Complex Automata Simulation Technique for Multi-Scale Multi-Science Systems

DESCRIPTION AND GOALS

The COAST project aims to develop a framework for modelling and simulation of multiscale complex systems.

COAST addresses the multi-scale modelling by using discrete models based on Cellular Automata (CA) and Agent Based Model (ABM), each on different scales. The basic modelling blocks are brought together in a *Complex Automaton*, in order to simulate a multi-scale multi-science process.

COAST is structured along 3 main lines:

- Mathematical formulation of a Complex Automaton, based on a Scale Separation Map and information exchange between different processes.
- Development of a COAST simulation environment.
- Validation using a challenging biomedical application related to coronary artery disease (in-stent restenosis).

A REAL BIOMEDICAL APPLICATION: IN-STENT RESTENOSIS IN CORONARY ARTERIES

A *stenosis* is an abnormal narrowing in a blood vessel. A possible treatment consists of deploying a metal mesh (*stent*) against the wall of the artery. An inflammatory response can lead to a restenosis (figure 2). It occurs in approximately 5-10% of patients following procedures involving stent deployment.

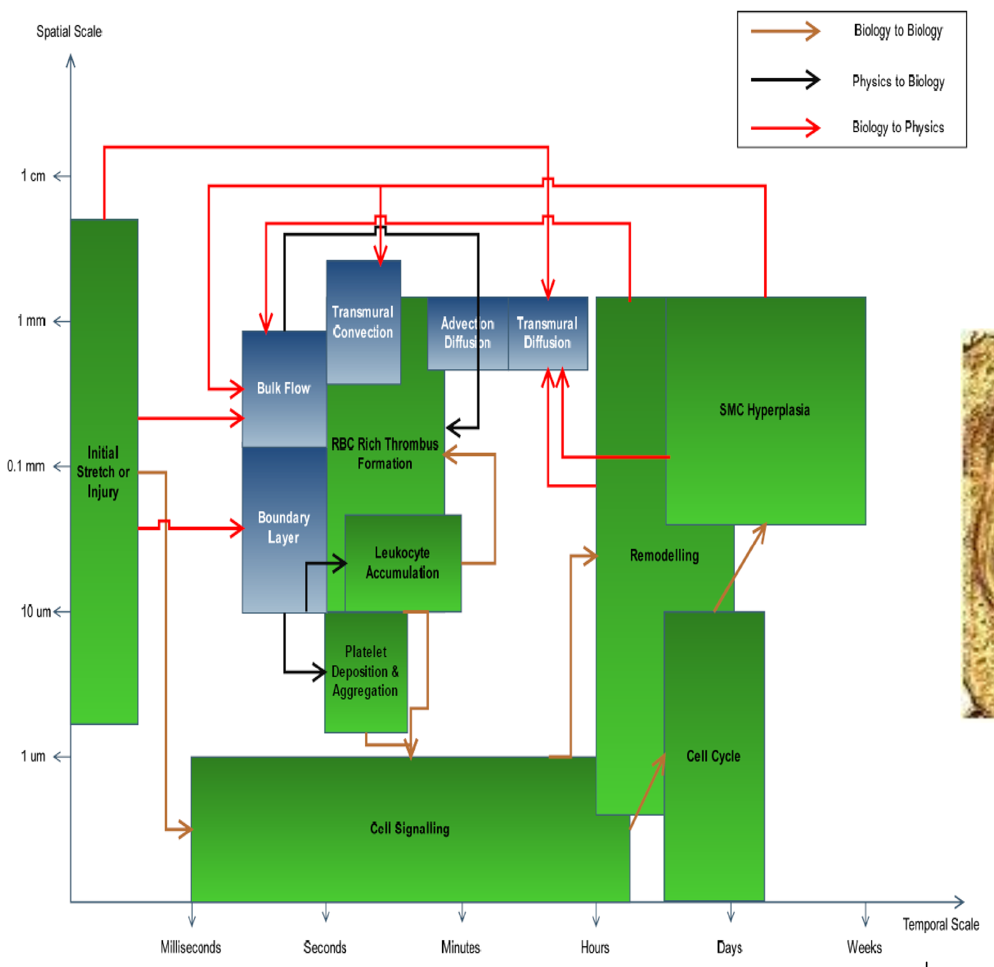

Figure 1: Presentation of all relevant processes of in-stent restenosis on a scale separation map inlcuding their mutual couplings

