D.2.5.1 – MAPPER Seasonal Schools

Project acronym: *MAPPER*

Project full title: Multiscale Applications on European e-Infrastructures.

Grant agreement no.: 261507

Due-Date:	M18
Delivery:	M18
Lead Partner:	LMU
Dissemination Level:	PU
Status:	Draft
Approved:	Q Board, Project Steering Group
Version:	final

DOCUMENT INFO

Date and version number	Author	Details
05.03.2012	Simone Ferlin	Draft
22.03.2012	Alma Erenstein	Review as part of QA procedure.

TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

No table of figures entries found.
No table of figures entries found.
No table of figures entries found.
No table of figures entries found.

1   MAPPER First Seasonal School

There will be two seasonal schools, one in February, 2012 and one programmed for the beginning of 2013. The first seasonal school in February, 2012 was initially discussed at the

second AHM in Poznan. The collection of ideas for speakers, guest speakers and suitable topics started right after the second AHM in October, 2010 in Poznan. Following that, several telephone conferences discussing about the seasonal school organization, i.e. venue, presentation topics, tutorials and hands-on sessions were discussed and fixed.

The planning for the second MAPPER Seasonal School in the beginning of 2013 has already started during the third AHM in London, U.K. in January 2012. The event will be possibly located at Lorentz Centre (http://www.lorentzcenter.nl) in Leiden, the Netherlands. The organisation group has to wait until the proposal for the venue is approved. The application's deadline on the proposal for the venue ends by May, 2012 and the response should come at latest July,1st, 2012.

2 Promotion of the MAPPER First Seasonal School 2012

The venue for the first MAPPER Seasonal School's event was the University College London (UCL) in London, United Kingdom.

For the promotion of this year's MAPPER Seasonal School a leaflet was designed, printed and they were displayed at the information counter and around the session room during the event. For the participants of the seasonal school, all project partners suggested names for guest speakers as well as invited other scientists from other related projects and potential future cooperations for the MAPPER project to attend the MAPPER first Seasonal School 2012 in London.

Additionally, a dissemination pack including one MAPPER folder, one pen, one lanyard and the MAPPER first Seasonal School leaflets was distributed during the seasonal school to all participants, including all project partners as well to local dissemination. The MAPPER first Seasonal School took place after the third AHM placed in the same venue in London, U.K. In 2011, the first MAPPER Seasonal School was also promoted at the Munich Network Management (MNM) Team booth, and by LMU during the International Supercomputing Conference (ISC11) and the Supercomputing Conference (SC11).

3 Organisation of the MAPPER First Seasonal School

The MAPPER Seasonal School 2012 took place at the University College London (UCL) in London, United Kingdom, right after the third AHM.

The MAPPER first Seasonal School started on 01 February 2012 in the morning and ended on 02 February 2012 in the evening. Besides other minor organizational details, i.e. certificates for the participants, venue, catering, suggestions for accommodation and directions; a social event was organised in the evening of February 01 to visit a very touristic traditional pub and restaurant in London.

Participants received a MAPPER dissemination pack, and the content of the first MAPPER seasonal school, including all presentations, has been added to the MAPPER website.

The MAPPER first Seasonal School 2012 was opened by Ilya Saverchenko followed by a set of sessions grouped under different topics, each containing a set of very interesting presentations.

3.1 Agenda

The First MAPPER Seasonal School's programme took place between February 01st-02nd, 2012.

February, 01. In the programme below, the title of the presentations links directly to the presentation on the MAPPER website.

- 09:00 - Welcome - Ilya Saverchenko
- 09:15 - Session 1: Multi-scale Computing – Introduction
  (presentations)
  1. The World is Multi-scale - Taxonomy of Multiscale Computing Communities - Peter Coveney
  2. The MAPPER Project - Alfons Hoekstra
  3. Interoperation of HPC and HTC grid infrastructures Daniel S. Katz, University of Chicago, ExTENCI
- 10:15 - Coffee Break
- 10:45 - Session 2: Multi-scale Modelling Concepts
  (presentations)
  1. Overview
  2. Scale Separation Maps
  3. Tightly and Loosely Coupled Multi-Scale Models
  4. Multi-scale Modeling Languages
  All presentations in session 2 were held by Bastien Chopard
- 11:30 – Lunch
- 12:30 - Session 3: User Tools for Multi-scale Modeling and Simulations
  (presentations + practical)
  1. Application Hosting Environment (AHE) - Stefan Zasada
  2. Coffee Break
  3. Multiscale Coupling Library and Environment (MUSCLE) - Joris Borgdorff
  4. Coffee Break
  5. Gridspace, Multiscale Application Designer (MAD) and Mapper Memory (MaMe) - Kasia Rycerz
- 19:30 - Social Event

February, 02:

- 09:00 - Session 4: Middleware and e-Infrastructures
  (presentations)

