D2.3 Project Communication Kit (M15)

Project acronym: *MAPPER*

Project full title: Multiscale Applications on European e-Infrastructures

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31-12-2011 v1.0	Christof Klausecker	Initial Version
24-09-2012 v2.0	M. Schiffers	Update

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1 Executive summary

This report is an updated version of the initial description of the MAPPER Communication Kit (MCK) [3]. The update can be summarized as follows:

- The MCK contains new material (see section 7)
- The MAPPER web site has additional information (see section 6.1)

All dissemination material is available for printing from the document section of the MAPPER project website [1]. High gloss leaflets can be ordered from the dissemination lead (LMU) by the individual partners. The project roll-ups are located at different partners to be circulated upon request.

2 Update Information

This document is an updated version of deliverable D2.3 (Project Communication Kit) [3]. The transition from version 1 to version 2 is as follows:

- new dissemination material has been added
- a section on the MAPPER web site has been added
- a reference to deliverable D2.3 (Initial Version of the Project Communication Kit) has been added

3 Mapper Communication Kit

Right from the beginning of the project, the MAPPER consortium started with the creation of dissemination material for the communication kit [2]. The current version of the communication kit consists of the following items:

- project folder
- project leaflet
- project application brochure
- project posters
- project roll-up
- Give-Away items
  - reflector stripes
  - lanyards
  - ballpoint pens

The communication kit will be updated and extended regularly through the course of the project.

3.1 Project Folder

The MAPPER folder (Figures 1 & 2) is designed for carrying all handout material plus business cards.

3.2 Project Leaflet

The MAPPER project leaflet consists of the MAPPER fact sheet and the project leaflet itself. The fact sheet (Figure 3 & 4) has been available for download from the project website already before the official start of the project and has been distributed at various occasions since. This fact sheet, which contains the most important information on the MAPPER project, has recently been superseded by the official project leaflet.
The project leaflet (Figure 5 & 6) provides an overview of MAPPER and builds the base for the corporate design strategy of the MAPPER consortium - future dissemination materials will use a similar design. In addition to PDF versions available for download and printing, high gloss printed project leaflets can be ordered from LMU, the leader of work package 2.

3.3 Project Application Brochure

The MAPPER Application Brochure describes the application of multi-scale services for various application communities. Currently, there is a general overview brochure available (Figure 7 & 8) for download from the project website and in printed form.

3.4 Poster

Currently there are two project posters available. The first poster (Figure 9) provides a general overview of the MAPPER project, the second one (Figure 10) is providing additional information for those interested in technical details. Both posters can be downloaded from the project website for printing.

4 Roll-up

To attract people to the MAPPER booth at conferences and exhibitions, a roll-up display (Figure 11 has been designed). It is available in three copies. Since project information material will be available at the booth, the roll-up itself contains only basic information and its design is kept simple.

5 Give-Away Items

For promotional purposes at exhibitions and conferences a set of give-away items has been designed. Figure 12 shows the currently available items: reflector tapes, lanyards, and (the logo of the) ball point pens.

6 Downloads

The PDF versions of dissemination print material is available from the public document section (`http://www.mapper-project.eu/web/guest/documents/`) of the MAPPER web site. The document sources are only available in the project internal section.

Item	Download link
fact sheet	`http://www.mapper-project.eu/documents/10155/22766/factsheet.pdf`
project leaflet	`http://www.mapper-project.eu/documents/10155/22766/leaflet.pdf`
project overview poster	`http://www.mapper-project.eu/documents/10155/22766/postero.pdf`
detailed project poster	`http://www.mapper-project.eu/documents/10155/22766/posterd.pdf`
roll-up	`http://www.mapper-project.eu/documents/10155/22766/rollup.pdf`

Table 1: Dissemination Print Material - Download Links

6.1 MAPPER Web Site

The MAPPER web site (`http://www.mapper-project.eu`) is regularly updated both for internal usage and for the general public. All dissemination material may be downloaded from the site (see 6). Additionally, the calendar of events (`http://www.mapper-project.eu/web/guest/calendar-of-events`) contains the events MAPPER is either participating or which are of special interest for multi-scale modeling.

