

# Programming and Execution of Multiscale Applications on Distributed Infrastructures

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<http://dice.cyfronet.pl>

## Goal

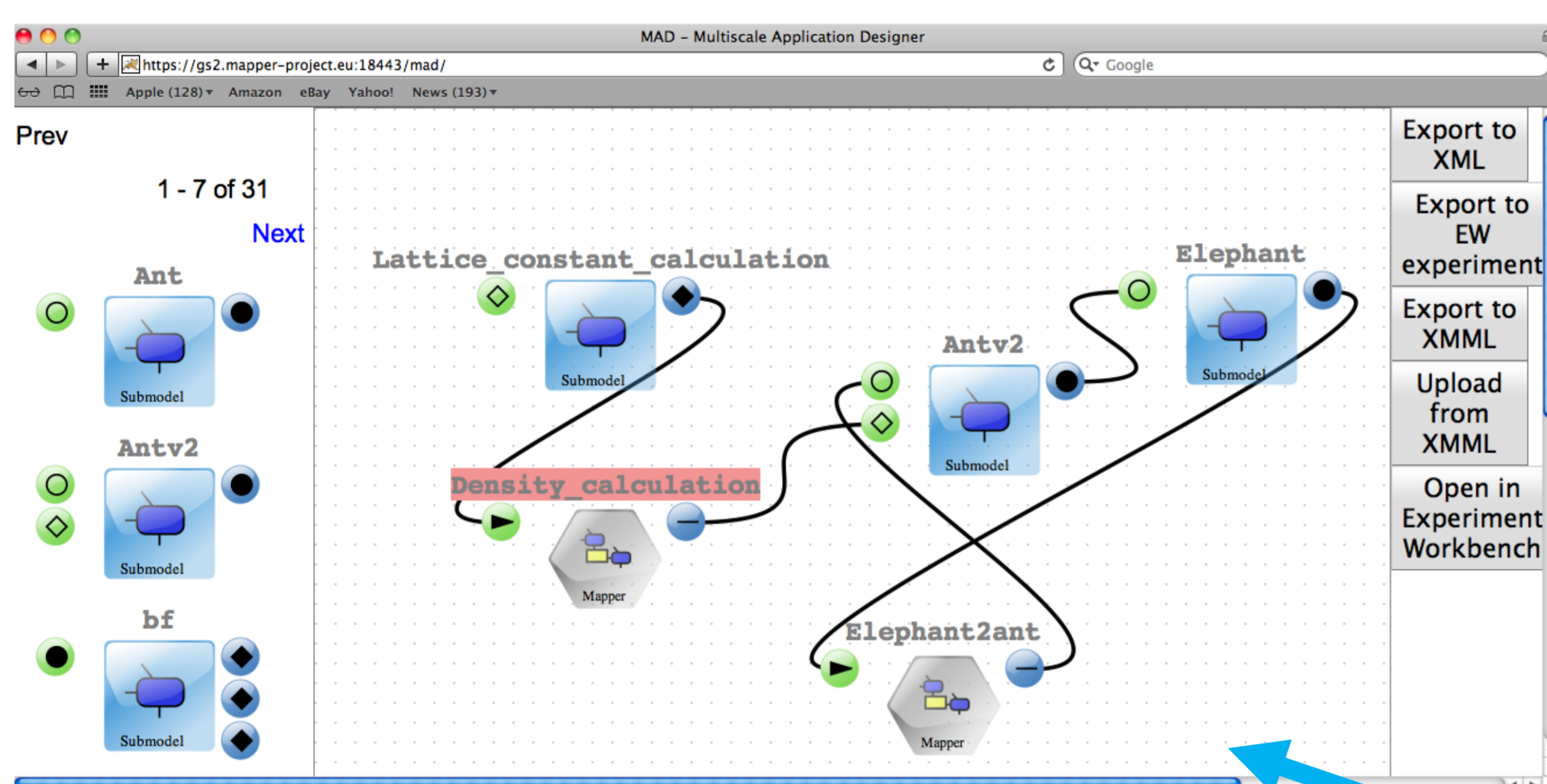
- the environment for composing multiscale applications
  - built from single scale models implemented as scientific software components
  - distributed in various European e-Infrastructures
- applications structure described in Multiscale Modelling Language (MML)
  - single scale sub-modules
  - scaleless converters
  - the coupling topology describing their connections