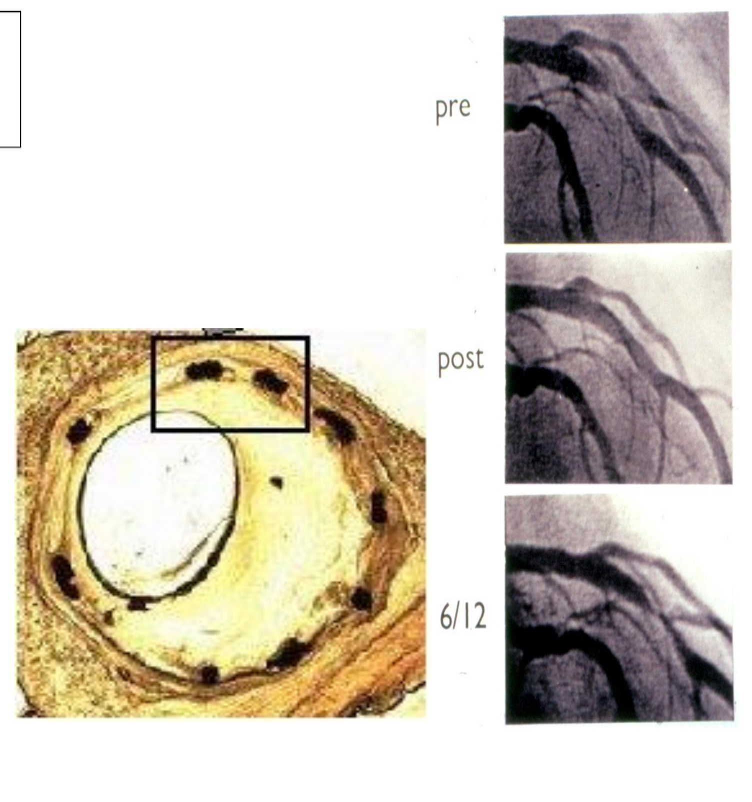

Figure 2: Section of a stented vessel narrowed by restenosis (left) and a typical course of in-stent restenosis (right): before and after stenting, until restenosis appears.

A Multiscale Multiscience Process:

The process can be categorized in various stages:

- initial injury;
- an inflammatory stage;
- granulation,
- extracellular matrix deposition
- finally blood vessel remodelling.

It is a multi-scale multi-science system, covering a range of phenomena from *biology* (cell signaling and cycles), *physics* (haemodynamics, convection-diffusion, transport), *chemistry* (drug uptake, reaction models) and *medicine*, and crossing many orders of magnitude in temporal and spatial scales (figure 1).

Validation:
The modelling of in-stent restenosis will be used to validate the COAST framework. One of the COAST goals is to develop a series of metrics to facilitate comparison between simulation data and *in vivo* data, in order to tune parameters in biological rule-set using subsets of experimental data.

EXAMPLE OF MULTI-SCALE MODELLING: FLUID-SUSPENSION COUPLING WITH HMC

Modeling of blood flow needs a detailed description of Blood Cells near the vessel wall but only a simplified bulk flow description inside the vessels, plus a proper coupling of these two different scales. Where those domains overlap we can think of a Hierarchical Model Coupling (HMC) [1] approach.

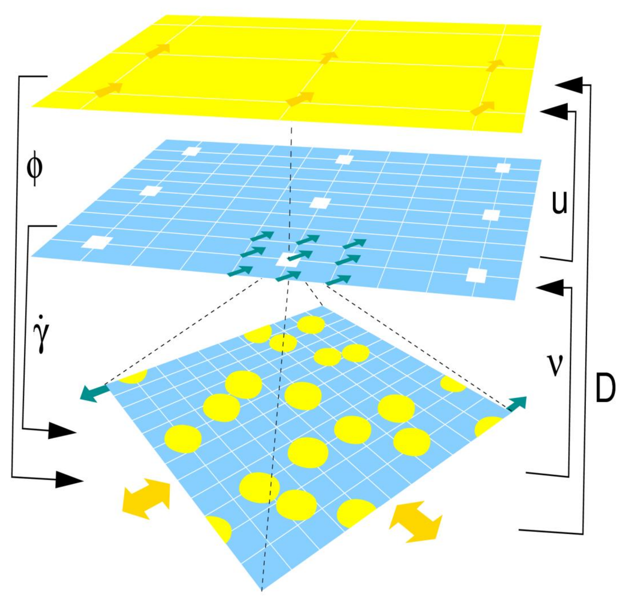

Figure 3: The HMC Suspension Coupling.