6.2 Plans for Additional Material

The MAPPER Project Communication Kit will be extended and updated regularly during the course of the project. Together with information on current MAPPER related events, like for instance information on MAPPER workshops and seasonal schools, the dissemination material will be distributed in the MAPPER project folder and via the MAPPER web site.

7 Appendix (Dissemination Material)

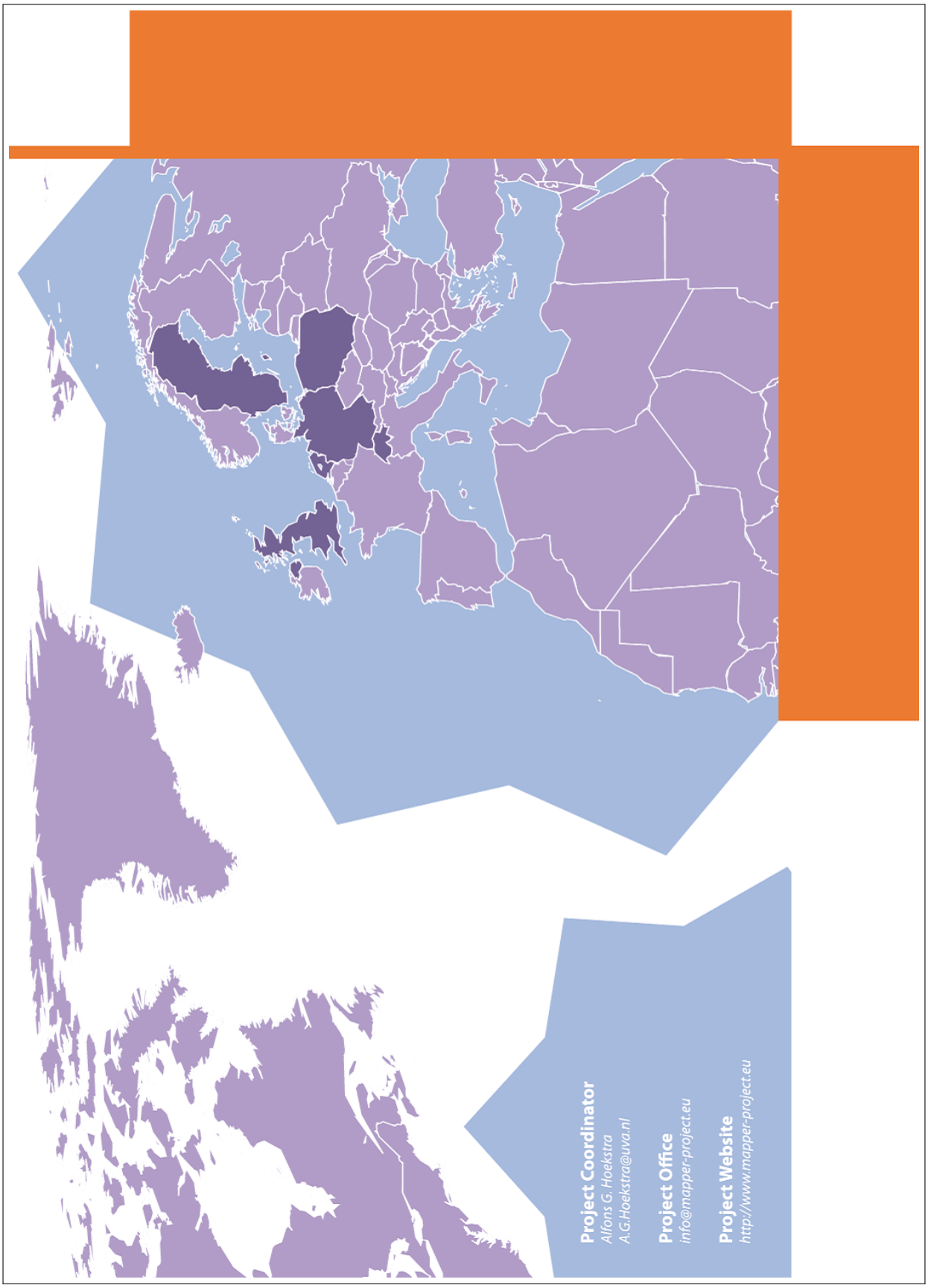


Figure 1: Project Folder (inside)

