e-infrastructure

Hands On Session 1: How to develop multiscale applications with MAD, MaMe and GridSpace Experiment Workbench?

CAPACITIES

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CYFRONET

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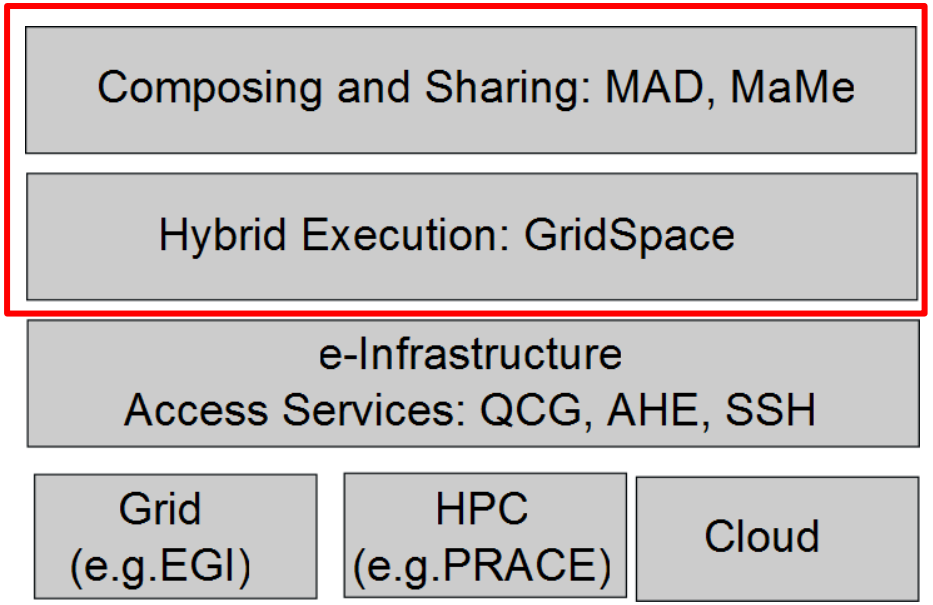
Plan

- Objectives and Requirements
- Idea of Multiscale Programming and Execution Tools
- Short demo based on Fusion application
  by Olivier Hoenen, IPP, MPG, Germany
- Hands on exercises

Objectives

- Design and implement an environment for composing multiscale simulations from single scale models
  - encapsulated as scientific software components
  - distributed in various European e-Infrastructures
  - supporting loosely coupled and tightly coupled paradigm
- Support composition of simulation models:
  - using scripting approach
  - by reusable “in-silico” experiments
- Allow interaction between software components from different e-Infrastructures in a hybrid way.