- 1. European e-Infrastructures - Ilya Saverchenko
  2. QosCosGrid (QCG) - Chris Kurowski
- 10:15 - Coffee Break
- 10:30 - Session 5: Related Tools and Approaches
  (external presentations)
  1. Integrated services for multiscale modelling of materials using the UNICORE middleware Ivan Kondov, KIT, MMM@HPC
  2. Workflow Interoperability Enables Interdisciplinary Research - G.Z.Terstyanszky, University of Westminster, SHIWA
  3. Scalable Software Services for the Life Sciences - Mihai Duta, University of Oxford, ScalaLife
- 12:00 - Lunch
- 13:00 - Session 6: Constructing and running a DMC Simulation
  (practical) - James Suter and Stefan Zasada
  1. Coupling of 2 codes
  2. Resource reservation
  3. Submission
  All presentations of session 6: Constructing and running a DMC Simulation
- 14:30 - Coffee Break
- 14:45 - Session 7: Survey and Outlook
  (discussion) - Alfons Hoekstra
  1. How projects and communities can benefit from MAPPER
  2. Future developments
  3. Presentation slides for session 7: Survey and Outlook
  All presentations of session 7: Survey and Outlook
- 15:45 - Wrap-up - End of school - Peter Coveney

The MAPPER first Seasonal School gladly welcomed the following external speakers:

- Mr. Daniel S. Katz, Senior Fellow in the Computation Institute (CI) at the University of Chicago and Argonne National Laboratory, and Open Grid Forum Area Co-director for Applications. He was the TeraGrid GIG Director of Science from 2009-2011. He presented current efforts in the project ExTENCI.
- Mr. G.Z.Terstyanszky, Reader in Computer Science and Software Engineering at the University of Westminster. He presented current efforts in the project SHIWA (Sharing Interoperable Workflows for Large-Scale Scientific Simulations on Available DCIs) .
- Mr. Ivan Kondov, Teamleiter SimLab NanoMikro in Performance assessment of different constraining potentials in computational Multiscale materials and biomolecular simulations at Simulation Lab NanoMikro, Karlsruhe Institute of Technology (KIT). He presented current efforts in the MMM@HPC project.
- Mr. Mihai Duta, Scientific Software Advisor for the Oxford Supercomputing Centre, the University's central high performance computing services. He presented current efforts in the project ScalaLife (Scalable Software Services for Life Science) .

As one can see the MAPPER first Seasonal School had a highly diverse programme with presentations, all-hands sessions with practical exercises and external representatives. More details on the agenda and the names of the presenters' can be found on the MAPPER website.

We believe with this to have taken an important step ahead with MAPPER in having started the integration and proliferation of MAPPER software and applications on distributed computing infrastructures.

Also, during the MAPPER first Seasonal School, evaluation forms were given to the participants in order to gather feedback about the event. The form and results can be found below in this section.

3.2 Pictures

Some pictures and video records were taken during the presentations and all-hands sessions in the MAPPER First Seasonal School 2012:

Figure 1: MAPPER First Seasonal School

Figure 2: Presentation Mr. Katz

4 MAPPER First Seasonal School: Participant's Feedback

In order to gather feedback to improve the next MAPPER seasonal school event, an evaluation form was prepared and handed out during the MAPPER first Seasonal School 2012.

The feedback given was very good: We thank the seasonal school participants for their participation as well as all people that helped with the organisation. Together with good

V1.1-D2.5.1 MAPPER seasonal schools-LMU-M18

venue organization, good presentations, tutorials and hands-on sessions the MAPPER first Seasonal School was a successful event.

The following diagrams show the outcome of the survey graphically:

4.1 Results

Here one can see the results of the evaluation forms separated by four categories:
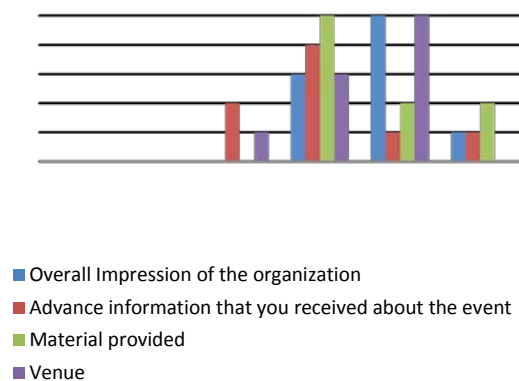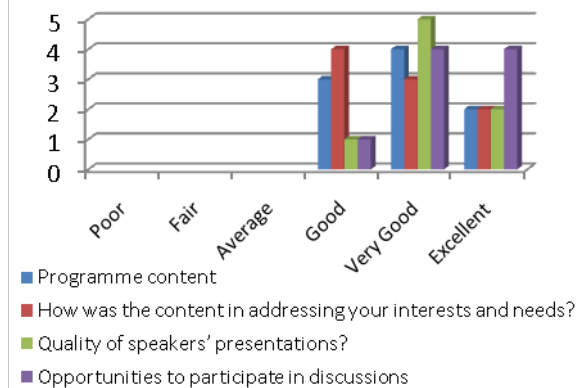

