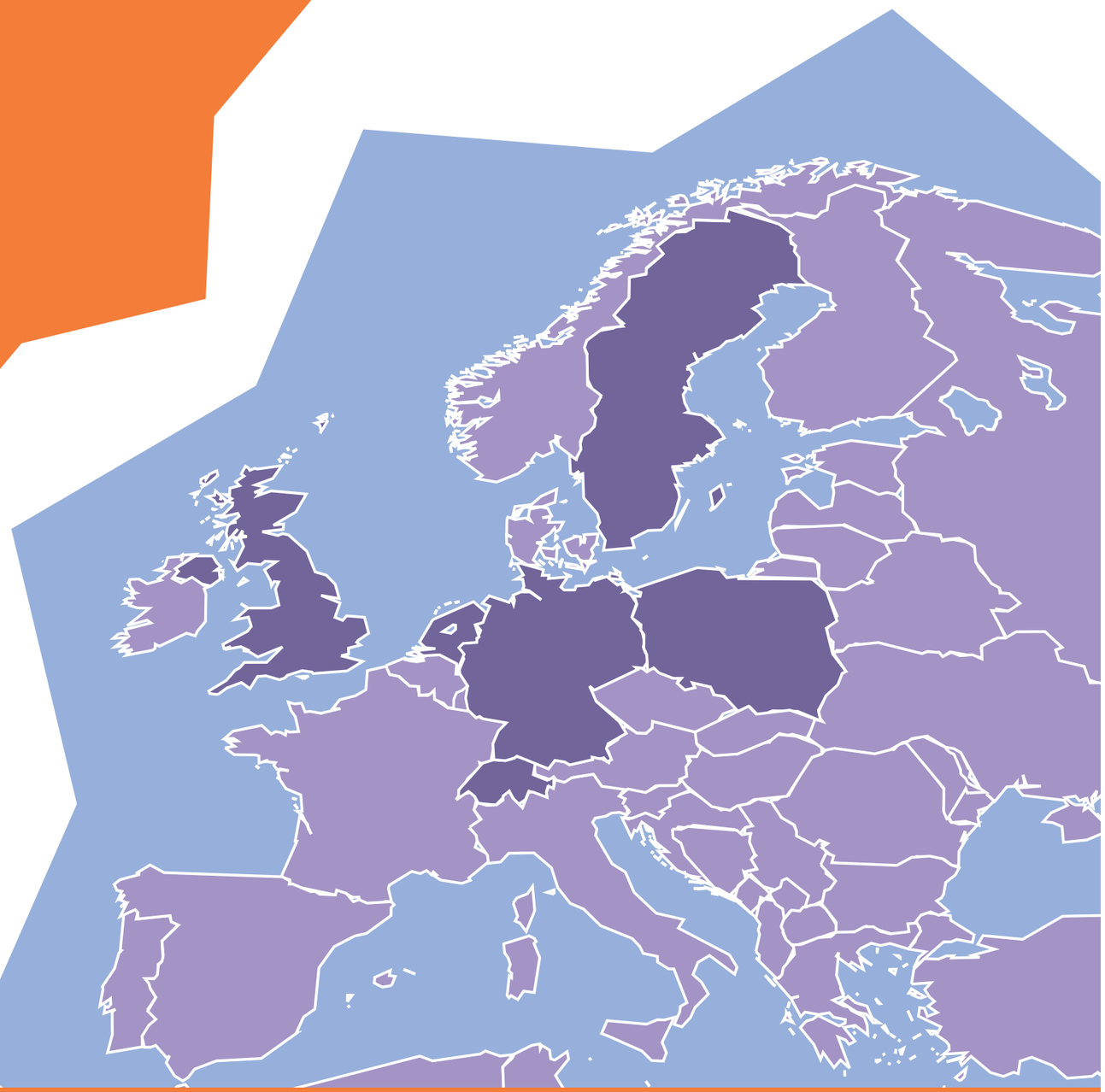


www.mapper-project.eu

MAPPER Applications

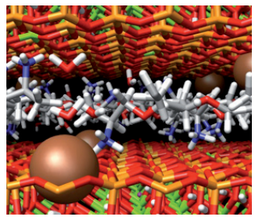
Multiscale APPlications on European e-infRastructures

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.

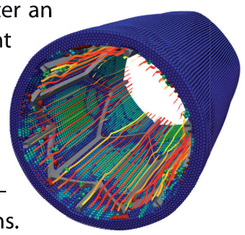
Simulation of Clay-polymer Composites *(Nanomaterials)*



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.

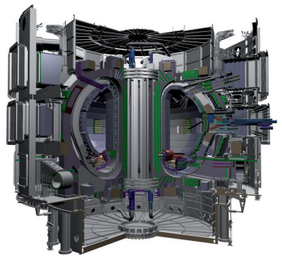


University of Amsterdam · UCL · University of Ulster · Poznan Supercomputing · Cyfronet · LMU Munich Network Management Team · Université de Genève · Chalmers · Max-Planck-Gesellschaft

e-infrastructure · Contract number: 261507 · Capacities

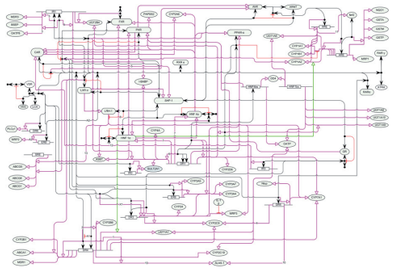
Equilibrium Stability Workflow *(Fusion)*

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.

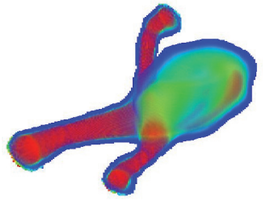


Bile Acid and Xenobiotic System *(Computational Biology)*

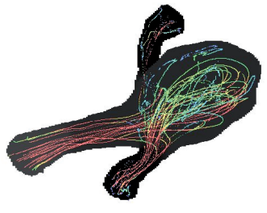
The bile acid and xenobiotic system (BAXS) defines an intricate physiological network that detoxifies and removes harmful xenobiotic and endobiotic compounds from the body while ensuring that primary bile acids (essential for the emulsification and absorption of dietary fats and fat-soluble vitamins) 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.

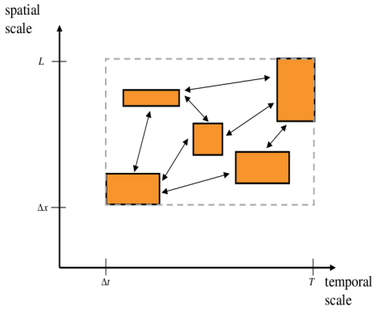
Both for HELENA and GEM a number of modules could be substituted, with differing tradeoffs of speed and accuracy/complexity). There are also some simple service modules in addition to these physics modules.

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.