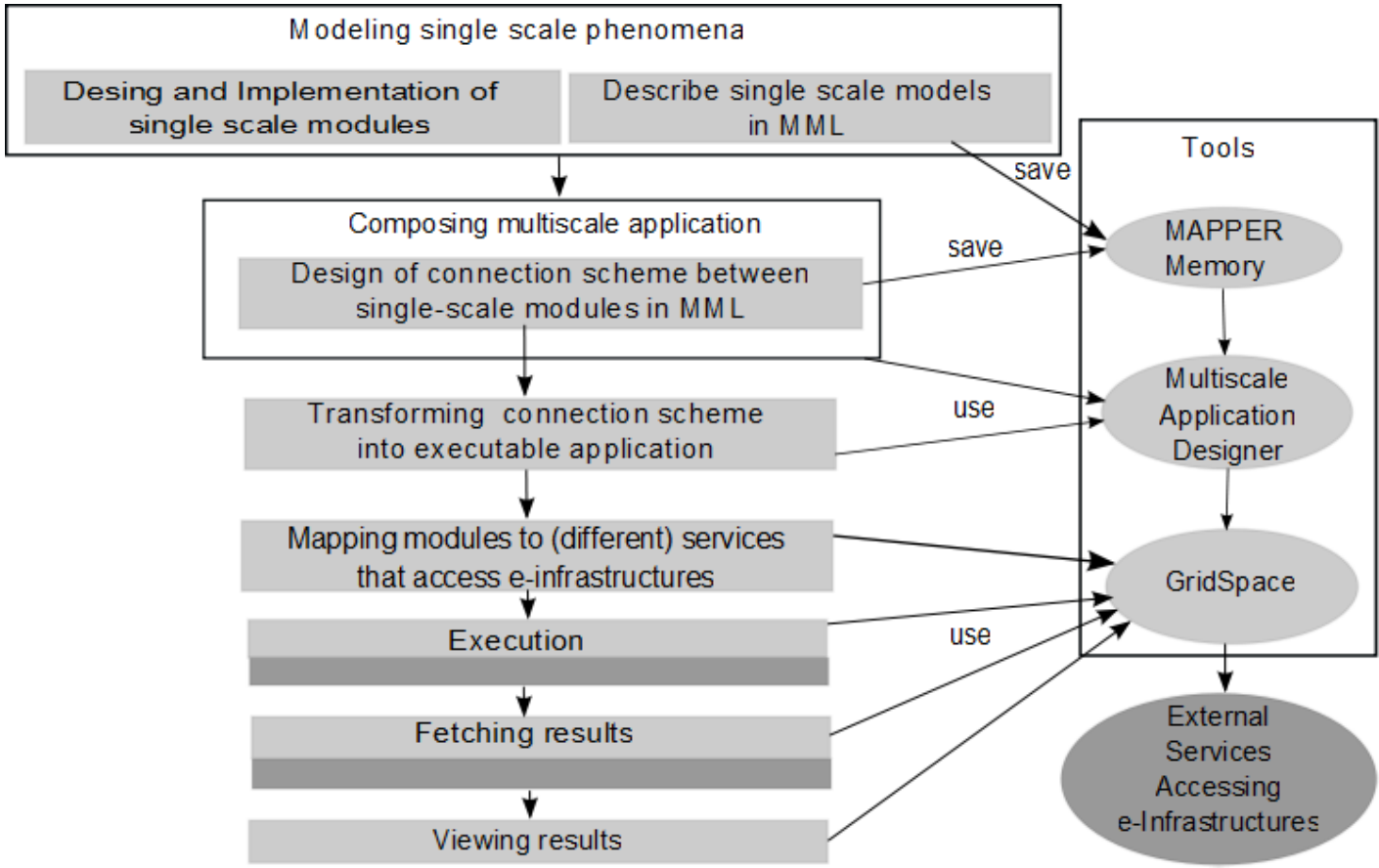


Requirements Analysis

- Focus on the multiscale applications that can be described as a set of connected, but independent single scale modules and mappers (converters)
- Support the variety of realizations of such applications in a unified way to:
  - Enable sharing of simulation modules
  - Support switching between different versions of the modules with the same scale and functionality;
  - Simplifying verification of modules against different realisations
  - Support building different multiscale applications from the same modules (reusability)
- Support computationally intensive simulation modules
  - requiring HPC and/or Grid resources,
  - often implemented as parallel programs
- Support tight (with loop), loose (without loop) or hybrid (both) connection modes

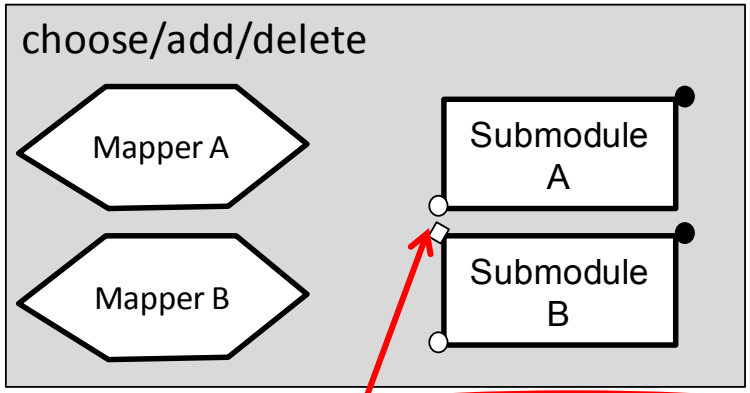
Building and Executing Multiscale Application

- Process of constructing multiscale application consists of different steps
- Most of these steps can be facilitated by:
  - Multiscale Modeling Language (MML)
  - programming and execution tools
  - services accessing e-infrastructure

