Lattice Boltzmann Workshop, Cemagref, 5.12.08

Schéma de Boltzmann sur réseau : méthodes et applications .
Lattice Boltzmann scheme: Methods and Applications

Comité d'organisation / Organizing Team

1. François Dubois (CNAM Paris et Univ. Paris Sud, Orsay)
2. Irina Ginzburg (CEMAGREF, Antony)
3. Pierre Lallemand (CNRS, L'ENS, Paris)

Programme/Schedule

- **9h-9h15** Michel Penel (Cemagref, France) Welcome
- **9h10-11h15**
  1. Dominique D'Humières (ENS Paris, France) : *Lattice Boltmann equations and Finite difference schemes*
  2. Jonas Tölke (T.U. Braunschweig, Germany): *Lattice Boltzmann simulations using Multiple GPUs and application to fluid-structure interaction*
  3. Pietro Asinari (Politecnico di Torino, Italy) : *Entropic multiple-relaxation-time lattice Boltzmann models*
  4. Martin Geier (U. Freiburg, Germany) : *The magic Boltzmann method*
- **11h15-11h45 Pause !**
- **11h45-12h45**
  1. Martin Rheinländer (U. Konstanz, Germany) : *Some aspects of stability and consistency of LBM*
  2. Benjamin Graille (U. Paris Sud, France) : *LB schemes for multi-temperature plasmas*
  3. Stéphane Dellacherie (CEA Saclay, France) : *A simple convergence result for the LBM method in the case of the heat equation*
- **12h45-14h15 Repas / Lunch !**
- **14h15-14h30** Yves Nédélec (Cemagref, Antony, France) : Presentation of Phyleau team in Antony
- **14h30-15h30**
  1. Jon Summers (U. of Leeds, United Kingdom) : *An evaluation of a multi-phase LB model for coating flows*
  2. Salvador Izquierdo (U. Zaragoza, Spain) : *Euler-characteristic boundary conditions for lattice Boltzmann methods*
  3. Denis Ricot (Renault Guyancourt, France) : *Application of Lattice Boltzmann Method in automotive industry*
- **15h30-16h00 Pause !**

- **16h-17h**

  1. Valérie Pot (INRA Grignon, France) : *Application of the TRT LB model to simulate pesticide transport in cultivated soils*
  2. Lyazid Djenidi (U. Newcastle, Australia) : *Lattice Boltzmann method, turbulence and micromixing*
  3. Frederic Kuznik (INSA Lyon, France) : *LBM based flow simulation using GPU*

  17h-18h Round table and Conclusions

ABSTRACTS

Dominique d'Humières & Irina Ginzburg

Laboratoire de Physique Statistique, École Normale Supérieure, Paris, France
and
Cemagref, Antony Regional Centre, HBAN, Antony, France

Lattice Boltmann Equations and Finite Difference Schemes

Lattice Boltzmann (LB) models are often presented by stressing their differences with more traditional numerical methods, such as finite differences. However it is known since a long time that BGK models reduce to finite-difference schemes when the relaxation time is equal to 1. It follows that the stability conditions known for finite-difference schemes can be used to study the stability properties of the BGK models and conversely. We extend this result for a subclass of the two-relation-time (TRT) models. For advection-diffusion LB models, this subclass has the same stability domain as BGK with $\tau = 1$ for any value of the diffusion coefficient.

In a second part, the steady TRT models are presented as link-wise central finite-differences. This result is used to explain how some unphysical dependencies of the macroscopic quantities (such as the permeability tensor) with the transport coefficients (such as the viscosity) can be removed by using a constant value for a "magic" combination of the relaxation times with suitable boundary conditions.

References:

1. D. d'Humières and I. Ginzburg. Viscosity independent numerical errors for Lattice Boltzmann models: from recurrence equations to "magic" collision numbers. *to appear in Computers & Mathematics with Applications*, 2008.

2. I. Ginzburg, F. Verhaeghe, and D. d'Humières. Com. Comp. Phys, 3:427–478, 2008.

3. I. Ginzburg, Phys. Rev. E, 77:0666704:1-12, 2008.

Jonas Tölke
Institute for Computational Modeling in Civil Engineering, Technische Universität Braunschweig, Germany

Lattice Boltzmann simulations using Multiple GPUs and application to fluid-structure interaction

A very efficient implementation of a Lattice Boltzmann (LB) kernel in three dimensions on a graphical processing unit (GPU) using the Compute Unified Device Architecture (CUDA) interface developed by nVIDIA is presented. A special memory layout for the D3Q13 model is developed. The propagation and collision process are combined in one step and a special design for a very fast data access is developed. Methods for the parallelization of the code for multiple GPUs within one PC are developed. The data is exchanged over the host (CPU) memory via the PCI-Express bus. A good parallel efficiency for three GPU cards is obtained. With this approach over one billion lattices updates per second are reached. As an example we compute solutions for the drag of a moving sphere in a circular pipe for Reynolds-numbers ranging from 1 up to 500 and with an LES model from 1000 to 10000. We developed methods and algorithms to integrate the GPU computing and fluid-structure interaction and present preliminary results.

