Computational Fluid Dynamics with the Lattice Boltzmann Method

Overview, computational issues and (biomedical) applications

Alfons Hoekstra
Computational Science
University of Amsterdam
A.G.Hoekstra@uva.nl
http://www.science.uva.nl/research/scs

This you (probably) know

Fluid velocity

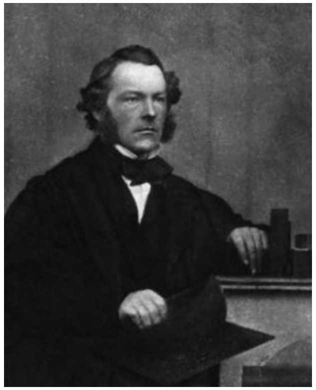
pressure

viscosity

$$\nabla \cdot \mathbf{u} = 0$$

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u}$$

- The Navier-Stokes Equations for an incompressible fluid.



Why an alternative?

CFD solvers are pretty good, aren't they?

The Boltzmann Equation - 1

Particle speed

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = \Omega(f)$$

$f(\mathbf{x},\mathbf{v})$: single particle distribution function

$\Omega(f)$: Boltzmann collision term (highly non-linear in f)

Collision term must satisfy conservation of mass, momentum and energy.

The Boltzmann Equation - 2

Macroscopic fields are obtained by taking velocity moments of *f*.

$$\rho(\mathbf{x}) = \int f(\mathbf{x}, \mathbf{v}) d\mathbf{v}$$

$$\rho(\mathbf{x})\mathbf{u}(\mathbf{x}) = \int \mathbf{v} f(\mathbf{x}, \mathbf{v}) d\mathbf{v}$$

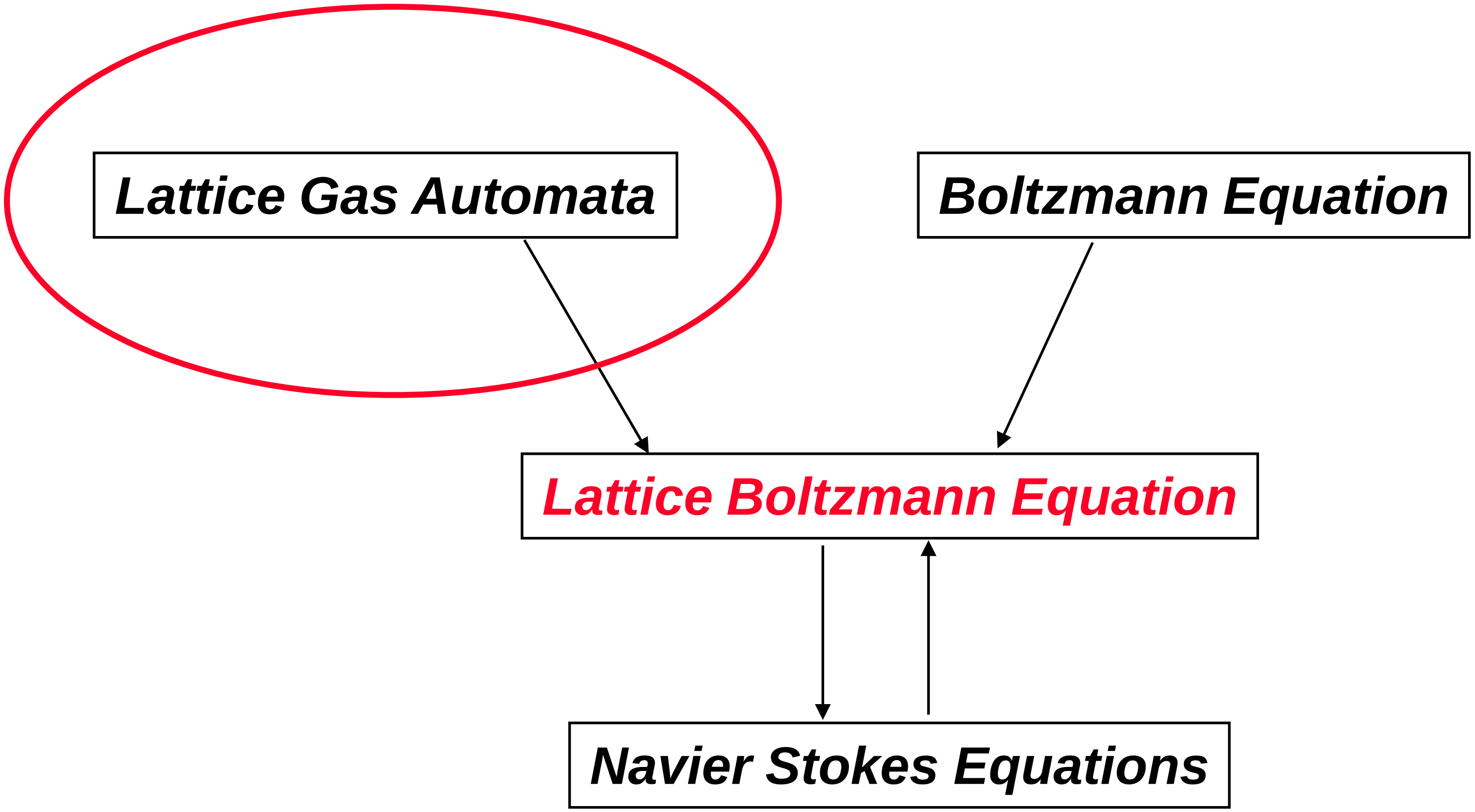
$$\rho(\mathbf{x}) e(\mathbf{x}) = \int 1/2 \left| \mathbf{v} - \mathbf{u}(\mathbf{x}) \right|^2 f(\mathbf{x}, \mathbf{v}) d\mathbf{v}$$

In the limit of low Knudsen and low Mach numbers, it can be shown that these fields obey the Navier-Stokes equations.

The Lattice Boltzmann Method

1. Discretize velocity space in a very small set of velocities;
2. Use a very simple collision operator, usually the BGK collision operator is applied;
3. Discretize space in a lattice with enough symmetry;
4. Use finite differencing for the differential operators
5. Choose the time step, lattice spacing, and discrete set of velocities, such that fit exactly, allowing streaming over the links of the lattice and collisions on the nodes.

Routes to the Lattice Boltzman Equation (LBE)

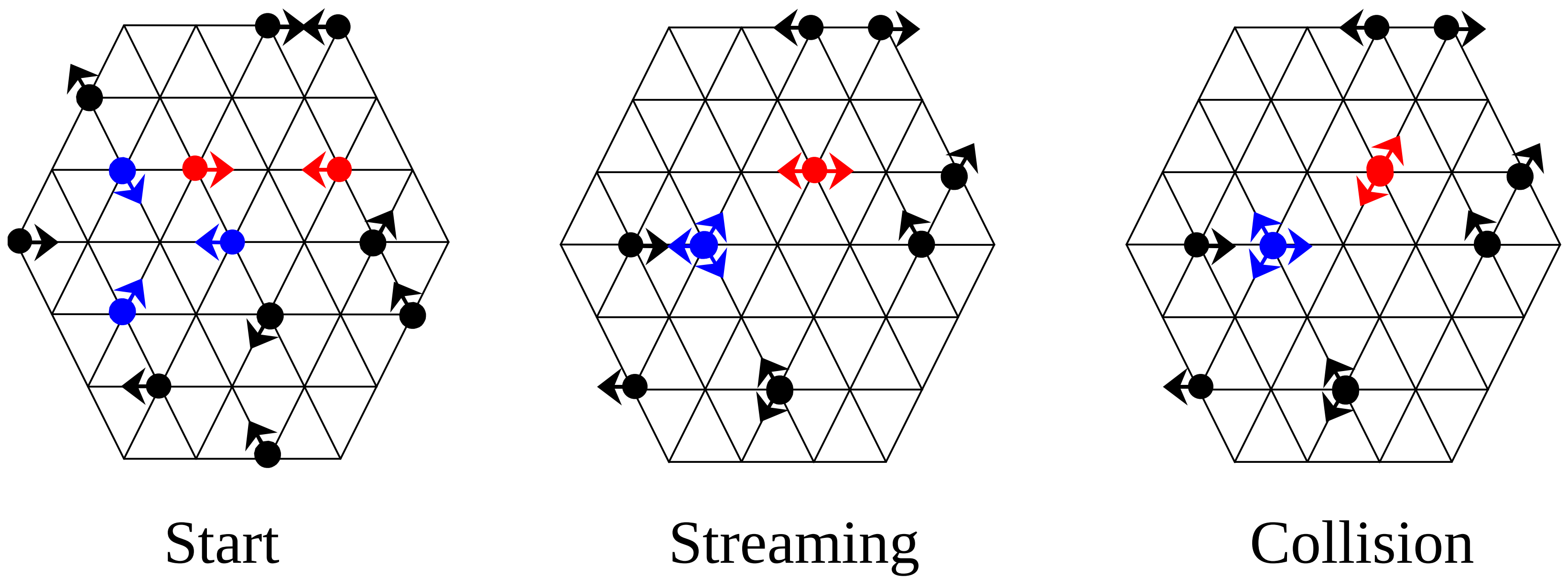


The Lattice Gas Cellular Automaton

U. Frisch et al., Phys. Rev. Lett 56, 1505 (1986)

- Regular lattice with enough symmetry.
- Particles live on the lattice.
  - Streaming over the links;
  - Collisions at the nodes;
    - conservation of mass, momentum, and energy.
- Very easy simulation, trivial for parallel computing.
- One can prove that this LGA recovers the Navier-Stokes equations.

The Hexagonal Lattice



Evolution Equation

State Vector

$$\mathbf{n}_i(\mathbf{x}+\mathbf{c}_i, t+1) = \mathbf{n}_i(\mathbf{x},t) + \Delta_i(\mathbf{n}(\mathbf{x},t))$$

streaming

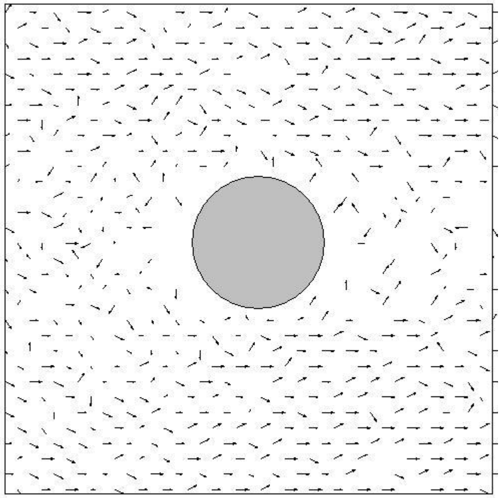
collision

Average occupation number $\quad f_i = \langle n_i \rangle$

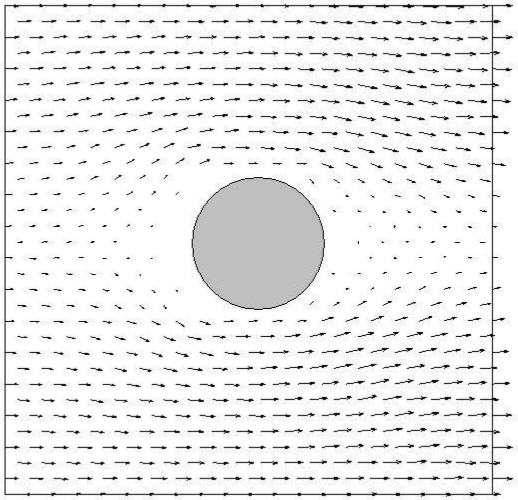
density $\quad \rho = \sum_{i=1}^{b} f_i$

velocity $\quad \rho\mathbf{u} = \sum_{i=1}^{b} f_i \mathbf{c}_i$

Flow past a Cylinder



single iteration



after averaging

Recover Hydrodynamics

1. Assume molecular chaos
2. Ensemble averaging and Taylor expansion of evolution equation
3. Apply mass and momentum conservation
4. Solve equations using Chapman-Enskog expansion

Ensemble Averaging

- Enemble averaging of the evolution equation leads to

$$\langle \mathbf{n}_i(\mathbf{x}+\mathbf{c}_i, t+1)\rangle = \langle \mathbf{n}_i(\mathbf{x},t)\rangle + \langle \Delta_i(\mathbf{n}(\mathbf{x},t))\rangle$$

- which becomes, using the definitions and the molecular chaos assumption

$$f_i(\mathbf{x}+\mathbf{c}_i, t+1) = f_i(\mathbf{x},t) + \Delta_i(f(\mathbf{x},t))$$

- This is the ***Lattice Boltzmann Equation***!

Lots of algebra

$$\frac{\partial f_i}{\partial t} + \frac{\partial f_i}{\partial \mathbf{x}_\alpha} \mathbf{c}_{i_\alpha} + \frac{1}{2}\Delta t \left(\frac{\partial^2 f_i}{\partial \mathbf{x}_\alpha \partial \mathbf{x}_\beta} \mathbf{c}_{i_\alpha} \mathbf{c}_{i_\beta} + \frac{\partial^2 f_i}{\partial t^2} + 2 \frac{\partial^2 f_i}{\partial t \partial \mathbf{x}_\alpha} \mathbf{c}_{i_\alpha} \right) = \frac{1}{\Delta t} \sum_{j=0}^{b} M_{ij} (f_j - f_j^{eq})$$

$$\frac{\partial f_i^{eq}}{\partial t_1} + \frac{\partial f_i^{eq}}{\partial \mathbf{x}_{1_\alpha}} \mathbf{c}_{i_\alpha} = \frac{1}{\Delta t} \sum_{j=0}^{b} M_{ij} f_j^{(1)}$$

$$\frac{\partial f_i^{eq}}{\partial t_2} + \sum_{j=0}^{b} (\delta_{ij} + \frac{1}{2} M_{ij}) \left(\frac{\partial f_j^{(1)}}{\partial t_1} + \frac{\partial f_j^{(1)}}{\partial \mathbf{x}_{1_\alpha}} \mathbf{c}_{i_\alpha} \right) = \frac{1}{\Delta t} \sum_{j=0}^{b} M_{ij} f_i^{(2)}$$

$$\sum_{i=0}^{b} \left[\frac{\partial f_i^{eq}}{\partial t_1} + \frac{\partial f_i^{eq}}{\partial \mathbf{x}_{1_\alpha}} \mathbf{c}_{i_\alpha} \right] = \frac{1}{\Delta t} \sum_{i=0}^{b} \sum_{j=0}^{b} M_{ij} f_i^{(1)} \qquad \frac{\partial \rho}{\partial t_1} + \frac{\partial \rho \mathbf{u}_\alpha}{\partial \mathbf{x}_{1_\alpha}} = 0$$

$$\sum_{i=0}^{b} \left[\frac{\partial f_i^{eq}}{\partial t_2} + \sum_{j=0}^{b} (\delta_{ij} + \frac{1}{2} M_{ij}) \left(\frac{\partial f_j^{(1)}}{\partial t_1} + \frac{\partial f_j^{(1)}}{\partial \mathbf{x}_{1_\alpha}} \mathbf{c}_{i_\alpha} \right) \right] = \frac{1}{\Delta t} \sum_{i=0}^{b} \sum_{j=0}^{b} M_{ij} f_i^{(2)} \qquad \frac{\partial \rho}{\partial t_2} = 0$$

$$\sum_{i=0}^{b} \mathbf{c}_{i_\alpha} \left[\frac{\partial f_i^{eq}}{\partial t_1} + \frac{\partial f_i^{eq}}{\partial \mathbf{x}_{1_\beta}} \mathbf{c}_{i_\beta} \right] = \frac{1}{\Delta t} \sum_{i=0}^{b} \mathbf{c}_i \sum_{j=0}^{b} M_{ij} f_i^{(1)} \qquad \frac{\partial \rho \mathbf{u}_\alpha}{\partial t_1} + \frac{\partial}{\partial \mathbf{x}_{1_\beta}} \sum_{i=0}^{b} \mathbf{c}_{i_\alpha} \mathbf{c}_{i_\beta} f_i^{eq} = 0$$

$$\sum_{i=0}^{b} \mathbf{c}_{i_\alpha} \left[\frac{\partial f_i^{eq}}{\partial t_2} + \sum_{j=0}^{b} (\delta_{ij} + \frac{1}{2} M_{ij}) \left(\frac{\partial f_j^{(1)}}{\partial t_1} + \frac{\partial f_j^{(1)}}{\partial \mathbf{x}_{1_\beta}} \mathbf{c}_{i_\beta} \right) \right] = \frac{1}{\Delta t} \sum_{i=0}^{b} \mathbf{c}_i \sum_{j=0}^{b} M_{ij} f_i^{(2)} \qquad \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \Pi = 0$$

$$\Pi_{\alpha\beta} = \sum_{i=0}^{b} \mathbf{c}_{i_\alpha} \mathbf{c}_{i_\beta} \left(f_i^{eq} + \sum_{j=0}^{b} (\delta_{ij} + \frac{1}{2} M_{ij}) f_j^{(1)} \right) \qquad \Pi_{\alpha\beta}^{(0)} = \rho c_s^2 \delta_{\alpha\beta} + \rho \mathbf{u}_\alpha \mathbf{u}_\beta \qquad \Pi_{\alpha\beta}^{(1)} = -c_s^2 \Delta t (-\frac{1}{\lambda} - \frac{1}{2})(\frac{\partial \rho \mathbf{u}_\alpha}{\partial \mathbf{x}_\beta} + \frac{\partial \rho \mathbf{u}_\beta}{\partial \mathbf{x}_\alpha})$$

Final Result

- To second order we find

$$\frac{\partial \mathbf{u}_\alpha}{\partial \mathbf{x}_\alpha} = 0$$

$$\frac{\partial \rho \mathbf{u}_\alpha}{\partial t} + \frac{\partial}{\partial \mathbf{x}_\beta} \Pi_{\alpha\beta} = 0$$

$$\Pi^{(0)}_{\alpha\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho \mathbf{u}_\alpha \mathbf{u}_\beta$$

$$\Pi^{(1)}_{\alpha\beta} = c_s^2 \Delta t \left(\frac{1}{\lambda} - \frac{1}{2}\right)\left(\frac{\partial \rho \mathbf{u}_\alpha}{\partial \mathbf{x}_\beta} + \frac{\partial \rho \mathbf{u}_\beta}{\partial \mathbf{x}_\alpha}\right)$$

- i.e., an incompressible fluid, with kinematic viscosity

$$\nu = c_s^2 \Delta t \left(\frac{1}{\lambda} - \frac{1}{2}\right)$$

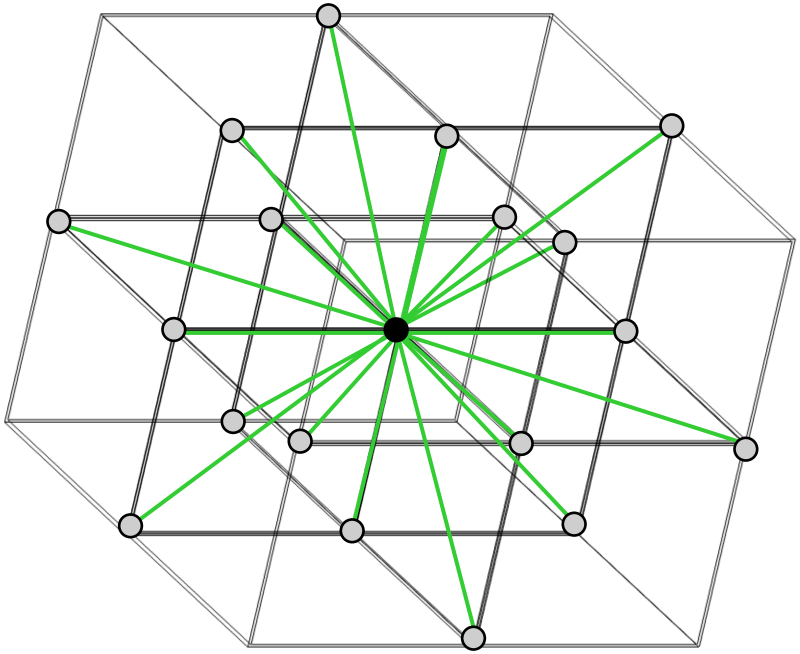
- Where λ is an eigenvalue of the linearized collision matrix

Properties of LGA

- Advantages
  - local interactions, i.e. inherent parallelism
  - binary operations, i.e. unconditionally stable
- Disadvantages
  - lack of Galilean invariance
  - noisy dynamics
    - note however that the noise contains a lot of interesting physics….