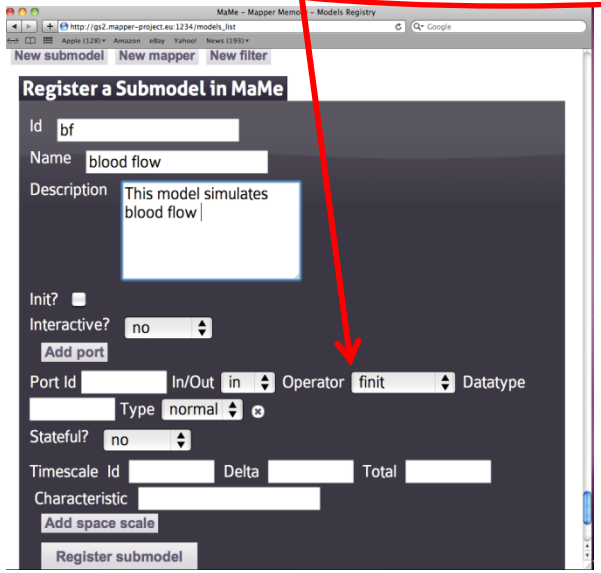


Mapper Memory (MaMe)

- Semantics-aware persistence store
- Records MML-based metadata about models and scales
- Supports exchanging and reusing MML metadata for
  - other MAPPER tools via REST interface
  - human users within the Consortium via dedicated Web interface

