

# Webinar #10 HemeLB - Simulation of cardiovascular flow on high performance computers



9 September 2019

The webinar will start at 1pm CEST



Presenter: Dr Jon McCullough (UCL) Moderator: Ben Czaja (UvA)



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675451 The webinar series is run in collaboration with:





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## Welcomel



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#### The Challenge of Medicine



Some of them anyway:

- Human body is comprised of multiple complex sub-systems
- Various factors further individualise each body - age, gender, weight, lifestyle, genetics, ...
- Many medical treatments are invasive and require all these to be considered on a case-by-case basis

Question: How can outcomes for patients be improved?

## Patient Specific Modelling

**Answer:** Assist clinicians' ability to understand how a course of treatment will impact a given individual

How: Simulating the patient using a personalised digital replica

#### Why:

- Multiple options for treatment can be investigated and the optimal course chosen for an individual
- Clinicians can treat a patient with greater confidence
- Digital models can provide non-traditional information about the patient
- Patients can have a clearer understanding of how a treatment will impact them

#### The Virtual Human

Non-invasive scanning technology has been available since 1970s:

- Computed Tomography (CT) scan
  - Images constructed from multiple x-rays
  - Generally better for bones, tumors, chest
- Magnetic Resonance Imaging (MRI)
  - Generally better for soft tissue, esp. brain
  - Images constructed from measuring atomic magnetic interactions

Quality and cost-efficiency is constantly improving with both techniques.

#### The Virtual Human

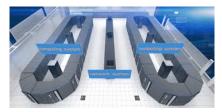


- Develop numerical models to predict behaviour of bodily components - organs, blood, nerves, ...
- Behaviour needs to be captured at multiple length scales
- Codes need to communicate at physiological interfaces
- Resolution needs to be high enough for clinical accuracy
- Ultimately, calculation time needs to be as short as possible

See CompBioMed's Virtual Humans film at https://youtu.be/1FvRSJ9W734

#### Computers - From Calculators to HPC

- Technological advancements have meant that computers have continually been getting faster<sup>1</sup>
- Largest supercomputer (Sunway TaihuLight, China) currently has over 10.5 million CPU cores
- Performance of top machines \$\mathcal{O}(10^{15} 10^{17})\$ floating point operations per second
- Exascale machines (>  $10^{18} flops$ ) anticpated in early 2020s



<sup>1</sup>Whether this continues is a whole different webinar

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#### Computers - From Calculators to HPC

- Simulations of full-humans at sufficient resolution currently demand the use of machines on this scale
- Developing codes that perform efficiently on machines of this size is challenging. Concerns include:
  - Communication between cores
  - Load balancing
  - Data visualisation
- Studying models of appreciable size becoming possible on desktop based machines - especially with GPU acceleration (another code issue).

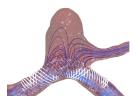
Example Simulation

Summary 000000

#### HemeLB - Purpose and Direction

HemeLB is a code developed with the vision of modelling a wide variety of vascular and blood flow problems

Within a virtual (and physical) human, blood flow around the networks of arteries and veins is vital for the communication of information (e.g. oxygen) around the body.



In a virtual human simulation, HemeLB will provide an interconnect between models for other organs - heart, brain, lungs, liver, ...

## HemeLB - History

The initial version of HemeLB was published in 2008, developed within CCS at UCL

Current support for HemeLB is, in particular, provided through -UKCOMES, CompBioMed CoE, QNRF and compute time used on ARCHER (UK), SuperMUC-NG (LRZ, GER), BlueWaters (NCSA, USA), ....



#### HemeLB - Capabilities and Case Studies

#### Features of HemeLB:

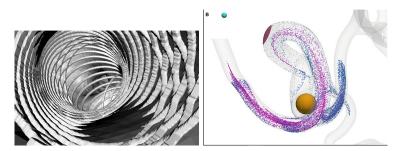
- C++ code parallelized using standard MPI communications
- CPU code (currently)
- Fluid flow solved using lattice Boltzmann method
- Multiple boundary condition options available
- Optimized for sparse geometries characteristic of vascular geometries
- Code execution designed to scale well on up to hundreds of thousands of cores

#### HemeLB - Capabilities and Case Studies

Applications of HemeLB:

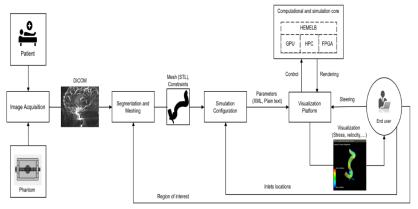
- Stent design
- Retinal vascular flow

- Cerebral blood flow
- Magnetic drug targetting



#### HemeLB - Capabilities and Case Studies

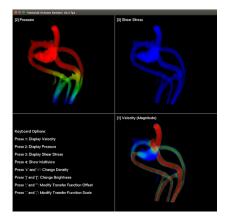
Applications of HemeLB: Aneurysm Pipeline