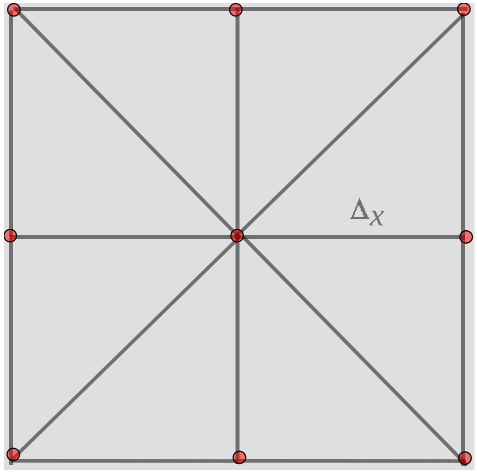
Lattice Boltzmann Method

- Apply directly the densities f_i.
- Use very simple collision operator
  - Lattice-BGK
- No need for averaging !
- Galilean Invariant by construction!



Example, the L-BGK D2Q9 model

- 2D square Lattice
- lattice spacing Δx and timestep Δt
- 9 discrete velocities
- BGK operator; single time relaxation towards equilibrium



$$\mathbf{c}_i = \frac{\Delta x}{\Delta t}\mathbf{e}_i \ , \ 0 \leq i \leq 9$$

$$\mathbf{e}_0 = 0$$

$$\mathbf{e}_i = \begin{pmatrix} \cos(\pi/2\,(i-1)) \\ \sin(\pi/2\,(i-1)) \end{pmatrix}, \ i = 1,3,5,7$$

$$\mathbf{e}_i = \sqrt{2}\begin{pmatrix} \cos(\pi/2\,(i-1) + \pi/4) \\ \sin(\pi/2\,(i-1) + \pi/4) \end{pmatrix}, \ i = 2,4,6,8$$

$$\Delta(f_i) = \frac{1}{\tau}\left(f_i^{eq} - f_i \right)$$

The L-BGK D2Q9 model

The resulting equations are

$$f_i(\mathbf{x}+\mathbf{e}_i\Delta x, t+\Delta t) = f_i(\mathbf{x},t) + \frac{1}{\tau}\left[f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)\right]$$

$$f_i^{eq} = \rho w_i\left[1 + 3\mathbf{e}_i\cdot\mathbf{u} + \frac{9}{2}(\mathbf{e}_i\cdot\mathbf{u})^2 - \frac{3}{2}u^2\right]$$

$$w_0 = 4/9,\ \ w_1 = w_3 = w_5 = w_7 = 1/9,$$

$$w_2 = w_4 = w_6 = w_8 = 1/36$$

Recover hydrodynamics from L-BGK

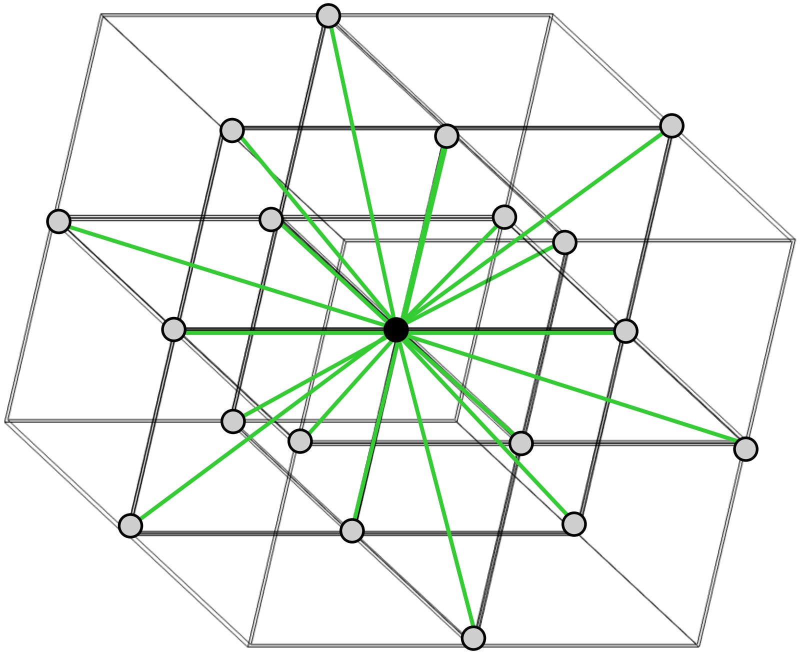
$$\rho = \sum_{i=0}^{8} f_i \qquad \rho \mathbf{u} = \sum_{i=0}^{8} f_i \mathbf{e}_i$$

Within the limits of low Mach and low Knudsen number, the Navier-Stokes equations are recovered, with

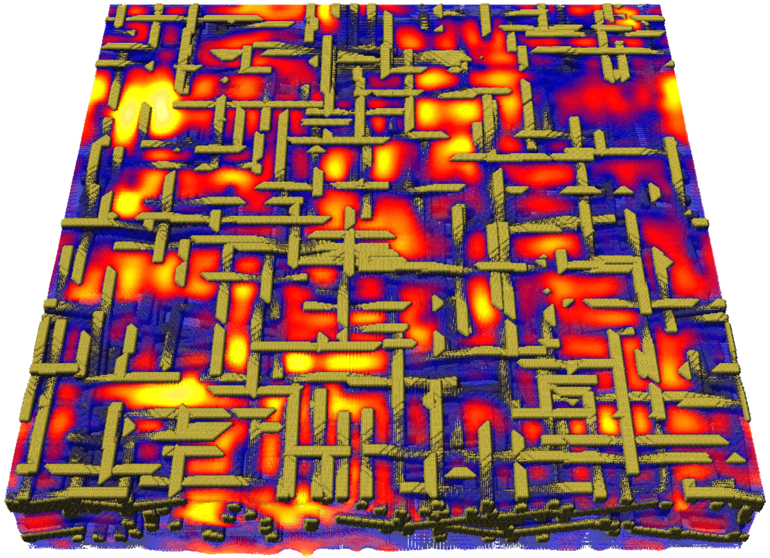
$$p = \rho/3 \Rightarrow c_s = 1/\sqrt{3}$$
$$\nu = (2\tau - 1)/6$$

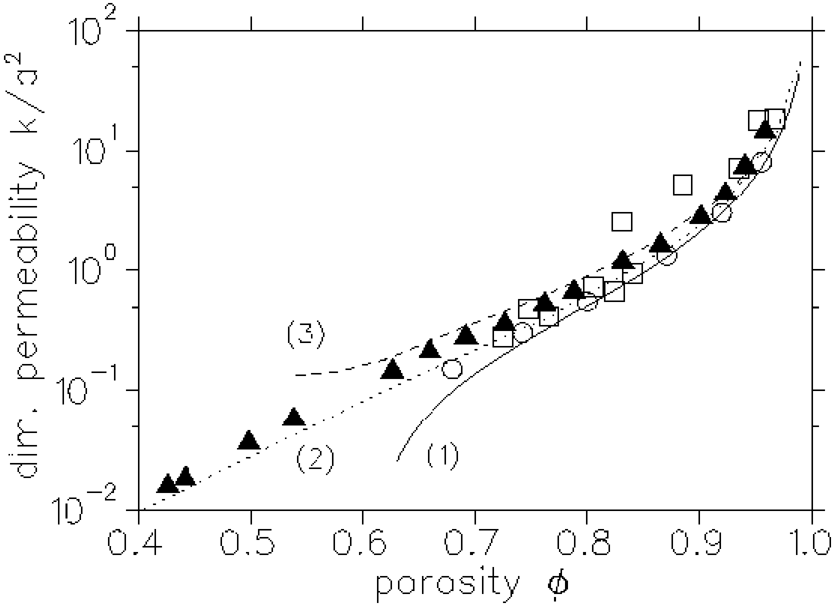
3D L-BGK

- 19 discrete velocities
- Same equations as in 2D
- D3Q19 L-BGK has been our workhorse for many years.



Permeability in a Random Fiber Web





Koponen A, Kandhai BD, Héllen E, Alava M, Hoekstra AG, Kataja M, Niskanen K, Sloot PMA, Timonen J. 1998. *Permeability of three-dimensional random fibre webs.* Physical Review Letters 80:716--9

Image Based CFD

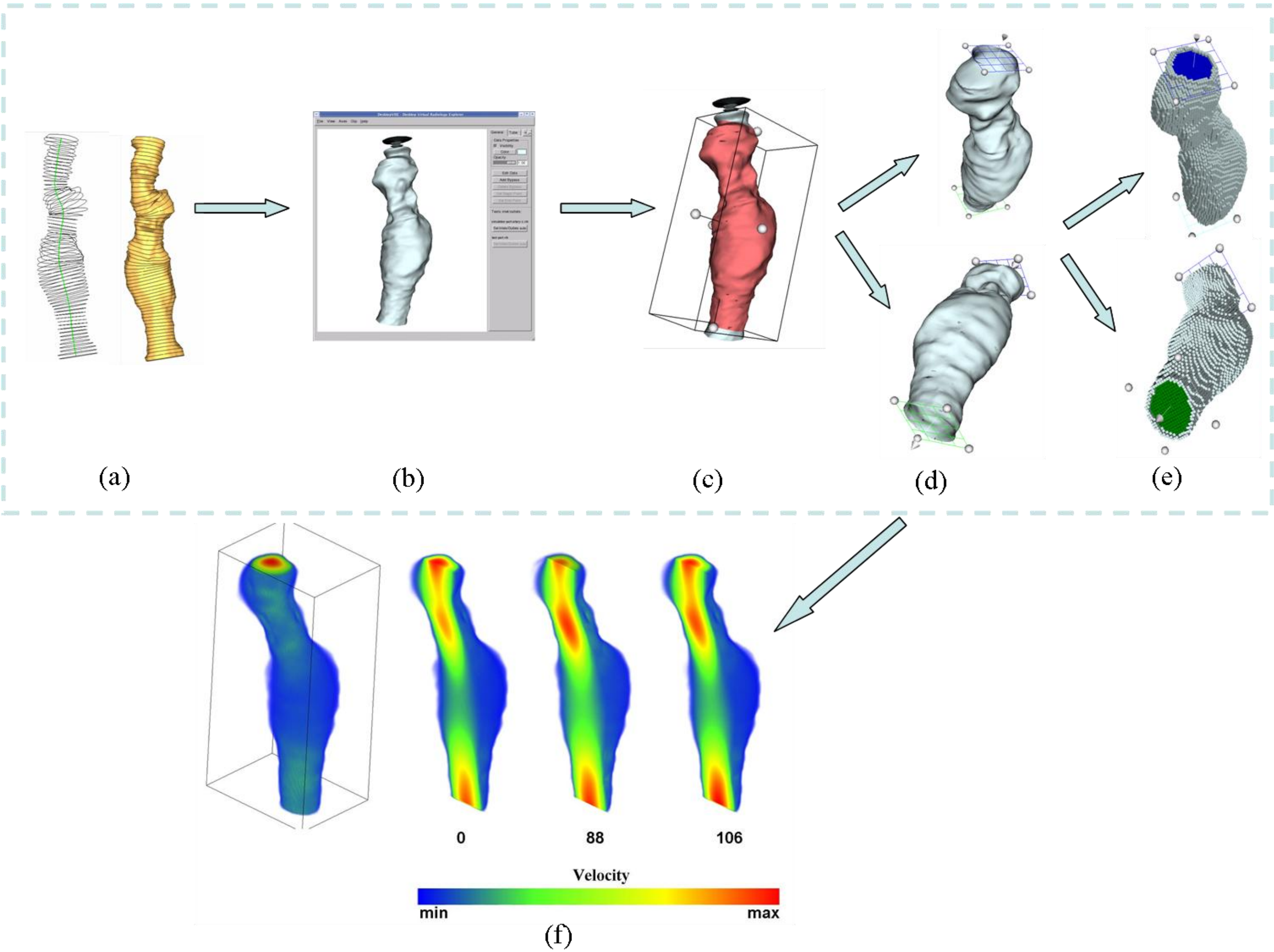
1. Segmentation of medical images
2. VR based system to change the images …
   - to add a bypass (*virtual surgical procedure*)

   … and to prepare the L-BGK lattice.
3. Image based CFD
   - For blood flow simulation
   - We use the Lattice Boltzmann Method
4. Visualisation kernels
5. A interactive problem solving environment to glue all this together
   - A grid based PSE

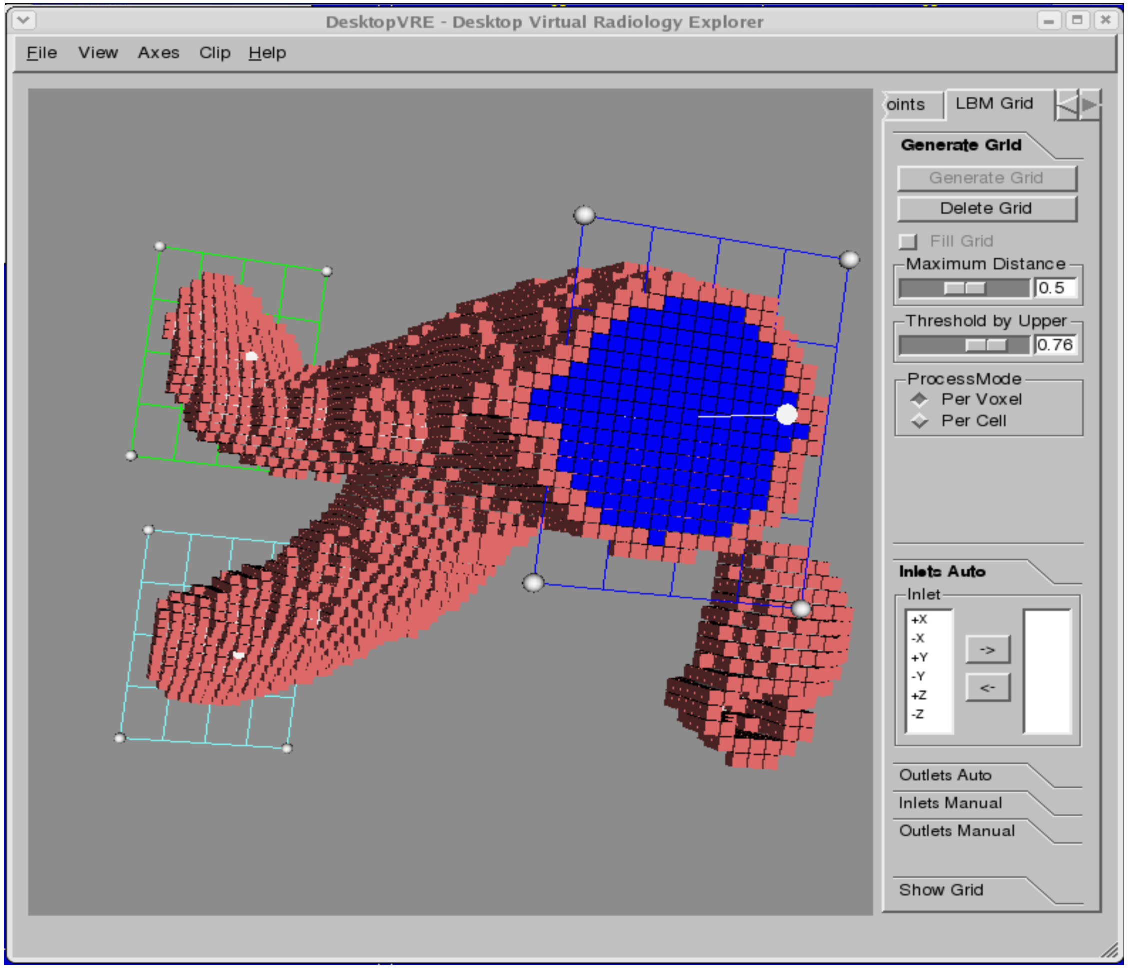
Ramos AT, Sloot PMA, Hoekstra AG, Bubak MT. 2004. An Integrative Approach to High-Performance Biomedical Problem Solving Environments on the Grid. Parallel Computing 30:1037—55

L. Abrahamyan; J.A. Schaap; A.G. Hoekstra; D.P. Shamonin; F.M.A. Box; R.J. van der Geest; J.H.C. Reiber and P.M.A. Sloot: A Problem Solving Environment for Image-Based Computational Hemodynamics, in V.S. Sunderam; G.D. van Albada; P.M.A. Sloot and J.J. Dongarra, editors, Computational Science - ICCS 2005: 5th International Conference, Atlanta, GA, USA, Proceedings, Part I, in series Lecture Notes in Computer Science, vol. 3514, pp. 287-294. Springer, Berlin, Heidelberg, May 2005. ISBN 3-540-26032-3.