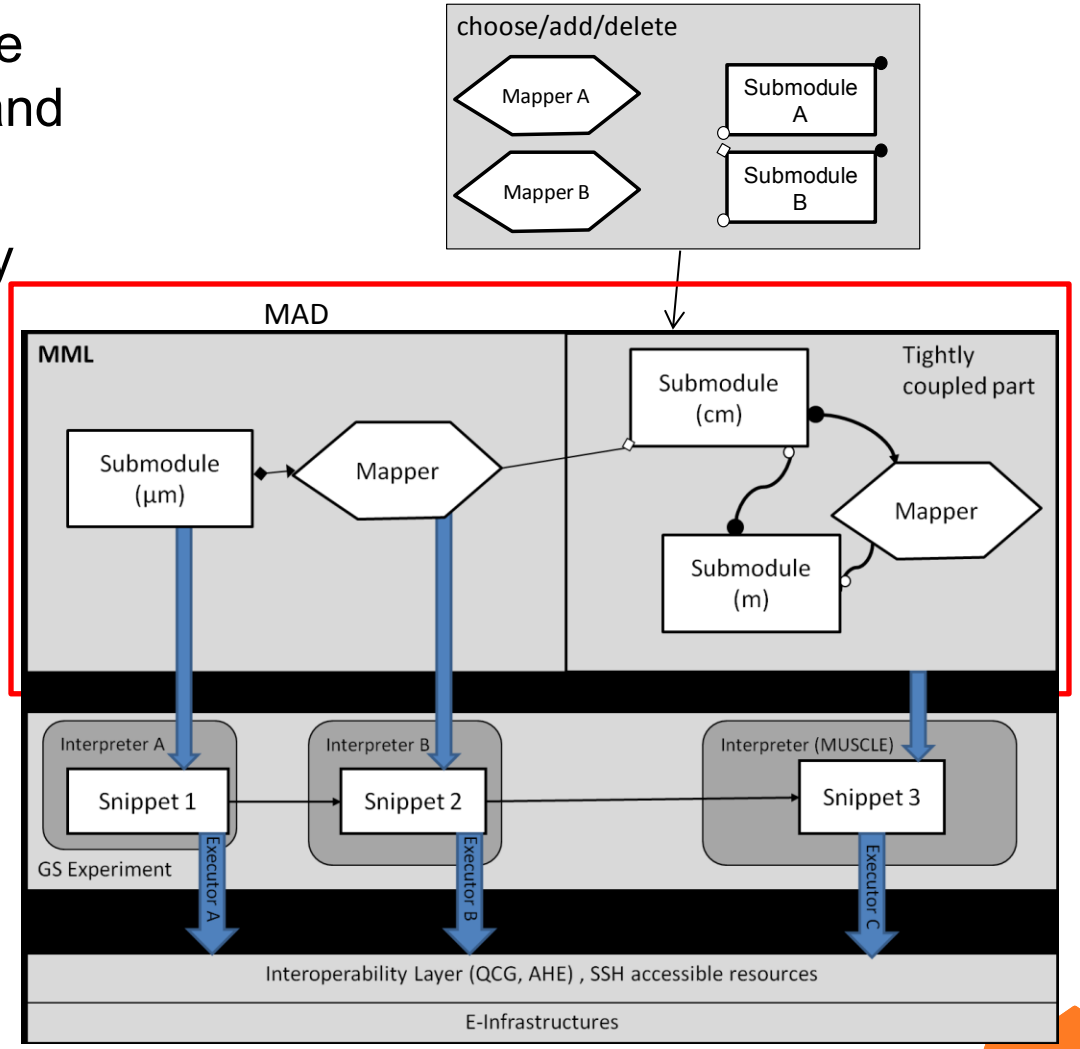


Ports and their operators



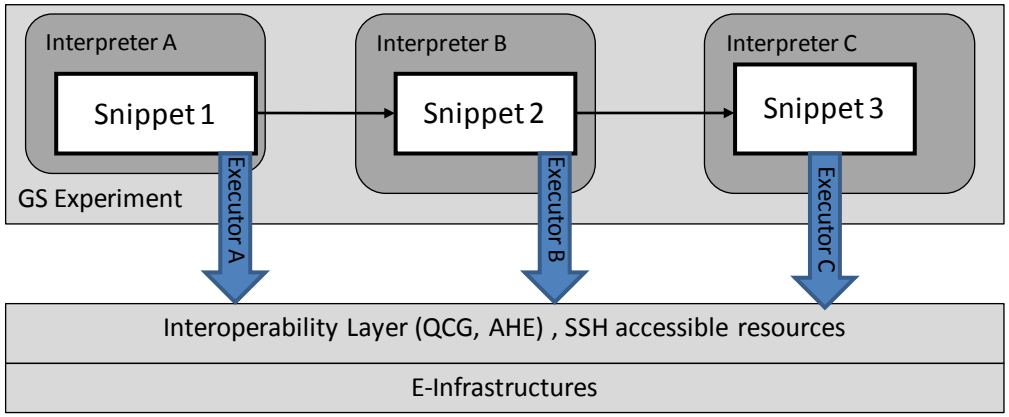
MultiscaleApplication Designer (MAD)

- Supports composing multiscale applications from submodels and mappers registered in MaMe
- Inport/export coupling topology represented in gMML to/from XMML file
- Transforms high level MML description into executable experiment for GridSpace Experiment Workbench

