# From computational experiments to services

Common aspects **ensured** or **streamlined** by GridSpace2

GridSpace2  
all about

From computational experiment to service  
(e.g. PL-Grid Plus domain service)

- Integration with common e-infrastructure
- User access management
- Respected intellectual property rights
- Cataloging, indexing
- Accessibility
- Re-usability, re-purpose
- Experiment availability
- Documentation availability
- Examples availability
- Monitoring
- Accounting
- Maintenance
- User support
- Quality assurance
- Security assurance



**Provisioning of services at little cost with GridSpace2 in platform-as-a-service model**



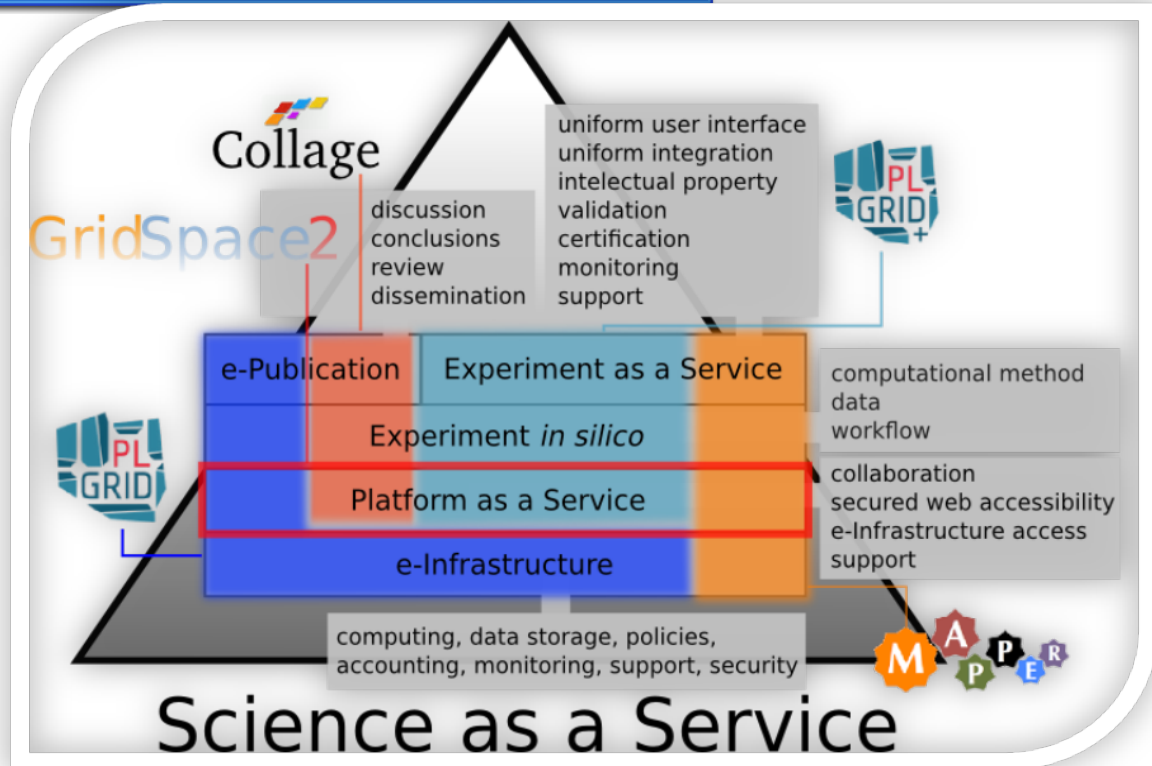
# From computational experiments to e-publications

Common aspects **ensured** or **streamlined** by GridSpace2

GridSpace2  
collaborative

From computational experiment to e-publication  
(e.g. Computers and Graphics  
Journal Special Issue)

- Scientific relevance
- Originality
- Reproducibility
- Verifiability
- Transparency
- Primary data and results availability
- Support for review process
- Publication factors
- Publishing medium

