





Deliverable D2.4.1 First Annual Dissemination Report

Project acronym: MAPPER

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Executive Summary

The First Annual Dissemination Report presents an overview of the dissemination activities of the MAPPER project for the first reporting period (October 2010 until September 2011). It describes how the work was done and which goals were achieved.

The key achievements of this reporting period are the delivery of the basic MAPPER dissemination material and the participation at events.

1. Introduction

MAPPER, grant number 261507, is an infrastructure project for the development and deployment of multiscale applications on European e-infrastructures. As there is no doubt that multiscale applications will be of interest to the broader scientific community, it is highly advisable to accompany MAPPER with corresponding dissemination and exploitation activities: Potential users need to be informed of the project's existence; students of technical sciences should be invited to support the project; and researchers of scientifically related domains should be educated regarding the benefits of the project.

Dissemination in MAPPER has the following objectives:

- Raise the awareness of the MAPPER project in the scientific community.
- Communicate the vision (abstract) and the project goals (concrete) of MAPPER across Europe and evangelize decision making bodies.
- Educate standardization bodies to discuss the requirements of multiscale applications more broadly, eventually leading to a standardization of architectures and their components. This effort should be visible worldwide with Europe recognized as leading the discussion.

The document will be updated annually. Updates will include the achieved goals related to dissemination, the attended conferences and events and information about scientific papers and posters produced by MAPPER members. This document (and all subsequent revisions) will be prepared by the dissemination team consisting of the following members:

- Bastien Chopard (UNIGE)
- Marian Buback (AGH)
- Derek Groen (UCL)
- Peter Coveney (UCL)
- David Coster (IPP)
- Ilya Saverchenko (LMU)
- Christof Klausecker (LMU)
- Michael Schiffers (LMU)
- Joris Borgdorff (UvA)
- Alexandru Mizeranschi (UU)
- Werner Dubitzky (UU)
- Tomasz Piontek (PSNC)
- Mariusz Mamoński (PSNC)
- Krzysztof Kurowski (PSNC)
- Pär Strand (CUT)

with Christof Klausecker as lead editor and contact point for the dissemination team. The dissemination team can be reached by emailing to wp2_ at_mapper-project.eu, the lead editor and individual team members can be contacted by using the email addresses given in the "contact information" section of this deliverable.

2. Objectives of the Dissemination Activities

Dissemination and outreach is a MAPPER networking activity which is completely handled in work package 2 (WP2). WP2 therefore focuses on the project objectives and results developed in the Service Activities (WP4-6) and the Joint Research Activities (WP7-8) by demonstrating the feasibility and benefits of MAPPER. Consequently, the main objectives of this WP are:

- to demonstrate the project solutions to stakeholders and to educate the stakeholders
- to raise project awareness in application communities, HPC communities, e-science communities
- to increase the involvement of user communities in European e-infrastructure
- to educate scientists in using the services provided by MAPPER

The specific means to achieve these objectives are

- preparation and distribution of adequate information material, including a webpage,
- · active participation in conferences,
- dedicated media work,
- offering dedicated training workshops

2.1. Description of Work

Dissemination plays an important role in every research and technological development project. For MAPPER the main activities will be targeted towards both promoting the project results and to evangelize interested communities, user groups and stakeholders, in the necessity of deploying and using the MAPPER enhanced infrastructure efficiently. It is very important for the project's success to reach all stakeholders, be they user communities, scientists, the press, or other authorities. This will be achieved by participating at dedicated conferences, by targeting workshops, by web portals, by printed media, and by exhibiting at specific fairs. As the final goal of the MAPPER project is to facilitate a new way of using supercomputing facilities at a pan-European level, this work package will also be responsible for training scientists and students in utilizing the infrastructure by offering a series of "schools". Work package 2 runs the following tasks:

• Task 2.1: Dissemination Action Plan. This task aims in the direction and management of all dissemination activities of the project. The task's objective is therefore the preparation of a detailed plan for the use and dissemination of foreground in which all dissemination actions are described. The action plan also contains for each task a success definition and a related measurement specification.

- Task 2.2: MAPPER Webpage and Communication Kit. For public relations, the MAPPER webpage at www.mapper-project.eu and the MAPPER Communication Kit will be prepared. The webpage will be the main source of public information for both, the project partners and the rest of the world. The MAPPER Communication Kit will be made available for distribution at conferences, seminars, workshops, and other occasions where a give-away may be beneficial. The kit consists of dedicated (if appropriate, targeted) leaflets, white papers, a project poster and electronic media (CD, DVD, Blu-ray). The leaflets will contain information similar to the public portion of the web site in a quality layout. It will advise the stakeholders of the existence of MAPPER as well as of its goals and achievements. The leaflets may be accompanied by other promotional material. White papers will be generated during the course of the project. They will be part of the communication kit upon release. The poster will showcase the project at specific locations. Electronic media will be integrated into the communication kit in cases the material is public. The kit will include a requestfurther-information card and a feedback form for success measurement. The kit also serves as input for task 2.4 as it can be customized as a press kit.
- Task 2.3: Press & Media Relations. All project partners will actively help in contacting their local press and in selecting focused media partners for greater coverage. Besides this regional focus, press and media with European presence will also be targeted by MAPPER success stories. This task utilizes the Communication Kit from task 2.2.
- Task 2.4: Annual MAPPER Seasonal Schools. This task is dedicated to the familiarization of all interested stakeholders with the MAPPER e-Infrastructure. During a series of hands-on seasonal schools the participants will learn how to use the infrastructure and how to benefit from it. The first one will be mainly targeted at project members, whereas the next one(s) will be more targeted at external participants.
- Task 2.5: Conference Participation. MAPPER will schedule events, such as workshops or targeted actions, at appropriate scientific conferences with the objectives to promote the MAPPER infrastructure and its benefits and to provide appealing use cases. The conferences will be determined in deliverable D2.2 of task 2.1. This task is responsible for delivering these workshops (preparation, execution, followup).

2.2. Dissemination Support within the Project

The dissemination workpackage is also responsible for information flow ("knowledge transfer") within the project consortium. It assists the management workpackage with presentation material and other items related to communication within the project. There were two meetings in this context: the project kick off meeting and the first All-Hands-Meeting (AHM). The project kick off meeting was held in Amsterdam (The Netherlands, 8-9 October 2010) with 23 participants. It was organized by the University of Amsterdam. Appendix 1 contains a picture and the agenda.

The first All-Hands-Meeting (AHM) was scheduled in Garching (Germany, 14-17 February 2011), organized by LMU with 33 participants joining the meeting. Appendix 10.2 contains pictures and the agenda.

The next AHMs are scheduled for October 2011 in Poznan and January 2012 ion London.

