

GridSpace2 - Comprehensive Platform for Managing e-Science Applications

Eryk Ciepiela (1), Daniel Hareźlak (1), Joanna Kocot (1), Marek Kasztelnik (1), Jan Meizner (1), Grzegorz Dyk (1), Piotr Nowakowski (1), Tomasz Gubała (1, 3), Tomasz Bartyński (1), Maciej Malawski (2), Marian Bubak (2, 3)

(1) AGH University of Science and Technology, ACC Cyfronet AGH, Krakow, Poland
 (2) AGH University of Science and Technology, Department of Computer Science, Krakow, Poland
 (3) Informatics Institute, University of Amsterdam, The Netherlands

Distributed Computing Environments Team
<http://dice.cyfronet.pl/>

Objectives

- Provide convenient web interface for managing e-science applications throughout their entire life-cycle including prototyping, authoring, sharing, operation, and evolution
- Provide generic interface to heterogeneous computational resources including PCs, private clusters, supercomputers, grid
- Allow for specifying and publishing e-science applications in a portable execution environment-agnostic format

Solution

Experiment Workbench

As a single user entry point to the GridSpace2, the Experiment Workbench facilitates exploratory writing, running and managing e-science experiments. URL-accessible experiments and their results can be shared, published and catalogued as any other web resources.

Experiment

E-science application is composed of code fragments called **snippets**, expressed in either general-purpose scripting programming language (e.g., Python, Ruby, Perl, Bash etc.), domain-specific language (e.g., quantum chemistry problem description, nanostructure description) or purpose-specific notation (e.g., for drawing plots). Snippets are evaluated by respective programs called **interpreters**.

Computational Resources

Behind the scenes a tremendous computational capabilities are enabled to be used by scientific applications including public e-infrastructure sites and private clusters. Depending on processing and interactivity demands the computations can be submitted to the server, cluster, grid e-infrastructure or executed within a user's web browser.