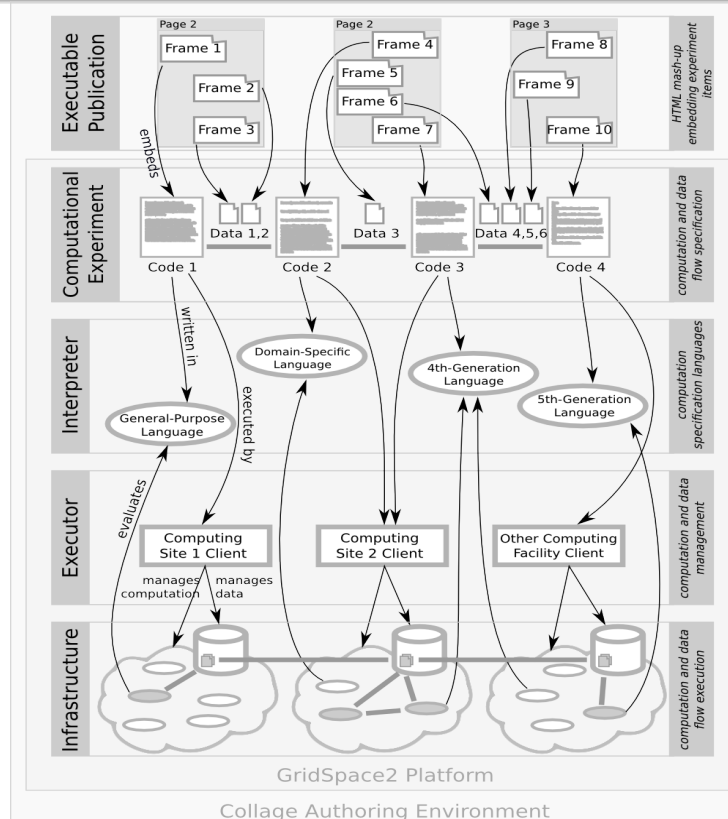


Provisioning of e-publications at little cost with  
GridSpace2 in platform-as-a-service model





# GridSpace2 and Collage Authoring Environment



## Extendability

- Various e-Infrastructures
- Range of interpreters
- Mash-ups on arbitrary web sites
- Pluggable in-browser data item visualization/manipulation modules

## White-box user experience

- Business logic codes as first class citizens
- Explicit, literate programming

## Platform concealing boiler-plate code

## Portable experiments

- Durable
- Sustainable

## Scalability

- Owing to web architecture

Experiments, code, data as URL accessible web resources



# GridSpace2 Platform and Collage Authoring Environment



Collage Authoring Workbench

You are logged in to **collage-exphost.elsevier.com** as **eciepiela**

**Files**

Menu

Upload files

arguments.txt  
collatz.exp.xml  
hwm.png  
iters.png  
last.png  
results\_raw.txt

Filter by file name

Path: eciepiela/collatz/

**Releases**

collage-exphost.elsevier.com: collatz/collatz collage-exphost.elsevier.com: hello

The Collatz Conjecture

Computing sequences for **Ruby 1.8.7** with collage-exphost.elsevier.com

Generating plots **GnuPlot 4.2.6** with collage-exphost.elsevier.com

```
set output 'collatz/hwm.png'
plot 'collatz/results_raw.txt' using 1:3 title "The biggest number (high water mark) reached when iterating"

set output 'collatz/last.png'
plot 'collatz/results_raw.txt' using 1:4 title "Value in last iteration"
```

1 input data defined for this code. 3 output data defined for this code.

**Output**

```
gnuplot> set output 'collatz/hwm.png'
gnuplot> plot 'collatz/results_raw.txt' using 1:3 title "The biggest number (high h water mark) reached when iterating"
```

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Acknowledgements

**Live demo**

<https://gs2.plgrid.pl/>

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# GridSpace2 Platform and Collage Authoring Environment

GridSpace2  
collaborative

GridSpace2 Experiment Portal | scientific computing e-services, scientific e-publications, and any web content enriched with interactive computing capabilities

ABOUT GRIDSPACE2 EXPERIMENT PORTAL

Search

Scientific e-Publications

Implementation of Algorithms of Quantitative Analysis of the Grain Morphology in Self-Assembled Hexagonal Lattices according to Hillebrand method

This work presents the implementation of a method proposed originally by Hillebrand et al. [1] of quantitative analysis of the grain morphology in self-assembled hexagonal lattices.

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eryk.ciepiela@cyfronet.pl Leszek Zaraska Grzegorz D. Sulka Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry, Jagiellonian University, Kraków, Poland [1] R. [...]

By Eryk Ciepiela

Parts by Eryk Ciepiela  
Eryk Ciepiela's Website

THIS WORK PRESENTS THE IMPLEMENTATION OF A METHOD PROPOSED ORIGINALLY BY HILLEBRAND ET AL. [1] OF QUANTITATIVE ANALYSIS OF THE GRAIN MORPHOLOGY IN SELF-ASSEMBLED HEXAGONAL LATTICES.