2.3. Description of Dissemination Deliverables

The following dissemination deliverables will be provided by the project:

Deliverable	Status
D2.1) MAPPER Home Page and mailing lists (due in month 3)	done
D2.2) Final Plan for the Use and Dissemination of Foreground This report will present a detailed plan and schedule for all dissemination actions. It will consist of the list of conferences/workshops and topics the project participants will take part in. D.2.2 will be delivered in month 3.	done
D2.3) Project Communication Kit The Communication Kit will be delivered in stages. The first stage will contain the project leaflet, the project poster and related support material. Both the poster and the leaflet will advise on the purpose of the project. The goal is to make stakeholders, as well as the general public, aware of the project, of the benefits of a Grid-based research infrastructure, and it indicates how to join the MAPPER Open Forum. The kit (or parts thereof) will be distributed during the project's lifetime at conferences, workshops and seminars to be identified in deliverable D2.2. The kit will be revised annually and delivered in months 6, 15 and 27.	
D2.4.1, D2.4.2, D2.4.3) Annual Dissemination Report	first

The annual dissemination reports reflect the work done in the lapsed project year	report
and reviews the actions to be performed in the coming year. Especially, it reports	D2.4.1
on the results as collected by the success measurements. The final dissemination	is this
report (M36) will summarize the work done during the complete project. It will	report
reflect the dissemination activities and evaluate them by taking into account the	
collected measurements. It will also contain a section on "Awareness and Wider	
Societal Implications" presenting horizontal project-related issues (including	
gender and science & society related aspects). Delivery of the reports will be in	
months 12, 24 and 36.	
D2.5.1, D2.5.2) MAPPER Seasonal Schools in months 18 and 30.	open

2.4. The MAPPER Home Page

The MAPPER home page is based on wiki technology and consists of three areas with the following restrictions:

- A public area for disseminating the project's purpose. This part is completely public
 for viewing, and it offers background information on each of the partners involved,
 and gives information on events taking place and the standardization work being
 done. Content can be included by every project partner.
- A semi-public area for describing how to deploy and operate MAPPER services. This
 area will include a step-by-step cookbook and offer pre-built packages and an
 accompanying distribution. This part of the webpage will be editable only by members
 of the project, but viewable for every registered user, i.e., user groups testing the
 deployment.
- A private area, which is only readable and writable by project partners. It serves as a communication medium and contains work in progress, such as draft deliverables, the technical annex, internal notes, and so on.

Figure 1 contains a screenshot of the MAPPER entry screen (http://www.mapper-project.eu/web/guest/home). For more detailed information we refer to deliverable D2.1 [1].

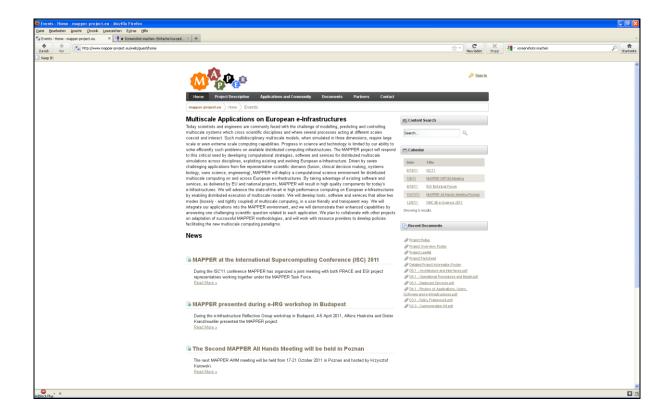


Figure 1: Screenshot of MAPPER home page

While the visitor statistics of the MAPPER website (starting August 2010) can be determined from Figure 2, the geographic distribution of the visits and the basic site usage are depicted in Figure 3¹ (same time period).

¹ All statistics are based on Google Analytics.

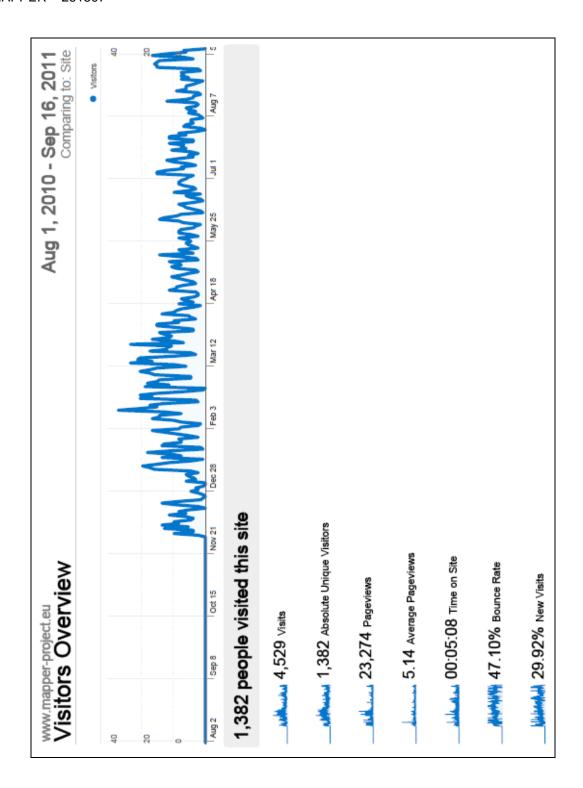


Figure 2: MAPPER web site visitor statistics

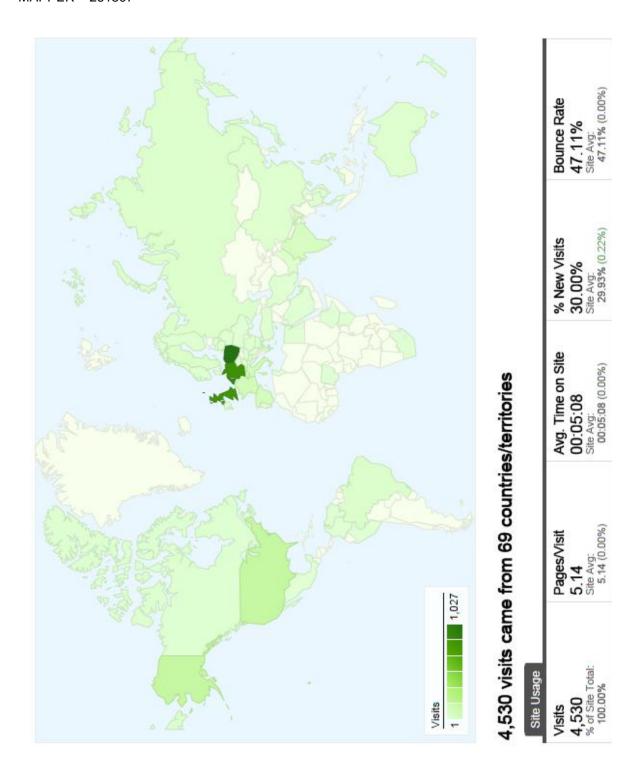


Figure 3: Geographic distribution of visits and site usage

3. Dissemination and Outreach

The MAPPER web site (see section 2.4. serves as the first contact point for all stakeholder groups. These groups are:

- scientists
- students
- system integrators
- industry experts
- standardization bodies

3.1. Scientists

Scientists may be most easily approached by visiting domain-specific conferences. These conferences include (but are not limited to) conferences on grid computing, distributed computing, network infrastructures, visualization, real-time applications, program frameworks, and conferences on specific application topics. As a matter of fact, MAPPER especially seeks to disseminate its experiences and prototypes to the application communities by participating conferences on fusion, hydrology, physiology, nanomaterials, computational biology, and similar conferences in related fields. Another possibility to approach scientists are the concertation activities organized by the European Commission. More information about events MAPPER took part can be found in section 0

3.2. Students

As students are tomorrow's scientists, it is very important to take care of their needs. Most likely students have never heard of multiscale applications during their studies, in fact it is quite common that they never were exposed to the term "grid computing". The MAPPER project has set out to organize seasonal schools in spring 2012 and 2013 where students have the possibility to learn what multi scaling and Grid computing are about. The number of participants will be a critical success factor.