The problem solving environment

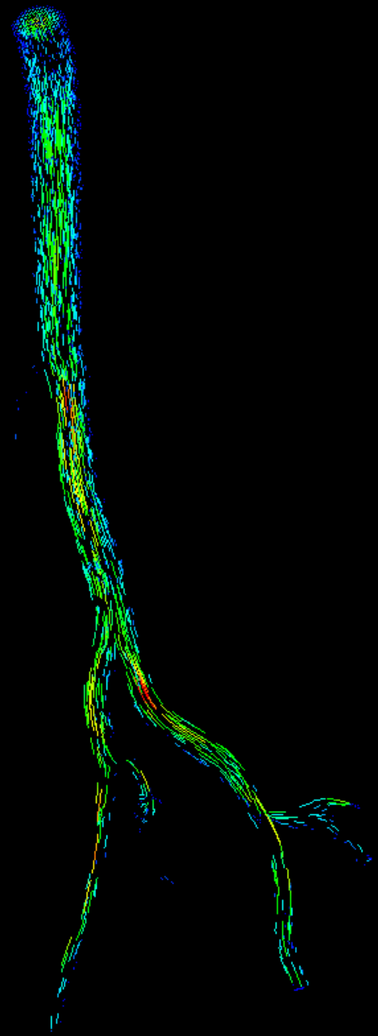


D-VRE

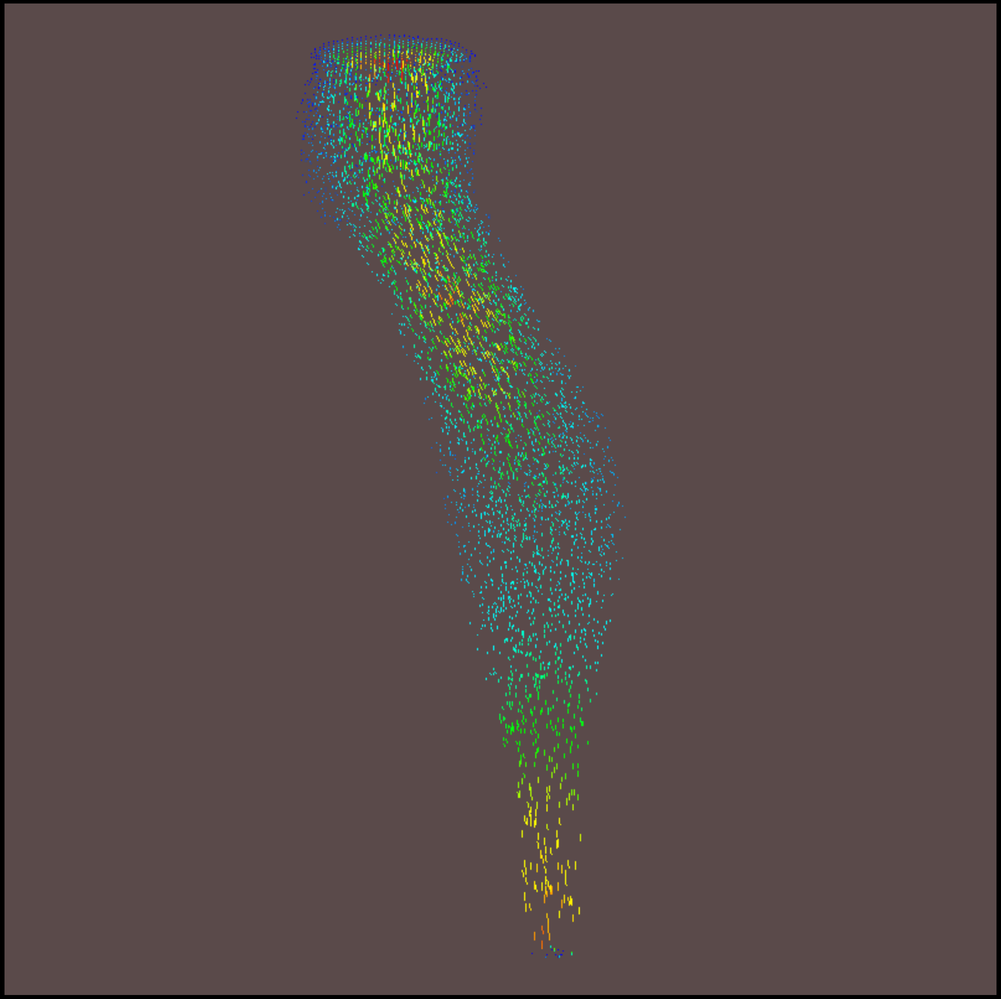


Step 4 : create computational mesh

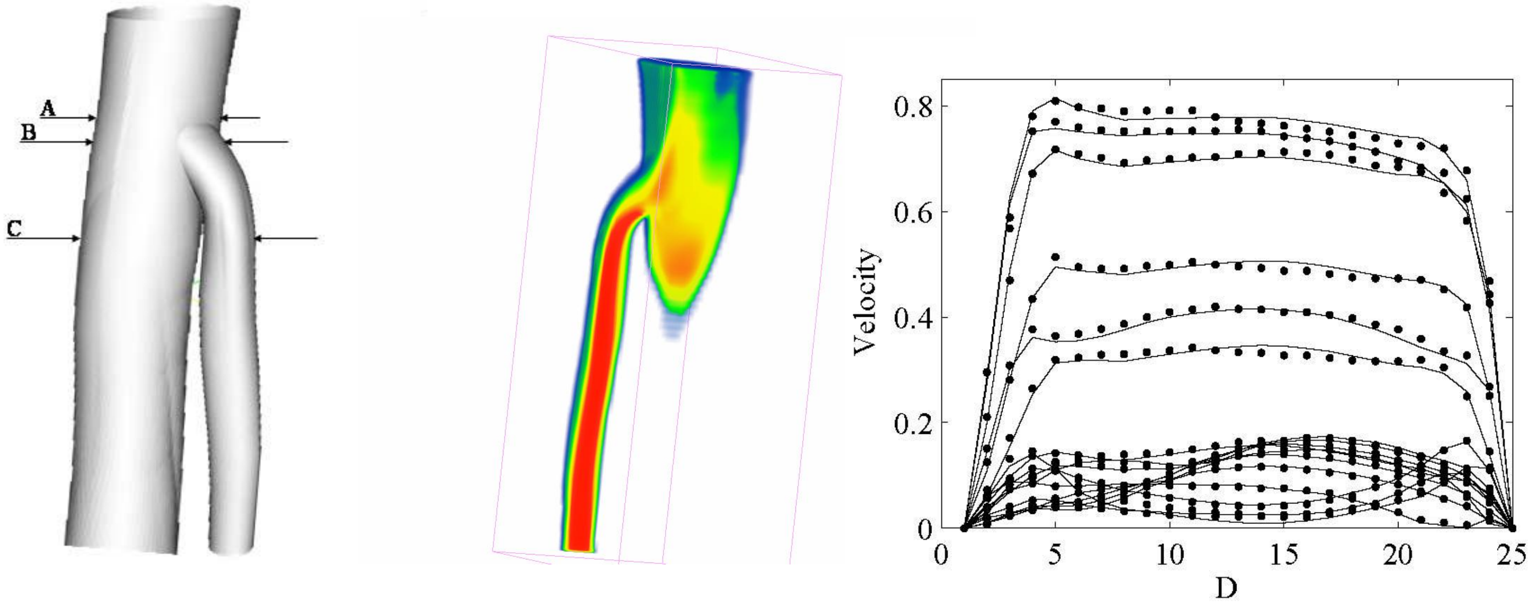
A few results : flow in the lower abdominal aorta



A few results : flow in an Abdominal Aorta Aneurysm

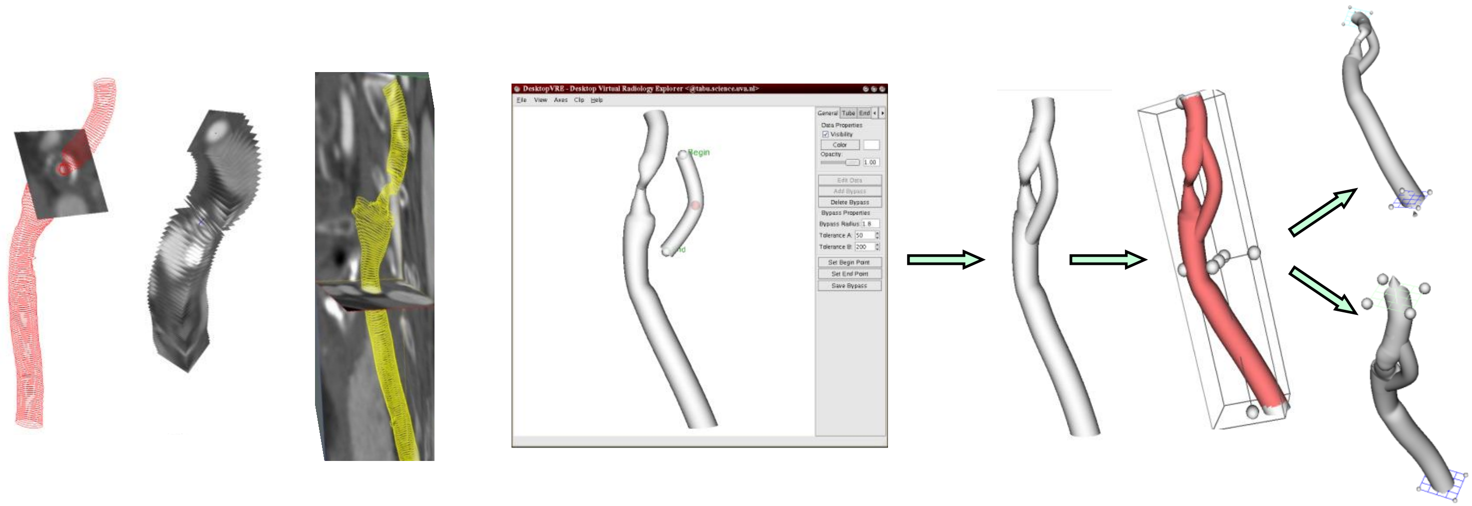


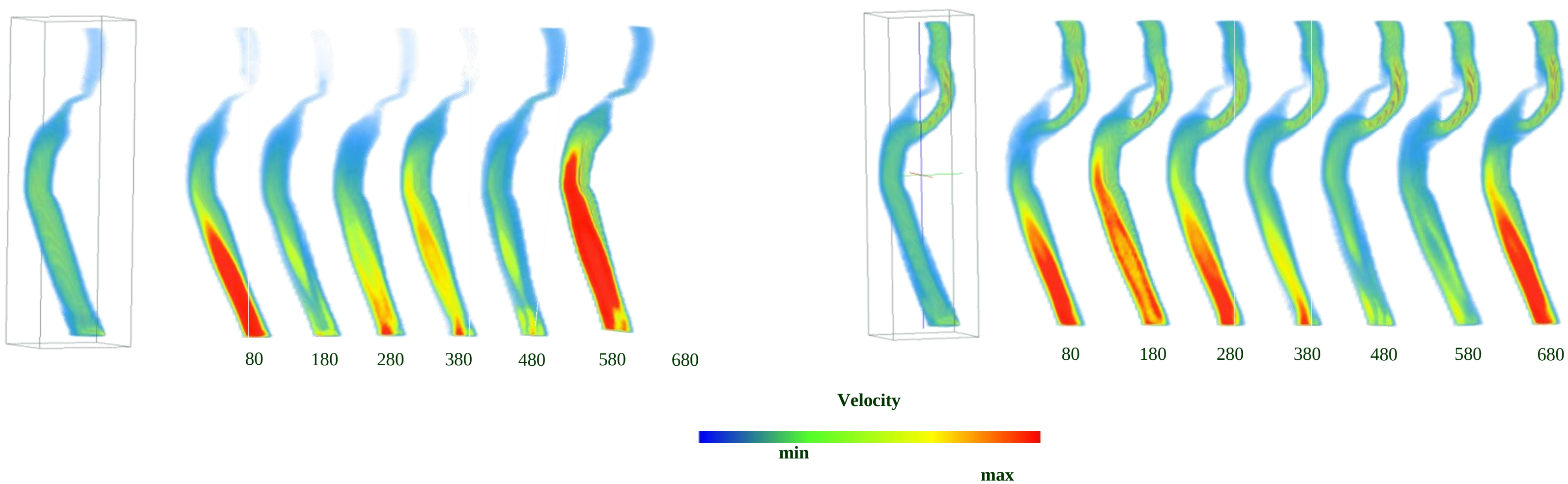
systolic flow in the superior mesenteric artery



Simulation of systolic flow in the superior mesenteric artery. The arterial structure (a); a snapshot of the simulation (b); a comparison of the velocity profiles between LBM (bullets) and FEM (solid lines) at the region and B at 0.04 second intervals throughout one systolic period, with velocities presented in m/s. (structure and FEM data from University of Sheffield, UK)

Carotid artery with stenosis





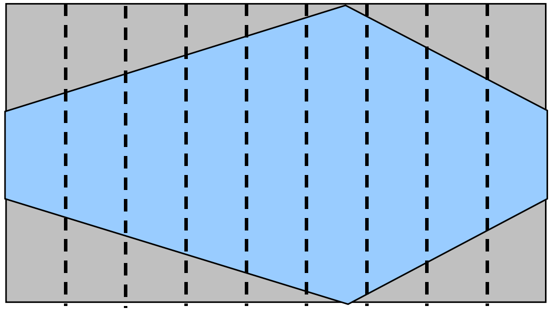
Parallelism

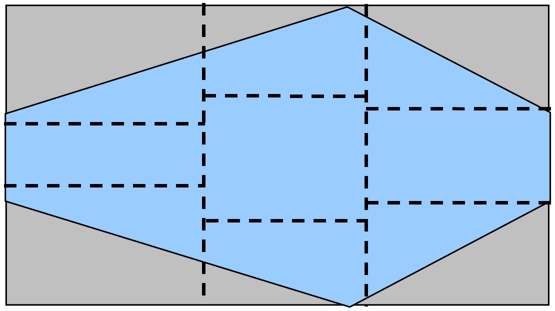
- Inherent local model → trivial parallelism
- Non-homogeneous domain
  - which decomposition ?
- Dynamically changing objects
  - load balancing
    - redundant scattered decomposition
    - dynamic load balancing

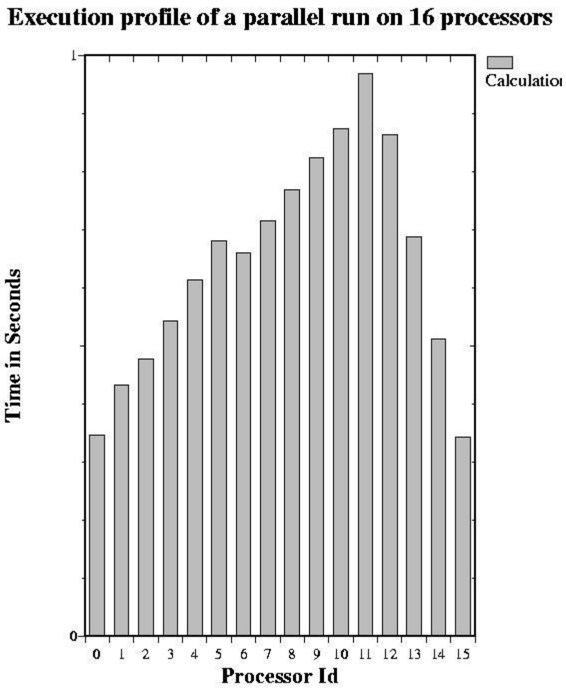
Kandhai BD, A. Koponen, Hoekstra AG, M. Kataja, J. Timonen, Sloot PMA. 1998. Lattice Boltzmann Hydrodynamics on Parallel Systems. Computer Physics Communications 111:14--26

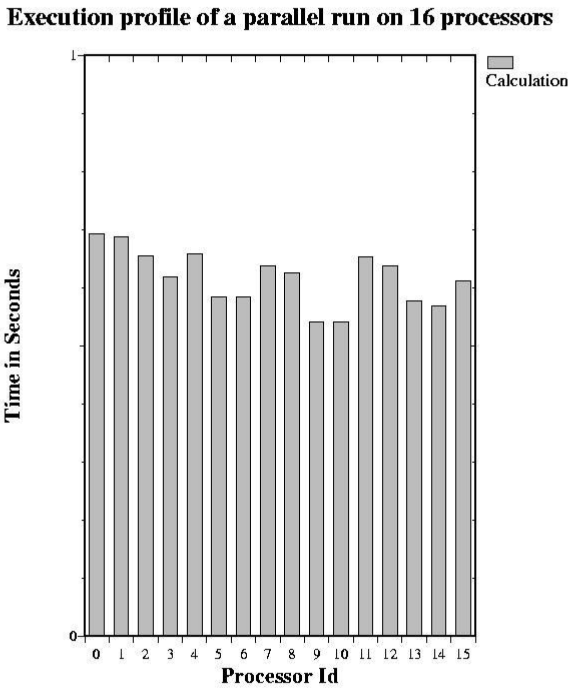
Non-Homogeneous domain

- Slice decomposition vs. ORB









slice

ORB

Parallel Sparse LBM

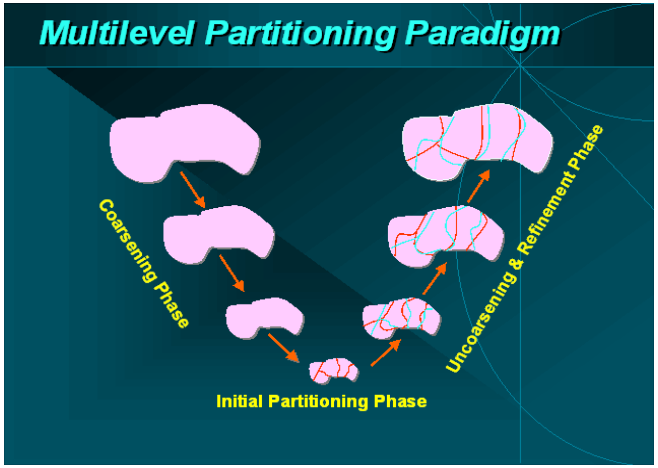
- Flow simulations in large and complex geometries are computationally intensive
  - e.g. porous media, or geometries from medical applications
- We need to
  - Minimize of computational time
    - ➔ Parallelization
  - Minimize of memory requirements
    - ➔ Sparse implementation

Parallel Sparse LBM

- The storage of density distributions is only for the fluid nodes
- The complete domain is mapped on an unstructured grid
- A sorted index list of fluid nodes is composed, where each node has the index list of its neighboring nodes
- 1D array is stored, where only 2*N*19 Reals are for density distributions and N*18 Integers for the adjacency list

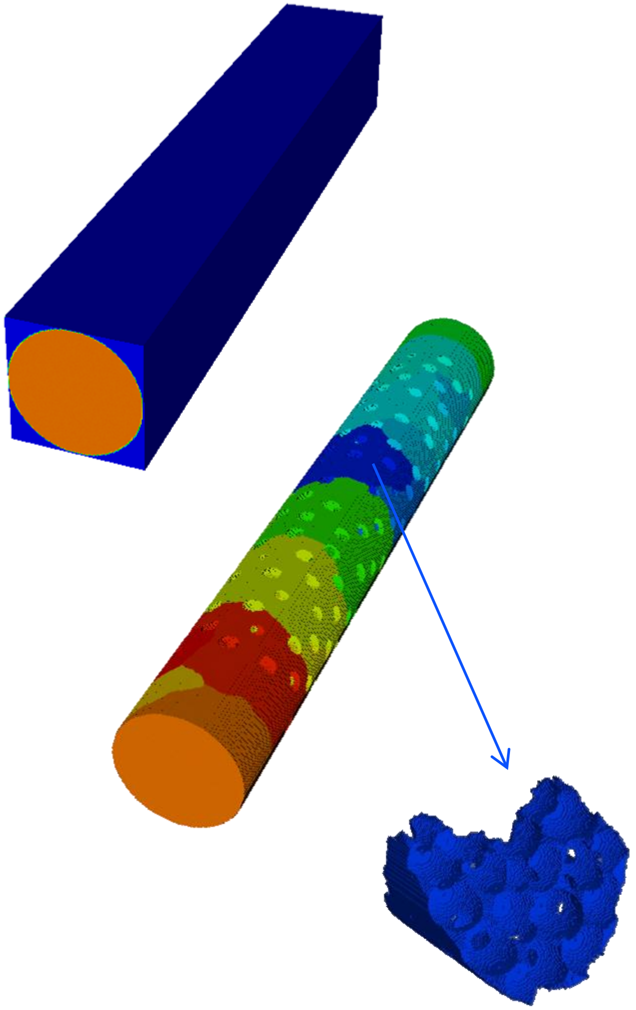
Graph Partitioning

- Keep the number of nodes on the sub graphs as equal as possible
  – to minimize load imbalance)
- Minimize edge-cut
  – reduce communication overheads
- We use multi-level partitioning strategies from the METIS library.
  – Fast
  – High quality partitioning



Partioning Algorithms

- Multilevel K-way
  - Coarsening only once
  - The coarsest graph is directly partitioned into k partitions
  - The uncoarsening phase is also performed only once.
- Multilevel recursive bisectioning (RB)
  - Perform recursive bisectioning on all phases of the multilevel graph partitioning.