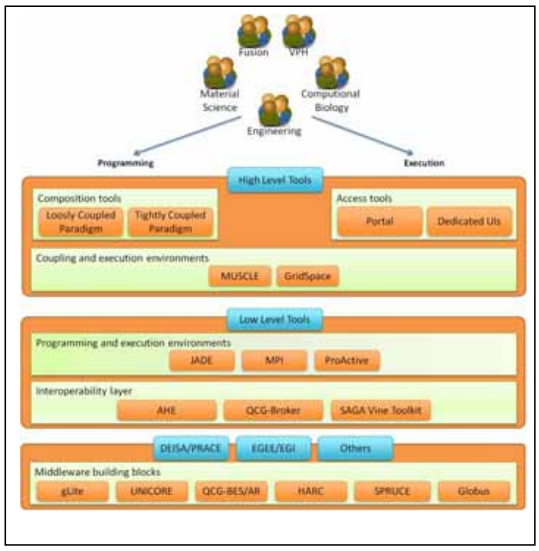
Figure 2: Project Folder (outside)

MAPPER

Multiscale **APP**lications on **E**uropean e-inf**R**astructures

Summary: Today scientists and engineers are commonly faced with the challenge of modelling, predicting and controlling multiscale systems which cross scientific disciplines and where several processes acting at different scales coexist and interact. Such multidisciplinary multiscale models, when simulated in three dimensions, require large scale or even extreme scale computing capabilities. The MAPPER project develops computational strategies, software and services for distributed multiscale simulations across disciplines, exploiting existing and evolving European e-infrastructure.

Objectives: Driven by seven challenging applications from five representative scientific domains (fusion, clinical decision making, systems biology, nano science, engineering), MAPPER deploys a computational science environment for distributed multiscale computing on and across European e-infrastructures. By taking advantage of existing software and services, as delivered by EU and national projects, MAPPER will result in high quality components for today's e-infrastructures. We develop tools, software and services that permit loosely and tightly coupled multiscale computing in a user friendly and transparent way. We integrate our applications into the MAPPER environment, and demonstrate their enhanced capabilities.



Action plan: MAPPER integrates heterogeneous infrastructures for programming and execution of multiscale simulations. We reuse as much of the existing infrastructural and software solutions as possible. The MAPPER solutions is developed on top of existing e-infrastructures without the necessity to modify already deployed components. The functionality to be delivered is realized as extensions to existing e-infra-structures. The integration is done using well defined APIs and standard based interfaces, thus reducing potential impact of changes on middleware level components.

***Networking activities*:** We create and maintain a stable management of the project, with strong internal and external communication and development of realistic plans for uptake and sustainability of MAPPER results during and after the lifetime of the project. We focus on targeted dissemination actions and a foresight study addressed to policy makers on the ICT concepts and technologies that facilitate multi-scale modelling approaches on large e-infrastructures.

continued overleaf

European Commission Information Society and Media

Project acronym:
MAPPER

Contract n°: RI-261507

Project type: CP-CSA

Start date: 01.10.2010

Duration: 36 months

Total budget:
3 272 777 €

Funding from the EC:
2 400 000 €

Total funded effort in person-month:
347

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UvA	NL
UCL	UK
UU	UK
PSNC	PL
CYFRONET	PL
LMU	DE
UNIGE	CH
CHALMERS	SE
MPG	DE

Keywords:
Distributed Multiscale Computing

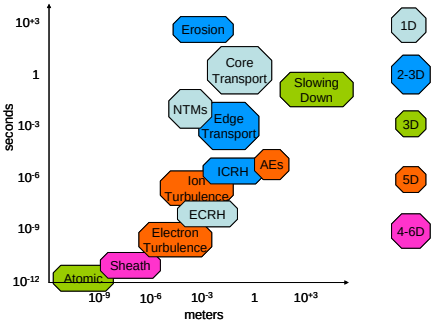
Collaboration with other EC funded projects:
EFDA
VPH-NoE
EUFORIA
MeDDiCa
PRACE
EGI-InSPIRE

Figure 3: Fact Sheet (front)

***Service activities*:** We distinguish two layers of services constituting the MAPPER environment. Users and applications communicate with services belonging to the interoperability layer, an abstract layer to grid resources managed by different middleware stacks. The interoperability services are responsible for providing concurrent access to resources controlled by different services synchronizing and orchestrating the execution of applications in the grid.