3.3. System Integrators and Industry Experts

These two communities will provide input to the requirements of the MAPPER software API and the shape of the software components to be developed so that they can easily be deployed and used on top of an e-infrastructure.

As soon as the design phase of the MAPPER project has ended, these groups will be targeted through workshops and seminars and will be taught on how to use and deploy the newly developed software components. As this will happen later in the project lifetime, no detailed plan has been created so far. However, it can be anticipated that the brochures

which will contain information on the deployment of the software components will play a critical role in this task.

3.4. Standardization Bodies

With regards to standardization, the MAPPER project leverages the work already begun in the Open Grid Forum (OGF) and similar bodies (see [2]. The standardization workpackage WP3 is responsible for technically interfacing with these bodies. However, for non-technical work, especially to increase the visibility of the standards, the MAPPER dissemination team will liaise with these bodies as well.

3.5. Gathering Feedback and Measurable Parameters

For future events MAPPER plans to distribute questionnaires and ask people to provide their feedback. Together with web site visitor statistics and event participation statistics the questionnaires will provide a very good indicator for the success of dissemination efforts, both quantitavely and qualitatively.

4. Dissemination Material

In order to be recognisable, MAPPER needs to build a strong corporate image, brand and style. These guidelines will be developed and enforced by the dissemination team when need arises, and documented on an internal space on the MAPPER web site as well as in updated versions of this document. For the time being, the following elements exist (for a more detailed discussion see also [3].

- A logo with very distinctive colors
- A matching color scheme
- Templates for slides and deliverables

These items will be discussed in the following sections.

4.1. MAPPER Logo



Figure 4: MAPPER logo

The logo art work is based on a set of colors to be used in all publications to ensure a homogeneous appearance of the project to the outside world. The colors and their use are given in the following table.

Color Name	R;G;B	Usage
orange	255;124;000	for the "M" background
dark red	167;074;069	for the "A" background
dark green	097;115;053	for the first "P" background
black	000;000;000	for the second "P" background
light blue	065;128;255	for the "E" background
purple	115;095;142	for the "R" background

4.2. Items to Be Disseminated

All items to be disseminated are subsumed under the label "MAPPER Communication Kit" (see also [3]). The communication kit consists of a folder, the project leaflet, dedicated project application brochures, project posters, project white papers, the scientific papers published by the project, visual and audio media galleries, press clippings, a project rollup, and a set of project related give-aways. Appendix 10.3 contains the actual status of the material. All give-away items, the folders, the leaflets, and the brochures are on stock at LMU. They can be ordered by the partners.

The posters are available for download from

- http://www.mapper-project.eu/documents/10155/22766/Project+Overview+Poster (for the overview poster) and from
- http://www.mapper-project.eu/documents/10155/22766/Detailed+Project+Information+Poster (for the detail poster).

The MAPPER rollup is available in three copies. One copy ist kept at LMU, the other copies are "on the road".

5. MAPPER Dissemination Channels

The MAPPER dissemination channels are described in deliverable D2.2 [3]. The achievements per channel are reported here.

5.1. MAPPER Home Page

See section 2.4.

5.2. Journals, Conferences and Workshops

During the reporting period MAPPER was presented at following occasions:

Category	Presentation
Talks	Multiscale modelling and simulation: Alfons Hoekstra, October
	2010, Invited lecture at 2010 Barcelona School on Biomedical
	Informatics, Barcelona, Spain
	2. Distributed Multiscale Computing for Biomedical Applications:
	Alfons Hoekstra, December 2010, Invited lecture, SARA
	Superdag, Amsterdam, the Netherlands
	3. Real Science at the Petascale: Peter Coveney and Derek
	Groen, December 2010, Presentation on the CCP5 Workshop:
	Algorithms and Architectures for Molecular Simulation, STFC in
	Daresbury, UK
	4. SAGA BigJobs in help of Multiscale Applications: Mariusz
	Mamonski, March 2011, Technical talk at Open Grid Forum 30
	(SAGA general session), Taipei, Taiwan
	5. Distributed Multiscale Computing: The MAPPER project: Alfons
	Hoekstra, April 2011, Presentation at the EGI User Forum,
	Vilnius, Lithuania
	6. Von Neumann Symposium: Peter Coveney, July 2010,
	Snowbird, Utah, USA
	7. PRACE Symposium: Peter Coveney, Ilya Saverchenko, Derek
	Groen, April 2011, Helsinki, Finland
	8. e-Science Institute: Peter Coveney, Edinburgh, UK
	9. Seminar on Clays and Clay-Polymer Nanocomposites: Peter
	Coveney, Department of Chemistry at Qatar University,
	February 2011
	10. Computational Biomedicine: A Challenge for the 21st Century:

Category	Presentation	
	Peter Coveney, RPI-NSF Workshop on Multiscale Modeling of	
	Complex Data, September 2011	
	11. Algorithms and Architectures in Molecular Simulation: Derek	
	Groen, Daresbury Laboratory, December 2010	
	12. PRACE/XSEDE Summer School: Derek Groen, Lake Tahoe,	
	California, USA, August 2011	
Papers (peer	1. Stefan J. Zasada, Derek Groen, Peter V. Coveney: Developing	
reviewed)	an infrastructure to support multiscale modelling and	
	simulation; Proceedings of the 2011 TeraGrid Conference:	
	Extreme Digital Discovery; Salt Lake City, Utah, USA; 2011	
	2. Swain M., Coti C., Mandel J. & Dubitzky W.: A topology-aware	
	evolutionary algorithm for reverse-engineering gene regulatory	
	networks, in Dubitzky W., Kurowski K., Schott B. (eds.), Large-	
	scale computing techniques for complex system simulations,	
	141-162, Wiley-VCH, 2011.	
Papers (non peer	Towards Distributed Multiscale Computing for the VPH: Alfons	
reviewed)	G. Hoekstra and Peter Coveney, Abstract accepted for the	
	VPH2010 conference (http://www.vph-noe.eu/vph2010)	
Extended	1. A framework for multiscale and multiscience modeling and	
abstracts	numerical sumulations: B. Chopard, J.L. Falcone, A. Hoekstra,	
	and J. Borgdorf, Unconventional Computation 2011 10th	
	International Conference on Unconventional Computation June	
	6 – 10, Turku, Finland	
Magazines and	1. MAPPER-Multiscale Applications on European e-	
newsletters	Infrastructures: Alfons Hoekstra, January 2011, VPH NoE	
	newsletter No 5	

In addition, MAPPER organizes and supports the First Workshop on Distributed Multiscale Computing in conjunction with the IEEE e-Science conference 2011 (December 5, 2011, Stockholm, Sweden). For more information on DMC we refer to http://www.computationalscience.nl/dmc2011/.