Performance Model

- Performance prediction model.
  - To analyze the parallel scalability
  - To find the sources of loss of parallel efficiency

$$T_p(N) = \frac{T_1(N)}{p} + \sum_i T_i(N)$$

$$\varepsilon_p(N) = \frac{T_1(N)}{p * T_p(N)} = \frac{1}{1 + \sum_i f_i}$$

$$f_i = \frac{p * T_i(N)}{T_1(N)}$$

Details in: Axner L, Bernsdorf J, Zeiser T, Lammers P, Linxweiler J, Hoekstra AG. 2008. Performance evaluation of a parallel sparse lattice Boltzmann solver. Journal of Computational Physics 227:4895-911

Fractional Overheads

1. Fractional communication overhead

$$f_{comm} = \frac{p * \max_j \{2d_j \tau_{setup} + 2e_j \tau_{send}\}}{N * \tau(N)}$$

2. Fractional load balance overhead

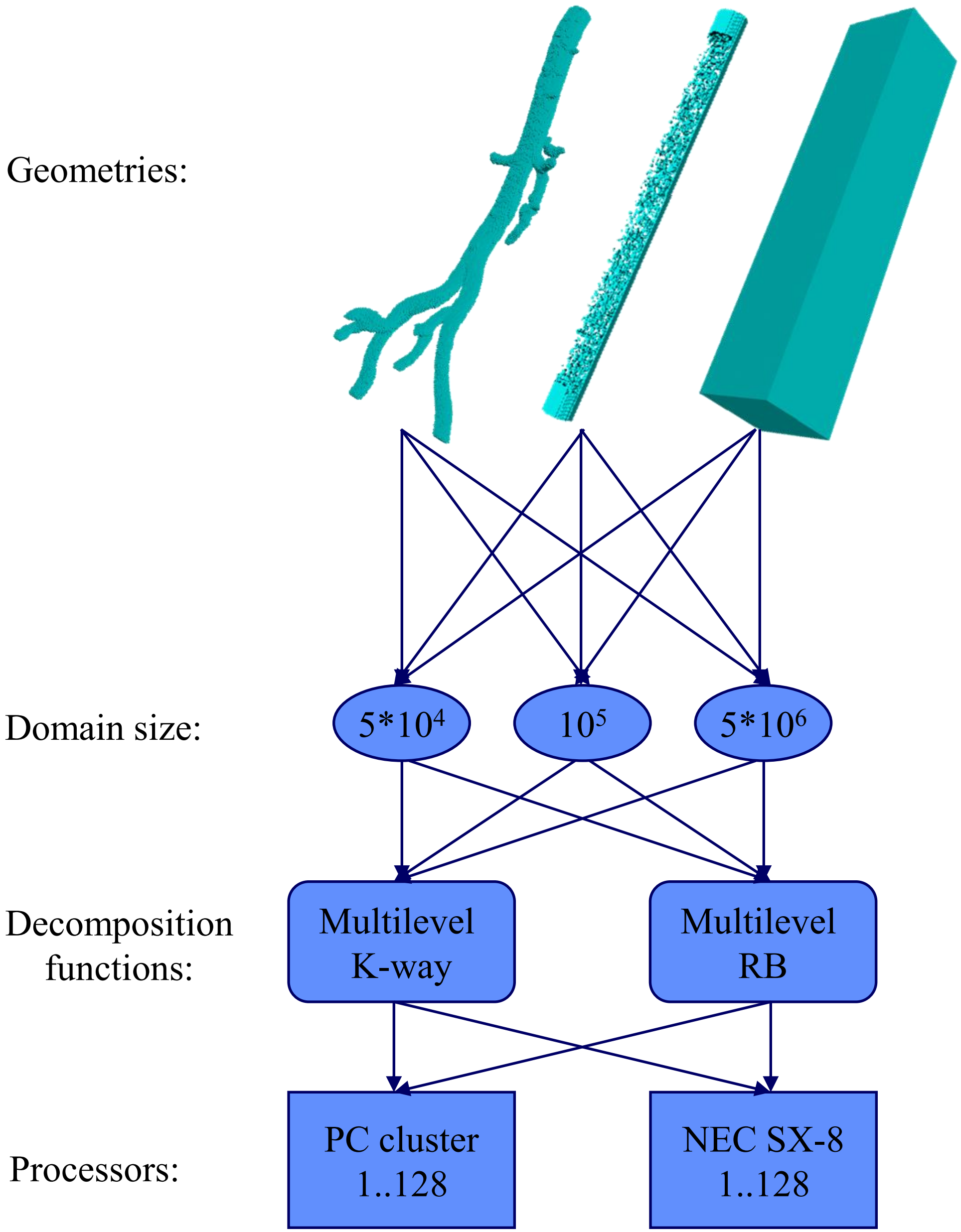
$$f_l = \frac{p * n_{\max}}{N} - 1$$

3. Fractional processor speed overhead

$$f_s = \frac{p * n_{\max}(\tau(n_{\max}) - \tau(N))}{N * \tau(N)} = \frac{p * n_{\max}}{N}\left(\frac{\tau(n_{\max})}{\tau(N)} - 1\right)$$

Details in: Axner L, Bernsdorf J, Zeiser T, Lammers P, Linxweiler J, Hoekstra AG. 2008. Performance evaluation of a parallel sparse lattice Boltzmann solver. Journal of Computational Physics 227:4895-911

Experiments



3 – different geometries
- Abdominal aorta (AA)
- Porous media (PM)
- Straight square channel (SSC)

3 – data sizes

2 – decomposition functions

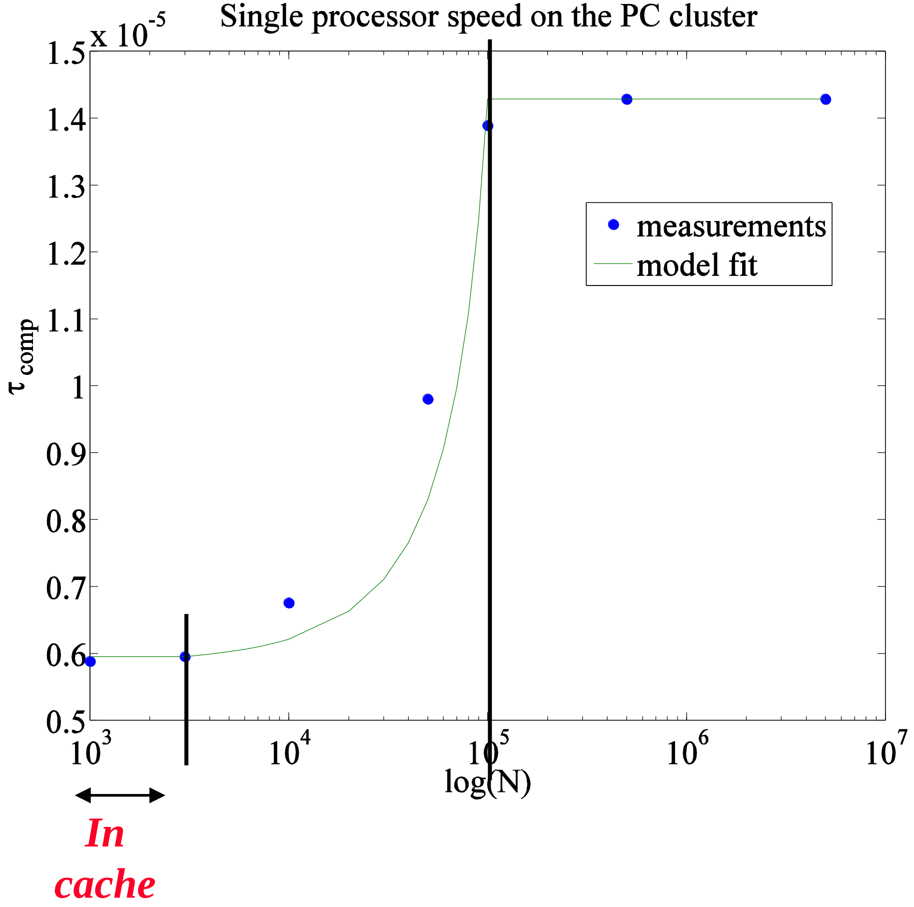
2 – PC cluster & NEC SX-8 machine
- with 1,2,4,16,32,64,128 processors

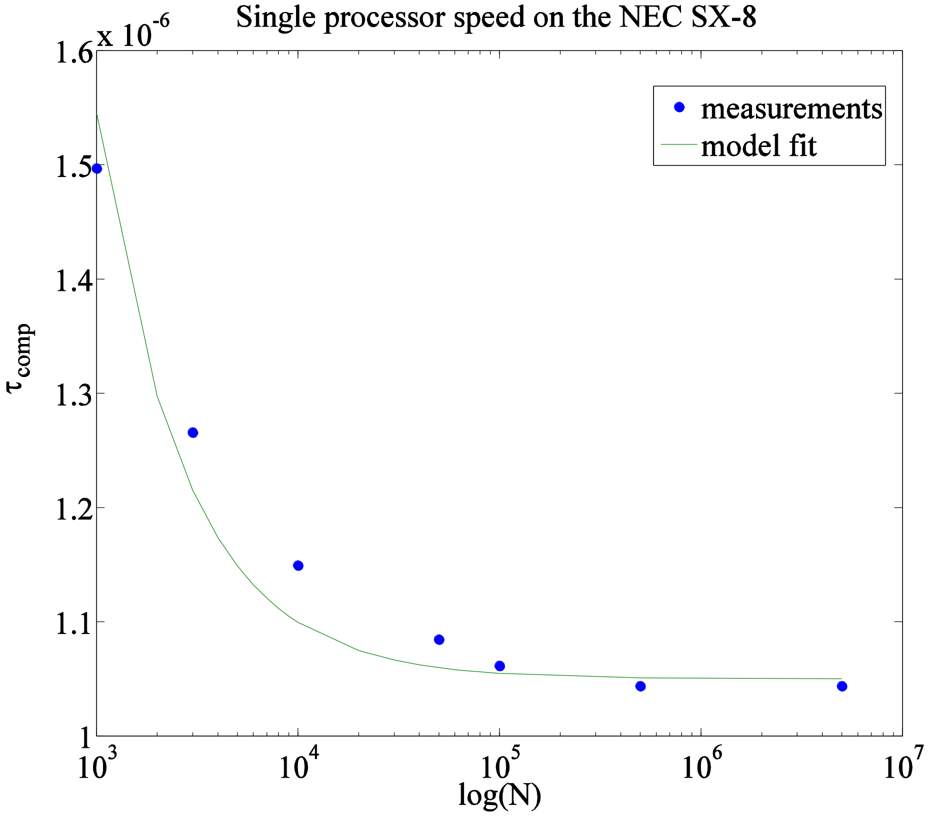
Total: 36 experiments on each of 1…128 processor

Full results in: Axner L, Bernsdorf J, Zeiser T, Lammers P, Linxweiler J, Hoekstra AG. 2008. Performance evaluation of a parallel sparse lattice Boltzmann solver. Journal of Computational Physics 227:4895-911

Single Processor Speed

- For PC cluster the discontinuity indicates that for the N < $3*10^3$ data sizes we see the cache effect which can give rise to a super linear speed-up.
- It is well-known that vector machines perform best for large data sizes.

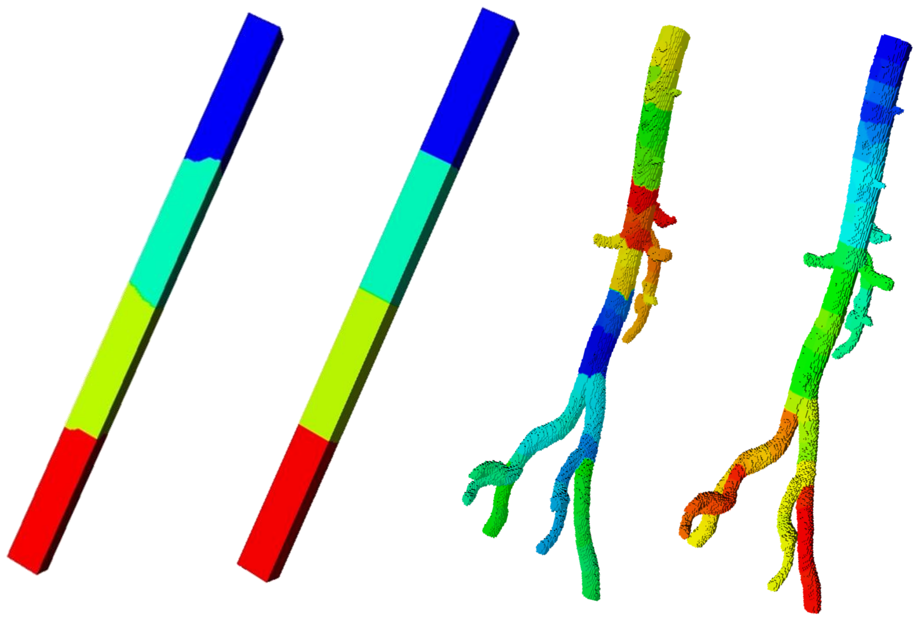


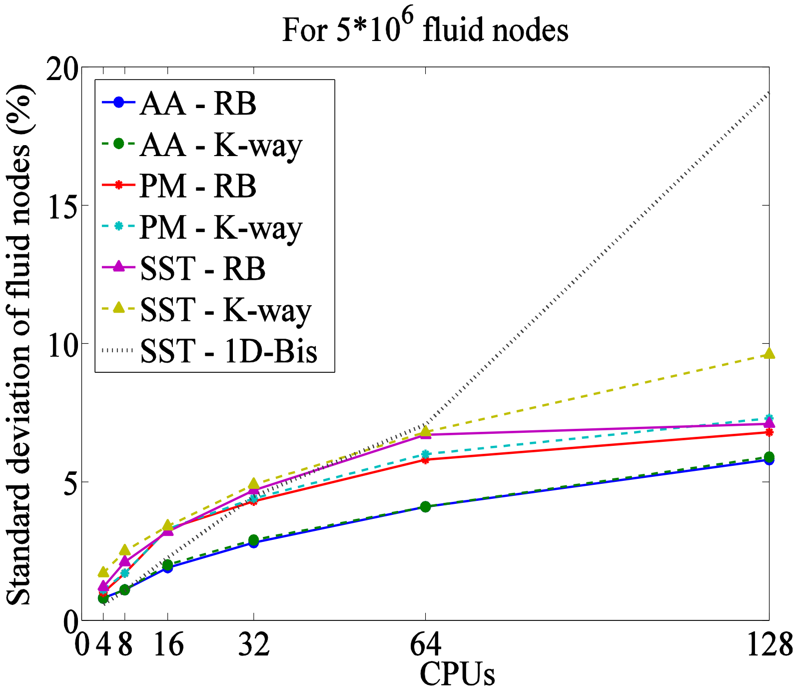


Partitioning

- The multilevel RB creates more sliced cuts between partitions, while the partitions of multilevel K-way are less structured and have curved cuts.

- From measurements of standard deviation of fluid nodes we hardly see difference between multilevel RB and multilevel K-way for all geometries except for SSC for a very large number of partitions.