Multiscale loosely and tightly coupled simulations are controlled by a broker and underlying computing access services developed in the FP6-ICT QosCosGrid project (http://www.qoscosgrid.org/). The broker is integrated with underlying middleware and its scheduling and co-allocation algorithms are tuned for specific needs of multiscale applications. Many of the services that we wish to use have been developed individually and do not necessarily interoperate. We ensure that these services do talk to each other where appropriate. We start working on application deployment as early as possible in the project. We therefore adopt a twin track approach in our service development activities. The fast track adapts, integrates and deploys a minimal set of infrastructure components to enable coupling of multi-scale applications. The deep track will do so for the higher level services required to realise the full and integrated MAPPER infrastructure, which will enable the coupling and launching of multi-scale component codes. MAPPER services evolve on the basis of a regular cycle of top-down and bottom-up analysis of existing e-infrastructure, MAPPER building blocks as well as new requirements defined by our multiscale user communities.

***Joint Research activities*:** The application portfolio is adapted to the MAPPER infrastructure. Our approach is that applications are up and running from the start of the project, with existing, easily adaptable and deployable tools in the fast track; the deeper track then produces enhancements which are fed into the user level fast track as and when ready. A number of programming and execution tools, dedicated to distributed multiscale computing, are developed. In the first phase of the project, the applications will have to rely on explicit coding of their multiscale simulations, but gradually programming tools are delivered that assist in this task. JRA tools allow interaction between software components from different e-infrastructures in a hybrid way.



Range of scales and processes involved in the fusion applications.

***User communities*:** MAPPER is driven by seven exemplar applications from five user communities (virtual physiological human, computational biology, fusion, hydrological engineering, nano material science), and these communities are specifically targeted. However, our solutions are generic and will enable distributed multiscale computing for any multiscale model fitting into our paradigm, and MAPPER therefore opens up to other user communities as well.

***International aspects*:** MAPPER partners have significant trans-Atlantic grid and HPC experience, and have been involved very actively in TeraGrid and with the US Department of Energy laboratories. We collaborate with the US TeraGrid to integrate infrastructures across the globe.

MAPPER - RI

e-infrastructure

Figure 4: Fact Sheet (back)

Fusion *Hydrology* *Physiology* *Nanomaterials* *Computational Biology*

***M**ultiscale **APP**lications on*
***E**uropean e-inf**R**astructures*

Today, scientists and engineers are commonly faced with the challenge of modelling, predicting and controlling multiscale systems that cross scientific disciplines and involve several interacting processes at different scales. Such multidisciplinary, multiscale models, when simulated in three dimensions, require large-scale or even extreme-scale computing capabilities. Driven by seven challenging applications from five representative scientific domains, the MAPPER project is developing computational strategies, software and services for distributed multiscale simulations across disciplines, exploiting existing and evolving European e-infrastructure.

Contract number: 261507

Figure 5: Project Leaflet (front)

Multiscale APPlications on European e-infRastructures

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.

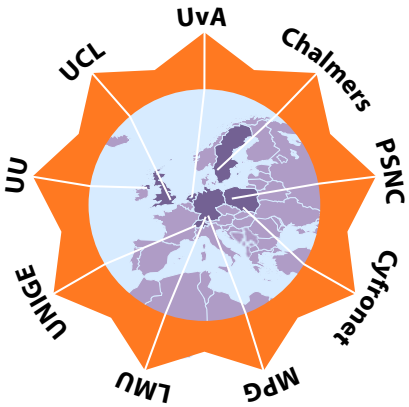
Technical Aspects

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 extreme-scale 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 6: Project Leaflet (back)

Equilibrium Stability Workflow *(Fusion)*

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 (HELENA) and a a linear MHD stability code (ILSA). Although listed as one application, several alternative workflows are possible which vary the profiles from the equilibrium code, recalculate the equilibrium for each case and then calculate the MHD stability. The equilibrium stability workflow application is a loosely coupled workflow where the data can be exchanged 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)*

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 can be 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 ligands 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 aneurysms 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, HemeLB, 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 equilibrium are:

HELENA	2D equilibrium solver (elliptic, no explicit time, but equilibrium time dependent).
GEM	3D gyrofluid turbulence code, calculates transport coefficients.
ETS	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)*

