UKCOMES/HEMELB MEETING

DATE: 29TH– 30TH MAY 2019

LOCATION: *ENGINEERING FRONT BUILDING, EXECUTIVE SUITE 103*

Day 1 – Wednesday 29th May 2019 Engineering Front Building, Executive Suite 103, UCL, London		
10:30	Peter V Coveney, UCL	**Welcome and introduction**
Software development, curation and future-proofing for exascale		
10:45	Robin Richardson, UCL	Development of HemeLB and adaptation to the clinic
11:15	Jianping Meng, STFC	Progress in developing high-level mesoscopic modelling system
11:45	**Remote**: Miguel Barnebeu, University of Edinburgh	Blood flow mesoscale simulations reveal an association between erythrocyte dynamics and vascular patterning in developmental vascular networks
12:15	General Discussion	
12:45	*Lunch*	
Parallel performance and scalability of the code; GPU implementations		
14:00	Alex Patronis, UCL	Preparing Initialisation for Extreme-scale Simulation.
14:30	Ulf Schiller, Clemson	Using HemeLB (on GPUs) to Simulate Cerebral Angioplasty and Drug Delivery
15:00	Ryan Marshall, University of Tennessee	TBA
15:30	Rupert Nash, University of Edinburgh	HemeLB's no hassle with the Hoff
16:00	*Break/Tea and Coffee – Further Discussions*	
Visualisation and Steering		
16:30	**Remote:** Sahar Soheillan, Qatar University	Interactive blood flow simulation and visualization pipeline for cerebral aneurysms
17:00	General Discussion	
19:00	*Dinner (costs not included)*	

Day 2 – Thursday 30th May 2019 Engineering Front Building, Executive Suite 103, UCL, London		
Implementation of features — colloidal particles, red blood cells		
09:00	Jon McCullough, UCL	Self-coupling of HemeLB: Recent developments towards simultaneous arterial-venous modelling
09:30	Timm Krüger, University of Edinburgh	HemeLB for red blood cells dynamics in complex geometries and inertial microfluidics
10:00	Yann Thorimbert, University of Geneva	Direct simulation of highly concentrated rigid spherical suspensions
10:30	*Break/ Tea and Coffee with further discussions*	
Implementation of features – LB flow simulations		
11:00	Ulf Schiller, Clemson	Coupling Brownian Particles and Polymer Chains to Lattice Boltzmann Fluids
12:00	Ioannis Zacharoudiou, Imperial College London	The impact of drainage displacement patterns and Haines jumps on CO2 storage efficiency
12:30	Edo Boek, Queen Mary University, London	Chemical mechanisms of dissolution of calcite by HCl and CO2 in porous media: Simulations and experiment
13:00	*Lunch*	
Extending our user base		
Round Table Discussion		
15:00	*Break/Tea and Coffee*	
Meeting Ends		

Abstracts:

Robin Richardson:

We give an overview of the state of HemeLB's development at CCS, and the future directions this could take, in particular with regards to merging development efforts that have somewhat diverged. On-going work towards bringing HemeLB into use in the clinic, particularly during surgical interventions, is presented. The challenges of validating the simulations against in-vitro and in-vivo measurements are discussed, as well as the problem of finding compact computational resources acceptable to hospitals.

Jianping Meng:

In this talk, we will discuss our progress in developing high-level mesoscopic modelling system (i.e., a domain specific language, DSL), where the project is split into two phases. In the first phase, we have been developing the function sequence that enables the user to combine the provided lattice Boltzmann models (e.g., various equilibrium functions and forces terms) to simulate a scientific problem. The second phase will provide the functionality for the researchers to use the DSL to define their own equilibrium functions and force term. A few examples will be utilised to demonstrate the usage of functionalities provided by the first phase.

Miguel Bernabeu

Alex Patronis:

In this talk I will discuss developments that allow HemeLB to operate on tens of billions of lattice sites distributed over hundreds of thousands of cores. Many changes have been made to the initialisation phase over the past couple of years: 1) move to associative containers from sequence containers (i.e. std::vector to std::map), 2) support for remote memory access offered by MPI 3.0, 3) support for reading of large data sets that exceed 32-bit MPI count, 4) move to other load-decomposition schemes; these enhancements will be described here. They allow for efficient initialisation and a drastically reduced memory footprint -- with falling memory per core on the latest generation of high-performance computing platforms, this represents important progress.