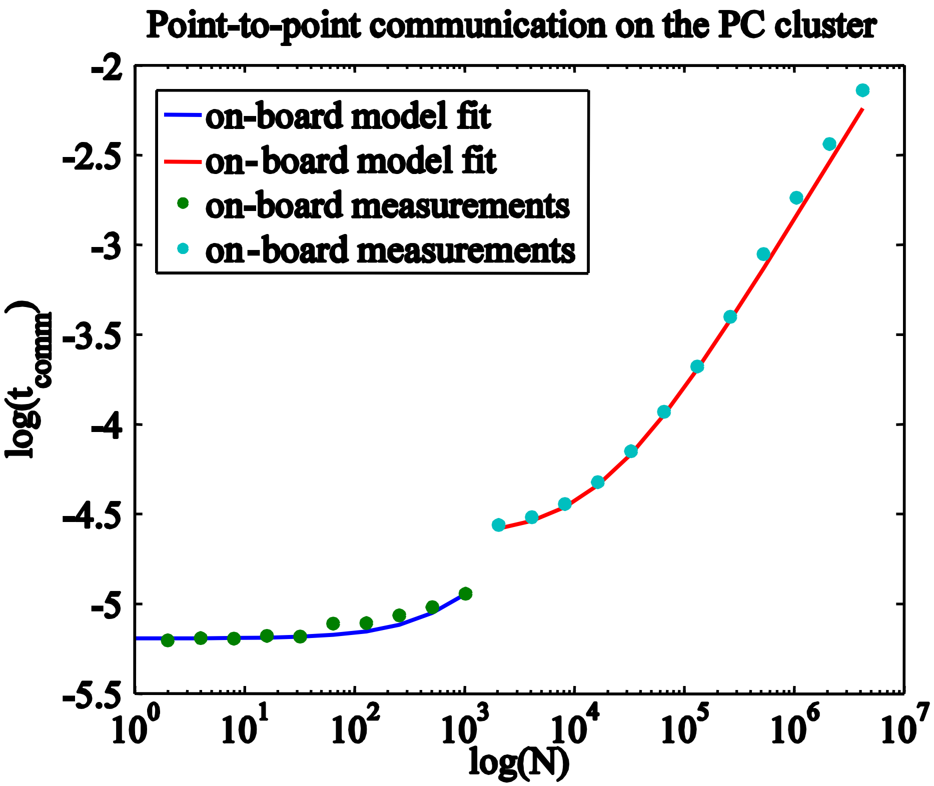


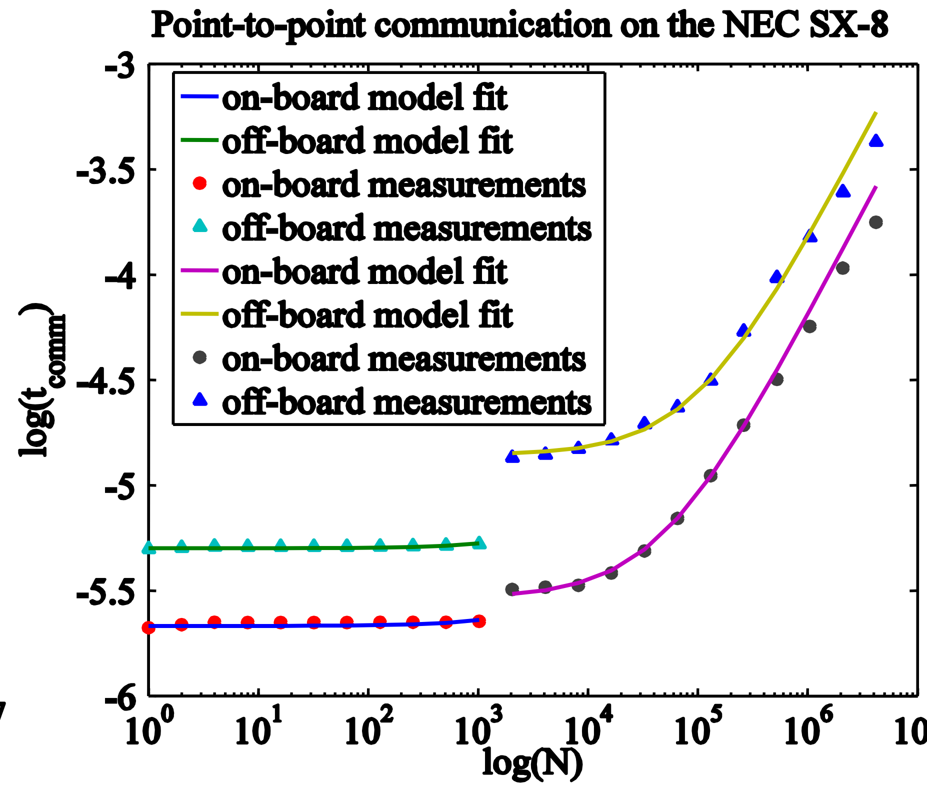
Dr. A.G. Hoekstra

Point to Point Communication

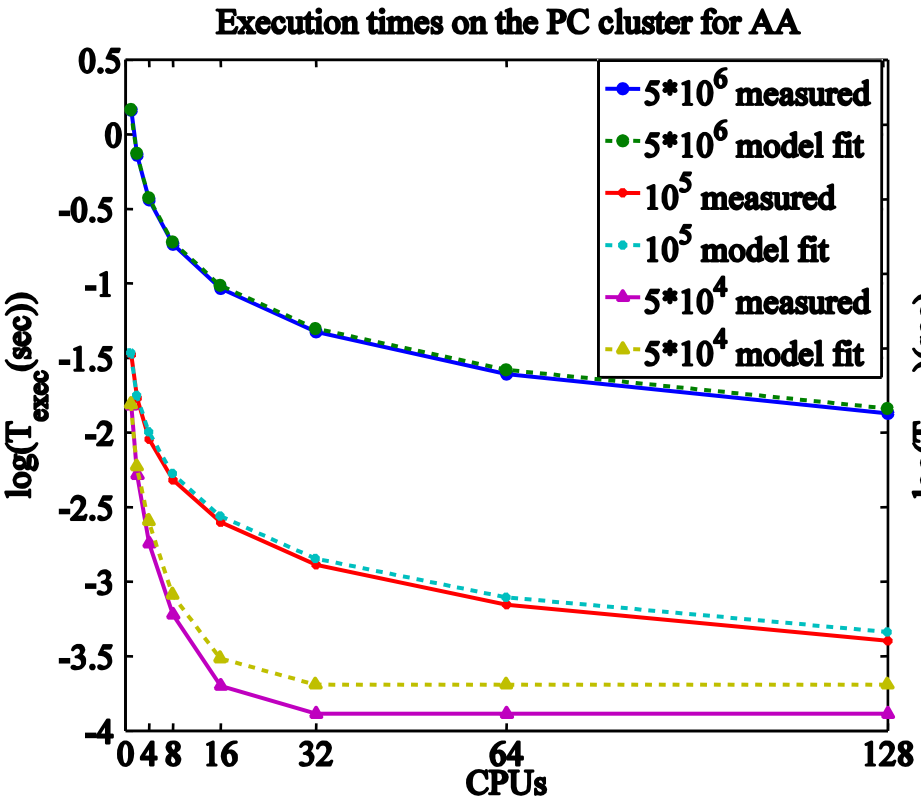
- The SX-8 vector machines have 8 processors per node, thus we distinguished between on-board and off- board communication times.

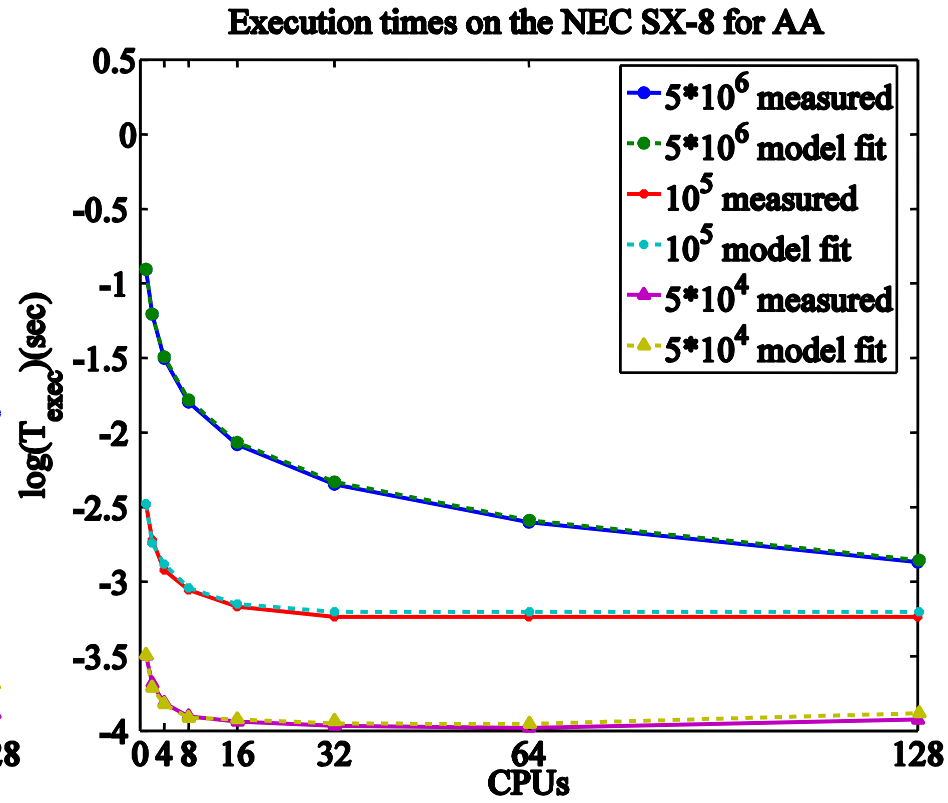
- After certain amount of data we see a discontinuity due to the buffer size on both PC cluster and SX-8 machine.



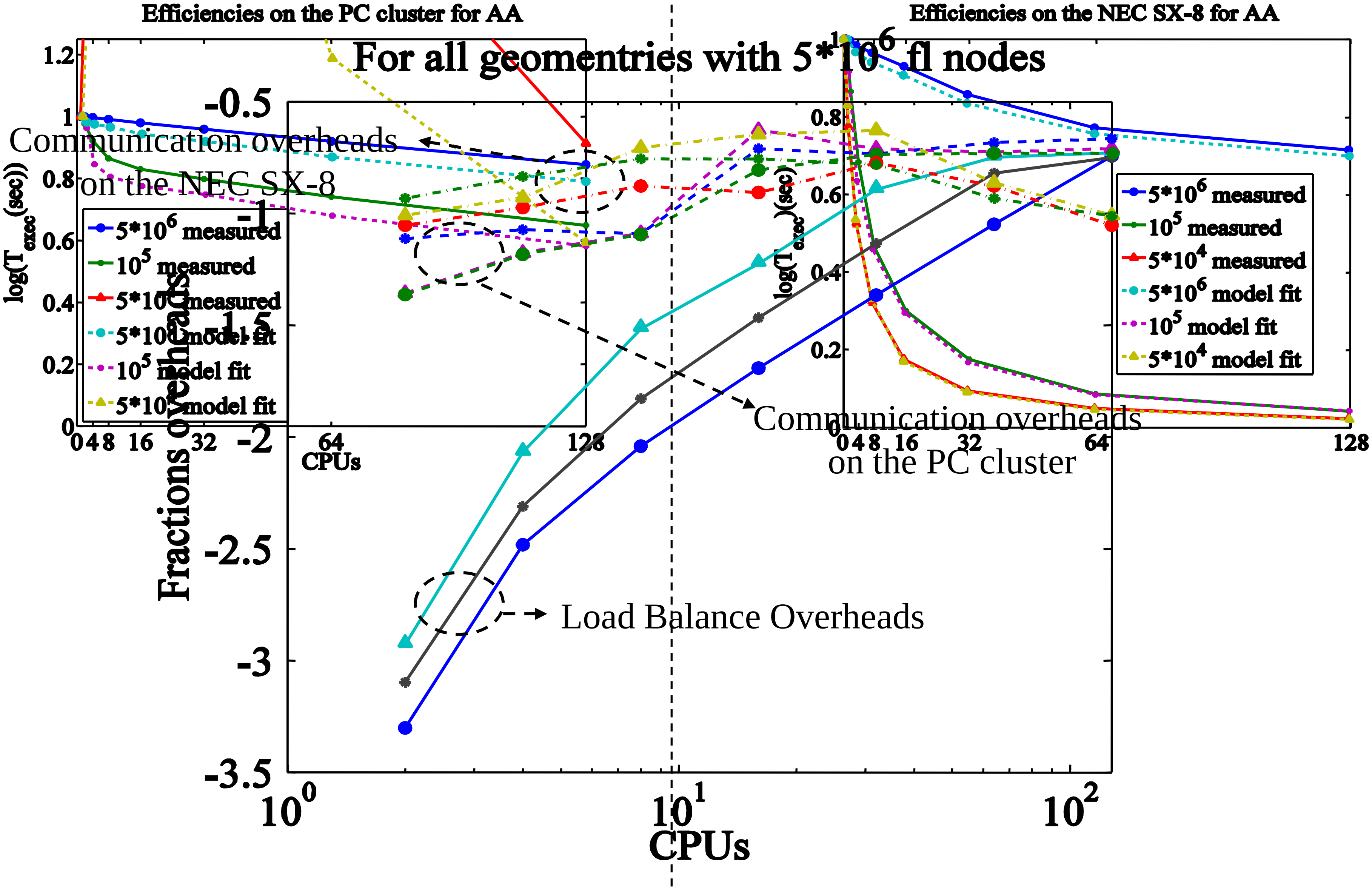


Execution Times





Performance measurements



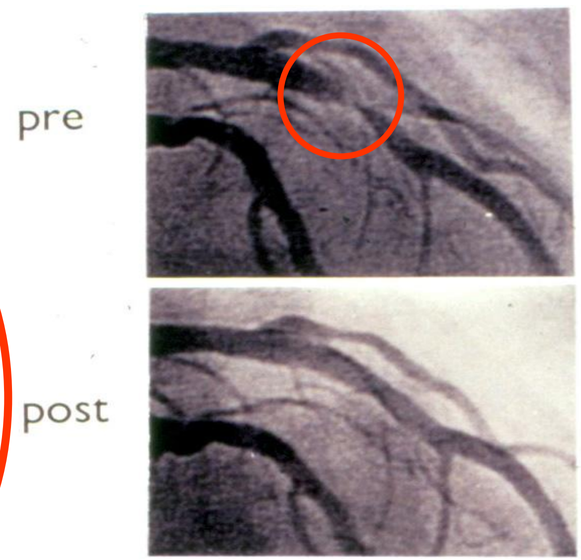
Dr. A.G. Hoekstra

MultiPhysics MultiScale

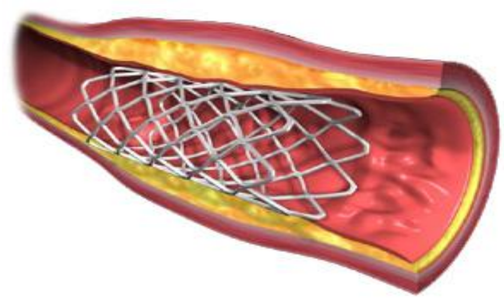
- We now use LBM as a solver in multiphysics multiscale applications
- Coupling LBM with solvers for
  - Diffusion
  - Reactions
  - Biological processes
  - Fluid-Structure interaction
- Multiscale modelling
  - Fast systolic flows (LBM) to slowly proliferating cells.

Example, in-Stent Restenosis

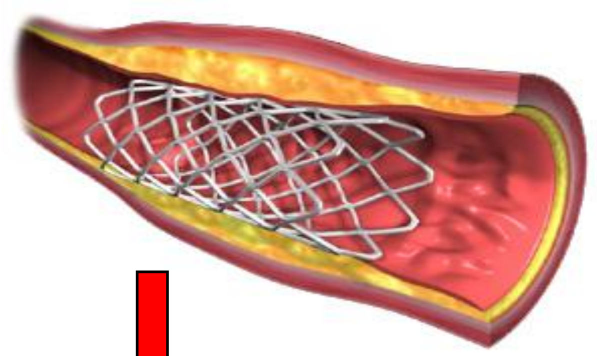
- stenosis: occlusion of blood vessels
- treated by stent-deployment

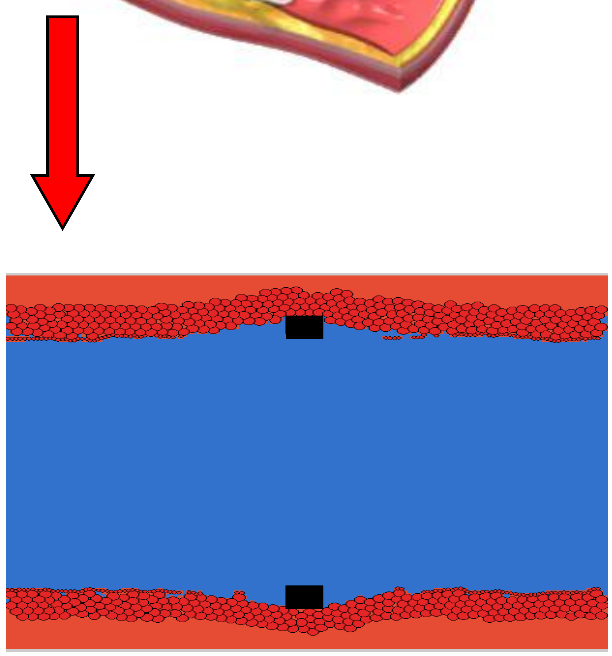


- (fast) periodic flow
- (slow) biological responses
- advection-reaction-diffusion
- tissue mechanics
- …



Simplified model

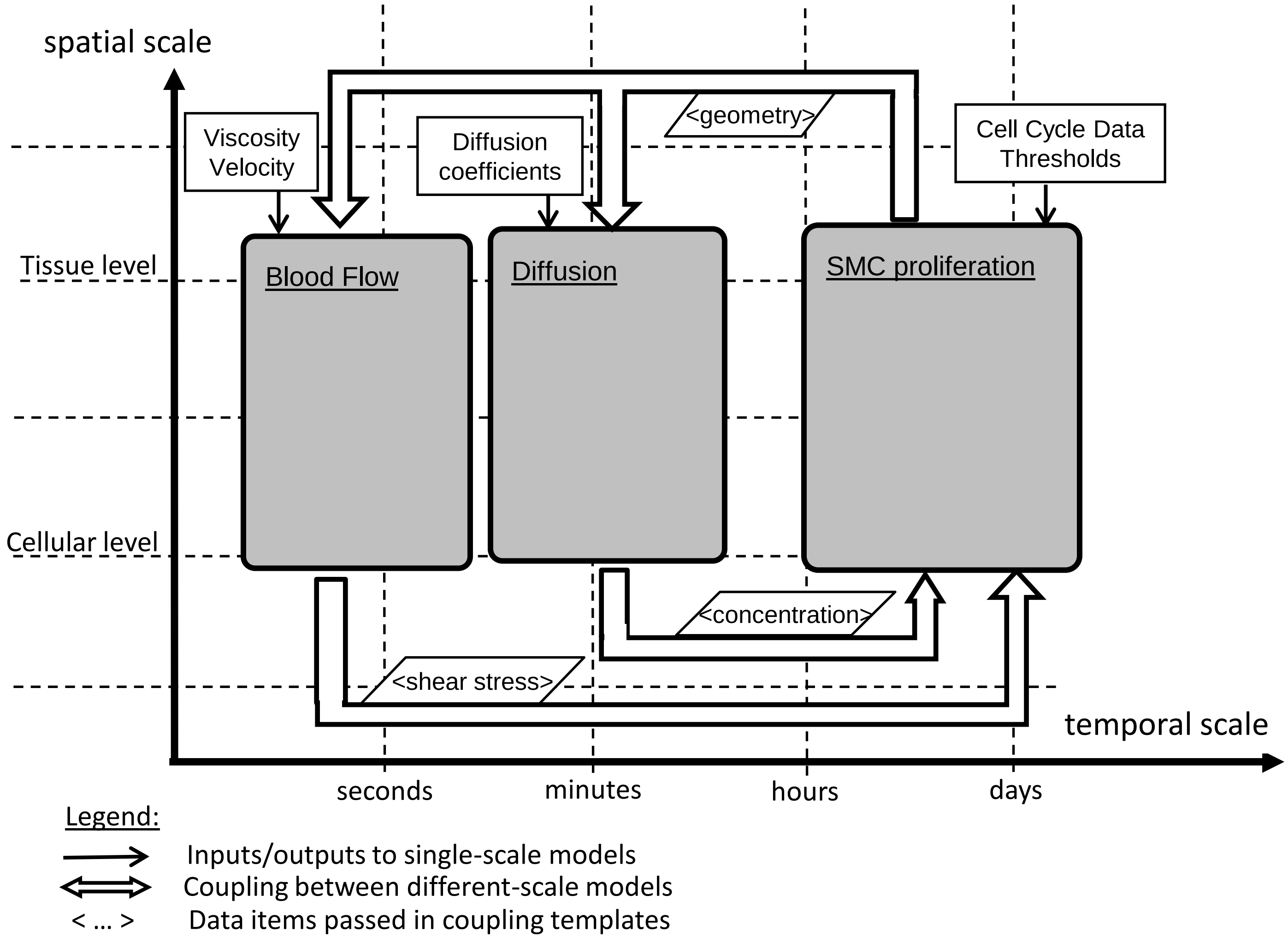




- 2D
- three single scale models
  - bulk flow (lumen)
  - smooth muscle cells (tissue)
  - drug diffusion (tissue)

