Multiscale Programming and Execution Tools

Katarzyna Rycerz(1,2), Eryk Ciepiela(2), Tomasz Gubała(2,3), Daniel Harężlak(2), Joanna Kocot(2), Grzegorz Dyk(2), Jan Meizner(2) and Marian Bubak (1,2,3)
(1) AGH University of Science and Technology, Department of Computer Science, Krakow, Poland
(2) AGH University of Science and Technology, ACC CYFRONET AGH, Krakow, Poland
(3) Informatics Institute, University of Amsterdam, The Netherlands

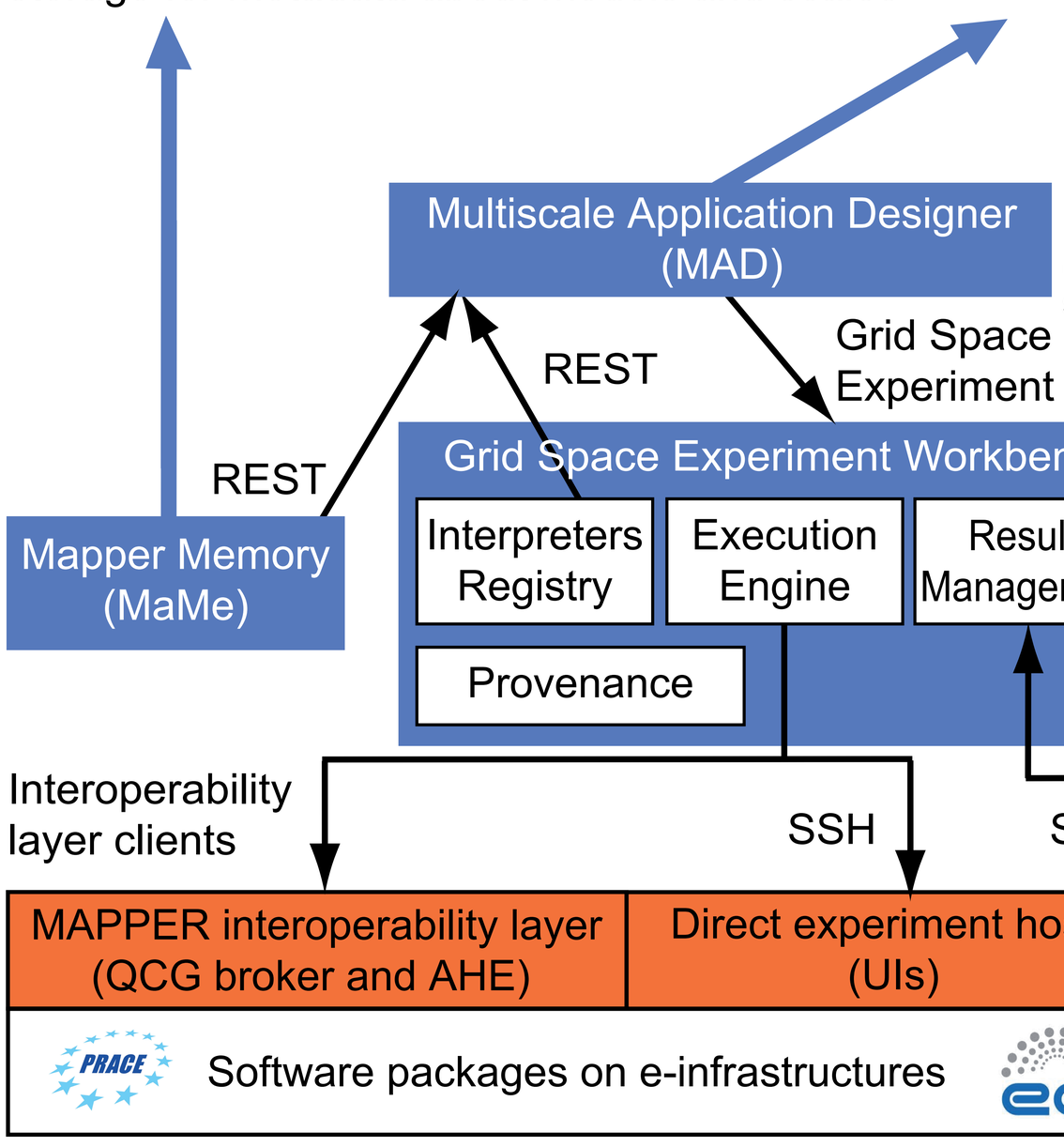
http://dice.cyfronet.pl

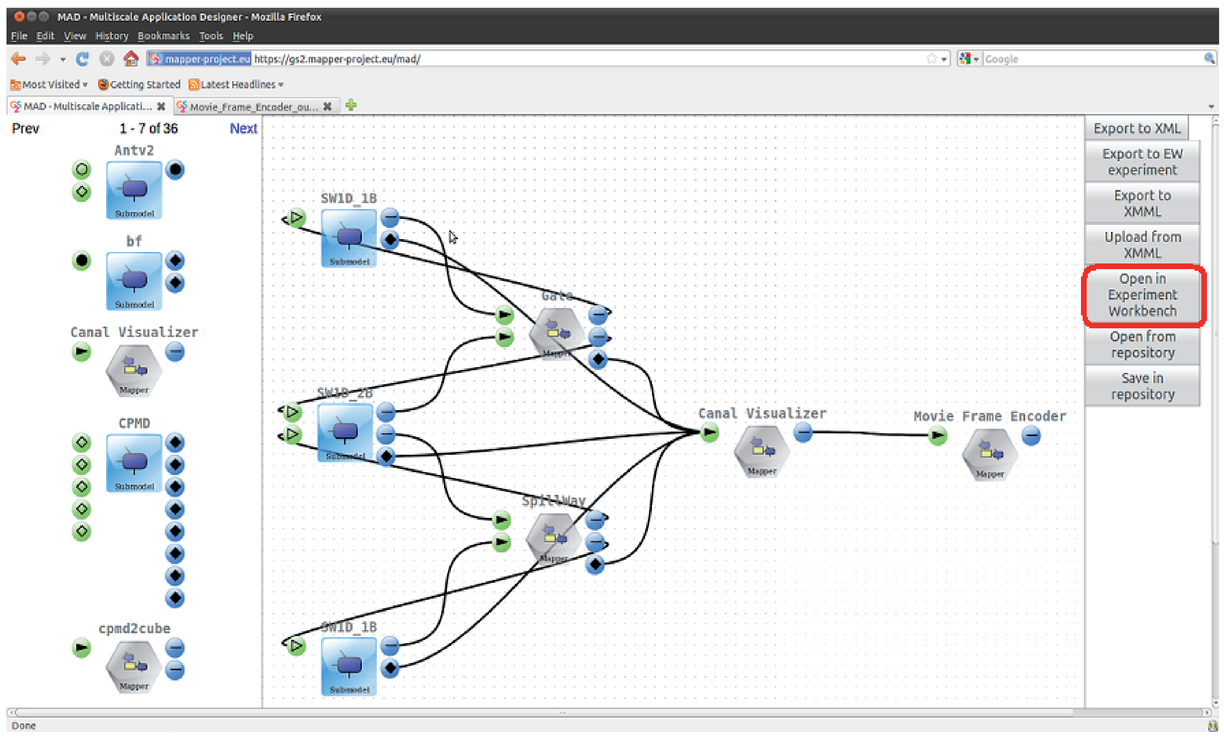
Goal

- 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-models
  - Scaleless converters
  - The coupling topology describing their connections

1 Register modules in MaMe http://gs2.mapper-project.eu/mame

MaMe is a **semantic-**aware persistent storage for metadata about models and scales





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

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

MAD is a user-friendly **visual composition** tool transforming high level MML description into executable GridSpace experiment

3 Execute experiment in GridSpace https://gs2.mapper-project.eu/ew

GridSpace Experiment Workbench (EW) supports **execution** and result management of generated experiments on e-infrastructures via interoperability layers using Interpreter-Executor model of computation

Interpreter - Executor Model

Interpreter: Software available in the infrastructure, e.g.:

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

Executor: A common entity of hosts, clusters, grid brokers, etc. capable of running software already installed

Support for Collaborative Work

- Enable sharing infrastructure-independent experiments
- Support reusability of simulation model implementations

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e-infrastructure
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