Scientific report (2011-2014)

Exploratory Research Project PN-II-ID-PCE-2011-3-056

KINETIC MODELS FOR MICRO-SCALE TRANSPORT PHENOMENA AND STRUCTURE FORMATION IN COMPLEX FLUIDS: IMPLEMENTATION ON GPU-BASED PARALLEL COMPUTING SYSTEMS

Objectives :

O I. Development of high order 3D models for phase-separating fluids, as well as of appropriate numerical schemes using the PETSc library for parallel computing on multi-core CPU systems (2011)

O II. Build up of a GPU-based computing system and implementation of LB models on this many-core system using the CUDA library (2012)

O III. Investigation of the phase transition dynamics and morphology in 3D systems using the GPU parallel computing system (2013-2014)

O IV. Application of 3D Lattice Boltzmann models to specific problems in microfluidics (2015)

Results :

O I. (October – December 2011)

O II. (January – December 2012)

A parallel computing code was developed in order to simulate the flow of a single phase fluid flow between two parallel plates. The code relies on a Lattice Boltzmann model based on the separation of variables in the phase space. The momentum vectors of the fluid particles were projected on the three Cartesian axes and the Gauss-Hermite quadrature method was used to calculate the macroscopic quantities of interest (fluid density, velocity and temperature fields). The set of distribution functions that resulted after the discretization of the phase space were solved using a flux limiter numerical scheme. This code was tested on the IBM Blue Gene / P parallel computing system at the West University of Timisoara.

A two-dimensional version of this code was used in 2011 to develop and test an original method of controlling the values of the transport coefficients (viscosity and conductivity) of the fluid. The method is based on adding an extra term to the BGK approximation of the collision integral, which appears in the right hand side of the Boltzmann equation. We studied the effects of the transport coefficients on the velocity and temperature profiles in Couette flow, as well as the effect of the Knudsen number on the slip velocity and the temperature jump at the channel walls, which are specific to microfluidics. A three-dimensional version was developed later and the results were compared to those obtained by the DSMC (Direct Simulation Monte Carlo) method existent in the literature, as well as to the results obtained using another Lattice Boltzmann model (SLB) involving the spherical coordinate system in the momentum space.

After the set-up of two new computing systems (2012), the first one equipped with an nVIDIA Quadro M4000 graphics card having 256 cores and 2GB internal memory and the second one equipped with four nVIDIA Fermi M2090 graphics computing units (GPUs), with 512 cores and 6GB internal memory each, the available facilities were substantially improved and more complex problems involving phase-separating fluids were addressed within the project. Specific numerical algorithms involving flux limiters and the corner transport upwind scheme were later implemented in order to improve the accuracy and the numerical stability of the Lattice Boltzmann codes designed for the GPU system, using the CUDA library, as well as their efficiency (computing speed).

The results were presented at three international conferences: 21st International Conference on Discrete Simulation of Fluid Dynamics (DSFD 2012) July 23-27, Bangalore (India), the CECAM Workshop on Fluid-Structure Interaction in Soft Matter Systems: from the Mesoscale to the Macroscale, November 27-30, Prato (Italy) and the Physics Conference TIM 12 held November 27-30 in Timisoara (Romania). The contribution to the DSFD 2012 conference, related to Gauss quadratures, was published in International Journal of Modern Physics C, vol. 25 (2014).

O III. (January 2013 – December 2014)

The three-dimensional version of the computer code based on Gauss-Hermite quadrature was extended for systems with phase separation (Iiquid-vapour). For this purpose, two versions of the force term describing the interparticle interaction were implemented in both the PETSc and the GPU versions of the parallel computing code used to investigate the phase separation in liquid-vapour system. Preliminary results show a good agreement with the van der Waals phase diagram, when run on a lattice with a small number of nodes and using the force term based on the derivatives of the Hermite polynomials. Later, the computation of the Minkowski functionals was included in the code and used to investigate the evolution of the morphology of the liquid/vapour phases during the phase separation process, as well as the growth of gas bubbles during the cavitation process. The use of a third-order Gauss-Hermite quadrature model that contains vectors whose Cartesian projections are expressed by irrational numbers required careful use of the corner transport upwind numerical scheme associated to a specific implementation of the diffuse reflection boundary conditions.