Ulf Schiller:

Vascular anomalies are often associated with changes in blood flow conditions which can be both cause or consequence of malformations. For example, vascular aneurysms are the result of vessel degradation associated with abnormal wall-shear stress conditions. The geometric distortion perturbs the blood flow through the parent vessel which can lead to rupture of the aneurysm. A possible treatment of aneurysms is the implantation of flow-diverting stents to stabilize the affected vessel and restore the original blood circulation. Aside from the immediate risks associated with angioplastic surgery, stenting procedures can lead to adverse effects such as restenosis and thrombosis. The latter can be mitigated by drug-eluting stents that prevent restenosis by local delivery of antiproliferative drugs, e.g., Paclitaxel or Sirolimus. Knowledge of the spatio-temporal drug distribution in the blood vessel is an important factor for assessing and improving the efficacy of different stent designs and drug coatings.

HemeLB has been successfully applied to simulate blood flow in patient-specific models of brain arteries that are reconstructed from three-dimensional angiography images. In this talk, I will describe our progress in extending the capabilities of HemeLB to virtually deploy vascular implants and study their effect on the blood flow. Moreover, to simulate drug delivery, we have implemented a lattice Boltzmann solver for the advection-diffusion equation that is coupled to the original solver for the flow field. I will present results on the drug distribution for different aneurysms and various commercial stent geometries and will discuss how the data can be used to optimize drug-eluting stents.

I will also briefly outline our efforts to use HemeLB on high-performance clusters with GPU acceleration. To this end, we have implemented a CUDA-kernel that supports the LBGK collision operator on several lattice types (D3Q15, D3Q19, D3Q27), and boundary conditions for walls and inlets/outlets. The GPU implementation integrates seamlessly with the existing HemeLB infrastructure for domain decomposition and parallelization via MPI. We are thus able to use a variable number of GPU accelerators per MPI rank. We have investigated how to maximize the performance of multi-GPU HemeLB through GPU over-subscription and block size. While we achieve a a single-GPU speedup of 18x (P100) and 67x (V100) for a large cerebral aneurysm geometry, the scalability of the multi-GPU implementation needs improvement which is an ongoing effort.

Ryan Marshall:

Rupert Nash:

HemeLB is now being used by biologists who have have experience with neither computational science nor high performance computing. Work by Bernabeu et al has led to the creation of PolNet, a containerised workflow for analysing cell-level biological activity during angiogenesis by correlating it with predictions from computational fluid dynamics. This tool has led to several publications, but use has been limited by running the HemeLB simulations on the client machine (typically a laptop or standard desktop).

We have designed a REST API for offloading the HPC part of the PolNet workflow to existing HPC systems (such as Cirrus at EPCC and Lisa at SURFsara) called the Hoff. This abstracts actions such as authentication, staging input and output files and starting simulations from pre-configured templates. The API is implemented by the hoff-server, a Python Flask application running on a secure VM, and the hoff-client, a small Python package which can easily be integrated into existing code.

We will present and overview of the architecture, implementation, and early results. We will outline how we plan to extend this to use IaaS cloud platforms as an alternative backend.

Sahar Soheillan

Intracranial or cerebral aneurysm is a malformation in a brain artery caused by a weakness in the inner muscular layer of blood vessel wall. It is one of the prevalent cerebrovascular disorders in adults worldwide. The most impressive treatment for brain aneurysms is interventional radiology treatments. These approaches are extremely dependent to the radiologist skill in recognizing the vascular geometry and estimating blood flow related information from the 2D and/or 3D medical images. Hence, accurate aneurysm detection and effective therapy planning are still remained as important clinical challenging interventions.