Example Simulation

#### HemeLB - Capabilities and Case Studies

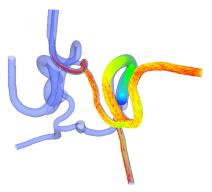
- Real time visualisation, using CUDA
- Current version displays pressure, shear stress and local velocity magnitude
- Frequent discussions with clinicians to see what visualisations make most sense to them



Example Simulatio

#### HemeLB - Capabilities and Case Studies

#### Play video - HemeLB flow in Circle of Willis



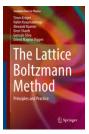
Example Simulation

#### HemeLB - Lattice Boltzmann Method

For further information on Lattice Boltzmann Method see CompBioMed Webinar #3 - Lattice Boltzmann method for CompBioMed (incl. Palabos) (Dr Jonas Latt, University of Geneva)

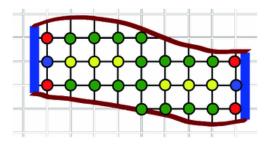
Many textbooks are also available e.g. The Lattice Boltzmann Method: Principles and Practice - Krüger *et al.* 





- Numerical method for solving Boltzmann equation
- Under certain conditions solves Navier-Stokes equations for fluid flow
- Localised algorithm has multiple advantages:
  - Easy to parallelise
  - Straightforward to use on complex boundary shapes
  - Adaptable for advanced flow physics multiphase, multi-component, non-Newtonian, thermal

- Determine lattice structure to use DnQm
  - n = dimensions
  - m = velocity directions
- Discretise domain into nodal locations using a regular cartesian grid
- Identify fluid sites and wall sites



At each site - assign distributions,  $f_i(\mathbf{x}, t)$ , in velocity direction i

- Represents the probability of fluid at site x moving in the i direction at a given point in time (t).
- Often simplified to f<sub>i</sub> for clarity
- At equilibrium, these are often determined through an approximation to the Maxwell-Boltzmann distribution

$$f(v) = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2kT}}$$

Evolution of flow computed by streaming and collision of distributions

1. Collision - HemeLB typically uses the BGK collision function

$$f_i^*(\mathbf{x},t) = f_i(\mathbf{x},t) - \frac{\Delta t}{\tau} (f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t))$$

- $f_i(\mathbf{x}, t)$  pre-collision distribution function
- $f_i^*(\mathbf{x}, t)$  post-collision distribution function
- au BGK relaxation time
- $f_i^{eq}(\mathbf{x}, t)$  equilibrium distribution function

Evolution of flow computed by streaming and collision of distributions

2. Streaming

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}, t)$$

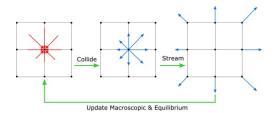


Image: A.R.G Harwood and A.J. Revell, Advances in Engineering Software (2017), Vol. 104, pp. 38-50.

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Local macroscopic properties determined by moments (sum of distributions weighted by velocity direction).

For hydrodynamics: Zeroth moment: Density  $\Rightarrow \rho = \sum_{i} f_{i}$ First moment: Momentum  $\Rightarrow \rho \mathbf{u} = \sum_{i} f_{i} \mathbf{c}_{i}$ Second moment: Stress tensor  $\Rightarrow$ 

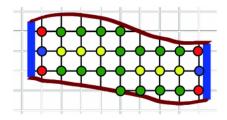
$$\mathcal{S}_{lphaeta} = -\left(1 - 1/(2 au)
ight)\sum_{i}\mathbf{c}_{ilpha}\mathbf{c}_{ieta}(f_{i} - f_{i}^{eq})$$

LBM hydrodynamics is only valid in low *Ma* limit, a result of this is:

Viscosity 
$$\Rightarrow \nu = \frac{1}{3} \left( \tau - \frac{1}{2} \right) \frac{(\Delta x)^2}{\Delta t}$$

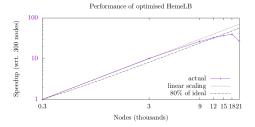
Boundary Conditions:

- Population values streaming in from outside the domain are unknown
- Construct unknown values based on desired boundary behaviour
- HemeLB allows for multiple options including solid walls and velocity or pressure based in/outlets



Example Simulation

#### HemeLB - Scaling Performance on HPC



Non-ideal performance seen due to:

- Load distribution between processors
- Reliability/performance of processors

- Frequency of I/O operations
- Communication between groups of nodes
- Architecture of HPC facility

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## HemeLB - Running a Simulation

HemeLB is designed to operate on large-scale high performance computers - university/regional/national clusters

Still able to be run on laptops with any unix-based environment

- Linux/Mac native
- Windows 10 WSL (Windows Subsystem for Linux)
- Windows 7 Sorry!