5.3. Seasonal Schools

Not applicable for the reporting period

5.4. Events

MAPPER participated in the Munich Network Management (MNM) Team's booth at the Supercomputing 2010 in New Orleans, USA, November 13-19 (booth 1360 in

Figure 24). MAPPER attracted more than 300 visitors.

MAPPER was also co-represented at MNM Team's booth at the International Supercomputer Conference (ISC) 2011 in Hamburg, Germany, June 17-21, with more than 100 visitors. A layout of the booth may be derived from Figure 25.

Appendix 10.4 has the floorplan for Supercomputing 2010 and a booth picture from ISC 2011.

5.5. Press and Media

Not applicable in the reporting period

5.6. Cross Project Dissemination

MAPPER shared ideas with other national and international projects as per the following table:

Project	URL
DRIHMS	http://www.drihms.eu/
DRIHM	To be announced
D-Grid	http://www.d-grid.de/
IGE	http://www.ige-project.eu/
Scalalife	http://www.scalalife.eu/
PL-Grid	http://www.plgrid.pl
EGI	http://www.egi.eu/
PRACE	http://www.prace-ri.eu/
VPH (in general), VPH-NoE,	http://www.vph-noe.eu/
VPH-SHARE	
ContraCancrum	http://www.contracancrum.eu/
InBiomedVision	http://www.inbiomedvision.eu/
EUDAT	http://www.csc.fi/english/pages/parade/whitepaper
CRESTA	http://cordis.europa.eu/fetch?CALLER=PROJ_ICT&ACTI
	ON=D&DOC=1&CAT=PROJ&QUERY=0132af13aed6:0
	9a9:258f5abd&RCN=100077

5.7. Local Dissemination

The Project Steering Group agreed on pursuing local dissemination as well. The first step to local dissemination is to setup a web site describing the MAPPER project in native language with a link to the English MAPPER home page. Having information on the MAPPER project localized is the first step to reach native stakeholder communities not fluent in English (for example local media). Localization is in progress. The current status of local dissemination activities will be reported in future versions of this document.

5.8. Concertation Activities

The European Commission regularly initiates concertation activities as platforms to bring together otherwise isolated projects. MAPPER is a strong supporter of these concertation activities and plans to participate in all of them as soon as the exact dates are announced. General Dissemination Roadmap

The following table lists all planned dissemination and outreach activities for the whole project duration, as they are currently planned.

If the "Key" column is encoded we use following codes:

- "D" denotes a formal MAPPER deliverable
- "O" denotes events MAPPER has organised / will organise (totally or partially)
- "S" denotes standardization events relevant for MAPPER
- "B" denotes events MAPPER is / will be represented with a booth

Please note that this table is subject to (frequent) changes and that several partners may be involved per activitiy.

Key	Month	Activity
	10/2010	Cracow Grid Workshop
S	10/2010	OGF30
	11/2010	e-Infrastructure Concertation Meeting
В	11/2010	International Conference for High Performance Computing,
		Networking, Storage and Analysis (SC)
D	12/2010	Deliverable D2.1 (Report on home page and mailing lists)
D	12/2010	Deliverable D2.2 (Report on final plan for the use and
		dissemination of foreground)
S	03/2011	OGF31
D	03/2011	Deliverable D2.3.1 (Report on Project Communication Kit)
	04/2011	European Geosciences Union General Assembly

Key	Month	Activity	
	04/2011	Open e-IRG Workshop	
	04/2011	EGI User Forum	
В	06/2011	International Supercomputer Conference (ISC)	
	06/2011	Federated Identity Management Workshop	
S	07/2011	OGF32	
	07/2011	EGI Technical Forum	
S	09/2011	OGF33	
D	09/2011	Deliverable D2.4.1 (First annual dissemination report)	
	11/2011	Cracow Grid Workshop	
В	11/2011	International Conference for High Performance Computing,	
		Networking, Storage and Analysis (SC)	
0	12/2011	DMC workshop at IEEE e-Science Conference	
D	12/2011	Deliverable D2.3.2 (Project Communication Kit Update)	
	02/2012	Euromicro International Conference on Parallel, Distributed and	
		Network-Based Processing (PDP)	
D	03/2012	Deliverable D2.5.1 (First seasonal school)	
	04/2012	European Geosciences Union General Assembly	
S	04/2012	OGF34	
	04/2012	EGI User Forum	
В	06/2012	International Supercomputer Conference (ISC)	
	07/2012	EGI Technical Forum	
S	09/2012	OGF35	
D	09/2012	Deliverable D2.4.2 (Second annual dissemination report)	
	10/2012	Cracow Grid Workshop	
0	12/2012	IEEE e-Science Conference	
D	12/2012	Deliverable D2.3.3 (Project Communication Kit Update)	
	02/2013	Euromicro International Conference on Parallel, Distributed an	
		Network-Based Processing (PDP)	
D	03/2013	Deliverable D2.5.1 (Second seasonal school)	
S	03/2013	OGF36	
	04/2013	European Geosciences Union General Assembly	
	04/2013	EGI User Forum	
В	06/2013	International Supercomputer Conference (ISC)	
	07/2013	EGI Technical Forum	

Key	Month	Activity
D	09/2013	Deliverable D2.4.3 (Third annual dissemination report)
S	09/2013	OGF37

6. Summary

In this document we summarized the dissemination activities performed during the respective reporting period. The general timeline for all dissemination activities is outlined in the dissemination roadmap.

The major dissemination achievements for the first reporting period (year 1 of the project) are the following:

- The MAPPER home page is up and running.
- The MAPPER Communication Toolkit is available in its first version
- MAPPER disseminated its vision, objectives and messages at several occasions, including the International Supercomputing Conference 2011 in Hamburg with a larger booth.

7. References

- [1] MAPPER Deliverable D2.1: MAPPER Home Page and mailing lists;

 http://www.mapper-project.eu/documents/10155/23424/D2.1+-+HomePage.pdf;
 2011
- [2] MAPPER Deliverable D3.2: Standardization Roadmap and First Sustainability Plan; To be published; 2011
- [3] MAPPER Deliverable D2.2: Final Plan for the Use and Dissemination of Foreground; http://www.mapper-project.eu/documents/10155/23424/D2.2+-+Dissemination+Plan.pdf; 2011

8. Abbreviations

AGH Akademia Górniczo-Hutnicza Cracow

AHM All Hands Meeting

API Application Programming Interface

CUT Chalmers University of Technology

EGI European Grid Infrastructure

HPC High Performance Computing

IPP Max-Planck-Institut für Plasmaphysik

ISC International Supercomputer Conference

LMU Ludwig-Maximilians Universität

MAPPER Multiscale Applications on European e-Infrastructures

MCK MAPPER Communication Kit

MNM Munich Network Management

OGF Open Grid Forum

PSNC Poznan Supercomputing and Networking Center

UCL University College London

UNIGE Université de Genève

UU University of Ulster

UvA Universiteit van Amsterdam

WP Work Package

9. Appendix

10.1 Pictures and Agenda of the Kick Off Meeting



Figure 5: MAPPER team at kick-off

MAPPER kickoff meeting

Amsterdam, the Netherlands

Faculty of Science, University of Amsterdam, Amsterdam, The Netherlands, October 7-8, 2010

Agenda

Day 1: Thursday, October 7, 2010 (room t.b.a.)