GridSpace2

You're logged in as plgciepiela@zeus.cyfronet.pl



Eryk Ciepiela

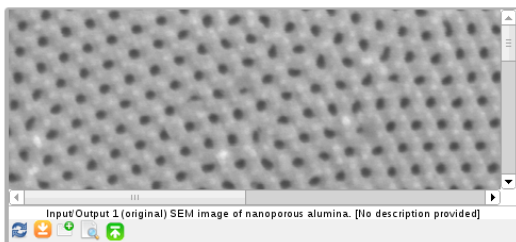
Academic Computer Centre CYFRONET, Kraków, Poland  
eryk.ciepiela@cyfronet.pl

Leszek Zaraska  
Grzegorz D. Sulka

Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry, Jagiellonian University, Kraków, Poland

[1] R. Hillebrand, F. Muller, K. Schwirn, W. Lee, and M. Steinhart, *Quantitative Analysis of the Grain Morphology in Self-Assembled Hexagonal Lattices* in ACS Nano, vol. 2, no. 5, pp. 913-920, 2008

Introduction



```
Source: Mathematica 8.0 Output
(* parameters to adjust !!! *)
minTol = 0.01 (* minimum value of tolerance for spreading algorithm *)
stepTol = 0.01 (* tolerance value step in for spreading algorithm *)
maxTol = 0.20 (* maximum value of tolerance for spreading algorithm *)
pdfNeighborhoodHops = 4 (* order of neighbours (order - how many hops from
one point to another) to include in PDF *)
domainMinimalSize = 7 (* domain minimal size, smaller are not considered a
domain *)
edgeLengthTolerance = 0.5 (* how much variation from the average distance
between pores we still consider as an edge between pores *)

(* end of parameters *)

Snippet 2 (your copy) Analysis of pore structure. Computing triangulation of pore mesh, color coding,
angle distribution function (ADF), pair distribution function (PDF) and domains for a range of
tolerance values.
```

The pore two-dimensional map from Input/Output 3 is then a subject for actual geometry computations carried out in Snippet 2. The resulting files include: the average orientation angle for each valid pore as defined in color coding method (Input/Output 5), angle values for estimation of Angle Distribution Function (ADF) (Input/Output 6), distances between pore pairs for estimation of Pair Distribution Function (PDF) (Input/Output 7) and domain partitioning of the map with respect to tolerances from a given range (Input/Output 8), triangulation of pore centers (Input/Output 9), and pore statistics (Input/Output 10).

1	1295.376	109.59	37
2	723.968	115.405	35
3	626.453	129.921	-1
4	1191.045	126.944	37
5	148.958	141.863	53
6	343.926	147.595	58
7	1090.485	147.075	38
8	528.376	164.017	45
9	981.623	165.162	38
10	1458.204	177.726	36
11	877.94	182.209	37
12	1353.942	194.663	37
13	771.463	198.343	36
14	242.802	197.785	38
15	434.72	204.439	56
16	1251.608	211.594	37

Input/Output 5 (original) Color coding. For each pore (coordinates in columns 1 and 2) the average orientation angle (column 3) from range [-30,30] is computed. For invalid pores the value is set to -40.

Live demo

<http://gs2.cyfronet.pl/epapers/hillebrand-grains/>

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# Science made possible by GridSpace2/Collage platform



- E. Ciepiela, L. Zaraska, G. D. Sulka: *GridSpace2 Virtual Laboratory Case Study: Implementation of Algorithms for Quantitative Analysis of Grain Morphology in Self-assembled Hexagonal Lattices According to the Hillebrand Method*. In: M. Bubak, T. Szepieniec, K. Wiatr (Eds) Building a National Distributed e-Infrastructure - PL-Grid - Scientific and Technical Achievements (2012)
- T. Jadczyk, M. Malawski, M. Bubak, I. Roterman: *Examining Protein Folding Process Simulation and Searching for Common Structure Motifs in a Protein Family as Experiments in the GridSpace2 Virtual Laboratory*. In: M. Bubak, T. Szepieniec, K. Wiatr (Eds) Building a National Distributed e-Infrastructure - PL-Grid - Scientific and Technical Achievements (2012)
- E. Ciepiela, T. Jadczyk, D. Haręźlak, M. Kasztelnik, P. Nowakowski, G. Dyk, M. Malawski, M. Bubak, I. Roterman: *Computations of Protein Hydrophobicity Profile as Virtual Experiment in Gridspace Virtual Laboratory*. In: Bio-Algorithms and Med-Systems (2012)
- L. Zaraska, W. J. Stępniewski, E. Ciepiela, G. D. Sulka: *The effect of anodizing temperature on structural features and hexagonal arrangement of nanopores in alumina synthesized by two-step anodizing in oxalic acid*. In: Thin Solid Films, accepted for publication (2013)
- L. Zaraska, W. J. Stępniewski, G. D. Sulka, E. Ciepiela, M. Jaskuła: *Analysis of nanopore arrangement and structural features of anodic alumina layers formed by two-step anodizing in oxalic acid using the dedicated executable software*. In: Applied Physics A, accepted for publication (2013)
- \*\*\*. In: *Computers & Graphics, Special Issue featuring Executable Papers*, to appear (2013)
- Your publication maybe?