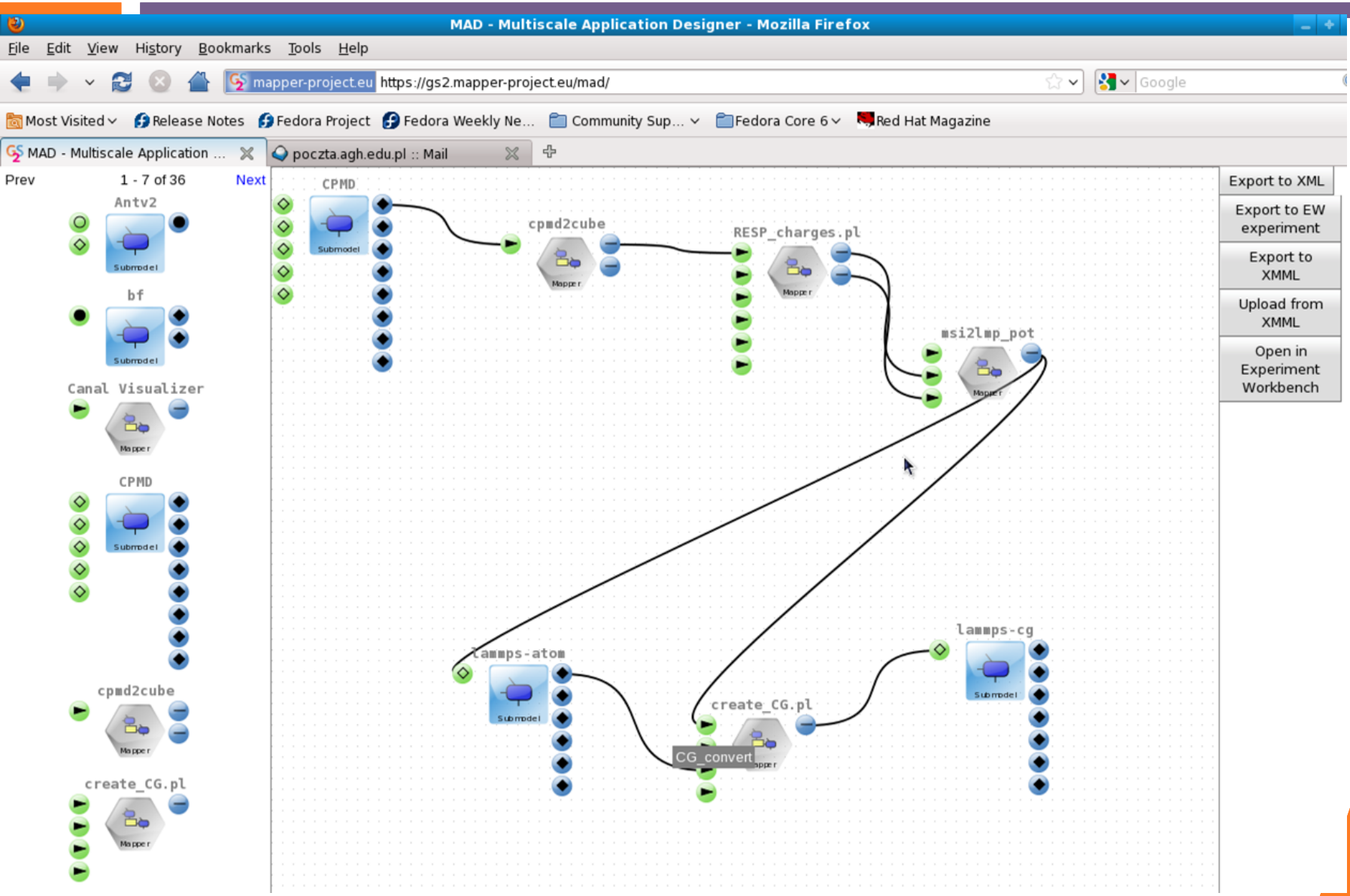


GridSpace Experiment Workbench

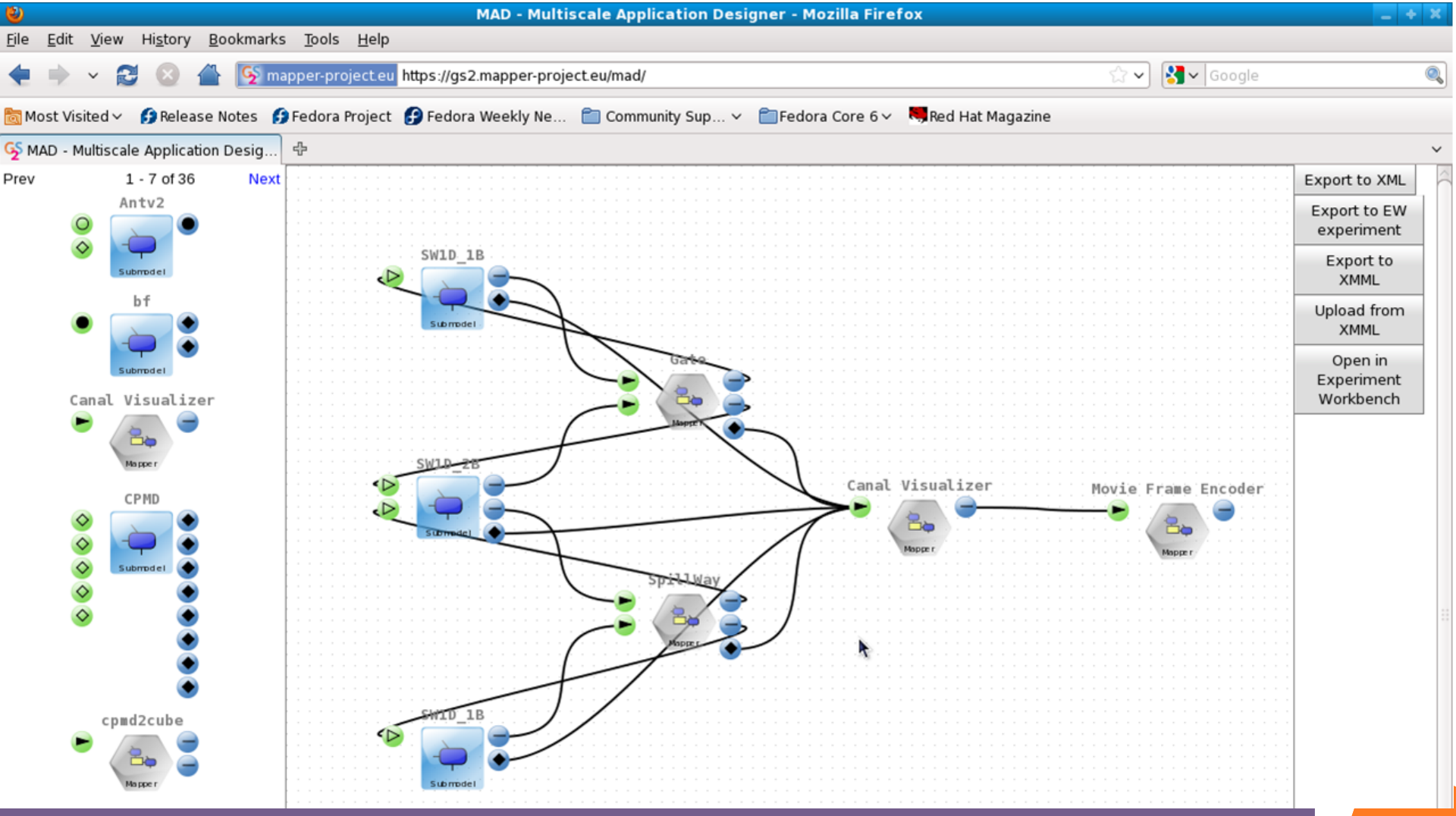
- Supports **execution and result management** of infrastructure independent experiments
- **Experiment** - application composed of code fragments called **snippets**, expressed in:
  - general-purpose scripting programming languages(Bash, Ruby, Perl etc.)
  - domain-specific languages (CxA in MUSCLE, LAMMPS, Matlab etc)
- Snippets are evaluated by respective programs called **interpreters**
- **Executors**- responsible for snippets execution on various computational resources – servers, clusters, grid via
  - direct SSH on UserInterface (UI) machine
  - Interoperability layer (QCG, AHE)
- Each snippet of the same experiment can be executed on different resource