08.30 - 09.00 Room open, coffee

09.00 - 09.30 Welcome, introduction, expectations (Alfons Hoekstra - UvA)

09.30 - 11.00 Introduction of MAPPER applications

(10 minutes for each application and 20 minutes in total for discussions)

Fusion (Par Strand - Chalmers and David Coster - MPG; 20 minutes)

Hydraulics (Bastien Chopard – UNIGE; 10 minutes))

Physiology (Peter Coveney – UCL and Alfons Hoekstra – UvA; 20 minutes))

Nanomaterial Science (Peter Coveny - UCL; 10 minutes) Computational Biology (Werner Dubitzky - UU; 10 minutes)

11.00 - 11.15 Short coffee break

11.15 - 12.45 Multiscale modelling and simulation

(30 minutes for each topic, including discussions)

Multiscale modelling paradigms (A. Hoekstra - UvA) Loosely coupled multiscale simulations - GridSpace (demonstration by CYFRONET)

Tightly coupled multiscale simulations - MUSCLE (introduction by UvA)

12.45 - 14.00 Lunch

14.00 – 15.00 Interoperability Layer (Introduction and demonstrations)

(30 minutes for each topic, including discussions)
The Application Hosting Environment (UCL)

QCG-Broker and the SAGA Vine Toolkit (POZNAN)

15.00 - 17.00 Parallel sessions (working/discussion sessions)

Services

Chair person - Michael Schiffers

Topics: 'fast' versus 'deep' track, what is the interoperability layer, what will be

integrated and when?

Expected outcome - A more detailed proposal on the architecture of the interoperability layer and the middleware building blocks, as well as

planning

17.00 - 18.00 Reporting, wrapping up

Applications

Chair person - Bastien Chopard

Topics: further qualifications of each application

Expected outcome - for each application, a first draft of a Scale Separation Map, computational requirements, and expected progress ('quantum leap') beyond state of the art.

Figure 6: Agenda kick off, day 1

Day 2: Friday, October 8, 2010 (room t.b.a.)

8.30 Room open, Coffee

09.00 - 10.00 Administrative and managerial issues (Isabelle Wartelle - UvA)

10.00 - 10.30 PSG Meeting Chair person - Alfons Hoekstra

Attendees: one formal representative for each partner, as mentioned on the grant agreement.

Topics: formalize management structure, decide on meeting agenda.

10.30 – 12.30 Dissemination and policy Chair Person – Michael Schiffers

Topics: Dissemination and policy related activities.

10.00 - 12.30 Technical working session

Topics: in depth technical discussion, split up in small working groups. Topics will emerge in day 1, but could involve issues related to MUSCLE and JADE, MUSCLE on Proactive or even on Gridspace; AHE vs QCG-Broker, how to execute on PRACE/EGI, etc.

Expected outcome – first conclusions, actions points, detailed planning of work to be

12.30 - 14.00 Lunch

14.00 – 15.00 two rooms are available for further discussion, take decisions, draft conclusions

15.00 - 16.00 reporting, agenda and work plan for the first 6 months of the project, meeting agenda.

16.00 Closing of meeting (note that two rooms remain available for further work)

Figure 7: Agenda kick off, day 2

10.2 Pictures and Agenda of the First All Hands Meeting



Figure 8: Snapshots from the Garching AHM

Day 1: Monday, February 14, 2011 (Room H.E.009 plenary sessions)

09:30 - 10:00 Opening, Presentation of the agenda and expected outcomes (Alfons Hoekstra)

- 10:00 12:30 **Applications** (session chair: Marian Bubak)
 - 1. The formal framework (characterization, MML; Joris Borgdorff and Bastien Chopard)
 - 2. Status update of each single application (20 minutes each)
 - characterization with SSM and MML
 - technical description of each application according to the template distributed during the kick-off meeting
 - current status of application development
 - 3. Wrapping up (Marian Bubak)
 - to which extend applications feed into the formal framework
 - · what is missing in the application descriptions
- 12.30 13.30 lunch

13:30 – 14:30 Demonstration of a first application on MAPPER (session chair: Marian Bubak)

- ISR application run with GridSpace on 1 node; with PBS system, usage of MUSCLE and MATLAB, collaboration with QCG (Joanna Kocot, Katarzyna Rycerz, Tomasz Gubała)
- ISR application run on production clusters using selected MAPPER fast track components and QoS capabilities (in particular advance reservation) - Mariusz Mamonski

14:30 – 15:30 Feedback on applications- discussions (session chair: Marian Bubak)

From the perspective of WP8 (programming and execution tools, Katarzyna Rycerz, Bastien Chopard)

From the perspective of WP4 – WP6 (services & operations – Chris Kurowski) From the perspective of WP1 (Management – Alfons Hoekstra)

15:30 – 17:00 **Services & operations** (session chair: Chris Kurowski)

- 15.30 15.45 Introduction to services & operations, introduction to the first e-infrastructure demonstration (Chris Kurowski)
- 15.45 16.15 Operations and deployment perspective on extended e-Infrastructures for MAPPER (Ilya Saverchenko)
- 16.15 16.30 Integration issues with selected fast-track components selected for the first demonstration (Mariusz Mamonski)
- 16.30 17.00 Adaptation of fast track components in the first demonstration (Stefan Zasada)
- 17:00 18:00 guest lecture by Anton Frank (LRZ) the PRACE and EGI projects, an update

Figure 9: Agenda AHM, day 1

Day 2: Tuesday, February 15, 2011 (Room H.E.009 plenary sessions)						
08.30 Room open, Coffee						
09.00 – 10.00 Programming & execution tools (session chair: Marian Bubak) Introduction of the idea of a multiscale application simulator (Katarzyna Rycerz), Introduction to the layer of programming and execution tools, presentation of the concept, introduction for discussion on Wednesday (Katarzyna Rycerz)						
10.00 – 10.30 Dissemination (Michael Shiffers)	Dissemination (Michael Shiffers)					
10.30 – 11.00 Management (Isabelle Wartelle)	0 – 11.00 Management (Isabelle Wartelle)					
11.00 – 12.30 Parallel sessions (Room H.E.008 and H	- 12.30 Parallel sessions (Room H.E.008 and H.E.009)					
PSG Meeting	Technical working session					
Chair person – Alfons Hoekstra Attendees: one formal representative for each partner, as mentioned on the grant agreement.	A short GridSpace tutorial (Joanna Kocot) MUSCLE, QCG tutorials (Joris Borgdorff + ?)					
Agenda will be distributed to PSG						
12.30 – 13.30 lunch						
13.30 – 14.15 Decision taking (session chair: Alfons Hoekstra) On all issues related to the fast track development On all issues related to middleware (as far as possible) On a workplan for the next project period						
14.15 – 15. 00 Lecture: The Euforia Project (David Coster, Par Strand).						
15.00 – 16.45 Guided tour through the Leibniz Supercomputing Centre						
16.45 – 17.30 Set up goals and agenda for next two days (Marian Bubak, Chris Kurowski)						

Figure 10: Agenda AHM, day 2

Day 3: Wednesday, February 16, 2011 (Room H.E.009 plenary sessions, H.E.008 for break-out sessions)

08.30 Room open, Coffee

09.00 - 10.00 Policy & Sustainability (Derek Groen, Werner Dubitzky)