The strategy used in developing the GPU code, as well as the optimization techniques implemented at this stage of the project were the subject of the MSc work (dissertation) defended by eng. Adrian Horga in June 2013 at the Department of

Computer Science and Software Engineering of the "Politehnica" University of Timisoara. The results related to the simulation of the liquid-vapour systems provided the grounds of the MSc work defended in July 2013 by another member of the team involved in the project, Mr. Tonino Biciusca, at the Department of Physics, West University of Timisoara. All these results were presented at three international conferences in 2013 and 2014 and submitted for publication to Comptes Rendus de Mecanique (2014). Another manuscript, related to the use of Lattice Boltzmann models for the investigation of the morphology of cell tissues (considered as two-phase fluid systems) and the influence of the viscosity on the evolution of these structures has been sent in 2014 for publication in the Biofabrication journal.

Given the features of this project, which aims to develop specific models for fluid systems that exhibit phase separation at the micro-scale, the implementation of boundary conditions with current LB models may generate significant errors when the value of Knudsen number is not negligible. To reduce the numerical errors during the implementation of the diffuse reflection boundary conditions, which involve the calculation of half-space integrals of the Boltzmann distribution function, a three dimensional (3D) Lattice Boltzmann model based on the Gauss-Laguerre quadrature method was elaborated in 2013. Two versions of this model were implemented : the first one is based on the series expansion of the equilibrium function, while the second one involves the direct projection of the distribution function on the orthogonal basis generated by the Laguerre polynomials. *The last one was published as a Rapid Communication in Physical Review E (April 2014).* Both models demonstrated the ability to capture specific effects at the micro-scale (velocity slip and temperature jump at the channel walls) when used in conjunction with the Shakhov collision term, as shown by comparison to Direct Simulation Monte Carlo (DSMC) results. Based on this experience, in 2014 another new Lattice Boltzmann model based on the half-range Hermite polynomials, defined on the half-axes of the Cartesian coordinate system, was introduced. Both the Laguerre and the Half-range Hermite Latice Boltzmann models allow to accurately compute the value of the incident particle flux at the flow channel wall, as well as the value of the emergent one. Computer simulation tests revealed that these models work well on the whole range of the Knudsen number (including the ballistic regime).

The investigation of micro-scale fluid flow using our Lattice Boltzmann models based on half-range quadratures were presented at four international conferences during 2013-2014. At this moment, two papers on this subject were already published and another one is accepted for publication. These results provide the basis for the investigation of specific problems in microfluidics, in accordance with the objective set for this project during 2015.

Scientific output :

International Journals:

1. B.Piaud, S. Blanco, R.Fournier, V.E.Ambrus, V.Sofonea
   Gauss quadratures - the keystone of Lattice Boltzmann models

International Journal of Modern Physics C 25 (2014) 1340016
DOI: 10.1142/S0129183113400160

2. V.E.Ambrus, V.Sofonea
   Implementation of diffuse reflection boundary conditions using lattice Boltzmann models based on half-space Gauss-Laguerre quadratures
   Rapid Communication
   Physical Review E 89 (2014) 041301(R)
   DOI: 10.1103/PhysRevE.89.041301

3. V.E.Ambrus, V.Sofonea
   Lattice Boltzmann models based on Gauss quadratures
   International Journal of Modern Physics C 25 (2014) 1441011
   DOI: 10.1142/S0129183114410113

4. V.E.Ambrus, V.Sofonea
   Application of Lattice Boltzmann models based on Laguerre quadratures to force-driven flows of rarefied gases
   accepted for publication in Interfacial Phenomena and Heat Transfer (November 2014)

5. A.Cristea, A.Neagu
   Shape changes of bioprinted tissue constructs simulated by the Lattice Boltzmann method
   submitted to Biofabrication (September 2014)

