

# Composing, Executing and Sharing Multiscale Applications in an Integrated Environment

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<http://dice.cyfronet.pl>

## Goal

- Build an environment for composing, executing and sharing multiscale applications
- Provide the ability to connect software modules to form complex, multiscale simulations
- Support hybrid distributed execution, i.e. different parts of the same application can be executed on various types of e-infrastructures i.e. on a grid (e.g. EGI), HPC (e.g. PRACE) or on a cloud
- Support a variety of possible configurations of multiscale simulations in a unified and non-invasive way

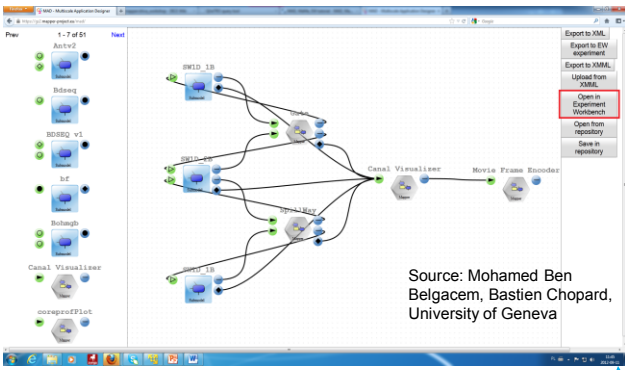
## Tools

- **MAPPER Memory** is a **semantic-aware persistence store** to record metadata about model sand scales
- **Multiscale Application Designer** is a user-friendly **visual composition tool** transforming high level MML descriptions into executable GridSpace experiments
- **GridSpace Experiment Workbench** supports **execution** and **result management** of generated experiments on infrastructures via interoperability layers
- **Provenance Tracking System** supports storing and providing detailed **information about experiment execution and its results**

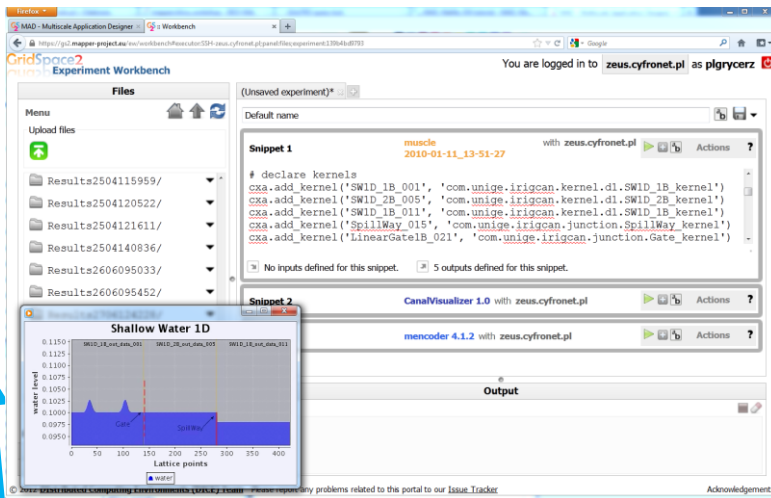
## 2. Compose Application in MAD <https://gs2.mapper-project.eu/mad>

## 3. Execute experiment in GridSpace EW <https://gs2.mapper-project.eu/ew>

## 4. View results



Source: Mohamed Ben Belgacem, Bastien Chopard, University of Geneva

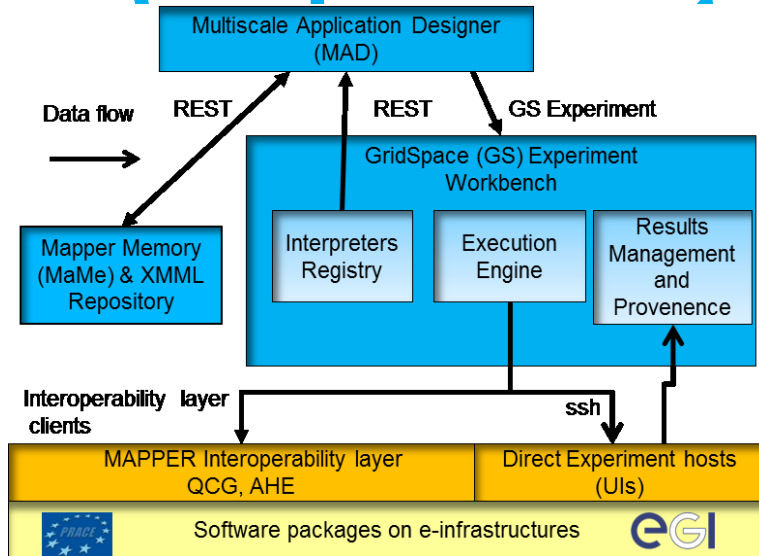


## 1. Register modules in MaMe, store information about MML-based applications structure <http://gs2.mapper-project.eu/mame>

### Used in simulation of

- blood flow
- irrigation canals
- clay-polymer nanocomposites,
- fusion
- gene-regulatory networks
- computational science dedicated to metallurgy

43 single-scale models and 38 mappers are already registered in the MaMe registry



## Conclusions

- Convenient composition of multiscale application variants
- Support for reusability of simulation models
- Easy usage of different resources in a single experiment
- Support for sharing infrastructure independent experiments
- Easy usage through Web interface
- Support for interactive execution
- Hierarchical code composition possible

## References

1. E. Ciepiela et al.: Exploratory Programming in the Virtual Laboratory, Proceedings of the International Multiconference on Computer Science and Information Technology p. 621–628, 2010
2. K. Rycerz and M. Bubak: Component Approach to Distributed Multiscale Simulations, SIMULTECH 2011, Noordwijkerhout, pp. 122-127, The Netherlands, 29-31 July, 2011
3. K. Rycerz et al.: Composing, Execution and Sharing of Multiscale Applications, Future Generation Computer Systems, in review

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