A detailed agenda will be drafted during the first two days, but the following topics are identified and should be worked on:

- Tightly vs. loosely coupled applications resource management perspective (parallel session with WP8 to be organised by Chris Kurowski)
- Fast track components which and why? (parallel session for WP4, WP5 and WP6 to be organised by Chris Kurowski)
- WP7-WP8 session (parallel session to be organised by Katarzyna Rycerz) Elaboration on the design of the layer of programming and execution tools and checking it against applications requirements (discussions)
- The current status of MAPPER e-Infrastructure what should be do next? (parallel session for WP4, WP5 and WP6 to be organised by Ilia Saverchenko)
- SSM and xMML descriptions of all applications (to be organised by Joris Borgdorff)

Moreover, were possible initial implementation, porting of applications, software development and testing should be pursued, so:

All day

technical meetings, collaborative code development, etc. Would it e.g. be possible to get a first application up and running in a rudimentary MAPPER environment. Would it be possible to already solve technical problems identified with applications, programming tools, middleware. Bring all programmers in MAPPER together and get work done

Day 4: Thursday, February 17, 2011 (Room H.2.007; Room H.2.002)

Morning session continue day 3 activity, with emphasis on technical work and code development.

A detailed agenda will be drafted during the first two days, but the following topics are identified and should also be worked on:

- New communication library for high-speed interconnections (a parallel session for WP4, WP5 and WP6 organised by Derek Groen)
- Technical review of Deep track components (parallel session for WP4, WP5 and WP6 organized by Stefan Zasada)
- Session on D 4.1 (a plenary session for all, organized by Derek Groen)
 - Plan of D 4.1
 - Contribution to D 4.1 from WP4 perspective
 - Contribution to D 4.1 from WP7 perspective
 - Contribution to D 4.1 from WP8 perspective (Tomasz Gubała)

After lunch wrapping it all up

Reporting on what has been achieved

Discussion on how to proceed, including a detailed planning

14.30 closing of meeting

14.30 – 18.00 Rooms are available for further working sessions.

Figure 11: Agenda AHM, days 3 and 4

10.3 Dissemination Items

10.3.1 Project Folder

The project folder serves as container for printed material. It is shown in Figure 12 and Figure 13.

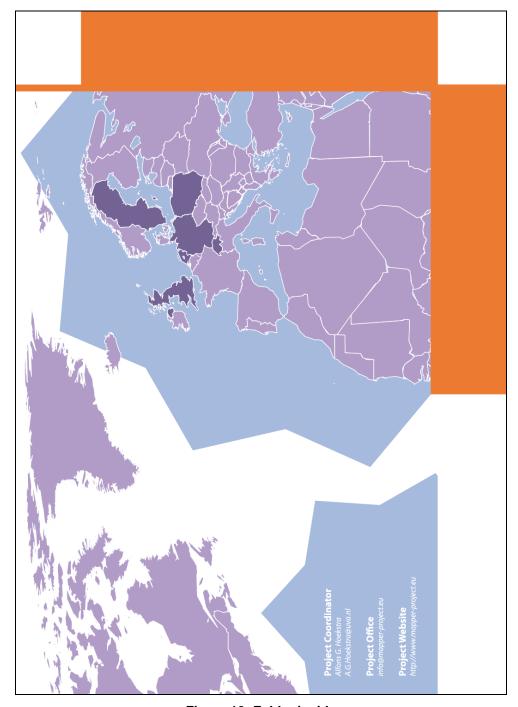


Figure 12: Folder inside

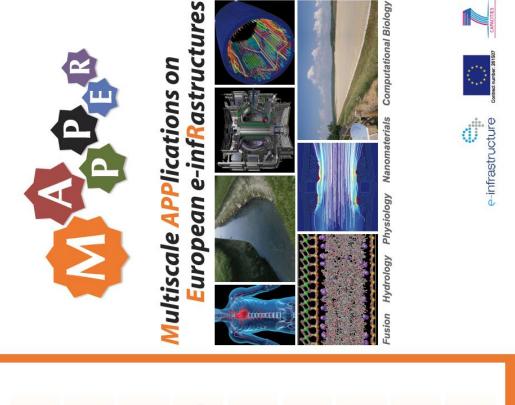




Figure 13: Folder outside

10.3.2 Project Leaflet

The MAPPER project leaflet contains basic information about the MAPPER project with the objective of making the recipient curious about the MAPPER project. The leaflet can be found in Figure 14 and Figure 15.

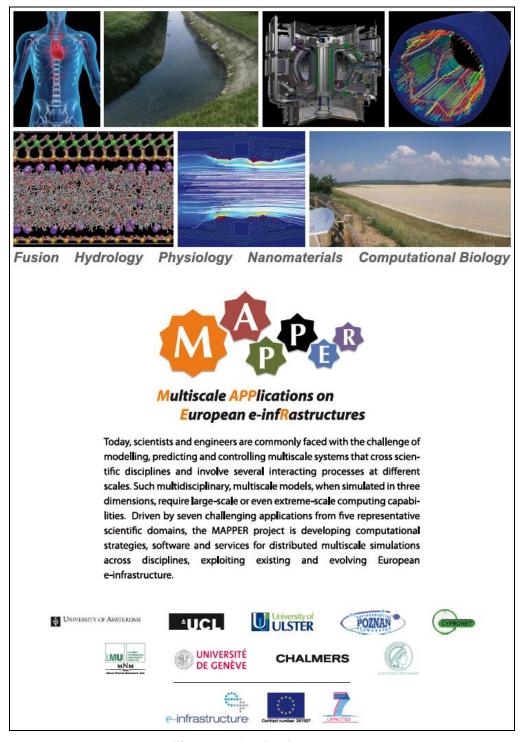


Figure 14: Leaflet front page

Multiscale APPlications on European e-infRastructures

MA DER

Objectives

MAPPER is developing strategies and will provide tools, software and services that permit loosely and tightly coupled multiscale computing in a user friendly and transparent way. This will be accomplished by deploying a computational science environment across European e-infrastructures.

User communities

MAPPER is driven by seven exemplar applications from five user communities:

- physiology
- computational biology
- fusion
- hydrology
- nano-material science

However, our solutions are generic and will enable distributed multiscale computing for any multiscale models fitting into our paradigm. In this way, MAPPER will be relevant to other user communities.

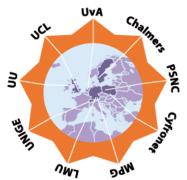
Technical Aspects

MAPPER integrates heterogeneous infrastructures for programming and execution of multiscale simulations. We reuse much of the functionality provided by existing software solutions - MAPPER is developed on top of existing e-infrastructures without the necessity to modify already deployed components. This is done by creating extensions using well defined and standardized interfaces, which reduce the potential impact of changes in middleware level components.

International Aspects

Multidisciplinary and multiscale models require extremescale computing capabilities. We have significant trans-Atlantic Grid and HPC experience and will work together closely with European resource providers and user communities.