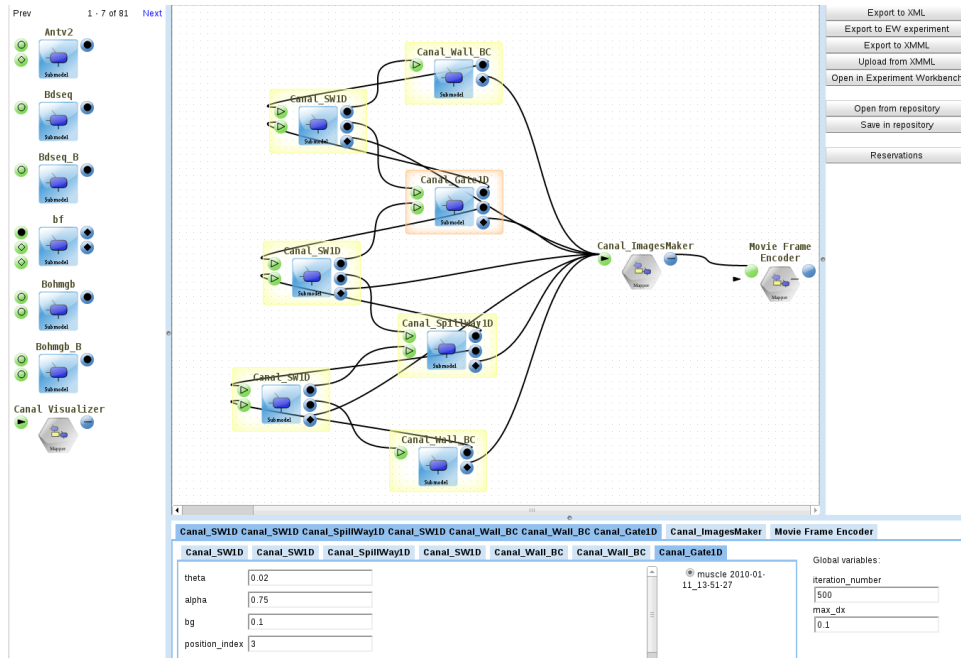
Pilot case studies for GridSpace2 and Collage

Publications made possible by GridSpace2

Executable publications powered by GridSpace2 and Collage



# Case study: Multi-scale applications in Mapper project



Multi-scale Application Designer



GridSpace2  
alias bac67

You are logged in to zeus.cyfronet.pl as plgciepieta

GridSpace2 Experiment Workbench

Files

Menu

Upload files

Files list:

- cacerts/
- certs/
- csmotifs/
- download/
- erlang-pbs/
- erlang/
- exps/
- logs/
- matlabdemo/
- mcr-r2012b/
- nanosstruct/
- phpprofile/
- profiles/
- Results0304123342/
- Results0304130734/
- Results0304142138/
- tj/
- tmp/
- tmpo/

Filter by file name

Path: plgciepieta/

Releases

Output

Movie Frame Encoder mencoder 4.1.2 with zeus.cyfronet.pl

```
mf://Movie_Frame_Encoder_in_img_id-054/* -mf
w=800:h=600:fps=25:type=png -ovc lavc -lavcopts
vcodec=mpeg4:mbd=2:trell -oac copy -o
Movie_Frame_Encoder_out_avi_movie_id-054
```

qsbus: waiting for job 27667773.batch.grid.cyf-kr.edu.pl to start  
qsbus: job 27667773.batch.grid.cyf-kr.edu.pl ready

Path: MEncoder SVN-r34896-snapshot-4.1.2 (c) 2000-2012 MPlayer Team

GridSpace2

# Conclusions



- Inefficient traditional model pushes scientists and research organizations to seek new business models for science
- Software-as-a-service model proved effective in IT market, science-as-a-service can too, especially in e-science
- E-science services are not only software and data but complete and consumable products
- Scientific findings and methods need new ways for communicating and disseminating to embrace reusability, verifiability, reproducibility, transparency, executability
- GridSpace2 is a platform-as-a-service that facilitates provisioning of experiment-as-a-service at low cost
- GridSpace2 support for multi-scale loosely-coupled applications in the Mapper project
- Collage Authoring Environment overlays GridSpace2 and enables executable scientific publications
- Collage Authoring Environment is integrated with Elsevier ScienceDirect portal



# Future Prospects



- In the context of PL-Grid Plus project GridSpace2 will be used as a platform for streamlined provisioning of domain services
- Collage Authoring Environment will empower special issue of “Computers and Graphics” journal featuring executable publications
- We’re supporting research teams in provisioning of services and e-publications



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