



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

K. Rycerz, E.Ciepiela, M.Pawlik, T.Gubała, D.Harężlak,  
J.Meizner, M.Bubak



03.06.13

CYFRONET

# Plan

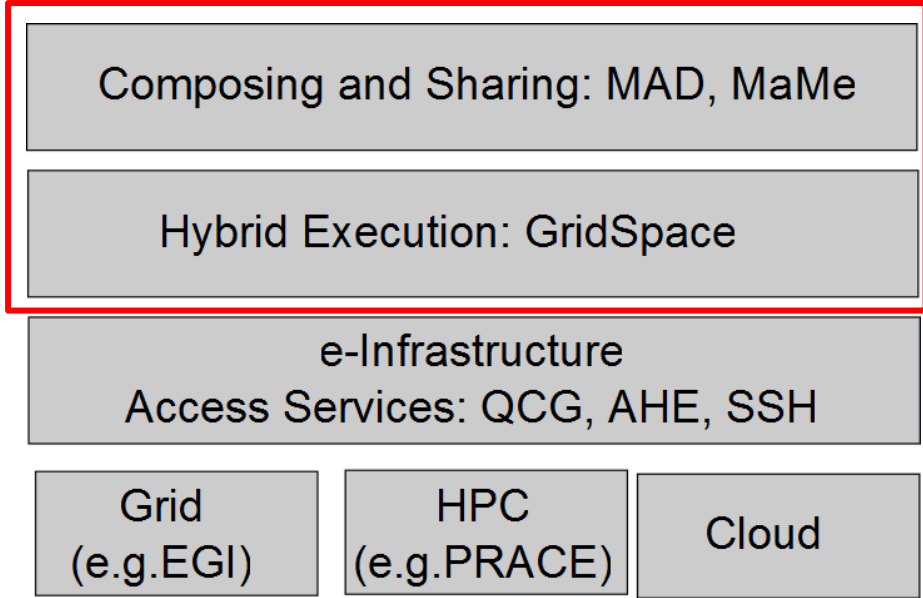


- Objectives and Requirements
- Idea of Multiscale Programming and Execution Tools
- Short demo based on Fusion application  
*by Olivier Hoenen, IPP, MPG, Germany*
- Hands on exercises