Embedded Experiment

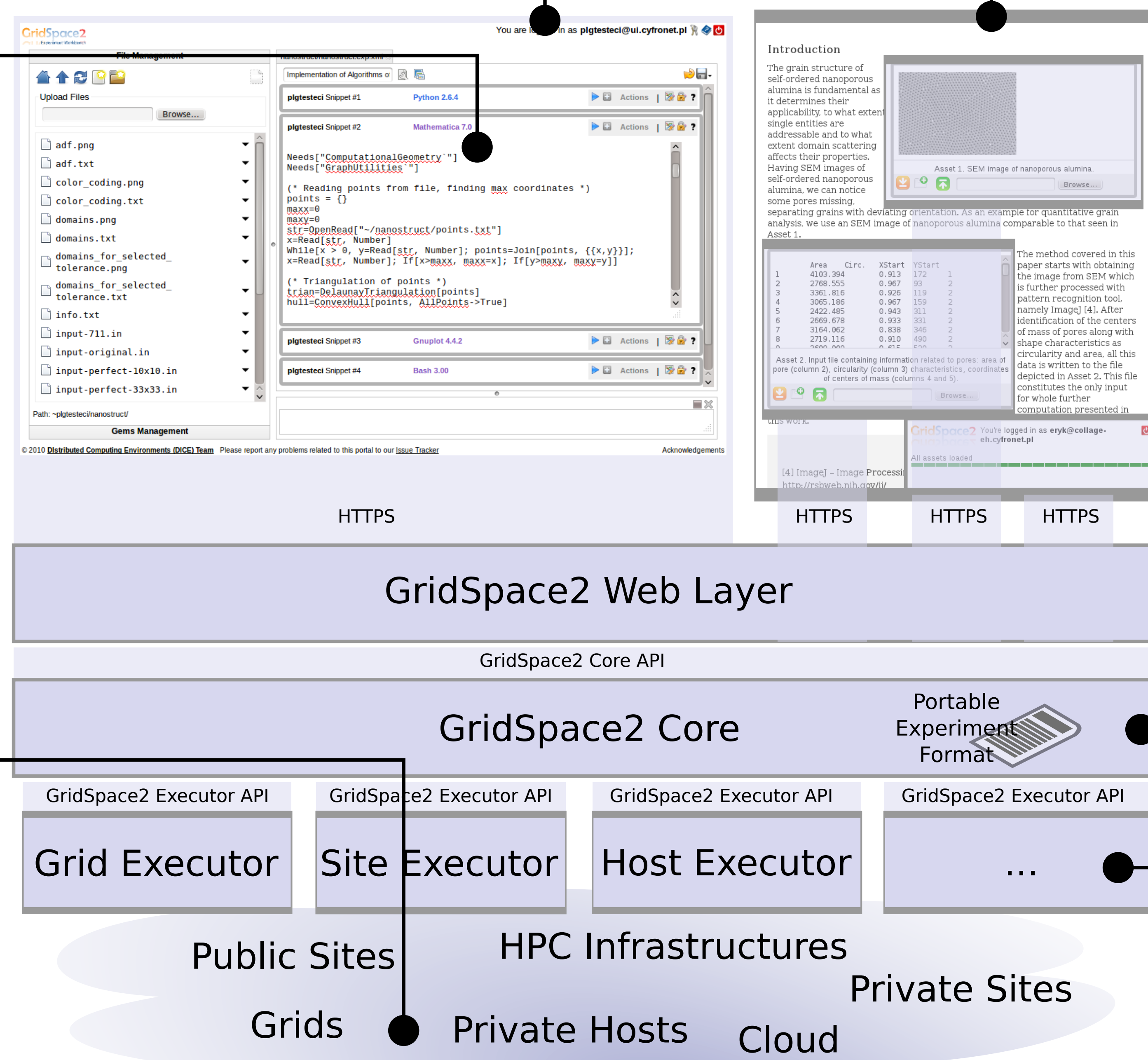
Published experiment can be embedded on arbitrary web sites owing to the Collage Authoring Environment feature and thus enrich web content by allowing experiment execution by one click trigger.

Core

GridSpace2 Core, that runs behind the web layer, is a Java library providing API for creating, persisting, managing and running experiments. It is configured by GridSpace configuration file which records all available interpreters and their installations on the underlying computational resources. The experiments are handled in execution environment-agnostic **portable format**, not dependent on execution environment - they are mapped to specific computational resources only at the execution step.