Providing clinicians with vascular geometries and fluid flow mechanical parameters such as velocity and pressure retrieved from the blood flow simulation, can help them to have the best prognosis and treatment for the patients. In fact, a reliable modeling and visualizing environment for measuring and displaying blood flow patterns in vivo can provide insight into the hemodynamic characteristics of cerebral aneurysms. In this work, we have developed a pipeline for cerebral blood flow simulation and real-time visualization incorporating all aspects, from medical image acquisition to real-time visualization and steering. The pipeline uses an improved HemeLB as its main computational core which is optimised for visualisation on GPU. It includes a real-time GPU based rendering engine capable of speeding up HemeLB for deployment in hospitals and clinical investigations. In addition, a visualization platform intended to ease access to the simulation environment is also designed. This platform allows clinicians to control the simulation operations and monitor the visualized results by providing access to different pipeline components.

Jon McCullough:

This talk will discuss recent developments within HemeLB as part of progress towards modelling interacting arterial and venous trees. This is proposed to occur through the coupling of multiple HemeLB simulations. Firstly, the physical and computational considerations and implementations for coupling HemeLB to itself will be articulated. The performance of this strategy is then demonstrated using a number of test cases of increasing complexity. Areas for further improvement of the process will also be outlined. Additionally, the incorporation of colloids within the HemeLB code for the study of magnetic drug targeting (MDT) will be briefly discussed.

Timm Krüger:

In blood flow in small vessels (<100 μm diameter) and microfluidic systems, red blood cells and other particles cannot be considered small compared to the vessel/channel dimensions and need to be taken into account explicitly. This generates massive challenges for any numerical modelling where the spatial resolution is determined by the particles and the overall simulation domain by the channel size, therefore leading to numerically expensive simulations. The ultimate aim is to find reliable constitutive models for particle behaviour in complex geometries so that particles need not be modelled explicitly. HemeLB, being a massively parallelised sparse-geometry lattice-Boltzmann tool, is able to simulate blood flow in complex geometries and microfluidic devices. I will talk about recent progress (e.g. blood flow in the retina) and provide an outlook for the next 5 years and beyond.

Yann Thorimbert:

The immersed boundary method (IBM) become popular among the lattice Boltzmann method (LBM) community, thanks to its formulation that does not require any adaptation of the fluid mesh, and is therefore particularly efficient in many cases.

Whereas GPU implementations of LBM are quite common, it is difficult to exploit GPUs architecture for IBM. Indeed, IBM requires a complex memory access pattern, which conflicts with the data broadcasting strategy of GPUs.

We propose new methods for the GPU implementation of a direct-forcing flavour of LBM-IBM (as proposed by [1]) in the CUDA language, enabling efficient simulations of large immersed surfaces. A performance comparison between our implementation and a CPU parallel implementation in Palabos is proposed, using a propeller geometry for test purposes.

References

[1] O. Keigo, K. Suzuki and T. Inamuro, Lift generation by a two-dimensional symmetric flapping wing: immersed boundary-lattice Boltzmann simulations, Fluid Dynamics Research 44, 045504, 2012.

Ulf Schiller:

Many soft matter systems are complex fluids that can be characterized as suspensions of micro- to nano-size objects in a solvent. The presence of the solute particles introduces a mesoscale structure that leads to interesting and sometimes unexpected dynamical behavior in these systems. A better understanding of the properties of complex fluids is not only interesting from a physics perspective, but it is also relevant for applications in materials science, chemical engineering, molecular biology, etc. In computer simulations, the solvent has to be explicitly taken into account in order to reproduce the hydrodynamic interactions between the solute objects, while at the same time the internal dynamics of the objects, e.g., polymers or cells, have to be resolved. This calls for a multiscale approach that combines mesoscopic methods for hydrodynamics with molecular dynamics techniques for particle based systems.

In this talk, I will review approaches for coupling particle-based molecular dynamics (MD) to the kinetics-based lattice Boltzmann method (LBM) that are capable of reproducing hydrodynamic interactions in soft matter. I will discuss how the LBM can be augmented with thermal fluctuations, an essential requirement for thermodynamic consistency in statistical equilibrium. I will then present a mesoscopic hybrid model for a polymer chain in solution, where the polymer is simulated with coarse-grained molecular dynamics and the fluid dynamics is solved using the lattice Boltzmann method. Results for the dynamic structure factor of a single polymer chain in solution show Zimm scaling and demonstrate that the method correctly captures long-range hydrodynamic interactions. This type of LB-MD coupling can naturally be extended to deformable particles such as red blood cells, as presented in other contributions to this meeting.