# 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.

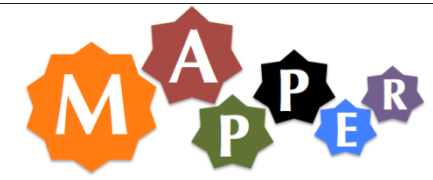


# Requirements Analysis

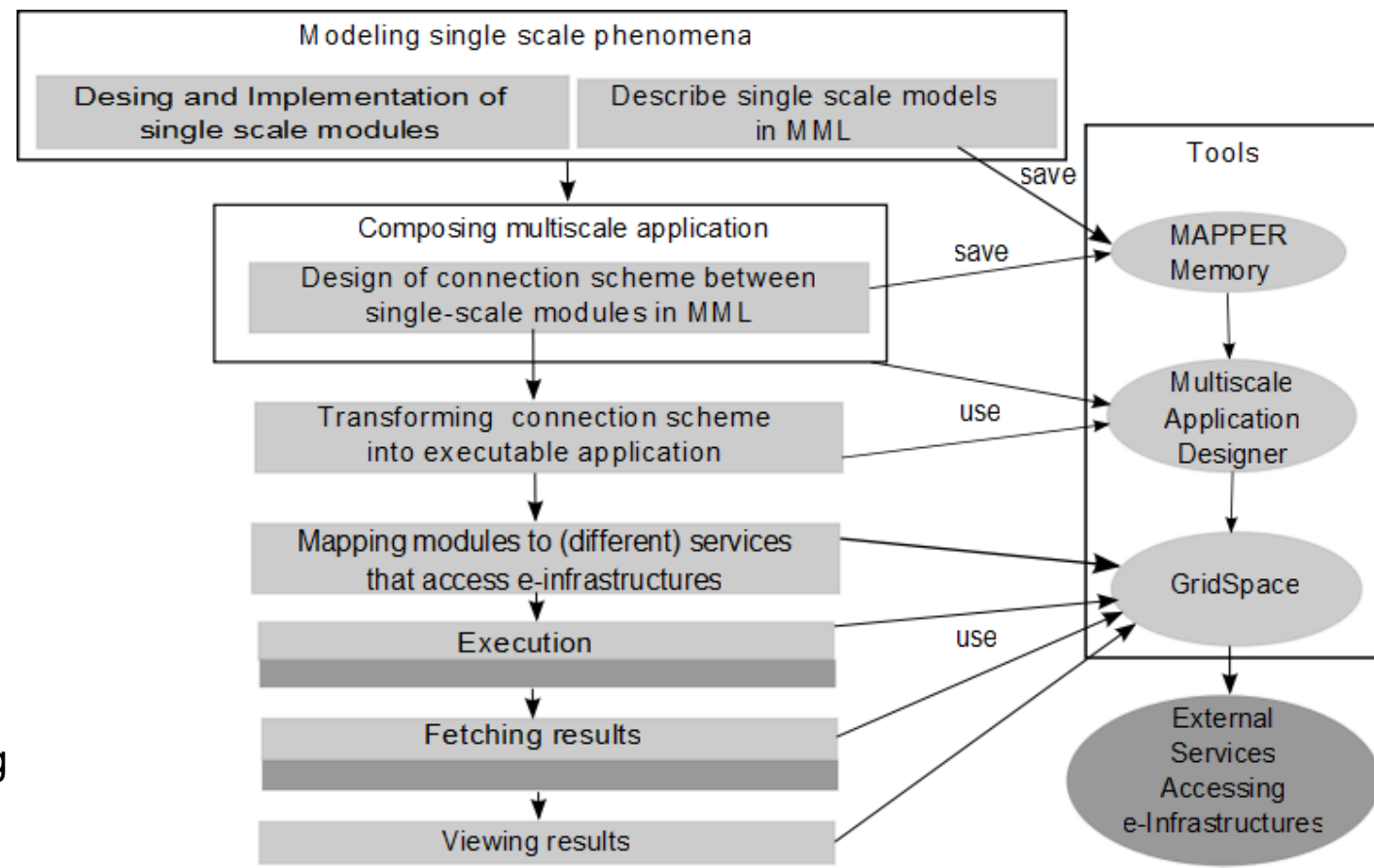


- Focus on the multiscale applications that can be described as a set of connected, but independent single scale modules and mappers (converters)
- Support the variety of realizations of such applications in a unified way to:
  - Enable sharing of simulation modules
  - Support switching between different 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



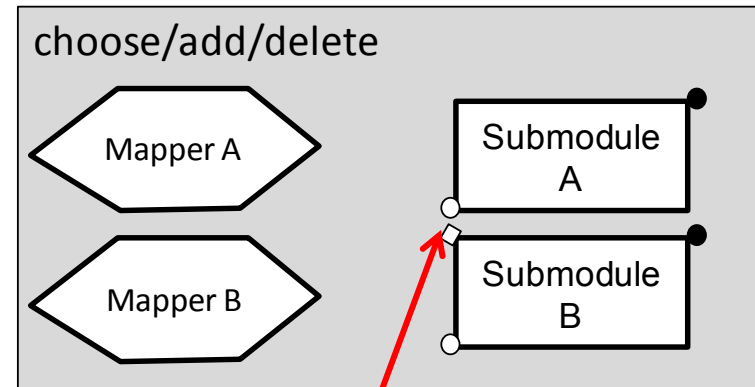
- Process of constructing multiscale application consists of different steps
- Most of these steps can be facilitated by:
- Multiscale Modeling Language (MML)
  - programming and execution tools
  - services accessing e-infrastructure