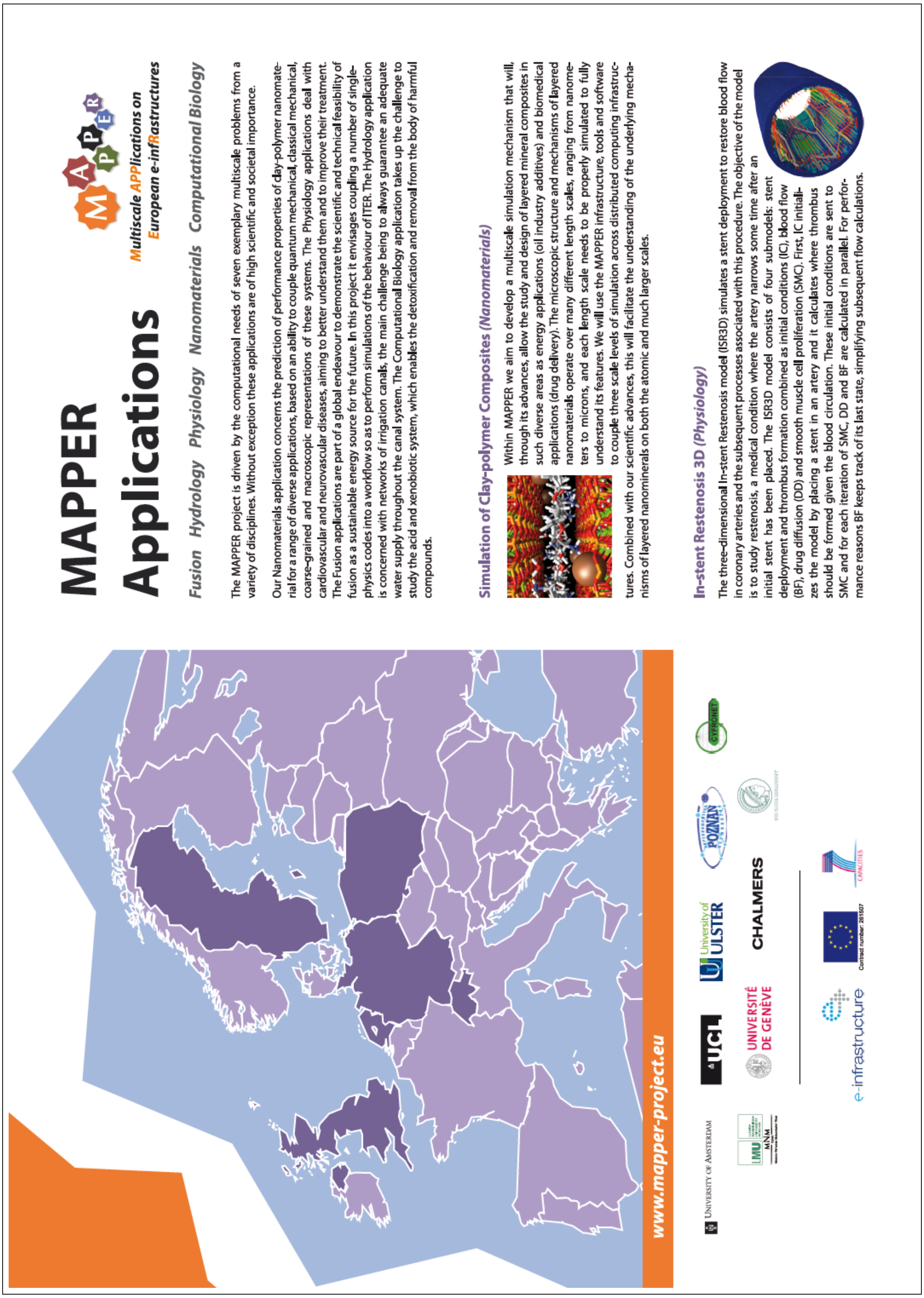
In a recent collaboration with ESISAR at Grenoble INP, France, UNIGE has developed multiscale models for the management of a network of irrigation canals. The problem remaining to be solved is the definition of appropriate actions (e.g. opening and closing gates) that need to be taken to always guarantee 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 approaches 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 computing.