Consortium



Project Information

Project acronym: MAPPER
Contract number: RI-261507
Project type: CP-CSA
Start date: 01.10.2010
Duration: 36 months

Keywords: Distributed Multiscale

Computing

Related Projects

EFDA VPH-NoE EUFORIA MeDDiCa PRACE EGI-InSPIRE

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Figure 15: Leaflet back page

10.3.3 Brochures

MAPPER aims at multiscale applications. The MAPPER application brochure contains a short description of these applications. Figure 16 and Figure 17 depict the brochure.



MAPPER Applications



Fusion Hydrology Physiology Nanomaterials Computational Biology

The MAPPER project is driven by the computational needs of seven exemplary multiscale problems from a variety of disciplines. Without exception these applications are of high scientific and societal importance.

Our Nanomaterials application concerns the prediction of performance properties of day-polymer nanomaterial for a range of diverse applications, based on an ability to couple quantum mechanical, classical mechanical, coarse-grained and macroscopic representations of these systems. The Physiology applications deal with cardiovascular and neurovascular diseases, aiming to better understand them and to improve their treatment. The Fusion applications are part of a global endeavour to demonstrate the scientific and technical feasibility of riskions as a sustainable energy source for the future. In this project it envisages coupling a number of single-physics codes into a workflow so as to perform simulations of the behaviour of ITER. The Hydrology application is concerned with networks of irrigation canals, the main challenge being to always guarantee an adequate water supply throughout the canal system. The Computational Biology application takes up the challenge to study the acid and xenobiotic system, which enables the detoxification and removal from the body of harmful compounds.

Simulation of Clay-polymer Composites (Nanomaterials)



Within MAPPER we aim to develop a multiscale simulation mechanism that will, through its advances, allow the study and design of layered mineral composites in such diverse areas as energy applications (oil industry additives) and biomedical applications (drug delivery). The microscopic structure and mechanisms of layered nanomaterials operate over many different length scales, ranging from nanometers to microns, and each length scale needs to be properly simulated to fully understand its features. We will use the MAPPER infrastructure, tools and software to couple three scale levels of simulation across distributed computing infrastructures. Combined with our scientific advances, this will facilitate the understanding of the underlying mechanisms of layered nanominerals on both the atomic and much larger scales.

In-stent Restenosis 3D (Physiology)

In-stem Restenoists 3D (Physiology)

The three-dimensional In-stem Restenois model (ISR3D) simulates a stent deployment to restore blood flow in coronary arteries and the subsequent processes associated with this procedure. The objective of the model is to study restenois, a medical condition where the artery narrows some time after an initial stent has been placed. The ISR3D model consists of four submodels: stent deployment and thrombus formation combined as initial conditions are usbmodels: stent deployment and thrombus formation combined as initial conditions (IC), blood flow (ISP), drug diffusion (IOP) and smooth muscle cell proliferation (SMC). First IC initial-zes the model by placing a stent in an artery and it calculates where thrombus should be formed given the blood circulation. These initial conditions are sent to SMC and for each iteration of SMC, DD and BF are activalated in parallel. For performance reasons BF keeps track of its last state, simplifying subsequent flow calculations.

Figure 16: Application borchure (outside)

Equilibrium Stability Workflow (Fusion)

The equilibrium stability workflow (*Pulson*)

The equilibrium stability workflow application is one of the scenarios used to simulate aspects of nuclear fusion processes. The equilibrium stability workflow consists of two subcodes: a magnetohydrodynamics (MHD) equilibrium code (*PEENA*) and a a linear MHD stability code (*PEENA*) and the consists as one application, several alternative workflows are possible which vary the profiles from the equilibrium code, recalculate the equilibrium stability workflow application is a loosely coupled workflow where the data can be exhanged via files or via structured objects defined by the *EFDA* Integrated Tokamak Modeling Task Force. Variants of the workflow can be defined which add additional components and then require multiple instances of the equilibrium and stability calculation modules.



Bile Acid and Xenobiotic System (Computational Biology)

Bile Acid and Xenobiotic System (Computational Biology)

The bile acid and xenobiotic system (BAXS) defines an intricate physiological network that detoxifies and removes harmful xenobiotic and endobiotic compounds from the body while ensuring that primary bile acids (essential for the emulsification and absorption of dietary fats and fat-soluble vitamins) are not eliminated and ane re-used. The results generated by using BAXS will help us to understand a range of physiological processes such as drug-drug interactions, intracrine hormone metabolism, xenobiotic clearance and cholesterol/lipid homeostasis. The BAXS involves the coordinated activities of many genes across multiple temporal and spatial scales. Basic BAXS processes and their time scales include the binding of iligands to nuclear receptors (hours), gene expression and regulation (hours), transporter protein (minutes) and metabolic enzyme activity (seconds). Spatially, BAXS components range from molecules (e.g., nuclear receptors) to organs (e.g., the liver). A comprehensive description of the interacting components that govern BAXS gene expression would enable the identification of regulatory nodes' as targets for treatment regimes, and understanding of the components impacting drug-drug interactions, and provide a framework for the design of large-scale, integrated prediction studies.



HemeLB (Physiology)



In this MAPPER application we are concerned with performing blood flow simulations of vessels in the brain in support of clinical neurosurgery. The behaviour of this blood flow plays a crucial role in the understanding, diagnosis and treatment of cardiovascular disease; problems are often due to anomalous flow behaviour in the neighbourhood of bifurcations and neurysms within the brain. Simulation offers the possibility of performing patient-specific, virtual experiments to study the effects of courses of treatment with no danger to the patient. For this work, we will use our lattice-Boltzmann code, Hemel.B, designed to simulate fluid flow in the sparse geometries of the human brain. The code can create visualizations from within a running simulation and send them to a viewing client on a workstation situated in, ultimately, a hospital. A clinician can then steer the parameters of the simulation while viewing the results. Away from the region of direct clinical interest, we require less accuracy in our hydrodynamical simulation and can therefore use a slightly more approximate but much faster method. Still further away, the rest of the circulatory system can be abstracted to a network model of the vasculature and a pump, i.e. the heart.



Transport Turbulence Equilibrium (Fusion)

The transport turbulence equilibrium application is a simplified and approximate version of a simulation of the full fusion core in a nuclear fusion reactor. The three main subcodes involved in transport turbulence equilibri-

2D equilibrium solver (elliptic, no explicit time, but equilibrium time dependent) 3D gyrofluid turbulence code, calculates transport coefficients. 1D transport code, calculates new profiles.

Both for HELENA and GEM a number of modules could be substituted, with differing tradeoffs of speed and accuracy/complexity). There are also some simple service modules in addition to these physics modules.

Irigation Canals (Hydrology)



In a recent collaboration with ESISAR at Grenoble INP, France, UNIGE has developed multiscale models for the management of a network of irrigation canals. The problem remaining to be solved is the definition of appropriate actions (e.g. opening and dosing gates) that need to be taken to always guarantee an adequate water supply throughout the canal system, whatever the external demands or perturbations may be, and with respect to constraints such as water height. We have identified four main sub-models in our application, where each sub-model can be instantiated several times inside the global model. The Complex Automata (CxA) formalism based on the lattice Boltzmann approach is used for the implementation of these submodels.