# 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



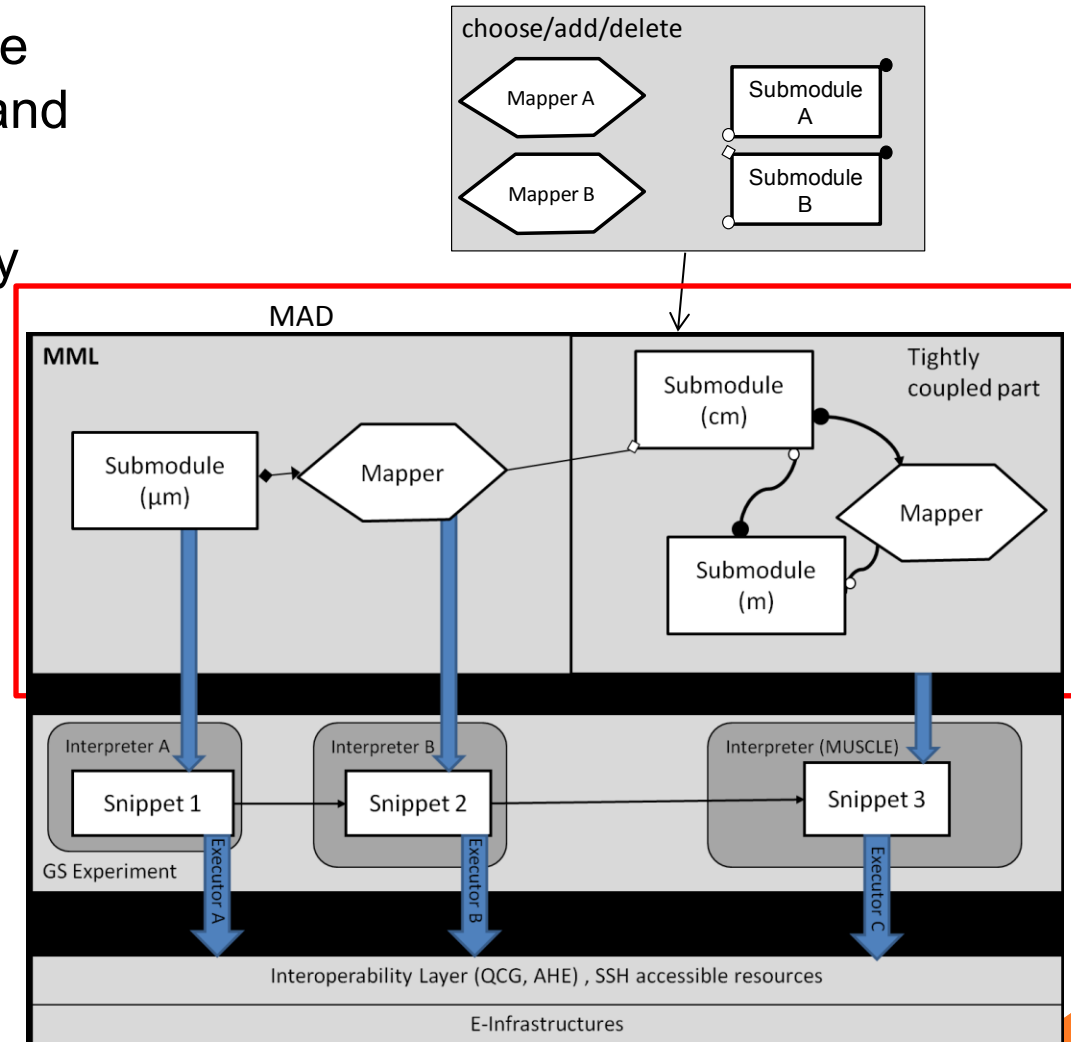
Ports and their operators

A screenshot of a web browser showing the 'Register a Submodel in MaMe' form. The form fields include: Id (bf), Name (blood flow), Description (This model simulates blood flow), Interactive? (no), Add port button, Port Id, In/Out (in), Operator (finit), Datatype, Type (normal), Stateful? (no), Timescale Id, Delta, Total, Characteristic, Add space scale button, and Register submodel button. A red arrow points from the 'Ports and their operators' text to the 'Add port' button.

# MultiscaleApplication Designer (MAD)



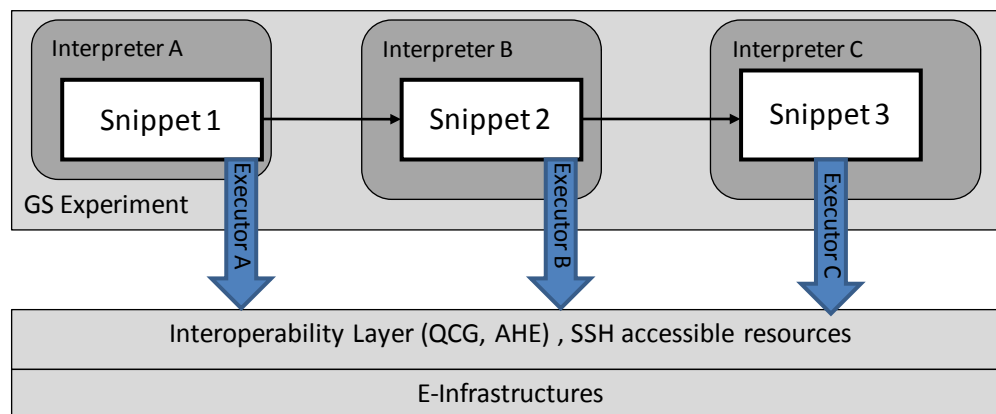
- Supports composing multiscale applications from submodels and mappers registered in MaMe
- Inport/export coupling topology represented in gMML to/from XMMML file
- Transforms high level MML description into executable experiment for GridSpace Experiment Workbench



# 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



MAD - Multiscale Application Designer - Mozilla Firefox

File Edit View History Bookmarks Tools Help

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

Most Visited Release Notes Fedora Project Fedora Weekly Ne... Community Sup... Fedora Core 6 Red Hat Magazine