The building blocks of a multiscale model are typically multiple single 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 composition 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 distributed multiscale computing for any multiscale models fitting into our paradigm, and MAPPER opens up to other user communities.

Figure 7: Project Application Brochure (inside)



MAPPER Applications

Multiscale APPlications on European e-infRastructures

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 clay-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 fusion 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)*

The three-dimensional In-stent Restenosis 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 restenosis, 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 (IC), blood flow (BF), drug diffusion (DD) and smooth muscle cell proliferation (SMC). First, IC initializes 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 calculated in parallel. For performance reasons BF keeps track of its last state, simplifying subsequent flow calculations.

Figure 8: Project Application Brochure (outside)

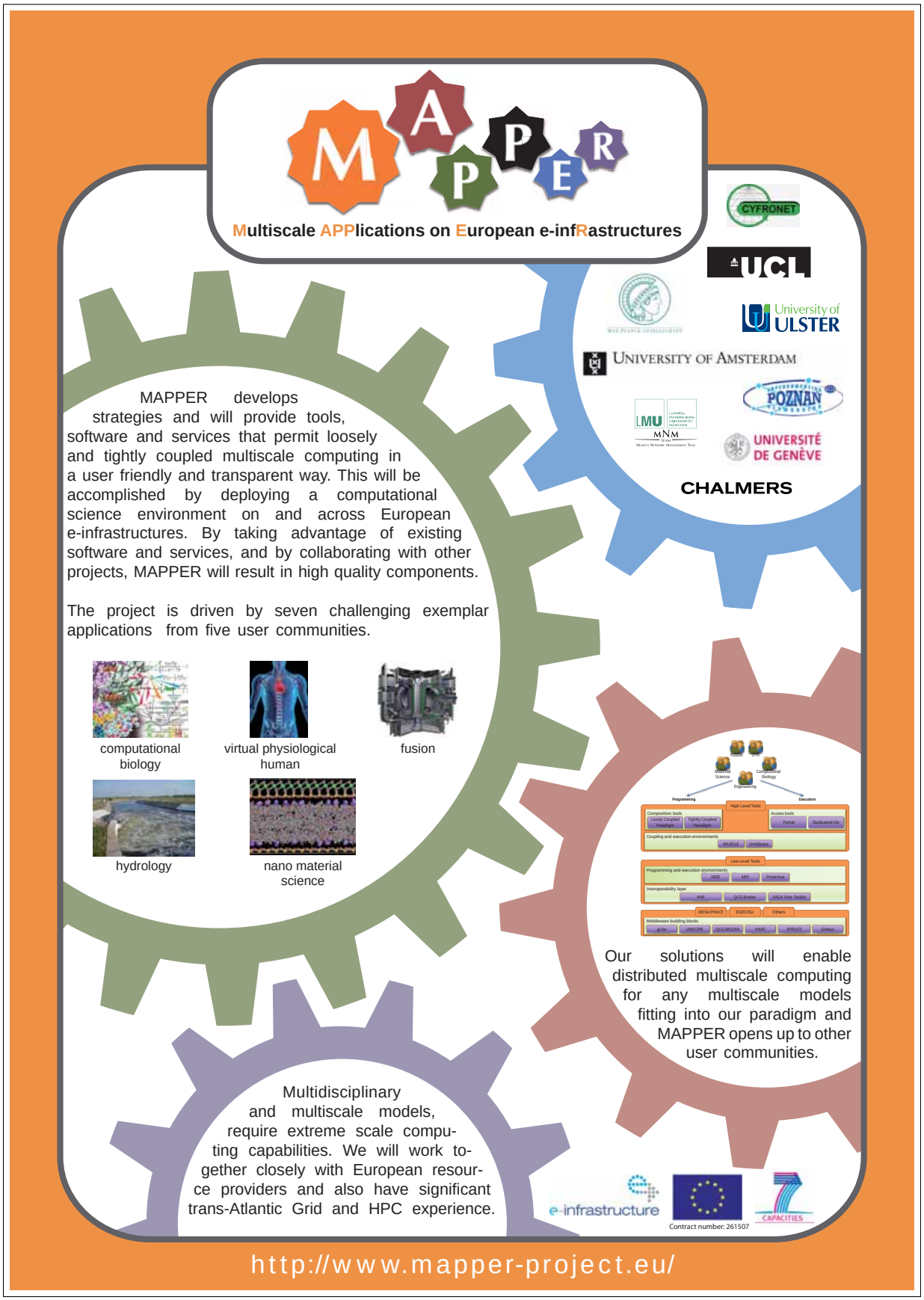


Figure 9: Project Overview Poster

www.mapper-project.eu

Multiscale APPlications on European e-infRastructures

Motivation

- Scientists are often faced with modelling **multiscale, multi discipline** systems
- Simulating such models in three dimensions requires large scale computing capabilities
- Existing modelling frameworks and middleware for distributed simulations do often not suffice

Ambition

- Develop computational strategies, software and services