Multiscale applications are present in a wide range of scientific and engineering communities, and by its nature, multiscale modelling is highly interdisciplinary. Traditional monoscale approaches have often proven to be inadequate, because many physical processes are inherently taking place across a range of spatial and temporal scales. As a result, there is a growing need to develop systematic modeling and simulation appro-sesses enabling to solve the broad range of scientific and engineering multiscale problems. With the emergence of methodologies for multiscale modelling and simulation, we start to grasp the full complexity of multiscale problems.

The building blocks of a multiscale model are typically multiple single scale models and their mutual multiscale couplings. The multiscale scale models and their mutual multiscale couplings. The multiscale model can be represented as a directed graph on a Scale Separation Map (SSM). The MAPPER project will further exploit the multiscale modelling methodology developed in previous projects by using the formalism of the SSM and the coupling templates to create compositi-on tools for multiscale simulations.

The seven presented applications have been developed in previous projects and are actively used. We will integrate them into the MAPPER environment. However, our solutions are generic and will enable distri-buted multiscale computing for any multiscale models fitting into our paradigm, and MAPPER opens up to other user communities.



Figure 17: Application brochure (inside)

10.3.4 Project Posters

MAPPER offers as per today two project posters. They available as download from the MAPPER home page. The overview poster is shown in Figure 18, the detailed poster is depicted in Figure 19.



Figure 18: Overview poster

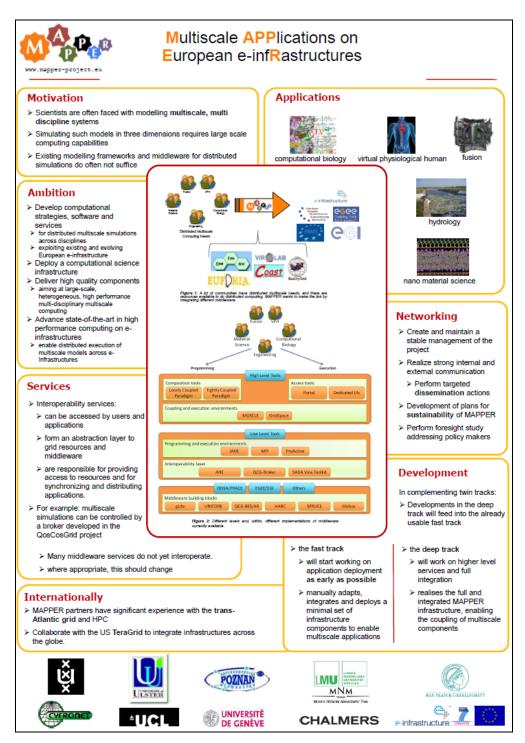


Figure 19: Detail poster

10.3.5 White Papers and Scientific Papers

White papers and scientific papers are not yet available.

10.3.6 Visual and Audio Media Gallery

The gallery is not yet available for the public audience.

10.3.7 Press Clippings

Press clippings are not yet available.

10.3.8 Project Rollup

MAPPER created three project rollups for dissemination purposes. The rollup is depicted in Figure 20.

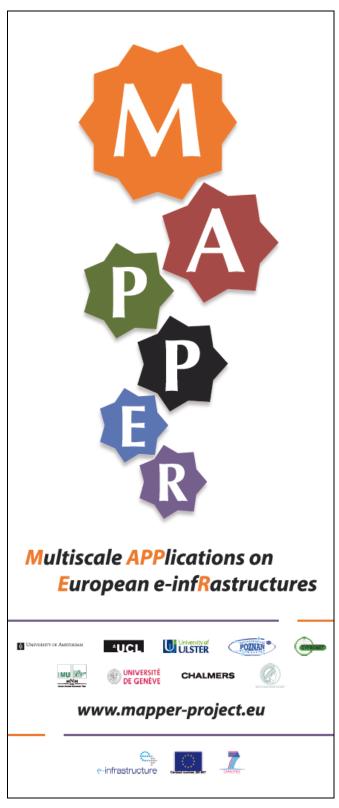


Figure 20: Rollup

10.3.9 Give-Away Items

These items have the purpose of remembering the MAPPER project. They contain a contact point for getting more information about the project. For the dissemination at booths, the MAPPER Seasonal School and other events ballpoint pens, reflector stripes, and lanyards have been created.

Figure 21 shows the inscription of a neon green reflector stripe.

Figure 22 shows the lanyard layout.

Figure 23 depicts the ballpoint pen inscription.

10.3.10 Event Calendar

The MAPPER Event Calendar will be updated constantly. It is available from the MAPPER homepage www.mapper-project.eu in the right navigation area.

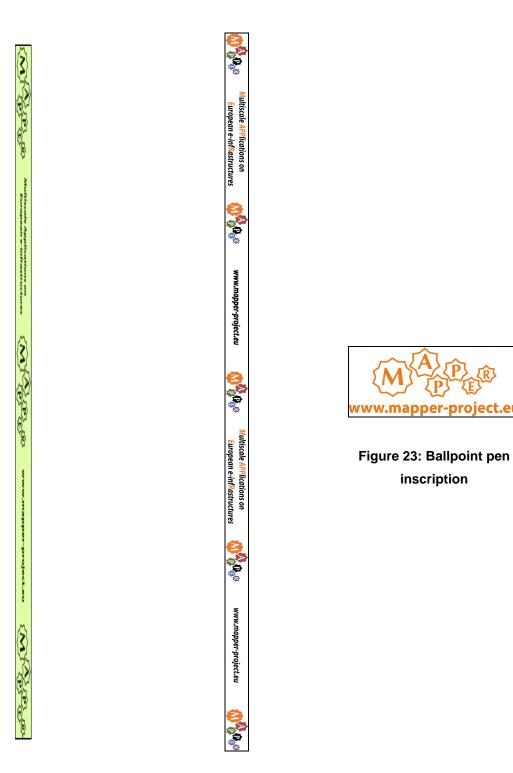


Figure 21: Reflector stripes

Figure 22: Lanyards

10.4 Booths at Events

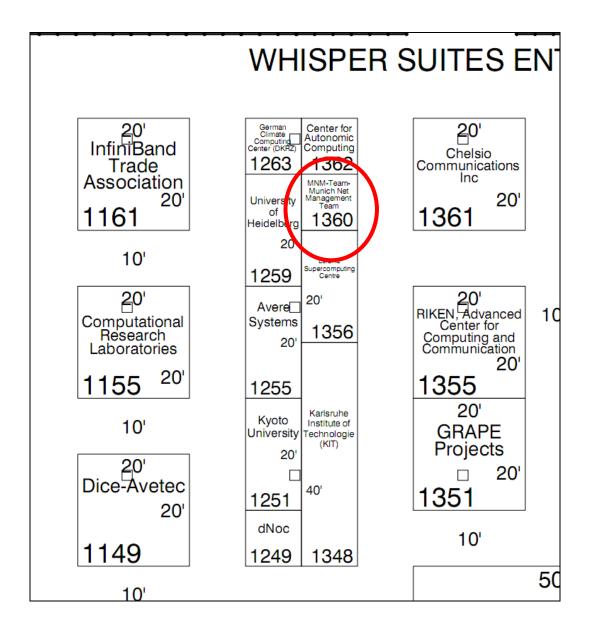


Figure 24: MNM booth at SC10 with MAPPER (excerpt from SC10 floorplan)



Figure 25: MNM booth at ISC 2011 with MAPPER