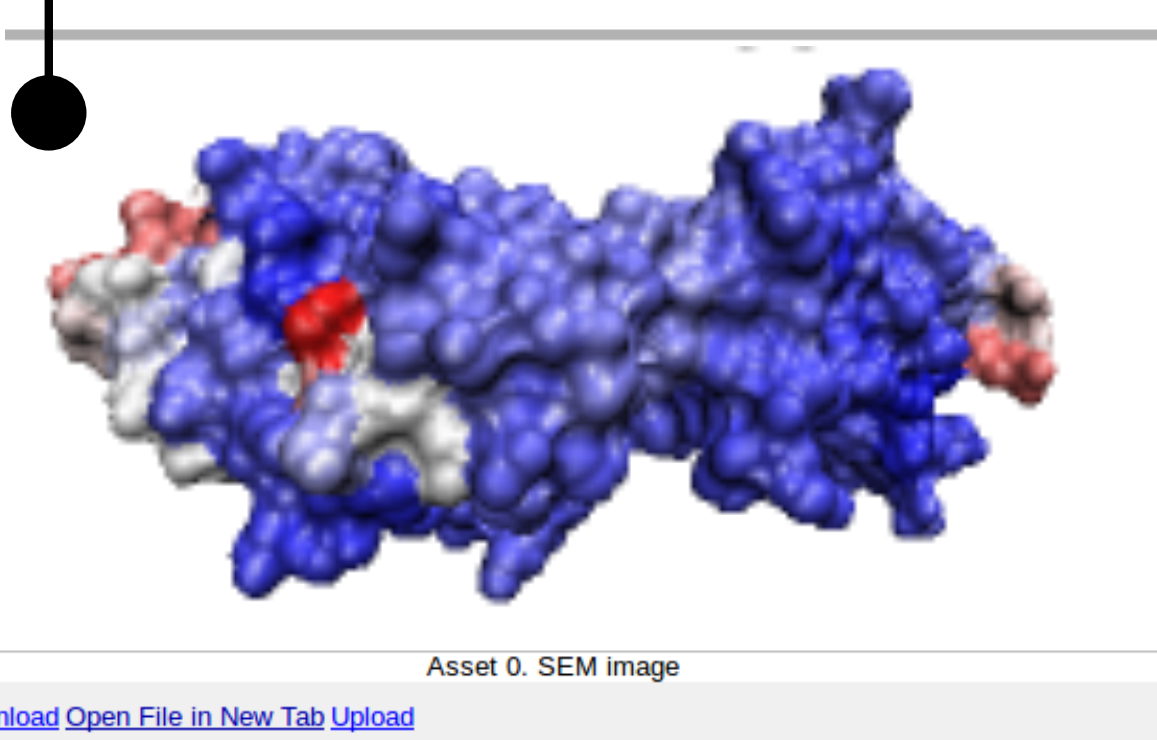
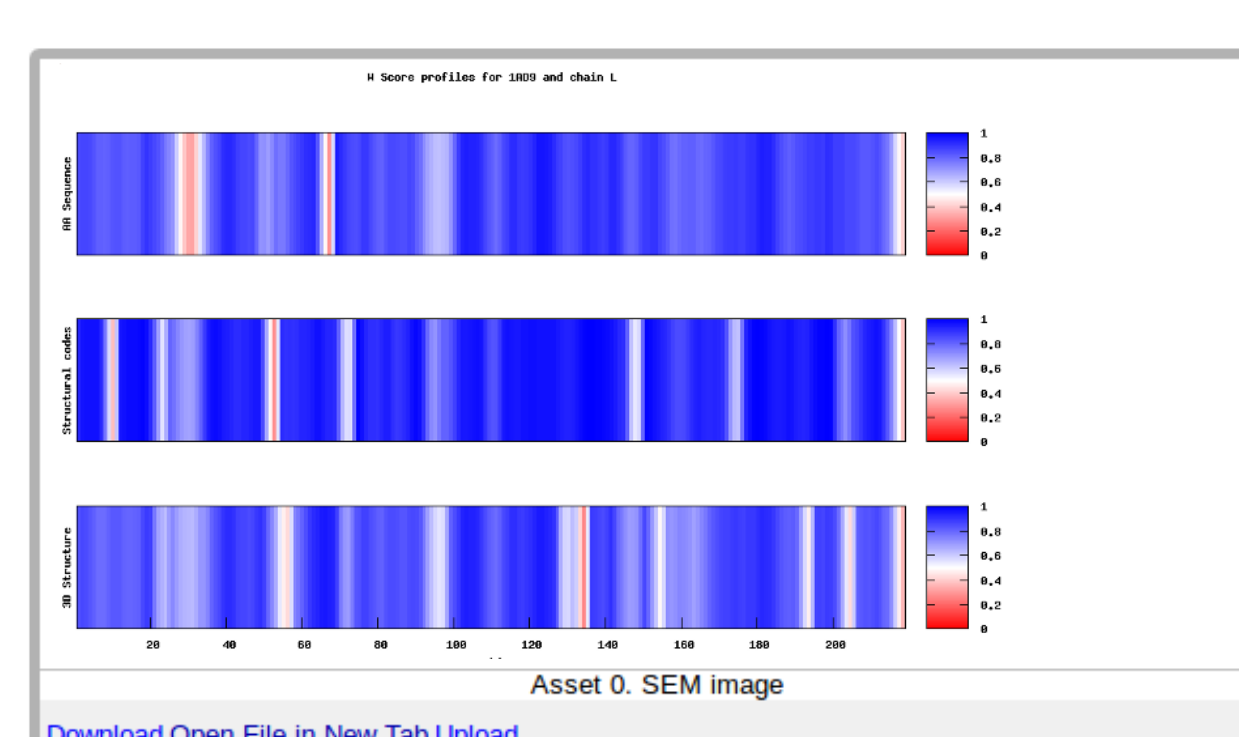
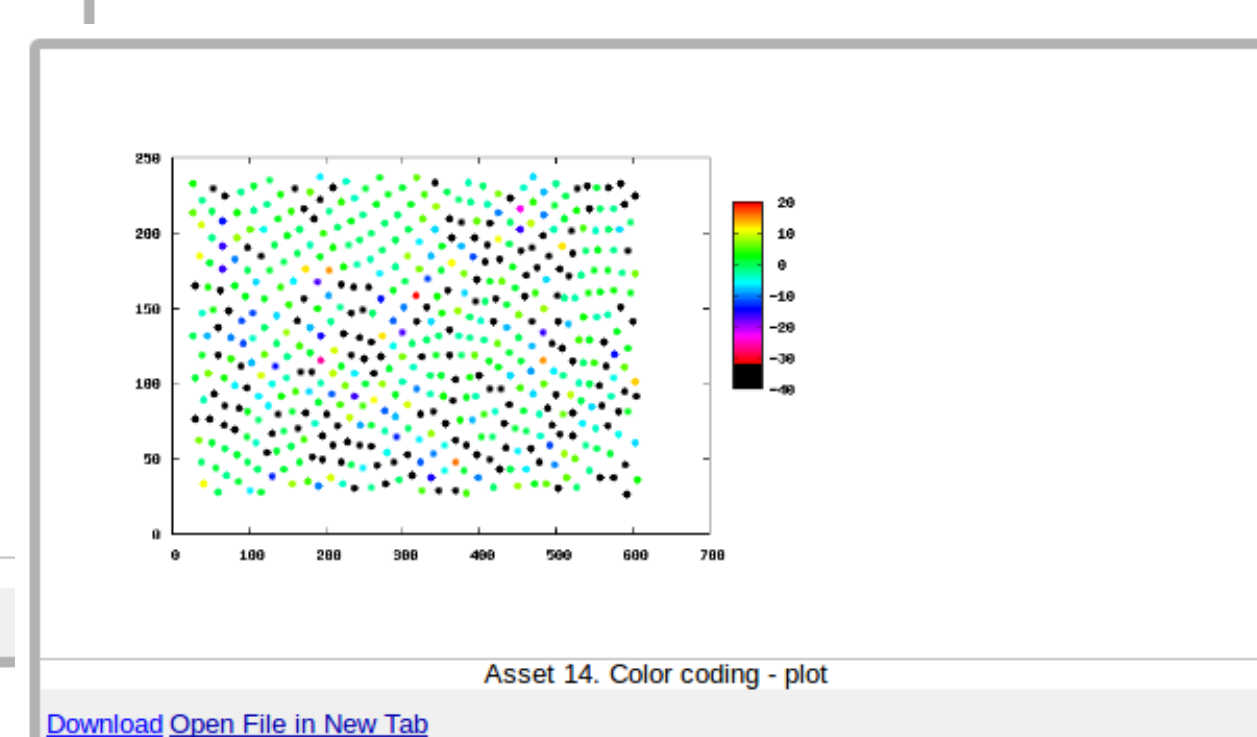
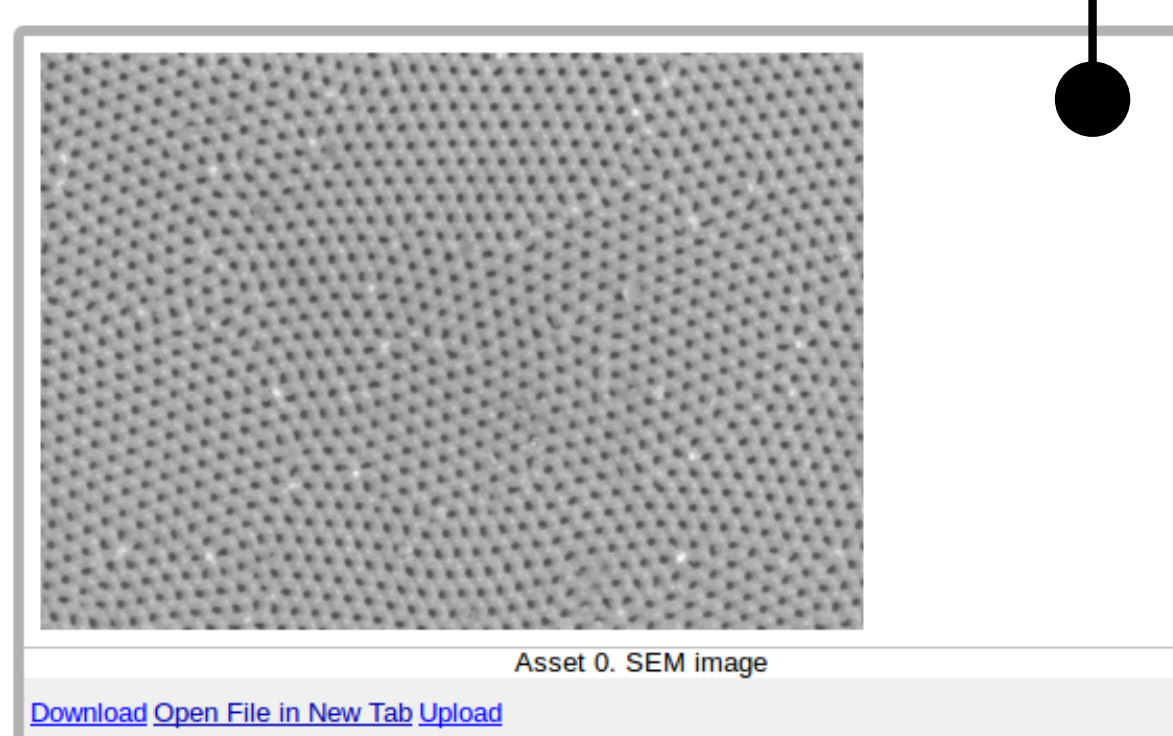
Executors

GridSpace2 Core dispatches computations to underlying computational resources. Executors deal with specifics of resource type, its interface, security mechanisms being used etc. The architecture of executors is open and allows for adding new and custom ones. At the execution step users decide how to arrange computations on the resources available by attributing executors to the snippets.



Example Applications

- Analysis of **nano-materials** and **protein structures** by using the specialized software installed on the PL-Grid e-infrastructure
- **Multiscale applications** that span over diverse resources and e-infrastructures



References

[1] GridSpace home site, <http://dice.cyfronet.pl/gridspace/>
 [2] E. Ciepiela, D. Hareźlak, J. Kocot, T. Bartyński, M. Kasztelnik, P. Nowakowski, T. Gubała, M. Malawski, and M. Bubak, "Exploratory programming in the virtual laboratory" in Proceedings of the International Multiconference on Computer Science and Information Technology, Wisla, Poland, 2010, pp. 621-628
 [3] P. Nowakowski, E. Ciepiela, D. Hareźlak, J. Kocot, M. Kasztelnik, T. Bartyński, J. Meizner, G. Dyk, M. Malawski: "The Collage Authoring Environment". In: Proceedings of the International Conference on Computational Science, ICCS 2011 (2011)