  - for distributed multiscale simulations across disciplines
  - exploiting existing and evolving European e-infrastructure
- Deploy a computational science infrastructure
- Deliver high quality components
  - aiming at large-scale, heterogeneous, high performance multi-disciplinary multiscale computing
- Advance state-of-the-art in high performance computing on e-infrastructures
  - enable distributed execution of multiscale models across e-Infrastructures

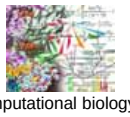
Services

- Interoperability services:
  - can be accessed by users and applications
  - form an abstraction layer to grid resources and middleware
  - are responsible for providing access to resources and for synchronizing and distributing applications.
- For example: multiscale simulations can be controlled by a broker developed in the QosCosGrid project
  - Many middleware services do not yet interoperate.
  - where appropriate, this should change

Internationally

- MAPPER partners have significant experience with the **trans-Atlantic grid** and HPC
- Collaborate with the US **TeraGrid** to integrate infrastructures across the globe.

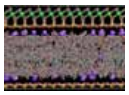
Applications


computational biology


virtual physiological human


fusion


hydrology


nano material science

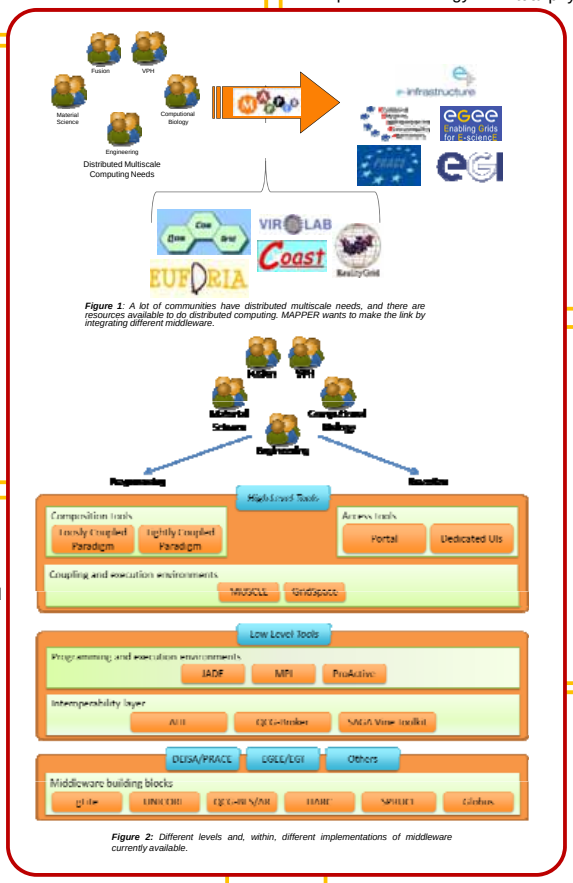


Figure 1: A lot of communities have distributed multiscale needs, and there are resources available to do distributed computing. MAPPER wants to make the link by integrating different middleware.

Figure 2: Different levels and, within, different implementations of middleware currently available.