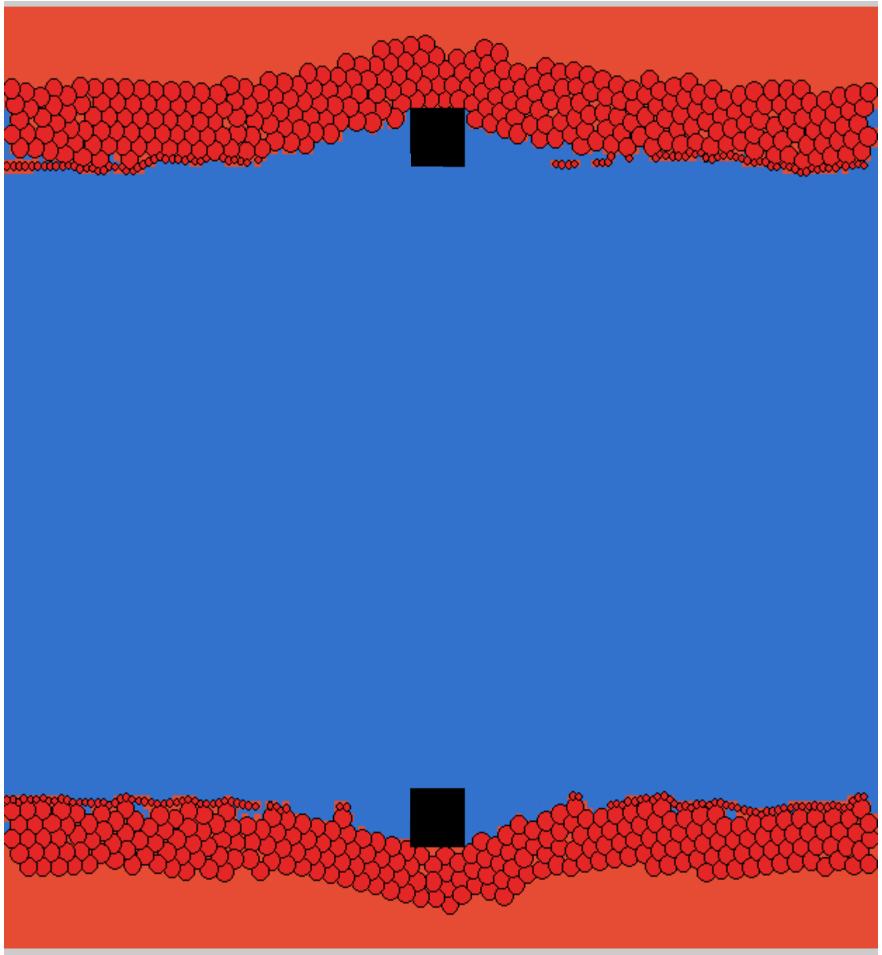
- initial conditions
- scale map
- connection scheme
  - details of single scale models and coupling templates

Scale Separation Map



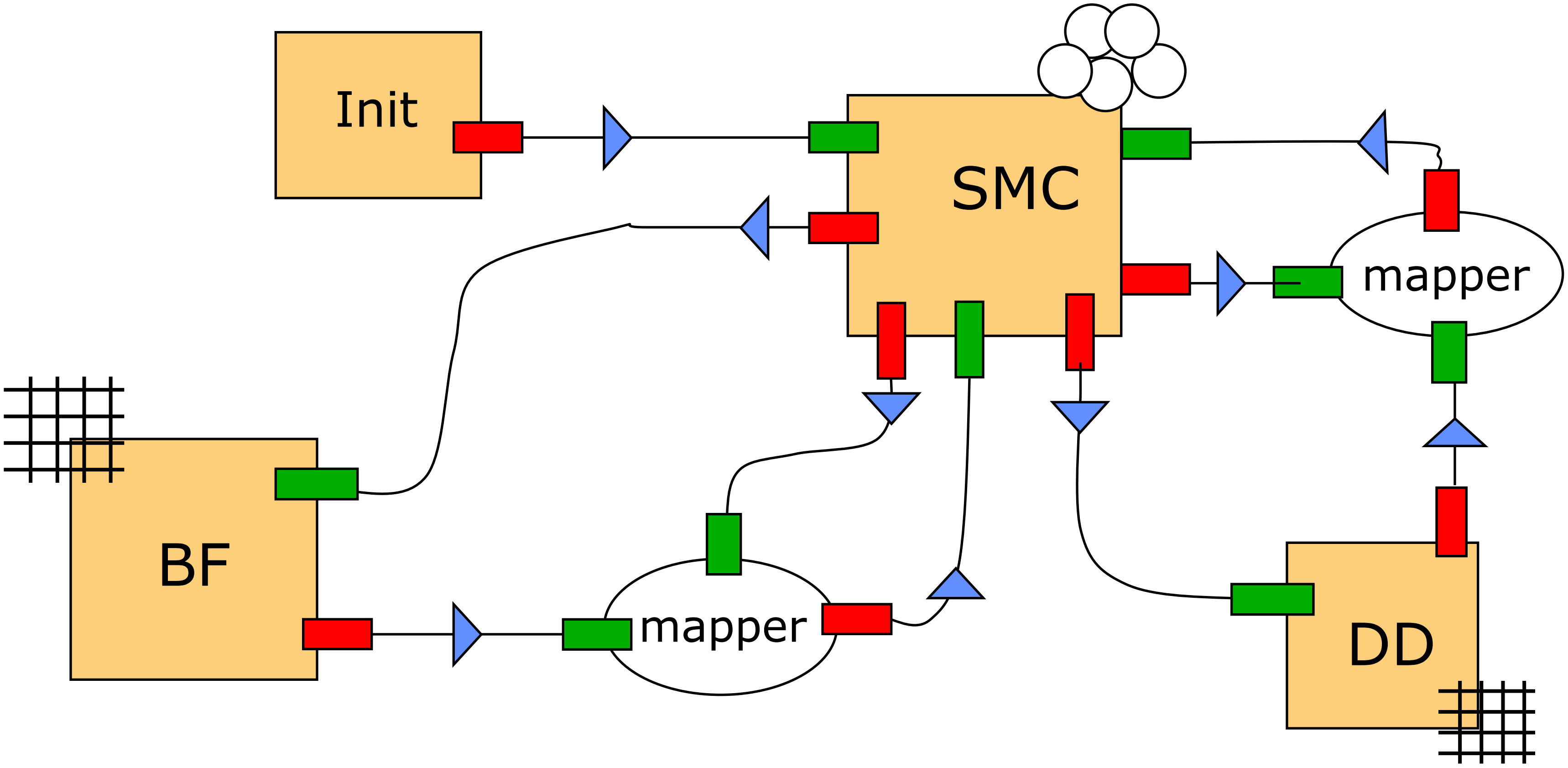
initial condition

- geometry:
  - 2D vessel: 1.5mm x 1mm
  - square struts, 90mm
  - tunica: 120mm
- initial conditions:
  - deployment + SMC relaxation

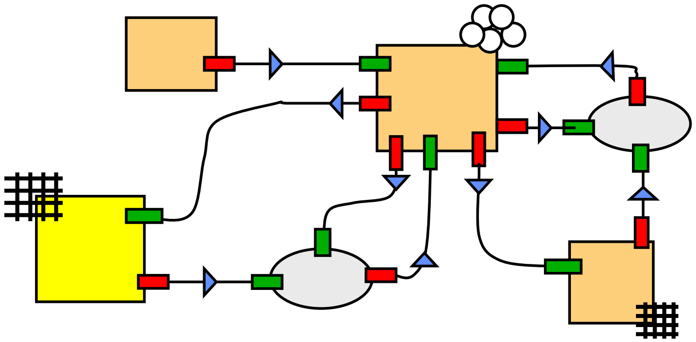


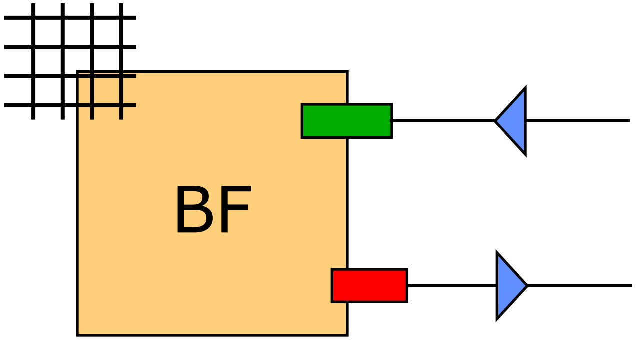
Dr. A.G. Hoekstra

CxA for ISR: Connection Scheme



Single Scale Models: bulk flow



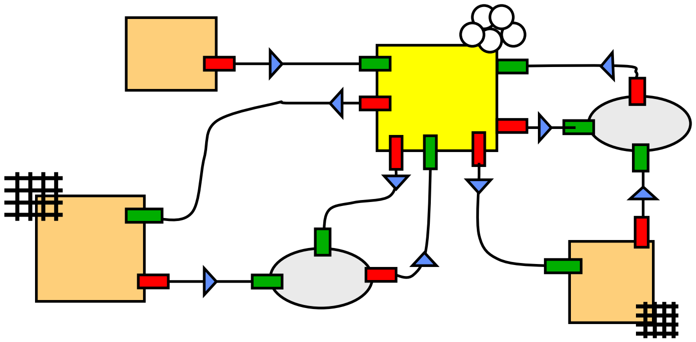


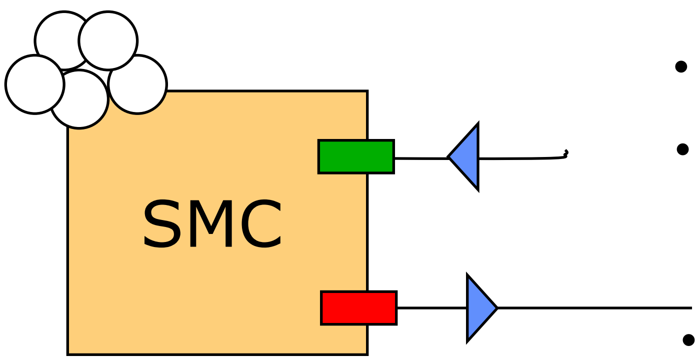
- Lattice Boltzmann Method

$$\Delta t = 10^{-5}\mathrm{s},\ \Delta x = 0.01\mathrm{mm}$$

- receive: geometry updates
- send: shear stress at boundary

Single Scale Models: SMC growth



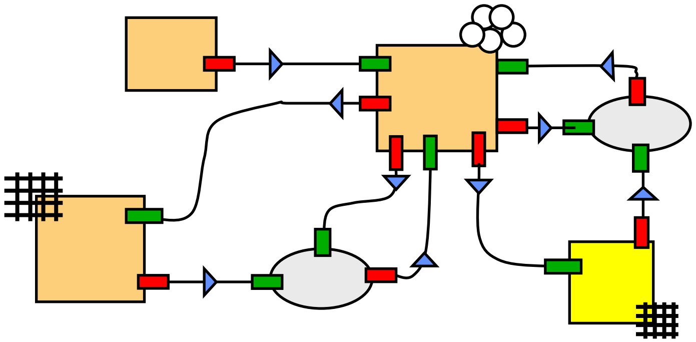


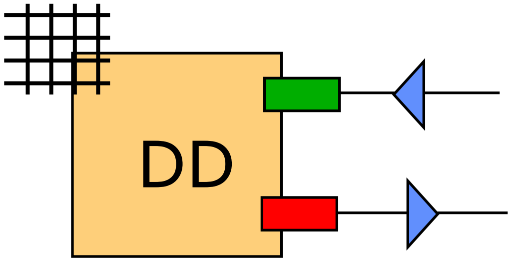
- Agent Based Model
- structural solver + biological rule-set

