Lattice Boltzmann Application Paradigms in Medical Physics

- some thoughts and concepts -

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Contributions from the EU funded projects COAST and @neurIST
please see http://complex-automata.org and http://www.aneurist.org/ for more details and references
Background: patient specific treatment planning

For certain diseases, a patient specific treatment (planning) is the standard procedure ...
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.... and we would hardly accept any cheaper „off the shelf“ alternatives!
Background: patient specific treatment planning

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Target Groups

• **Fundamental research** (scientists, biologists, ...)
  - blood flow in cerebral aneurysm
  - blood coagulation, thrombus formation
  - in-stent re-stenosis

• **Medical physics device industry** (engineers, ...)
  - stent positioning and design

• **Clinical application** (clinicians)
  - cerebral aneurysm rupture risk assessment
  - cerebral aneurysm treatment planning
Scientists at the Los Alamos National Laboratory and in France have developed a new computerized method to predict the flow of air and fluids that may improve the aerodynamics of cars and planes, track weather systems more reliably and expedite development of "Star Wars" weapons.

The new method of predicting flow dynamics, still in the early testing stage, could allow relatively unsophisticated computers to make calculations that can now be done only by new-generation supercomputers over days or weeks.

According to the method’s developers, this has led researchers and defense specialists to question whether the discovery may not be of great value to the Soviet Union, which lags behind the United States in computer sophistication and capacity.

Brosi Hasslacher of the Los Alamos laboratory, who created the new computer model in collaboration with Uriel Frisch of the Observatoire d’Nice in France, said Defense Department officials at the lab questioned whether his technical paper, expected to be published in the next few weeks in Physical Review Letters, should be classified to keep it out of Soviet hands.

But, he said, everyone quickly decided that the basic mathematics are in an area of research well-
Simulation Paradigm

linear tool-chain vs coupled simulation
Example: tool-chain from the @neurIST project

Problem classification: linear tool-chain

For certain cases (e.g. blood flow in vessel geometries) we can consider a linear tool-chain, applying one simulation tool for which we typically have to perform pre-processing to define the boundary conditions and post-processing for providing meaningful data to the clinicians.

Pre-processing
(imaging, segmentation, meshing, boundaries)

Simulation

Post-processing
(visualisation, data extraction, derived data production)
Problem classification: linear tool-chain

For certain cases (e.g. blood flow in vessel geometries) we can consider a *linear tool-chain*, applying *one simulation tool* for which we typically have to perform pre-processing to define the boundary conditions and post-processing for providing meaningful data to the clinicians.

More often, physiological systems can only be described in terms of *coupled systems* acting on *various time- and length-scales*.
Multi-scale example: blood coagulation

What happens if you cut yourself?

- the clotting cascade is initiated, which eventually leads to a clot formation via platelet aggregation
- clotting occurs on a time scale of minutes, the flow below seconds
Problem classification: multi-agent coupled simulation

For most biomedical cases (e.g. blood clotting, ...) we must consider a **coupled simulation**, applying **various simulation tools** which often (but not always) operate on disjunct time- and length-scales.

Initialisation (imaging, segmentation, meshing, boundaries) → Simulation Agent 1

Simulation Agent 1 → Simulation Agent 2 → Post-processing (visualisation, data extraction, derived data production)

Simulation Agent 1 → Simulation Agent 3

Simulation Agent 1 → Simulation Agent 4

Simulation Agent 1 → Simulation Agent 5
Problem classification: multi-agent coupled simulation

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**Initialisation** (imaging, segmentation, meshing, boundaries)

**Simulation Agent 1**

**Simulation Agent 2**

**Simulation Agent 3**

**Simulation Agent 4**

**Simulation Agent 5**

**Post-processing** (visualisation, data extraction, derived data production)
Scale separation and scale map

Scale separation and scale map
Blood coagulation from flow past a stenosis

Experiment with tracer (black ink)

Experiment: Medical Physics, University of Sheffield
Blood coagulation from flow past a stenosis

LB flow simulation on 4 CPU of a NEC SX-8

\( l_x \times l_y \times l_z = 1214 \times 98 \times 98 \)

1.6*10^6 iterations for 12s

real time required several CPU-days

Experiment with tracer (black ink)

Experiment: Medical Physics, University of Sheffield
Proximity condition

For general geometries, additional rules must be applied:

- Proximity condition: clotting is only allowed in contact with a solid surface, otherwise a detached clot might develop

Clot formation past a stenosis. The colour indicates the age of the clot (green=young)
Shear stress condition

High wall shear stress prevents clots from growing, the structure is „washed away“.

• Shear stress condition: Clots are only allowed to grow below a certain shear stress threshold.

Milk clotting model (shear stress condition): clot downstream of a stenosis, colour indicates age of clot (red=young)
Coagulation simulation and experimental results

The shape of the experimental milk clot has great similarities with the numerical simulation.

Numerical simulation of clotting processes: A lattice Boltzmann application in medical physics
Mathematics and Computers in Simulation, Volume 72, Issues 2-6, 9 September 2006, Pages 89-92
J. Bernsdorf, S.E. Harrison, S.M. Smith, P.V. Lawford, D.R. Hose

Applying the lattice Boltzmann technique to biofluids: A novel approach to simulate blood coagulation
J. Bernsdorf, S.E. Harrison, S.M. Smith, P.V. Lawford, D.R. Hose

Application and validation of the lattice Boltzmann method for modelling flow-related clotting
S.E. Harrison, S.M. Smith, J. Bernsdorf, D.R. Hose, P.V. Lawford
Coagulation simulation and experimental results

The shape of the experimental milk clot has great similarities with the numerical simulation.

PhD thesis of Sarah Harrison, University of Sheffield
Cerebral aneurysm
Flow simulation and visualisation
CA treatment

Figure 2. (A) Anterior-posterior view of angiogram showing an aneurysm at the terminus of the basilar artery. (B) Comparable view after embolization of the aneurysm using detachable platinum coils.
Multi-scale simulation of CA treatment

Coupled multi-scale multi-physics simulation

- time scale
  - milliseconds
  - seconds
  - minutes

- space scale
  - μm
  - mm
  - cm

- flow
- advection diffusion
- clotting

blood-biology
Multi-scale simulation of CA treatment

Coupled multi-scale multi-physics simulation

- flow
- advection diffusion
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Space scale:
- cm
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Multi-scale simulation of CA treatment

Coupled multi-scale multi-physics simulation

Dr. Jörg Berndorf, Applied Supercomputing in Engineering

Donnerstag, 17. Februar 2011
Multi-scale simulation of CA treatment

Coupled multi-scale multi-physics simulation

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Multi-scale simulation of CA treatment

Coupled multi-scale multi-physics simulation
Coupling scheme for a distributed multi-scale simulation
Issues

Within our recent projects, we had a variety of „practical difficulties“:

- multiple non-mesh-aligned transient in- and outlets
- local mesh refinement in the presence of a (growing) solid fraction at fine/coarse boundary
- extremely small time-step (several $10^6$ iterations / cardiac cycle)
- automatic (or non expert’s) setting of reasonable simulation parameters
- numerical stability (BGK and TRT)
- maturity of turbulence model (Smagorinsky without wall function??)
- load balancing with multi-scale simulations

... I don’t believe that all these points are just „implementation issues“.
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... I don't believe that all these points are just „implementation issues“. 

... but I do believe we need to address them all in order to succeed!
Thank You!