Does require familiarity of command line interface

#### HemeLB - Running a Simulation

Installation and compilation:

- Tools needed for compilation: CMake, MPI (e.g. OpenMPI), GCC
- Other dependencies installed as part of initial compilation process - see online/README instructions
- LBM parameters configured into compilation flags lattice choice, collision kernel, wall and in/outlet boundary conditions
- Download HemeLB source code from www.hemelb.org
- Install and compile code as per instructions
- Test case in examples see website tutorials

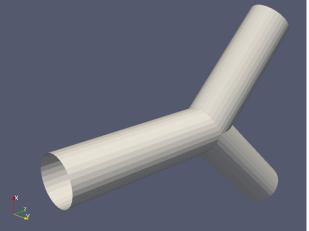
HemeLB

Example Simulation

Summary 000000

#### HemeLB - Running a Simulation

Flow due to a pressure gradient through a bifurcation



#### HemeLB - Running a Simulation

```
<2xml version="1 0"?>
<hemelbsettings version="3">
  <simulation>
    <step length units="s" value="1e-5"/>
    <steps units="lattice" value="5000"/>
    <stresstype value="1"/>
    <voxel size units="m" value="5e-5"/>
    <origin units="m" value="(0.0,0.0,0.0)"/>
  </simulation>
  <geometry>
    <datafile path="bifurcation.gmy"/>
  </geometry>
  <initialconditions>
    <pressure>
      <uniform units="mmHg" value="0.001"/>
    </pressure>
  </initialconditions>
  <monitoring>
    <incompressibility/>
  </monitorina>
```

Lattice Boltzmann parameters

Geometry file

Initial conditions

Example Simulation

#### HemeLB - Running a Simulation

```
<inlet>
    <condition subtype="cosine" type="pressure">
      <amplitude units="mmHg" value="0.0"/>
      <mean units="mmHg" value="0.001"/>
      cohase units="rad" value="0.0"/>
      coeriod units="s" value="1"/>
    </condition>
    <normal units="dimensionless" value="(4.15565e-13,1.44689e-12,1)"/>
    <position units="lattice" value="(165.499,35.8291,3)"/>
</inlets>
<outlets>
    <condition subtype="cosine" type="pressure">
      <amplitude units="mmHq" value="0.0"/>
      <mean units="mmHq" value="0.0"/>
      <phase units="rad" value="0.0"/>
      <period units="s" value="1"/>
    <normal units="dimensionless" value="(0.707107,-2.4708e-12,-0.707107)"/>
    <position units="lattice" value="(26.2137.35.8291.372.094)"/>
  </outlet>
    <condition subtype="cosine" type="pressure">
      <amplitude units="mmHq" value="0.0"/>
      <mean units="mmHg" value="0.0"/>
      <phase units="rad" value="0.0"/>
      <period units="s" value="1"/>
    </condition>
    <normal units="dimensionless" value="(-0.707107.-4.27332e-12.-0.707107)"/>
    sition units="lattice" value="(304,784,35,8291,372,094)"/>
</outlets>
```

Inlet boundary conditions

Outlet boundary conditions

#### HemeLB - Running a Simulation

```
<properties>
<propertyoutput file="whole.dat" period="100">
<propertyoutput file="whole" />
<field type="whole" />
<field type="pressure" />
</propertyoutput>
<propertyoutput file="inlet.dat" period="100">
<propertyoutput file="inlet.dat" period="100">
<propertyoutput file="inlet.dat" period="100">
<propertyoutput</pre>
</propertyoutput>
</propertyoutput>
</properties>
</hemelbsettings>
```

Data output information

#### HemeLB - Running a Simulation

Execute with: mpirun -n N <hemelb executable address> -in <input file \*.xml address> -out <output directory address>