$$\Delta t = 1h, \; \Delta x = 6\mu\mathrm{m}$$

- receive: shear stresses, drug concentration
- send: cell positions and radii

Single Scale Models: drug diffusion



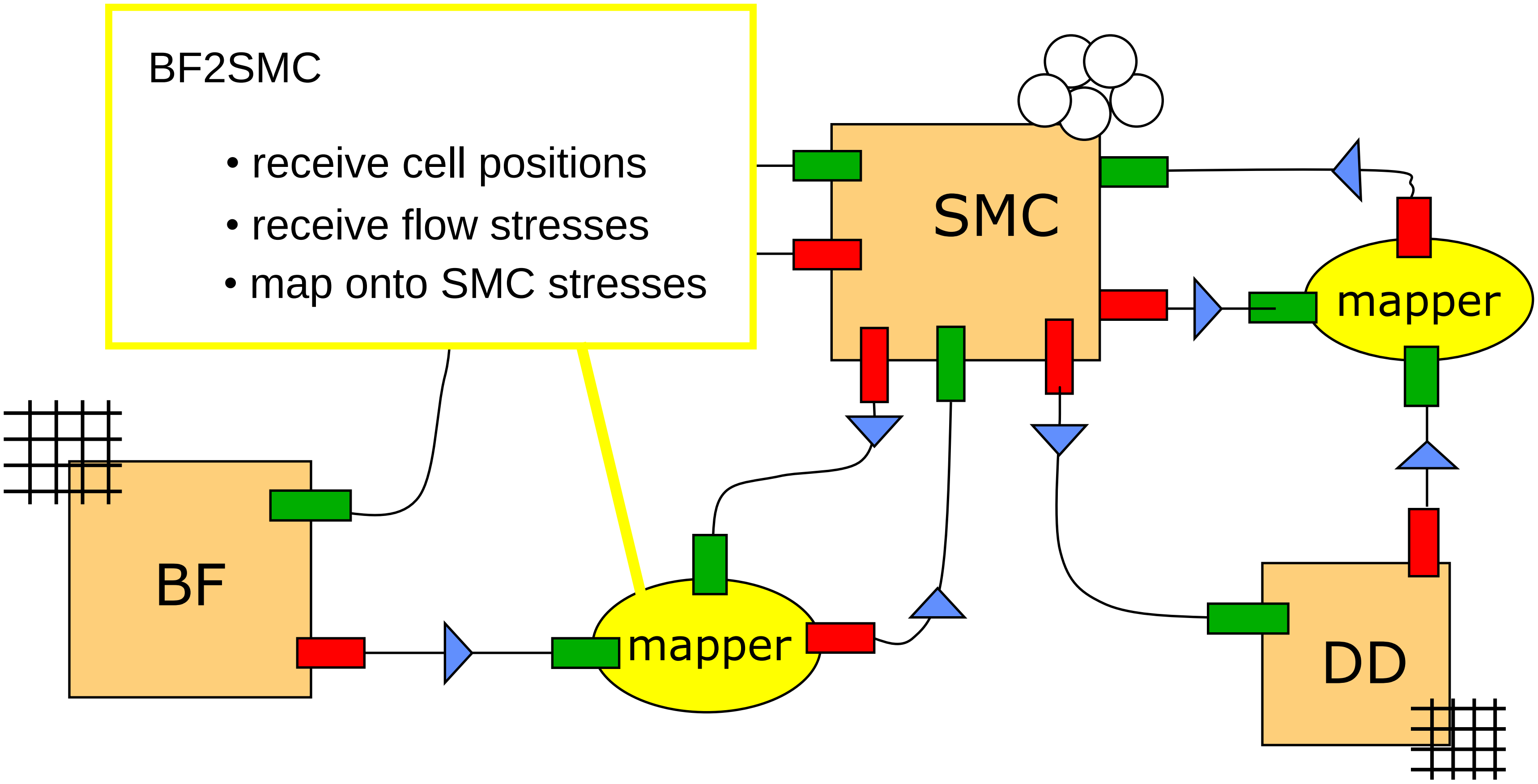


- Finite Difference
- SOR to determine steady state

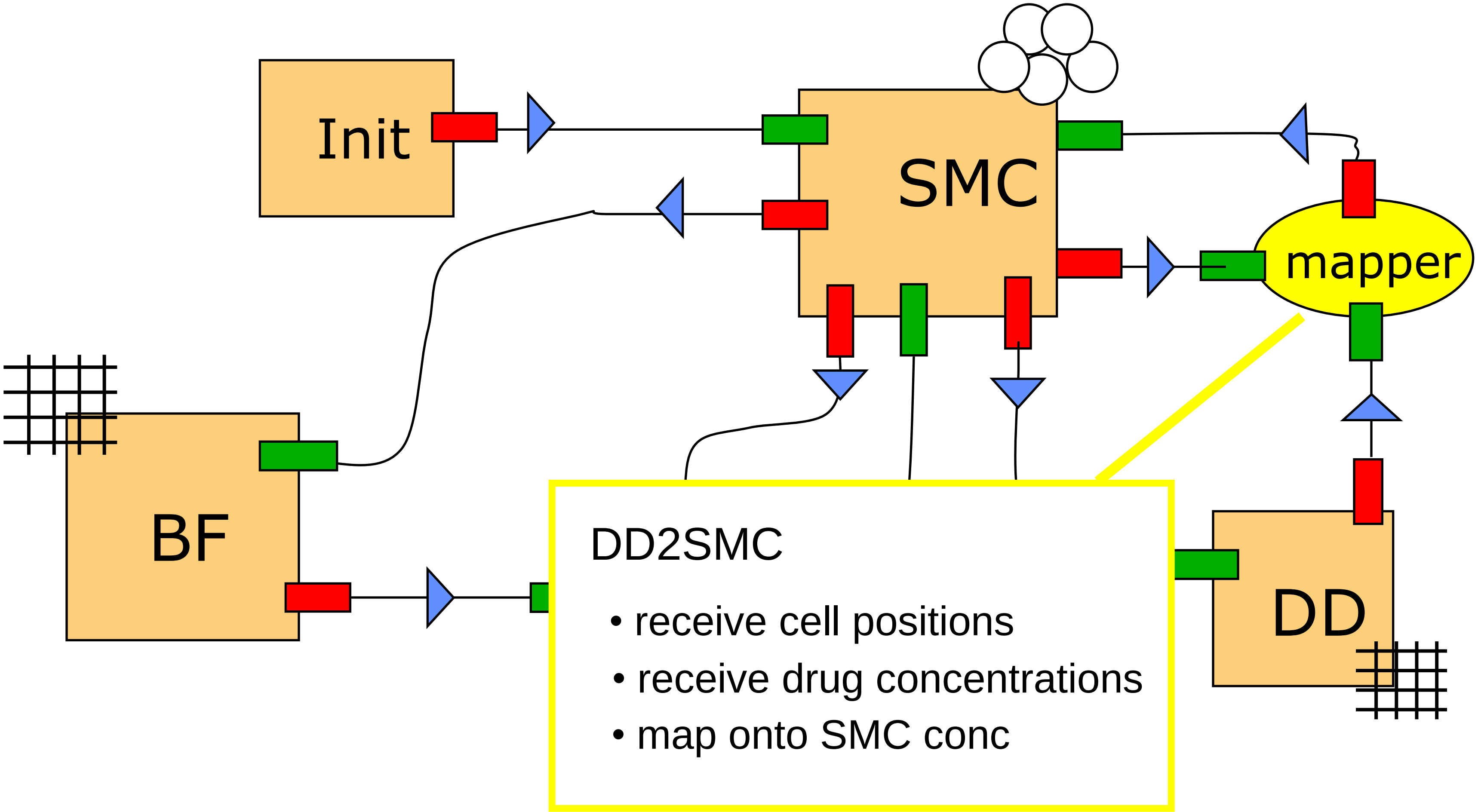
$$T = 1h,\ \Delta x = 0.01\mathrm{mm}$$

- receive: geometry information
- send: drug concentrations

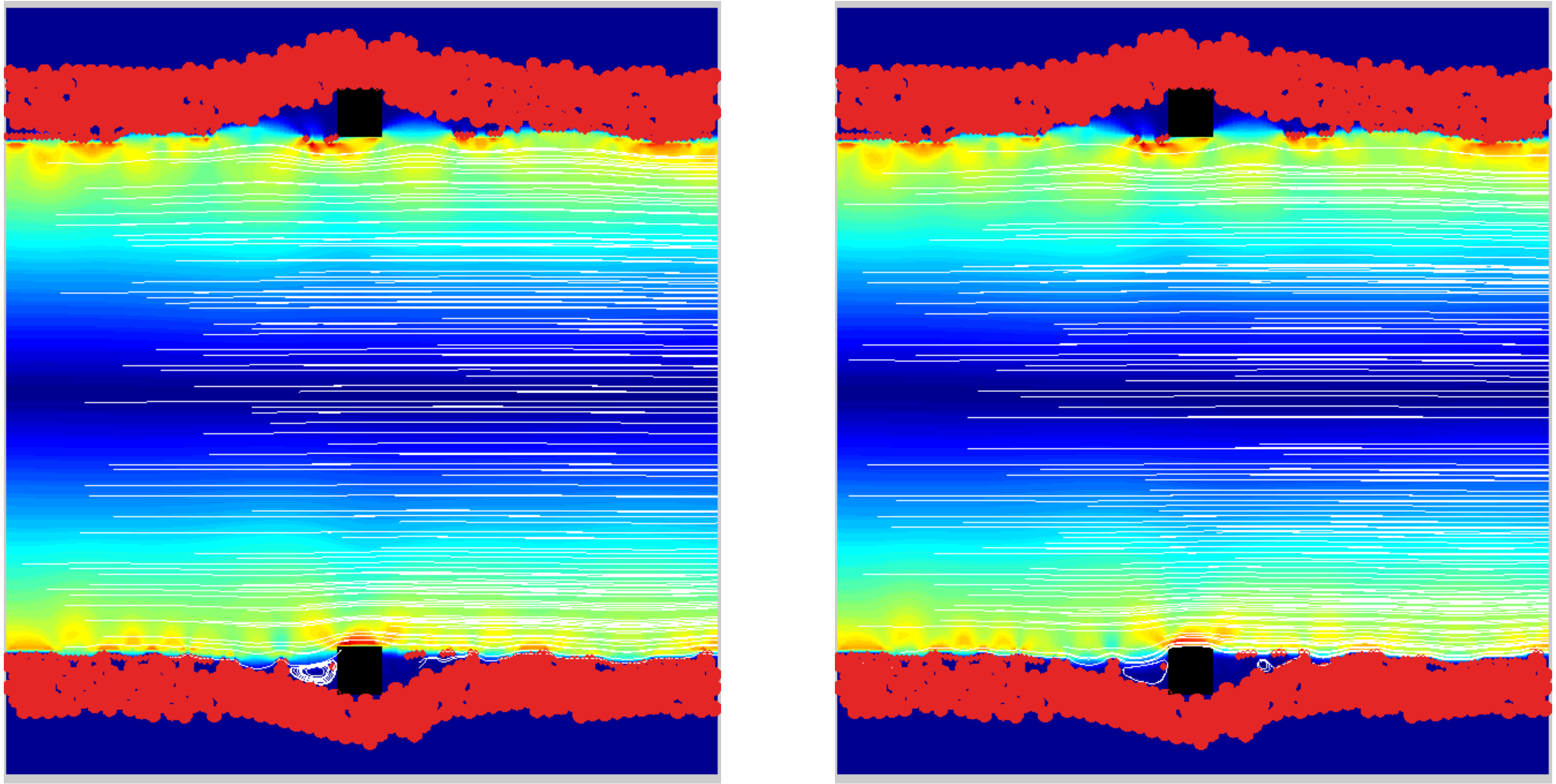
Mappers


BF2SMC
• receive cell positions
• receive flow stresses
• map onto SMC stresses
SMC
mapper
BF
mapper
DD

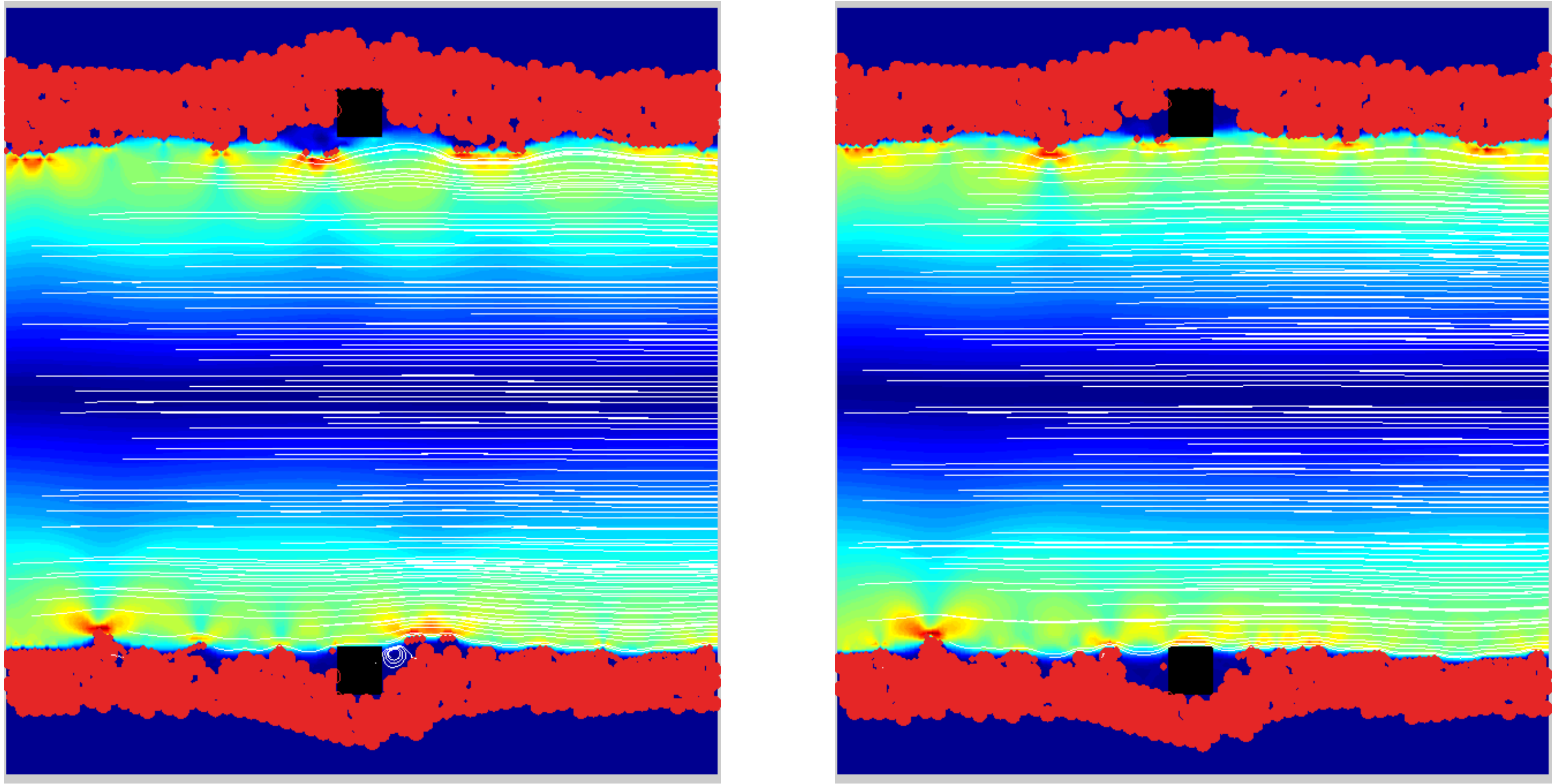
Mappers


Init
SMC
mapper
BF
DD
DD2SMC
• receive cell positions
• receive drug concentrations
• map onto SMC conc