## Tools features

- **MaMe** is a **semantic-aware** persistence store to record metadata about models and scales
- **MAD** is a user-friendly **visual composition** tool transforming high level MML description into executable GridSpace experiment
- **GridSpace Experiment Workbench (EW)** supports **execution** and **result management** of generated experiments on e-infrastructures via interoperability layers using Interpreter-Executor model of computation

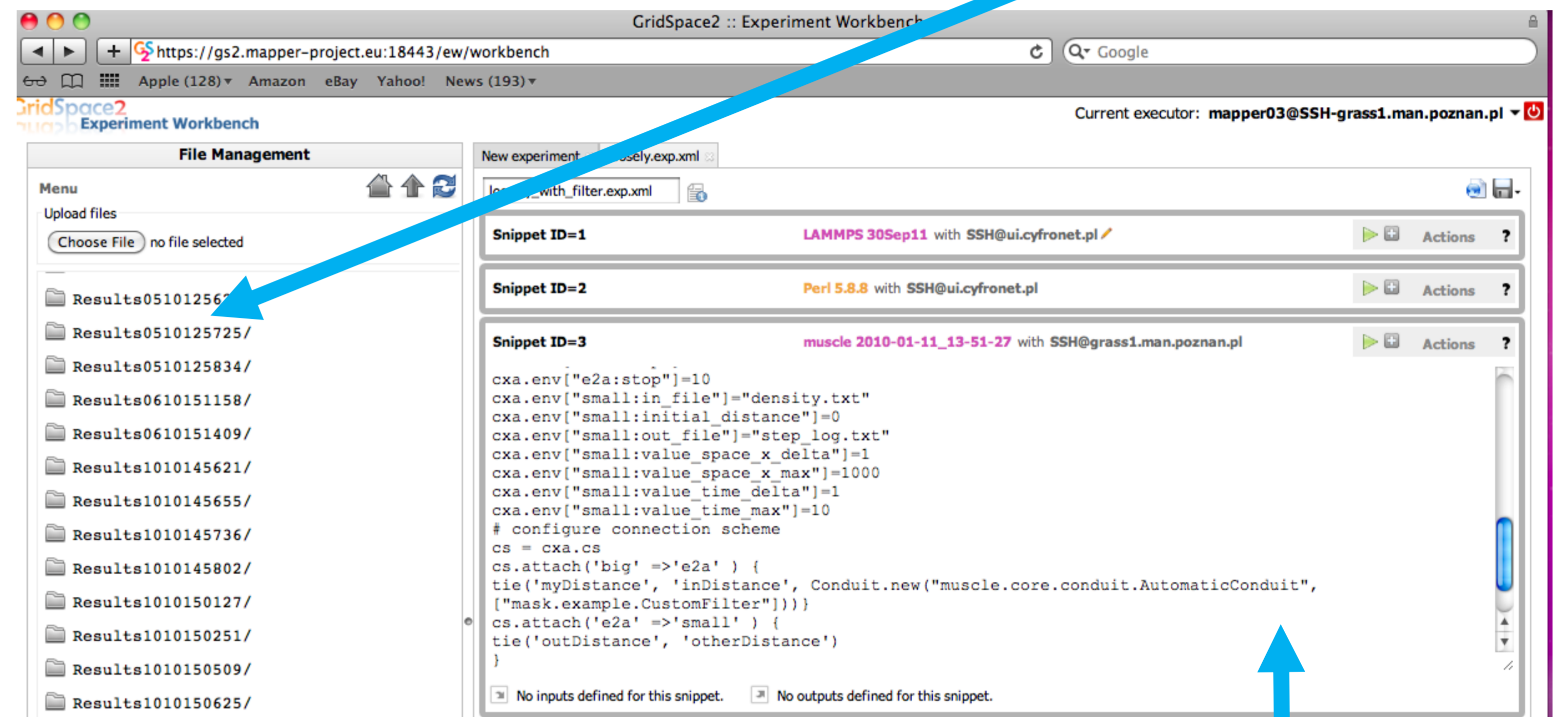
## 2. Compose Application in MAD

<https://gs2.mapper-project.eu/mad>



## 3. Execute experiment in GridSpace EW

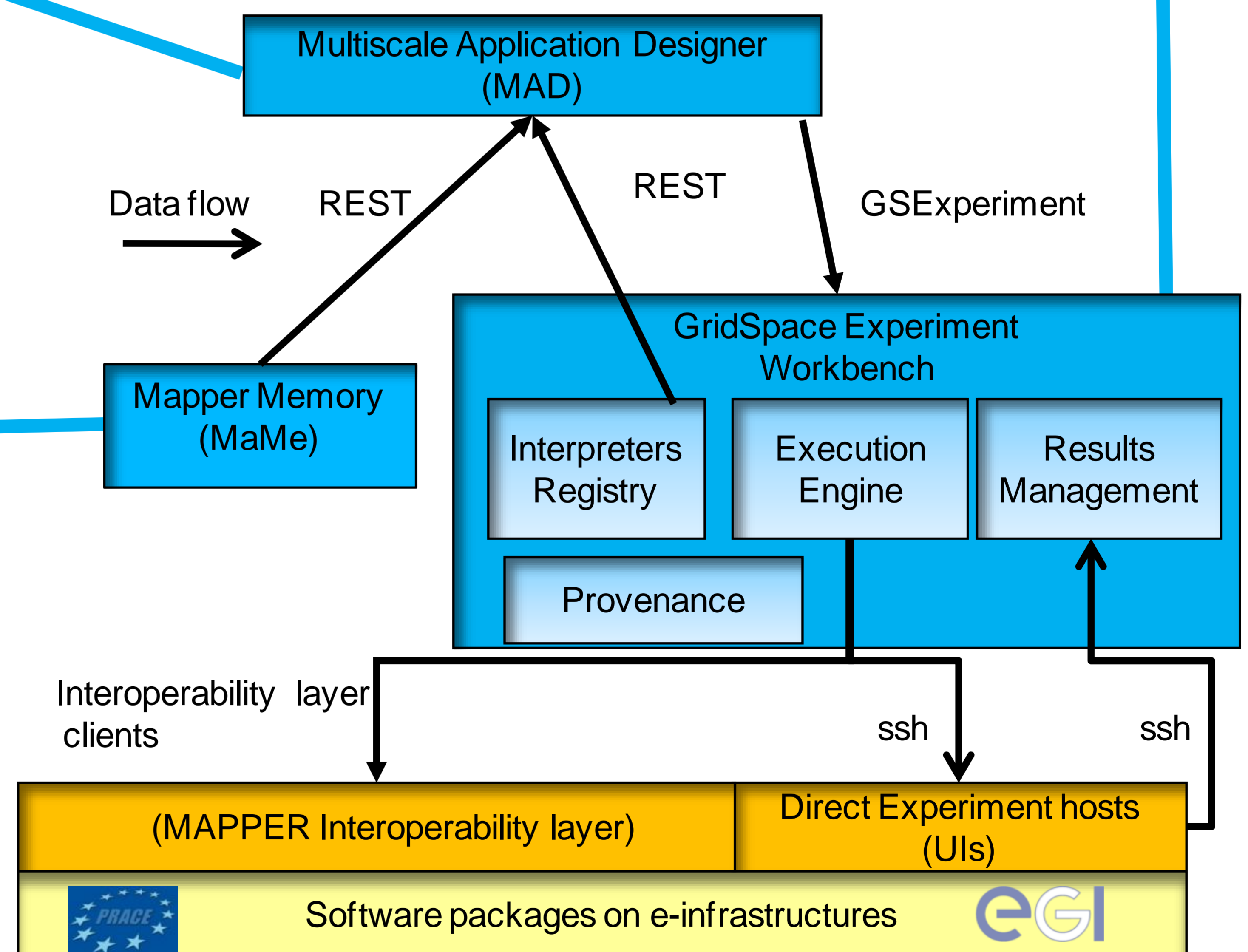