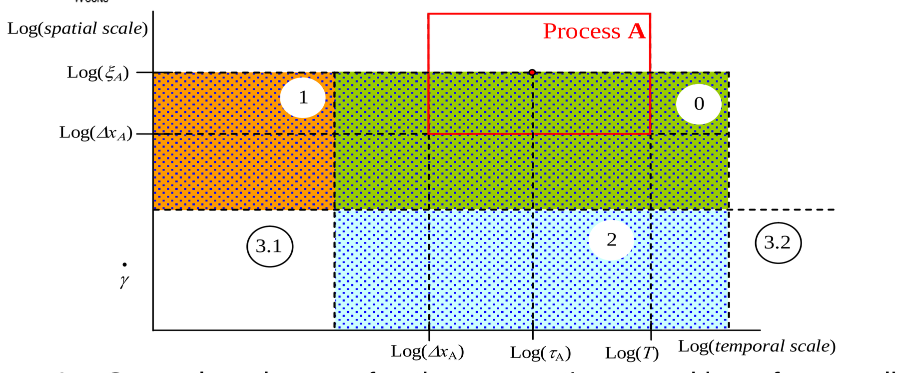

Figure 4a: General scale map for the automatic proposition of a coupling mechanism. Given a process A, we identify 5 possible regions where another process B can be placed. HMC (figure 3) corresponds to region 3.1.

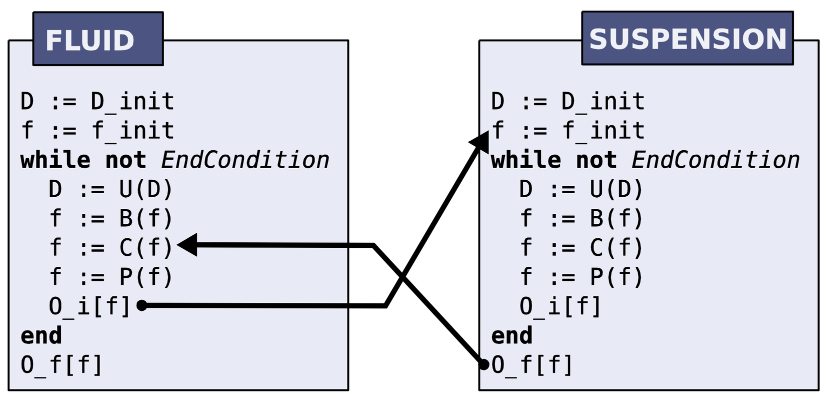

Figure 4b: Coupling mechanism of execution loops for the HMC suspension example. **D** stands for domain, while **f** denotes the state of the system.

- The middle blue layer (figure 3) holds pressure and velocity fields of a non-Newtonian fluid.
- To obtain an apparent viscosity v(**r**,t) we open up micro-pockets where, receiving as parameters the shear rate and the particle density from the macro-scale, shear flow experiments of fully resolved suspension are carried out, using a lattice Boltzmann approach.
- The macro-scale (yellow layer) resolves advection and diffusion of particles, to address the particle density Φ using the *local* self-diffusivity D and the velocity field u from the fluid layer. This is essential to allow for important effects of complex flow on local particle concentrations and vice versa.

The HMC approach presents an efficient method particularly if numerous other realistic details are incorporated (deformability of particles, varying particle sizes etc.). Instead of costly pre-sampling only relevant regions are sampled and micro-scale simulations are carried out only if interpolation would give insufficient accuracy.

[1] Weinan E and Bjorn Engquist, Comm. Math. Sci. 1(1), 87-132, 2003

COMPLEX AUTOMATA FRAMEWORK

Constructing a Complex Automaton:
Cellular Automata (CA) and Agent Based Models (ABM) are often seen as efficient discrete models for the dynamics of complex systems. They are characterized by an execution loop in form of local collision, propagation and boundary condition operators, which allows particularly favourable and efficient implementations.
COAST will bring together different CA and ABM models on the different scales in a single framework called *Complex Automaton*.

Scale Separation Map:
The multi-scale model is based on a scale separation map (example in Fig. 1), constructed placing the different sub-systems on a Cartesian plane according to their relevant space and time scales. COAST will investigate the different ways of placing a process B relative to a process A on the scale map (figure 4a), the definition of general *coupling templates* (figure 4b) and the consequences on the resulting Complex Automaton, both from the analytical and from the practical point of view.

Simulation environment:
A task of COAST is the development of a general Complex Automaton simulation framework based on JADE, providing elements such as coupling libraries which can be embedded into different existing software, in order to allow a wide range of applications.

Bibliography

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◦ A. Hoekstra, E. Lorenz, J.-L. Falcone, and B. Chopard, “Towards a Complex Automata Framework for Multi-scale Modeling: Formalism and the Scale Separation Map”, in Computational Science – ICCS 2007 (LNCS vol. 4487, Springer Verlag) 2007, pp. 922-930.
◦ www.complex-automata.org

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