Loosely Coupled Example - Nano Polymer Simulation in MAD



Tightly Coupled example – canal application



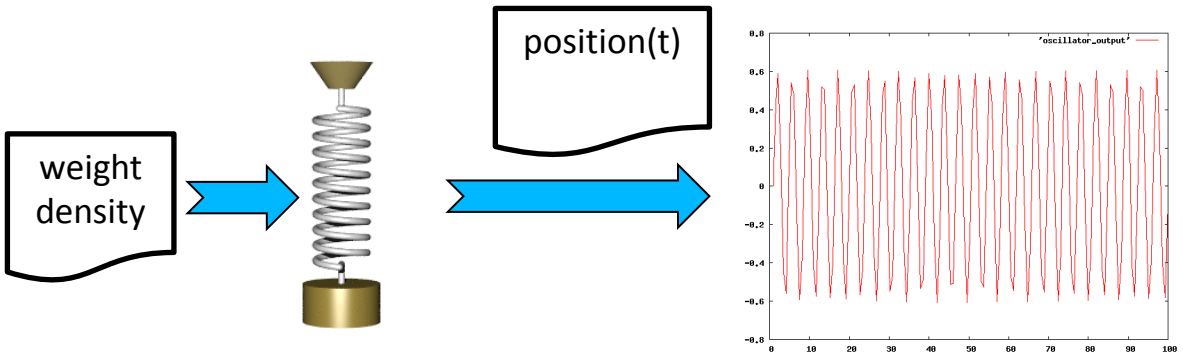
See also:

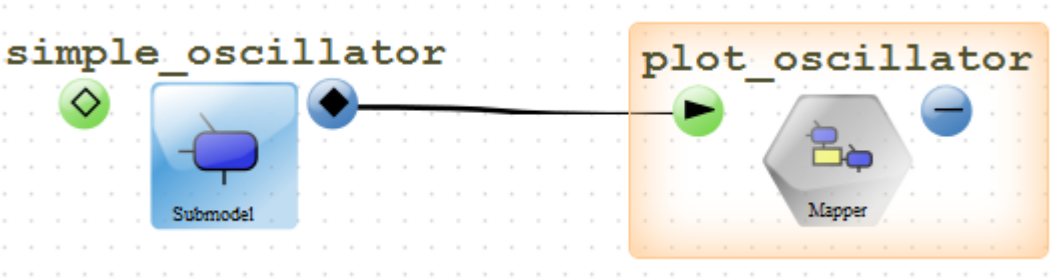
- http://dice.cyfronet.pl
- http://dice.cyfronet.pl/projects/details/Mapper
- E. Ciepiela et al.: Exploratory Programming in the Virtual Laboratory, Proceedings of the International Multiconference on Computer Science and Information Technology p. 621–628, 2010
- K. Rycerz and M. Bubak: Component Approach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