Networking

- Create and maintain a stable management of the project
- Realize strong internal and external communication
  - Perform targeted **dissemination** actions
- Development of plans for **sustainability** of MAPPER
- Perform foresight study addressing policy makers

Development

In complementing twin tracks:

- Developments in the deep track will feed into the already usable fast track
- the **fast track**
  - will start working on application deployment **as early as possible**
  - manually adapts, integrates and deploys a minimal set of infrastructure components to enable multiscale applications
- the **deep track**
  - will work on higher level services and full integration
  - realises the full and integrated MAPPER infrastructure, enabling the coupling of multiscale components

Figure 10: Detailed Project Poster

Figure 11: Roll-up Display

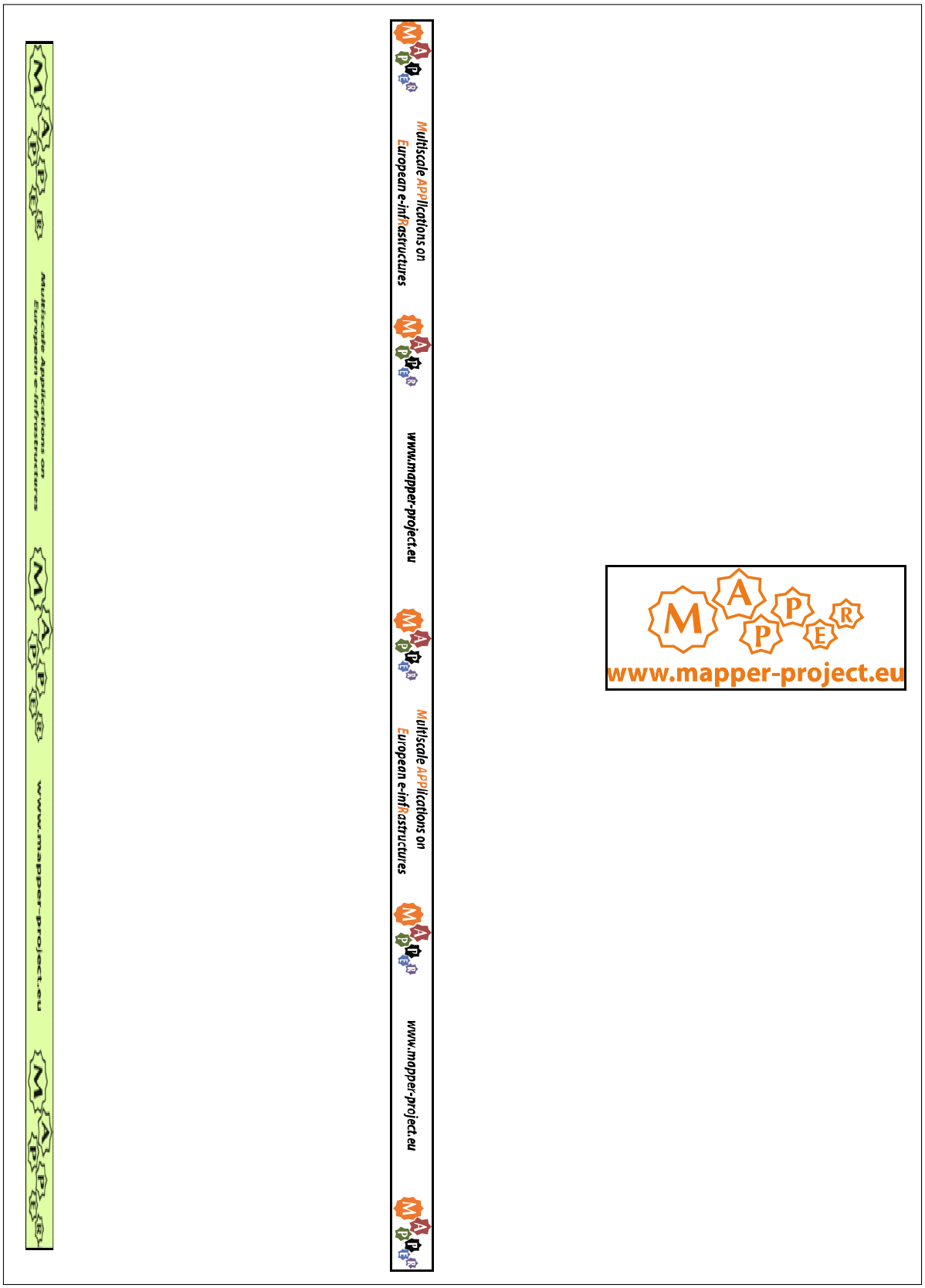


Figure 12: MAPPER Give-Away Items

References

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

[2] Deliverable D2.2 Dissemination Plan

[3] Deliverable D2.3 Initial Version of the Project Communication Kit