MAD - Multiscale Application ... poczta.agh.edu.pl :: Mail

Prev 1 - 7 of 36 Next

Antv2 Submodel

bf Submodel

Canal Visualizer Mapper

CPMD Submodel

cpmd2cube Mapper

create\_CG.pl Mapper

CPMD Submodel

cpmd2cube Mapper

RESP\_charges.pl Mapper

msi2lmp\_pot Mapper

lamps-atom Submodel

CG\_convert Mapper

lamps-cg Submodel

Export to XML

Export to EW experiment

Export to XMML

Upload from XMML

Open in Experiment Workbench

The screenshot displays the MAD Multiscale Application Designer interface. On the left, a vertical toolbar contains icons for various components: Antv2, bf, Canal Visualizer, CPMD, cpmd2cube, and create\_CG.pl. The main workspace shows a workflow diagram with several nodes: CPMD (Submodel), cpmd2cube (Mapper), RESP\_charges.pl (Mapper), msi2lmp\_pot (Mapper), lamps-atom (Submodel), CG\_convert (Mapper), and lamps-cg (Submodel). Lines connect these nodes, indicating the flow of data or processes. A mouse cursor is visible over the msi2lmp\_pot node. On the right side, there is a vertical menu with buttons for 'Export to XML', 'Export to EW experiment', 'Export to XMML', 'Upload from XMML', and 'Open in Experiment Workbench'. The browser window title is 'MAD - Multiscale Application Designer - Mozilla Firefox' and the address bar shows 'https://gs2.mapper-project.eu/mad/'.

# Tightly Coupled example – canal application



MAD - Multiscale Application Designer - Mozilla Firefox

File Edit View History Bookmarks Tools Help

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

Most Visited Release Notes Fedora Project Fedora Weekly Ne... Community Sup... Fedora Core 6 Red Hat Magazine

MAD - Multiscale Application Desig...

Prev 1 - 7 of 36 Next

Antv2 Submodel

bf Submodel

Canal Visualizer Mapper

CPMD Submodel

cpmd2cube Mapper

SW1D\_1B Submodel

SW1D\_2B Submodel

SW1D\_1B Submodel

Gate Mapper

Spillway Mapper

Canal Visualizer Mapper

Movie Frame Encoder Mapper

The screenshot shows the MAD software interface. On the left is a component palette with icons for Antv2, bf, Canal Visualizer, CPMD, and cpmd2cube. The main workspace contains a flow diagram with submodels (SW1D\_1B, SW1D\_2B, SW1D\_1B) and mappers (Gate, Spillway, Canal Visualizer, Movie Frame Encoder) connected by arrows. On the right is a sidebar with export and upload options.

# 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

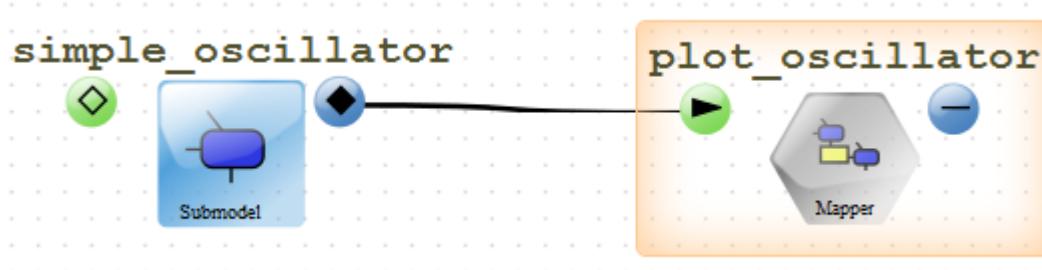
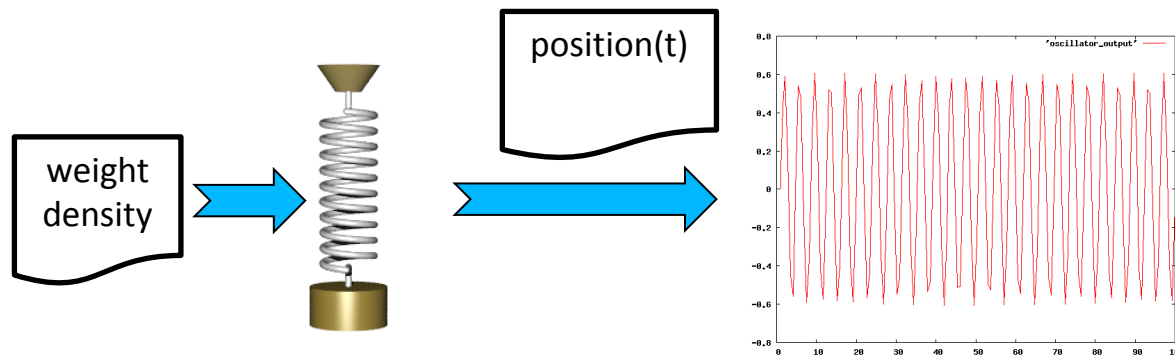