Fusion application demo

Hands on exercises - step1

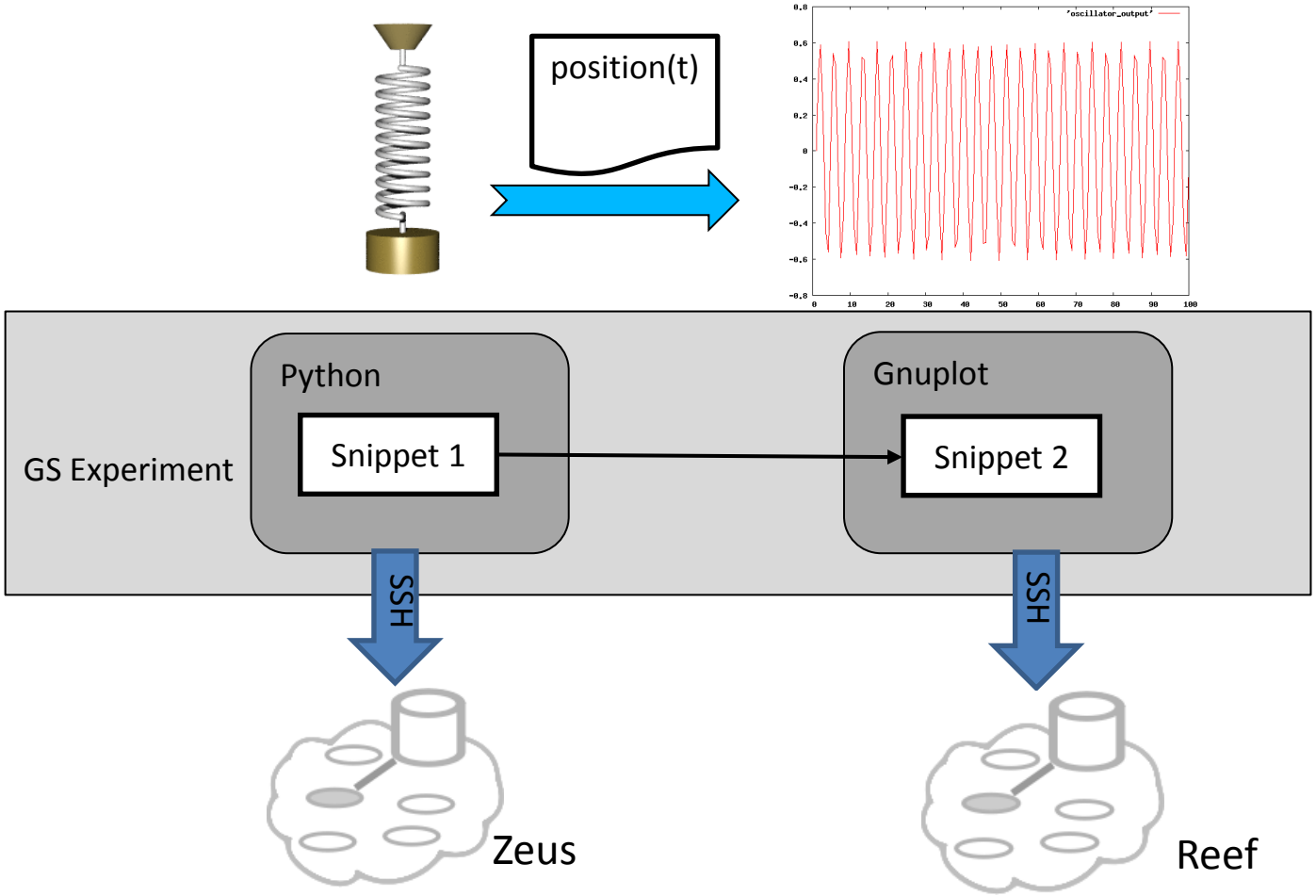
- http://www.mapper-project.eu/ -> Events, conferences, training->Multiscale Summer School-> Exercises & Hands on ->Hands On 1
- Step 1 – simple oscillator simulation and plot





Hands on exercises – step 2

- simple oscillator simulation and plot distributed



Hands on exercises – step 3

- Building multiscale application