- Overall Impression of the organization
- Advance information that you received about the event
- Material provided
- Venue

Figure 3: Organisation of the Event

- Programme content
- How was the content in addressing your interests and needs?
- Quality of speakers' presentations?
- Opportunities to participate in discussions

Figure 4: Programme and Presentations

- Selection of the sessions' content
- How was the content in addressing your interests and needs?
- Quality of the tutorial and hands-on sessions
- Opportunities to participate in discussions
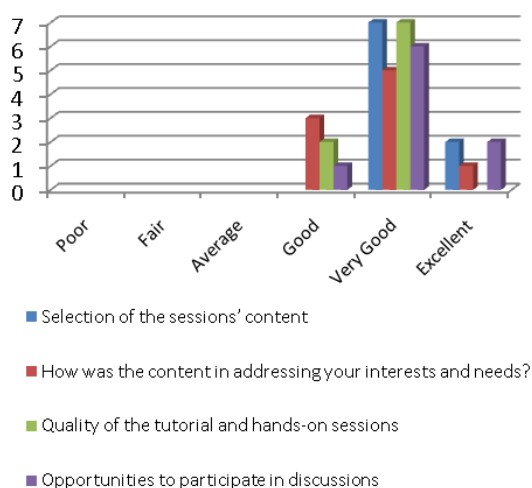
Figure 5: Tutorial and hands-on sessions

- Overall Impression of the event
- Opportunities to develop new ideas
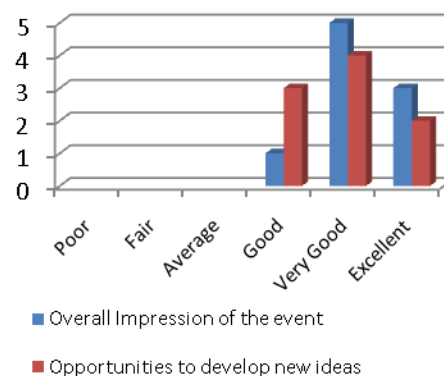
Figure 6:Overall impression of the event

4.2 Evaluation Forms

In the following, the evaluation forms distributed to all seasonal school participants show the different categories that were evaluated:

- Organization of the event
- Programme and presentations
- Tutorials and hands-on sessions
- Overall impression of the event

Each category contained 2 to 4 questions that can be seen in figures 3 to 6.

The last field in the form was about "general comments", that means, any improvements that were not mentioned in the four categories and could be valuable for future seasonal school, e.g., from scientific presentations over Internet connection to catering service was left for the participants to freely give their opinions.

In summary, the most important message left to the organisation group from participants was: *"I would like to see more external speakers and organisations giving talks and all-hands sessions."*

We are looking forward to improving this aspect in near future, which we have already started during the first seasonal school by having external representatives in the participants group of the seasonal school.

Below one can see the evaluation form that was distributed to all participants during the MAPPER First Seasonal School 2012:

Evaluation Form

MAPPER Seasonal School 2012

1st and 2nd February 2012 – UCL, London, U.K.

Organization of the event	Poor	Fair	Average	Good	Very good	Excellent
1. Overall Impression of the organization						
2. Advance information you received about the event						
3. Material provided						
4. Venue						
Programme and presentations	Poor	Fair	Average	Good	Very good	Excellent
5. Programme content						
6. How was the content addressing your interests?						
7. Quality of speakers' presentations?						
8. Opportunities to participate in discussions						
Tutorial and hands-on sessions	Poor	Fair	Average	Good	Very good	Excellent
9. Selection of the sessions' content						
10. How was the content in addressing your interests?						
11. Quality of the tutorial and hands-on sessions						
12. Opportunities to participate in discussions						
Overall impression of the event	Poor	Fair	Average	Good	Very good	Excellent
13. Overall Impression of the event						
14. Opportunities to develop new ideas						

General comments

Suggestions for improvement: Sessions, speakers, organisation etc.

V1.1-D2.5.1 MAPPER seasonal schools-LMU-M18

5 MAPPER Second Seasonal School 2013: Promotion

After the decision to locate the MAPPER Second Seasonal School 2013 in Leiden, the Netherlands, and fixing a date for the event expected for the beginning of 2013, flyers will be prepared in the same way as in 2011 for the first seasonal school in order to promote the MAPPER Second Seasonal School.

We will thus focus on inviting representatives of related projects and communities that MAPPER can collaborate with to either give presentations or to take part during the next seasonal school. Thus, enhancing MAPPER's visibility and integration on available e-infrastructures.

For the time being, we are sure to promote the next seasonal school again during the International Supercomputing Conference (ISC'12) in Hamburg, Germany and, later on, in November, at the Supercomputing Conference (SC'12) in Salt Lake City, US due to the positive resonance observed last year. Furthermore, suggestions and cooperative work of the MAPPER scientists, while they present their own work in other events, will be very valuable to improve the audience for next year.