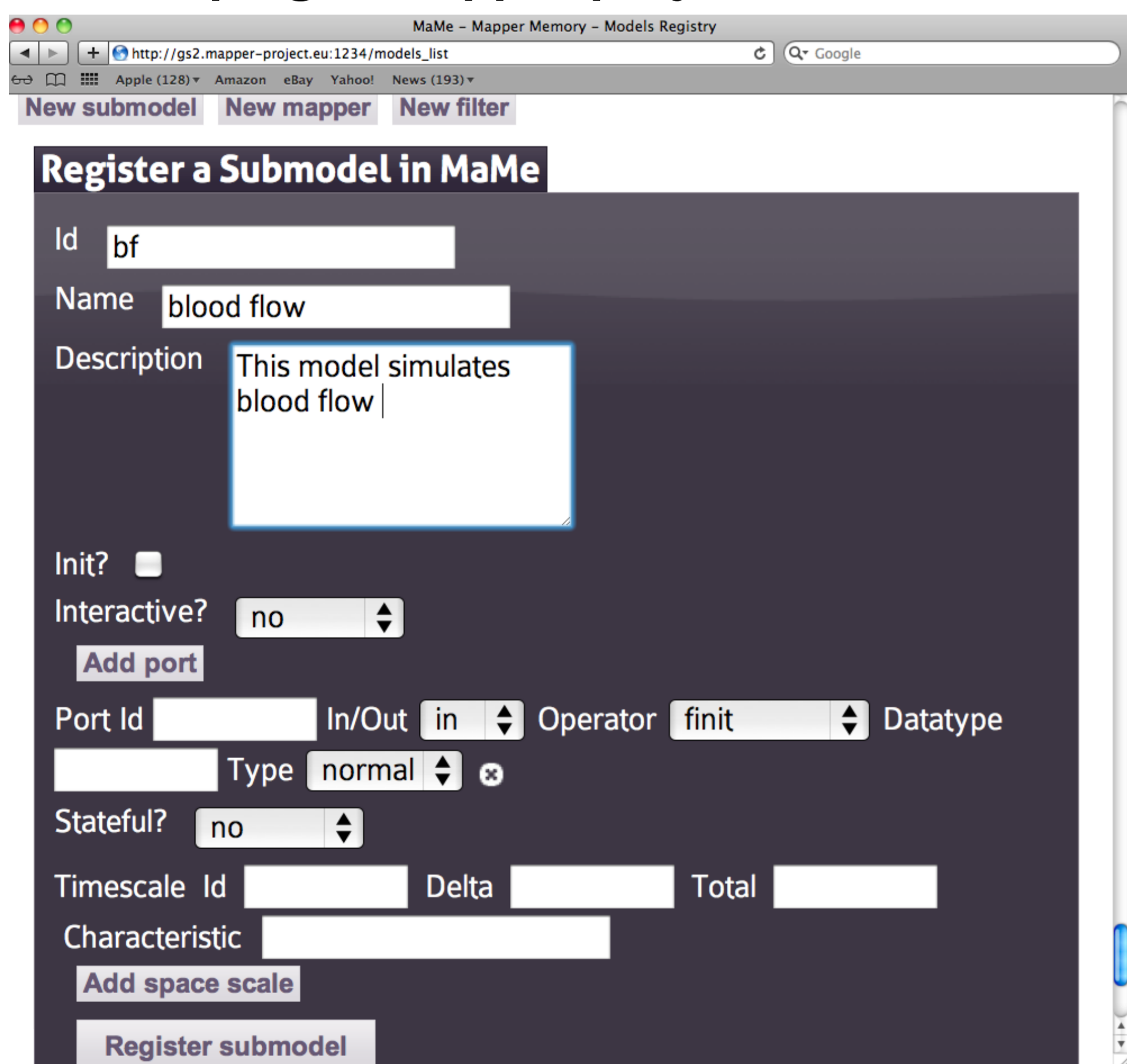
<https://gs2.mapper-project.eu/ew>



## 4. View results

## 1. Register modules in MaMe

<http://gs2.mapper-project.eu/mame>



## Interpreter – Executor model

**Interpreter** - a software package available on the infrastructure, e.g.:

- Multiscale Coupling Library and Environment (MUSCLE)
- Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

**Executor** - a common entity for hosts, clusters, grid brokers, etc. capable of running software which is already installed (represented as Interpreters).

## Support for collaborative work

- enabling sharing infrastructure-independent experiments
- supporting reusability of simulation models implementations

## References

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- K. Rycerz and M. Bubak: Building and Running Collaborative Distributed Multiscale Applications, in: W. Dubitzky et al.(Eds), Chapter 6, Large Scale Computing, J. Wiley and Sons, 2012
- K. Rycerz and M. Bubak: Component Approach to Distributed Multiscale Simulations, SIMULTECH 2011, 1st International Conference on Simulation, Modeling Technologies and Applications, Noordwijkerhout, pp. 122-127, The Netherlands, 29-31 July, 2011

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