TRank 0000000 6.799901e-01 5. 0000000055328 kB1 :: INITIALISE
[Mark 0000000 6./999014:01 5, 00000000053528 KB] :: INIINLISE
[Rank Dobbion, 0.501200701.3, D0000000055328 kB] ::> loading input and decomposing geometry
Rank 0000000, 0.002000000, s. 00000000000000000000000000000
Rank dobdodo, 7.01582e-01 z, opdobdodos94 kaj ::> reading premble
Rank dobbodd, 7.017149-01 S. 000000000099+ kB ::> reading beader (start)
Rank 0000000, 7.042514-01 a, 0000000006664 kg 1: reading header (and)
Rank 0000000, 7.04214 - 01, 0000000006616 kB ::> non-enty blocks: 5330
Rank dobbodd, 7.840304-01 s, 000000000655 kb] : total blocks: 18450
TRank 0000000, 7,050843e-01 5, 00000000066636 kB1 :: ratto: 0,288889
[Rank 0000000, 7.051701e-01 s, 000000000066636 kB] :: sites: 2010048
[Rank 0000000, 7.052528e-01 s. 0000000000000 kB] ::> blockInformation.slze(): 5330
(Rank 0000000, 7.053350e-01 s, 00000000066636 kB] :: flutdSttesOnEachBlock.stze(): 0
[Rank 0000000, 7.054173e-01 s, 0000000000006 kB] :: blockWeights.size(): 0
(Rank 0000000, 7.054991e-01 s. 000000000066536 kB] ::
Rank 0000000, 7.081596e-01 s, 00000000066636 kB] ::> not optinising decomposition
[Rank 0000001, 7.0900900-01 s, 00000000017200 kB] ::> load distribution: 0.000281
[Rank 0000000, 7.082588e-01 s, 00000000066666 kB] ::> basic decomposition (start)
[Rank 0000000, 7.095788e-01 s, 00000000007592 kB] ::> basic decomposition (end)
[Rank 0000000, 7.090923e-01 s, 00000000007592 kB] ::> read blocks (start)
[Rank 0000001, 7.282304e-01 s, 0000000017784 kB] ::> blockInformation.size(): 5330
[Rank 0000002, 7.281983e-01 s, 00000000017412 kB] ::> blockInformation.size(): 5330
[Rank 0000003, 7.222003e-01 s, 00000000016404 kB] ::> blockInformation.size(): 1931
[Rank 0000000, 2.023984e+00 s, 00000000694832 kB] :: ···-> read blocks (end)
[Rank 0000000, 2.1215500+00 s, 00000000095148 kB] ::> lattice data
[Rank 0000000, 3.151832e+00 s, 00000002014288 kB] ::
[Rank 0000000, 3.151998e+00 s, 00000002014288 kB] ::> gathering lattice information (end)
[Rank 0000000, 4.372778e+00 s, 00000002312332 kb] ::> neighbouring data wanager
[Rank 0000000, 4.373169e+00 s, 00000002312332 kB] ::> lattice-Boltzmann model
Rank 0000000, 4.620966e+00 s, 00000002672220 kB] ::
[Rank 0000000, 4.621000e+00 s, 0000002672220 kB] :: INITIALISE FINISHED
[Rank 0000000, 4.663895e+00 s, 00000002672220 kB] :: SIMULATION STARTING
[Rank 0000000, 4.663959e+00 s, 0000000272220 kB] ::
[kank obdobdo, 2.2009436491 %, dobdobc.22000 kb] :: time %tep obd0220 :: write_inage_t0_ctk o [Rank 0000000, 2.20094364e01 %, d00000270260 kb] :: time %tep 0000200 :: write_inage_t0_ctk o
[Rank 0000000, 2.2009010701 3, 0000002072000 KB] II the step 000000 II GUI 9.50000, natretative_press_otil 0.000, Natretative_pres
[Rank 0000000, 4.0/10/10/10/10, 0000000/272666 KB :: the step 000040 Mite_imgg_[0_01ks relative press diff: 0.000. Na: 0.000. max vel phys: 7.528757e-05
Rank 0000000, 5.772616+01 , 00000002672660 kB :: the step 000000 :: wite inset to state of the other and the other
Rank dobbodd, 5.772624+01 5, 0000002072000 kB] :: the step 0000000 :: tau: 0.54000 nax relative press diff: 0.000. Na: 0.000, nax vel phys: 0.581018+05
[Rank 0000000, 7.520723e+01 s, 00000002672660 kB] :: time step 0000000 :: write image to disk 0
Rank 0000000, 7.520713e-01 , 0000000272600 KB :: time step 000000 :: tau: 0.54000, max relative press diff: 0.000, Na: 0.000, max vel phys: 1.292713e-04
[Rank 6000000, 9.2004690+01 S, 0000002072000 kb] :: time step 0001000 :: write inage to disk 1
Rank 0000000, 9,288484e+01 5, 00000002672660 kB] :: time step 0001000 :: tau: 0.565000. max relative press diff: 0.000. Na: 0.000. max vel phys: 1.336011e-04
[Rank 0000000, ].104421e+02 s, 00000002672936 kB] :: time step 0001200 :: write image to disk 0
Rank 0000000 1,1044224-02 5, 00000002/2225 kB :: time step 0001200 :: tau: 0.540000 max relative press diff: 0.000. Na: 0.000, max vel phys: 1.3300114-04
Rank 0000000, 1,283911e+02 s, 00000002673572 kB] :: time step 0001400 :: write inage to disk 0
[Rank 0000000 1 2010110+02 x 00000002033572 kt] ·· time step 0001400 ·· tau: 0 560000 pay celative press diff: 0 000 Na: 0 000 may yel phys: 1 3300110-04