6. T.Biciusca, A.Horga, V.Sofonea
   Simulation of liquid-vapour phase separation on GPUs using Lattice Boltzmann models with off-lattice velocity sets
   submitted to Comptes Rendus de Mecanique (November 2014)

Conference presentations

1. B.Piaud, S. Blanco, R.Fournier, V.E.Ambrus, V.Sofonea
   Gauss quadratures - the keystone of Lattice Boltzmann models
   oral presentation
   21st International Conference on Discrete Simulation of Fluid Dynamics
   July 23 - 27, 2012, Bangalore (India)

2. V.Sofonea, V.E.Ambrus
   Diffuse Reflection Boundary Conditions and Lattice Boltzmann Models for Microfluidics
   oral presentation
   CECAM Workshop Fluid-Structure Interactions in Soft-Matter Systems: From the Mesoscale to the Macroscale, November 26 - 30, 2012, Prato (Italy)

3. T. Biciusca, V. Sofonea
   Lattice Boltzmann simulation of phase separation in liquid - vapour systems
   poster presentation
   Physics Conference TIM-12, November 27 - 30, 2012, Timisoara (Romania)

4. V. E. Ambrus, V. Sofonea
   Lattice Boltzmann models derived by Gauss quadratures and microfluidics applications
   oral presentation
   Seminar held June 17, 2013, LAPLACE Laboratory, Paul Sabatier University, Toulouse (France)

5. V. E. Ambrus, V. Sofonea
   Lattice Boltzmann Models based on Gauss Quadratures
   oral presentation
   22nd International Conference on the Discrete Simulation of Fluid Dynamics
   July 15 - 19, 2013, Yerevan (Armenia)

6. T. Biciusca, V. Sofonea
   Lattice Boltzmann simulation of phase separation in liquid - vapour systems
   poster presentation
   10th International Conference for Mesoscopic Methods in Engineering and Science (ICMMES), July 22 - 26, 2013, University of Oxford (United Kingdom)

7. V. E. Ambrus, V. Sofonea
   Applications of the Laguerre Lattice Boltzmann Models to Couette flow
   oral presentation
   Physics Conference TIM-13, November 21 - 24, 2013, Timisoara (Romania)

8. V. E. Ambrus, V. Sofonea
   Application of Lattice Boltzmann Models based on Laguerre Quadratures in Complex Flows
   oral presentation
   5th International Conference on Heat Transfer and Fluid Flow in Microscale (HTFFM-V), April 22 - 25, 2014, Marseille (France)

9. V. T.Biciusca, A.Horga, V. Sofonea
   Simulation of liquid-vapour phase separation on GPUs using Lattice Boltzmann models with off-lattice velocity sets
   oral presentation
   23rd International Conference on Discrete Simulation of Fluid Dynamics (DSFD)
   July 28 - August 1, 2014, Paris (France)

10. V. E. Ambrus, V. Sofonea
    Lattice Boltzmann models based on half-space quadratures and the corner transport upwind method
    oral presentation
    23rd International Conference on Discrete Simulation of Fluid Dynamics (DSFD)
    July 28 - August 1, 2014, Paris (France)

11. T. Biciusca, A. Horga, V. Sofonea
    Lattice Boltzmann approach to multiphase fluids using massively parallel systems
    oral presentation
    Physics Conference TIM-14, November 20 - 22, 2014, Timisoara (Romania)

12. A. Cristea, A. Neagu
    Bioprinted tissue constructs simulated by the Lattice Boltzmann method
    Oral presentation
    Physics Conference TIM-14, November 20 - 22, 2014, Timisoara (Romania)

MSc works:

1. Tonino Biciusca
   Lattice Boltzmann models for multiphase systems
   West University of Timisoara, Department of Physics (2013)

2. Adrian Horga
   Fluid dynamics simulation with lattice Boltzmann models using CUDA enabled GPGPUs
   "Politehnica" University of Timisoara, Department of Computer and Software Engineering (2013)