CxA for ISR: preliminary results

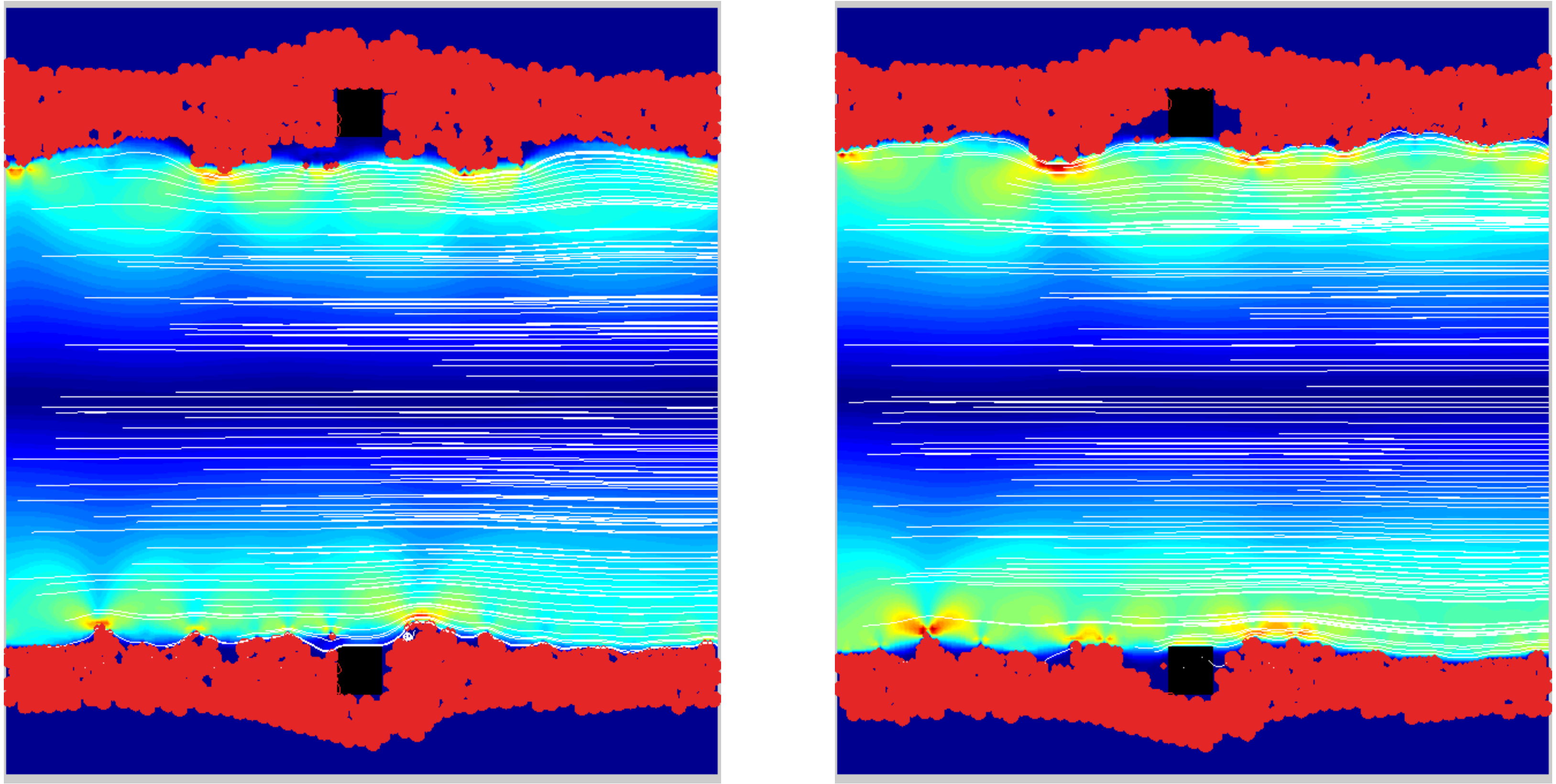


CxA for ISR: preliminary results



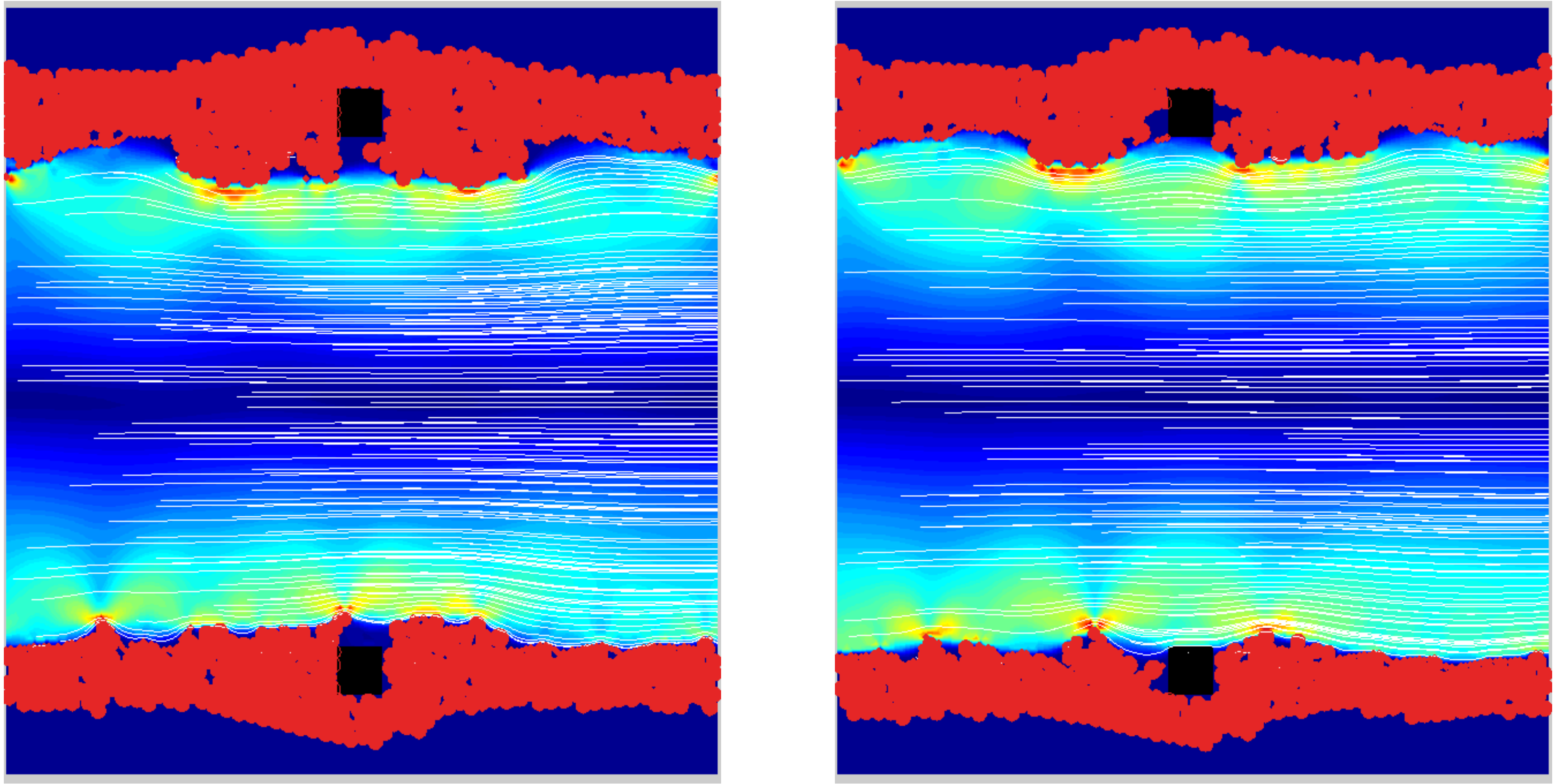
time = 2 days

CxA for ISR: preliminary results



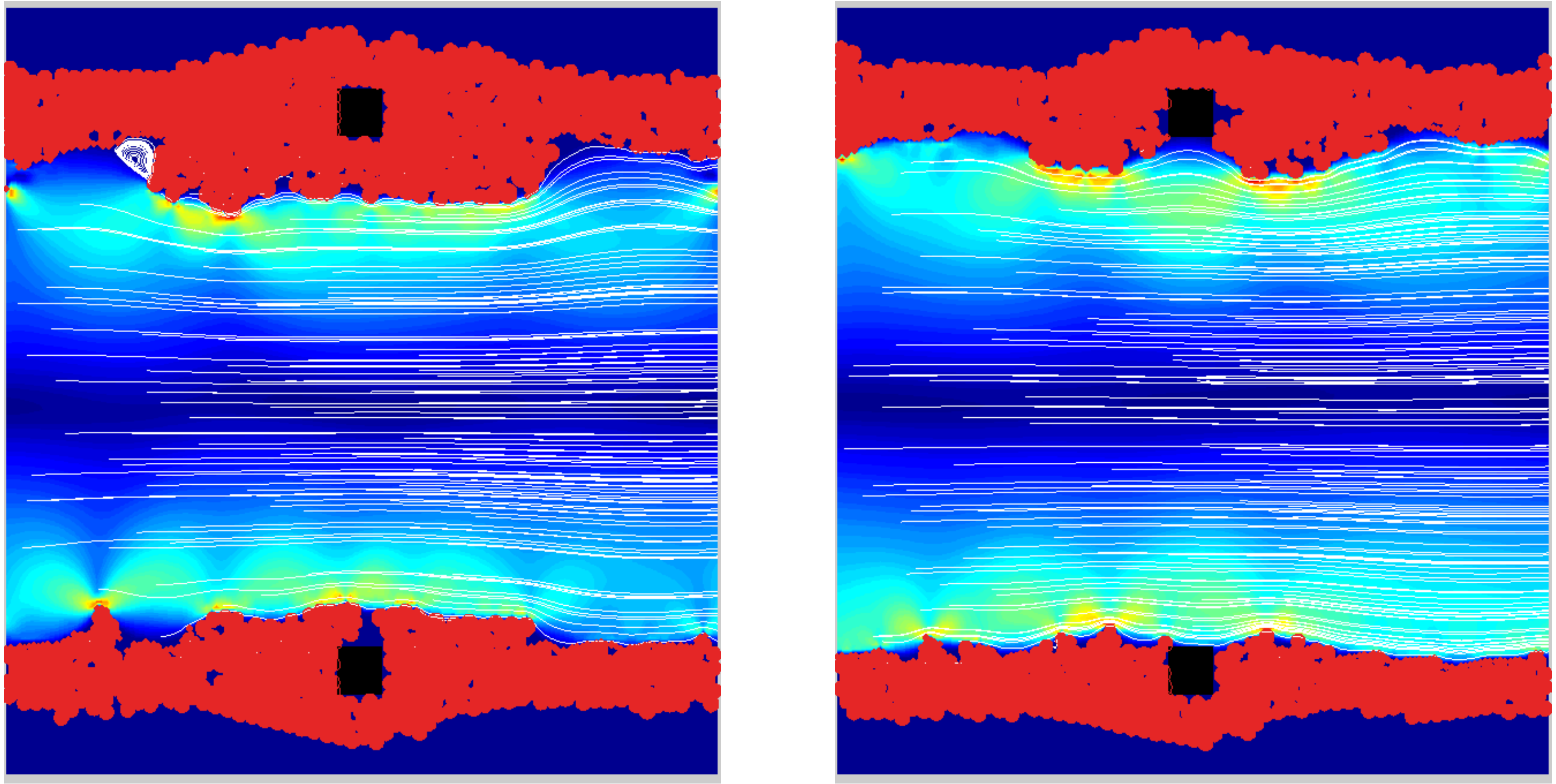
time = 4 days

CxA for ISR: preliminary results



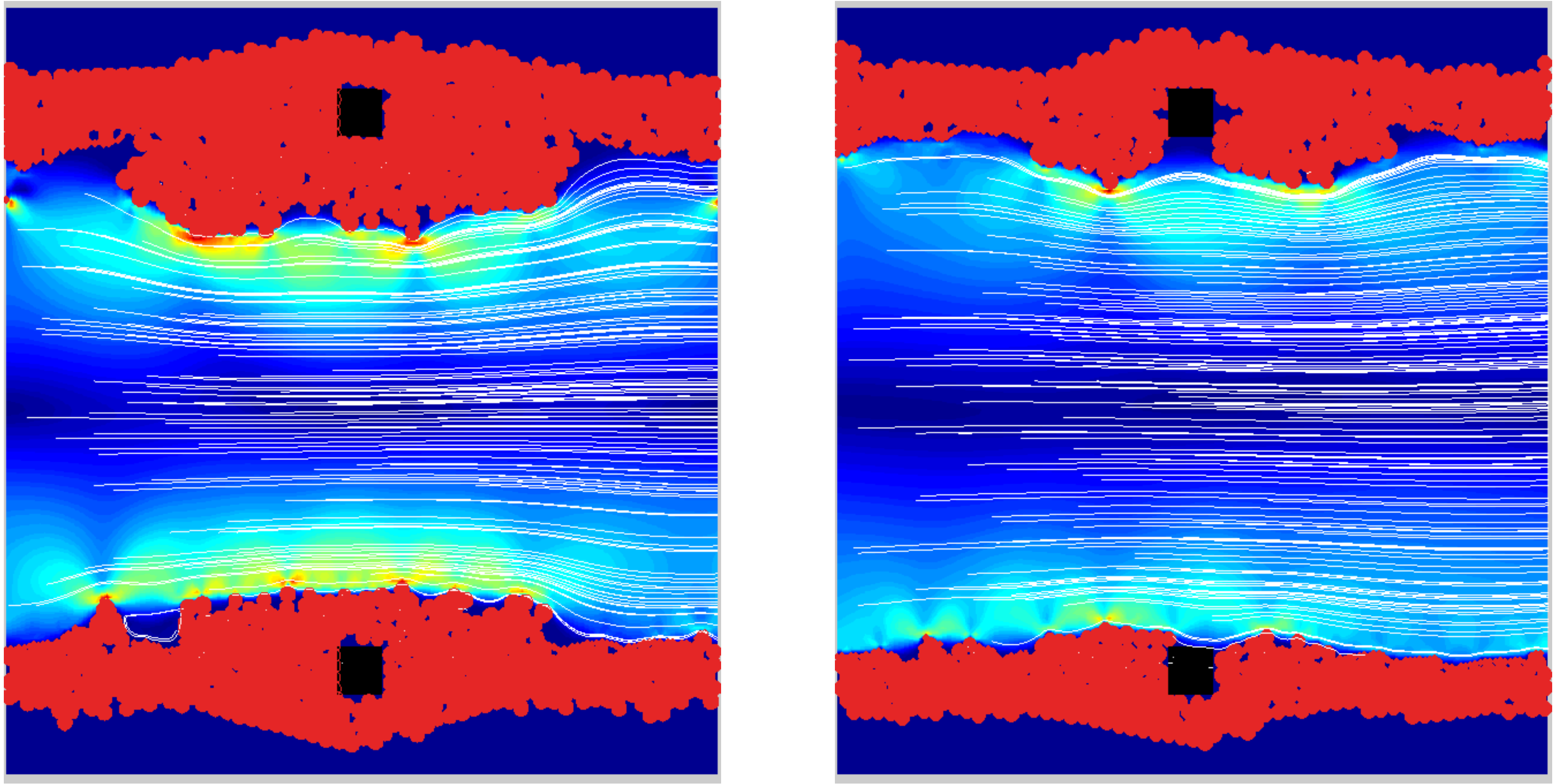
time = 6 days

CxA for ISR: preliminary results



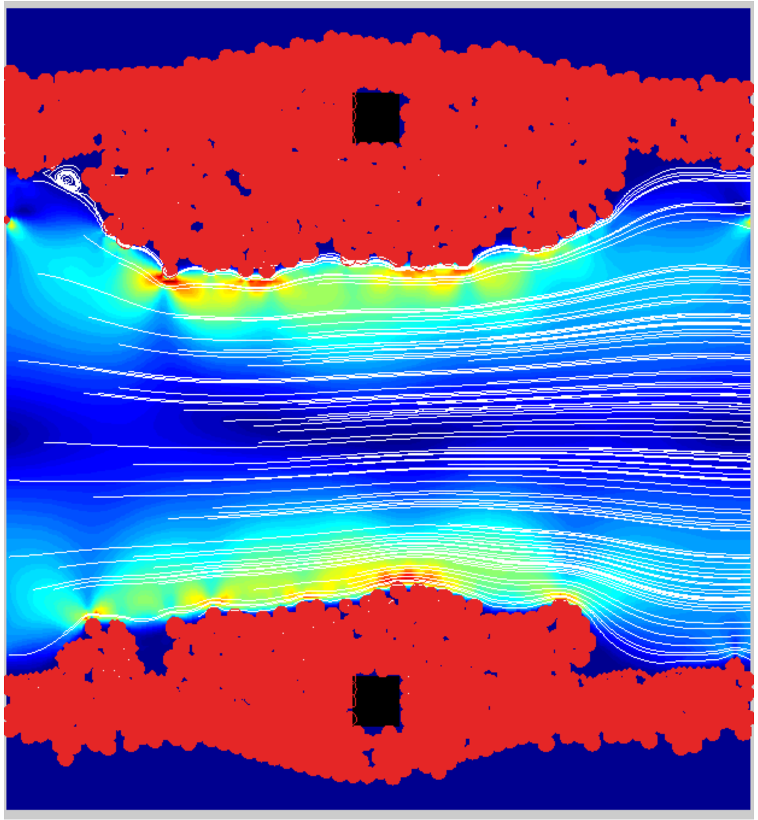
time = 8 days

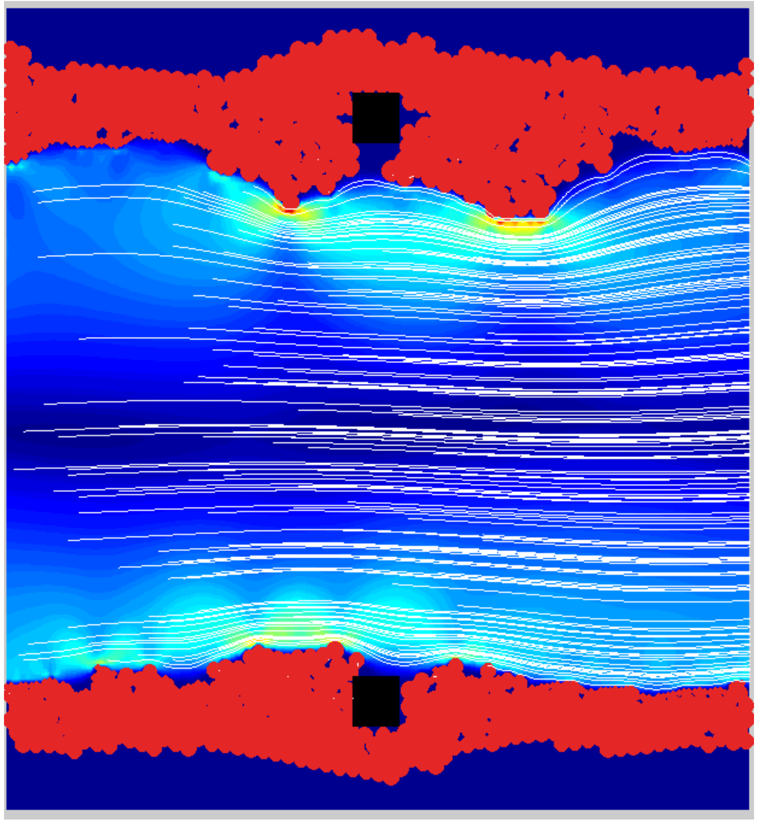
CxA for ISR: preliminary results



time = 10 days

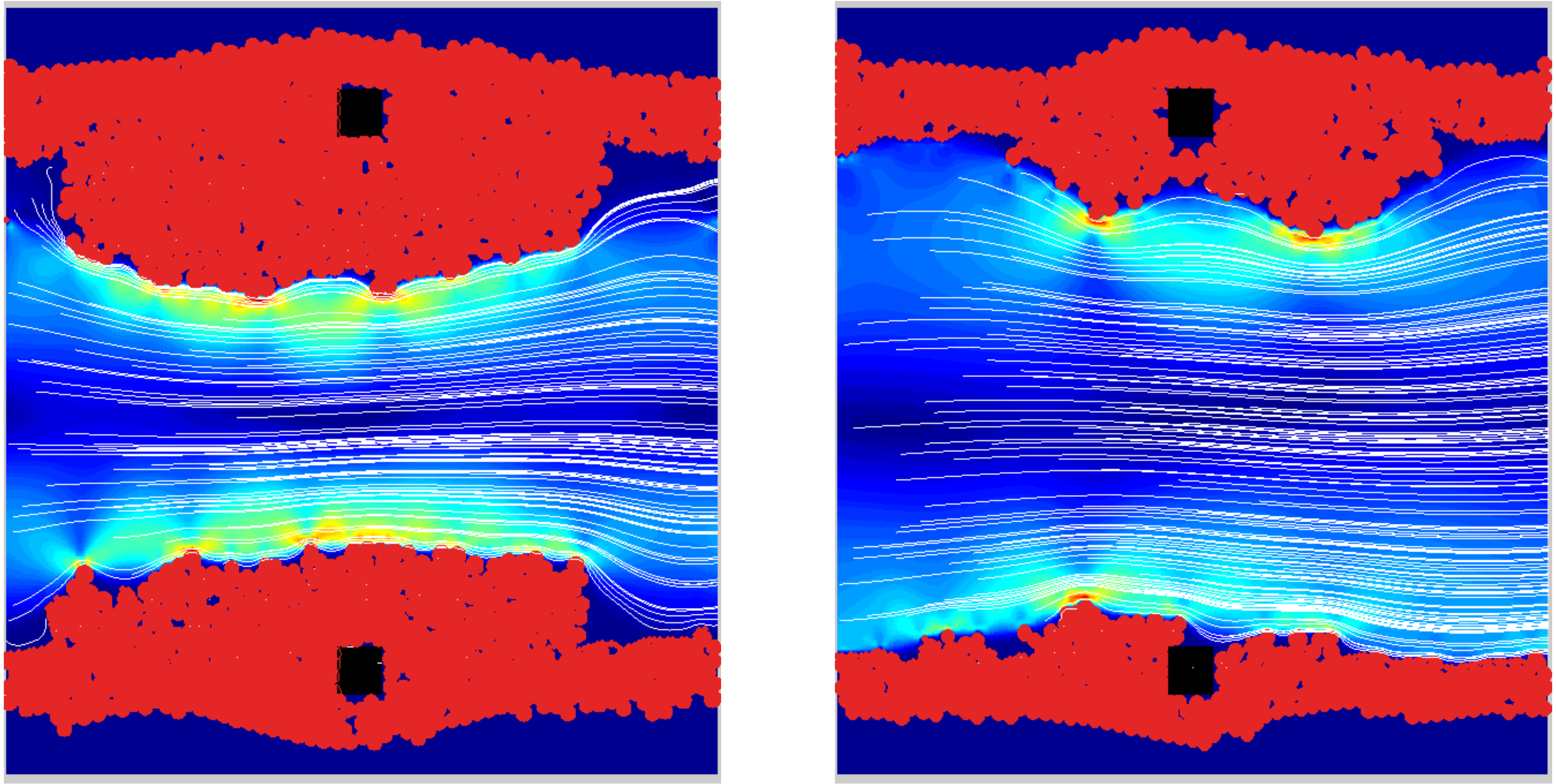
CxA for ISR: preliminary results





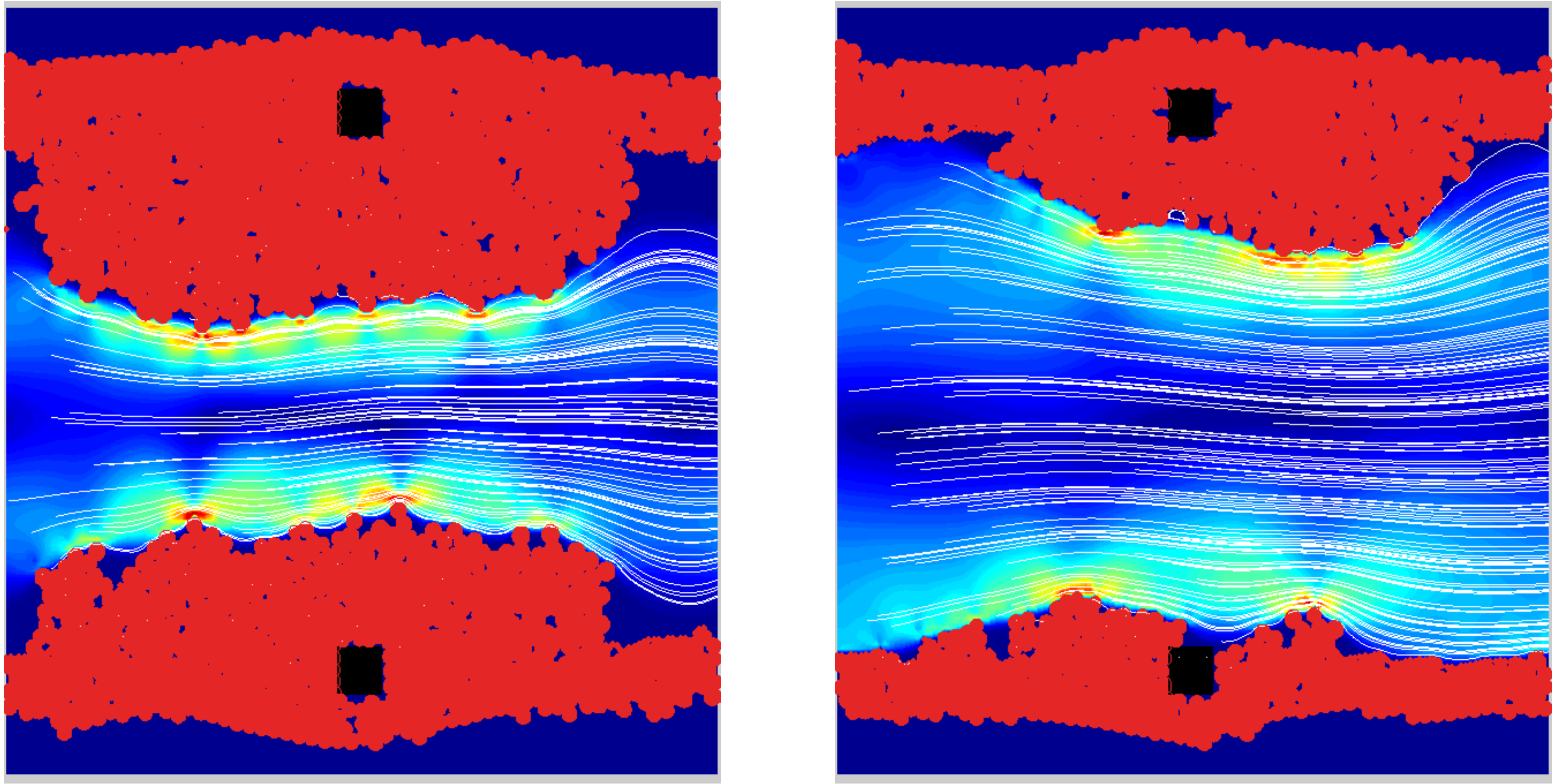
time = 12 days

CxA for ISR: preliminary results



time = 14 days

CxA for ISR: preliminary results



time = 16 days

Final Remarks

- LBM is a powerful CFD solver for incompressible flows
  - Multiphase
  - Multicomponent
  - Turbulence
- LBM can also be used to model other phenomena
  - Compressible, thermal, non-newtonian flows
  - Shallow water equations
  - Diffusion
  - Waves
- Computationally well understand
  - Serial, parallel, distributed computing
  - Also on GPU, FPGAs, Cell processer
- Active Community
  - Two dedicated annual conferences (DSFD, ICMMES)
  - Many applications in physics, chemistry, biology, biomedicine

Section Computational Science

Universiteit van Amsterdam

Acknowledgements

- Drona Kandhai
- Antti Koponen
- Abdel Monim Artoli
- Lilit Axner
- Alfons Caiazzo
- Eric Lorenz
- Joost Geerdink
- Members of the LBM development consortium

and many others