#### Took approx. 8min on N=4

J. McCullough (UCL-CCS)

The hemeXtract tool converts the output.dat file to human-readable format (1). (2) splits this into stepwise files for visualisation in paraview

(1) hemeXtract -X output.dat > readable-output.txt

(2) bash paraviewProcessing.sh readable-output.txt
paraview-file-name

Paraview is a widely-used visualisation package www.paraview.org/

- 1. Import paraview-file-nameXX.txt files: File  $\rightarrow$  Open  $\rightarrow$  Navigate
- to folder  $\rightarrow$  double-click on paraview-file-name..txt (type GROUP)
- 2. Click green apply button on LHS

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	2 2 180.000000 0.006730 E.001330 E.001330 E.001330 0.00000e+80 0.000000e+80 0.00000e+80 0
	3 3 1 100.000000 0.008/300 8.002/300 0.000000+00 0.000000+00 0.000000+00 0.000000+00 1.000000
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3. Change default comma (,) in Field Delimeter Characters to a space ( )

4. Click green apply button on LHS (this is a recurring theme in Paraview)

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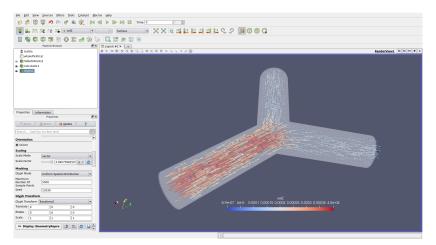
- 5. Filters  $\rightarrow$  Alphabetical  $\rightarrow$  Table To Points
- 6. Change Y Columns to 'gridY' and Z columns to 'gridZ'
- 7. Click green apply button on LHS

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- 8. Ensure RenderView panel is active and click on eye next to TableToPoints1 in Pipeline
- 9. Change rendering option from 'Solid Colour' to 'velZ'
- 10. Use Play and rescale options to watch time evolution

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Can do plenty more with Paraview - glyph and streamline examples



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#### HemeLB - Future Developments

HemeLB is constantly developing - accuracy and scalability always of concern.

- Coupling to itself and other physiological codes
- Elastic walls capture the variable shape of vessels
- GPU implementation enable HemeLB to take advantage of performance advantages of GPU architecture

### Summary

HemeLB is numerical code designed for solving blood flows within human-scale vasculatures.

- Optimised for the sparse geometries
- Highly scalable performance on over 300,000 cores
- Demonstrated capability for simulating highly complicated vasculatures
- Will communicate between multiple codes for simulation of a full virtual human
- Get more information from the HemeLB website www.hemelb.org

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  - CompBioMed CoE (EU Horizon 2020 (Grant Nos. 675451 and 823712))

Developers of HemeLB in P.V. Coveney's CCS group at UCL include: M.D. Mazzeo, S. Manos, G.M. Doctors, M.O. Bernabeu, R.W. Nash, D. Groen, H.B. Carver, J. Hetherington, T. Krüger, U.D. Schiller, S. Schmieschek, A. Patronis, R.A. Richardson, J.W.S McCullough

#### Selected Publications

- M. D. Mazzeo and P. V. Coveney, "HemeLB: A high performance parallel lattice-Boltzmann code for large scale fluid flow in complex geometries", Computer Physics Communications, 178, (12), 894-914, (2008).
- D. Groen, J. Hetherington, H. B. Carver, R. W. Nash, M. O. Bernabeu, P. V. Coveney, "Analyzing and Modeling the Performance of the HemeLB Lattice-Boltzmann Simulation Environment", Journal of Computational Science, (2013), 4 (5), 412–422.
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#### Image References

- Slide 3 http://www.sciencekids.co.nz/pictures/humanbody/humanorgans.html
- Slide 5 https://stanfordhealthcare.org/medical-tests/p/pet-mri-scan.html
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#### To pose a question, you can write your question in the "Questions" tab



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