Ioannis Zacharoudiou

Injection of CO_2 deep underground into porous rocks, such as saline aquifers, appears to be a promising tool for reducing CO_2 emissions and the consequent climate change. During this process CO_2 displaces brine from individual pores and the sequence in which this happens determines the efficiency with which the rock is filled with CO_2 at the large scale. At the pore scale, displacements are controlled by the balance of capillary, viscous and inertial forces. We simulate this process by using multi-GPU free energy lattice Boltzmann simulations to directly solve the hydrodynamic equations of motion on a three dimensional geometry reconstructed from micro-CT images of Ketton limestone and consider fluid flows in a range of capillary numbers *Ca* and viscosity ratios.

The simulations show the three types of fluid displacement patterns, at the larger scale that have been previously observed in both experiments and simulations, namely viscous fingering, capillary fingering and stable displacement [1]. Here we examine the impact of the patterns on storage efficiency and then focus on slow flows, where displacements at the pore scale typically happen by sudden jumps in the position of the interface between brine (wetting fluid) and CO_2 (non-wetting fluid), termed as Haines jumps [2,3]. We demonstrate that numerically we capture the main features of the jumps: i) sharp increase in the non-wetting fluid velocity, ii) sharp drop in the pressure signal and iii) extensive fluid rearrangement. The fluid velocity during these abrupt events is orders of magnitude higher than the average fluid velocity, with maximum Reynolds number of the order 10^1, necessitating the use of a full Navier-Stokes solver in order to capture the dynamics of Haines jumps. Examining the displacement efficiency, during these jumps the fluid in surrounding pores can rearrange in a way that prevent later displacements in nearby pores, potentially reducing the efficiency with which the CO_2 fills the total available volume in the rock [4].

References

[1] Lenormand, R., Touboul, E. & Zarcone, C. Numerical models and experiments on immiscible displacements in porous media. Journal of Fluid Mechanics 189, 165–187, https://doi.org/10.1017/S0022112088000953 (1988).

[2] Berg, S. et al. Real-time 3D imaging of Haines jumps in porous media flow. Proceedings of the National Academy of Sciences 110, 3755–3759, https://doi.org/10.1073/pnas.1221373110 (2013).

[3] Zacharoudiou, I. & Boek, E. S. Capillary filling and Haines jump dynamics using free energy Lattice Boltzmann simulations. Advances in Water Resources 92, 43–56, https://doi.org/10.1016/j.advwatres.2016.03.013 (2016).

[4] Zacharoudiou, I., Boek, E. S., & Crawshaw, J. The impact of drainage displacement patterns and Haines jumps on CO_2 storage efficiency. Scientific reports, 8(1), 15561, https://doi.org/10.1038/s41598-018-33502-y (2018).

Edo Boek:

We use a pore-scale dissolution model to simulate the dissolution of calcite by HCl and CO2 in two different systems and compare with experiment. The model couples flow and transport with chemical reactions at the mineral surface and in the fluid bulk. Firstly, we inject HCl / CO2 through a single channel drilled through a solid calcite core as a simple validation case, and as a model system with which to elucidate the chemical mechanisms of the dissolution process. The overall dissolution rate is compared to a corresponding experiment. Close agreement with experimental and simulated dissolution rates is found, which also serves to validate the model. We also define a new form of effective Damkohler number which can be obtained from simulated chemical distributions and show how this gives a more precise measure of the balance of transport and reaction. Secondly, we inject HCl / CO2 into a Ketton carbonate rock core at high flow rate, which leads to wormhole formation, and compare to experiment. The simulation matches the experimental mass dissolution rate extracted from the micro-CT images, and predicts the resulting morphological changes reasonably well. The permeability change though is greater in the experiment than in the simulation, and this is shown to be due to more elongated wormhole formation in experiment. Possible reasons for this are discussed, including uncertainties in diffusion coefficients, and calcite density variations and micro-porosity in the Ketton grains. The distribution of chemical species from the simulation then permits a detailed understanding of the rate-controlling mechanisms at work, including the relative importance of the H + –calcite and H 2 CO 3 –calcite dissolution pathways.