# Fusion application demo

# Hands on exercises - step1



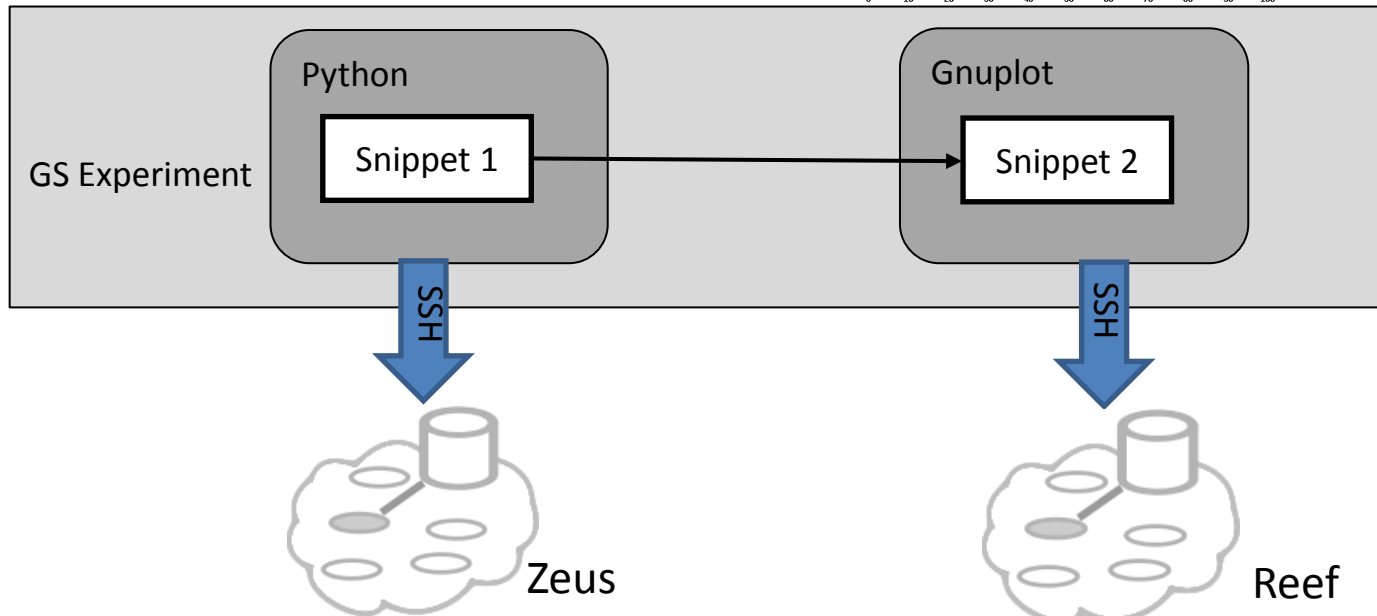
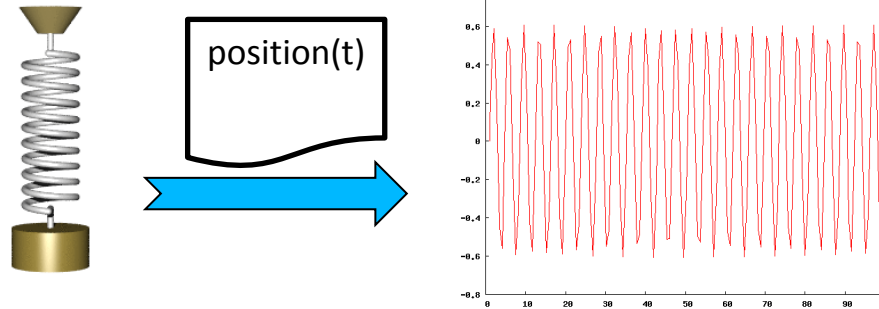
- <http://www.mapper-project.eu/> -> Events, conferences, training->Multiscale Summer School-> Exercises & Hands on ->Hands On 1
- Step 1 – simple oscillator simulation and plot



# Hands on exercises – step 2



- simple oscillator simulation and plot distributed



# Hands on exercises – step 3



- Building multiscale application