References:

1. Jonas Tölke *Implementation of a Lattice Boltzmann kernel using the Compute Unified Device Architecture developed by nVIDIA*, Computing and Visualization in Science, 2008. DOI: 10.1007/s00791-008-0120-2.

2. J. Tölke and M. Krafczyk: *TeraFLOP Computing on a Desktop PC with GPUs for 3D CFD*, Int. J. of Computational Fluid Dynamics, 22(7): 443-456 (2008).

Pietro Asinari and Ilya V. Karlin
Department of Energetics, Politecnico di Torino, Italy
and
Institute of Energy Technology, ETH Zurich, 8092 Zurich, Switzerland
School of Engineering Sciences, University of Southampton, UK

Entropic multiple-relaxation-time lattice Boltzmann models

Generalized Maxwell distribution function is derived analytically for the lattice Boltzmann (LB) method. All the previously introduced equilibria for LB are found as special cases of the generalized Maxwellian. The generalized Maxwellian is used to derive a new class of multiple-relaxation-time LB models with tunable bulk viscosity and prove the H–theorem for them. Finally some numerical tests are reported in order to prove the stability enhancement and the recovered accuracy.

Martin Geier
University of Freiburg, Germany

The Magic Boltzmann Method

We discuss two methods to enhance the convergence of the lattice Boltzmann method: Relaxation of cumulants and ”magic” relationships between collision rates. Both method are found to improve simulation results but a formal justification for their use and an analysis of their range of applicability is still missing. We present this as a challenge for the community to turn magic into science.

Stéphane Dellacherie and Christophe Le Potier
CEA-Saclay, France

A Lattice Boltzmann Method applied to the heat equation

We show how to conscruct two LBM schemes to solve the heat equation $\partial_t \rho = \nu \partial^2_{xx} \rho$. This construction allows to clearly recover the classical "magic" formula in the field of LBM schemes

$$\nu = \left(\widehat{\varepsilon} - \frac{1}{2} \right) c_s^2$$

(c_s=pseudo sound velocity of the lattice) that links the physical diffusion ν (conductivity in the case of the heat equation) to a kind of time collision $\widehat{\varepsilon}$ of a discrete velocity Boltzmann system. Then, we prove that there is a deep connection of the proposed LBM schemes with a particular class of Du Fort-Frankel type schemes which are finite-difference schemes. Thus, we prove the convergence in L_∞ of these LBM schemes with periodic, Neumann or Dirichlet boundary conditions. We also prove that it is possible to verify an unconditionally discrete maximum principle by modifying the Dirichlet boundary condition. This discrete maximum principle allows to obtain a LBM scheme which is robust when the mesh is rough. At last, we show and we explain some "strange" properties of the proposed LBM schemes. These "strange" properties clearly limit the applicability of the unconditionally stability property of the proposed LBM schemes. We think that this last remark should be quite general in the field of LBM schemes.

Jonahatan Lewis Summers & Michael W. T. Wilson
Institute of Engineering Thermofluids, Surfaces and Interfaces (iETSI), School of Mechanical Engineering, University of Leeds, Leeds, UK.

An evaluation of a multiphase LB model for coating flows

The production of liquid film coatings is used in many industries, from speciality papers, to functional packaging, from cosmetics to adhesives. All processes have to displace a gas in order to deposit a liquid film at high speed, which gives rise to the dynamics of wetting. Attempts to model the dynamic wetting process are explored and in particular the development of multiphase LB model is used in an attempt to capture the physical phenomena of forced wetting failure, contact line hysteresis and natural wetting.

A. R. Davies, J. L.Summers, and M. C. T.Wilson, *On a dynamic wetting model for the finite-density multi-phase lattice Boltzmann method*. Int. J. of Computational Fluid Dynamics, 20(6):415-427, 2006.

Salvador Izquierdo
University of Zaragoza, Spain

Euler-characteristic boundary conditions in lattice Boltzmann methods

The lattice Boltzmann (LB) method solves the isothermal compressible Navier-Stokes equation in the incompressible and continuous limit (low Mach and Knudsen numbers). It has been extensively shown that the choice of initial and boundary conditions influences the accuracy of the method. However, even if the spurious behaviors of these conditions in the form of small numerical waves and/or initial layers are suppressed, it is still necessary to formulate a mechanism to suppress the physical pressure waves generated in the bulk of the fluid (e.g. due to vortex shedding) when they arrive to an open boundary. The aim is that the truncation of the physical domain made by these open boundaries does not bear an influence on the behavior of the process. And, further, it is necessary to guarantee not only a good behavior in terms of wave suppression, but also a correct preservation of the order of the method. The techniques for artificial boundary modeling may be classified in two main groups [1]: Characteristic boundary conditions and absorbing layers. We suggest that some sort of these nonreflecting boundaries should be applied for most of the simulations with LB methods, including those where it is desired to recover the incompressible solution. A formulation will be presented of a characteristic boundary condition for the standard LB method which is based on the characteristics of the Euler equations and their extension to the Navier-Stokes ones; these are the so-called Navier-Stokes characteristic boundary conditions, developed by Poinsot and Lele [2]. With respect to the similar conditions used in finite-difference or finite-volume implementations, some corrections are needed to compensate the isothermal compressible nature of standard lattice Boltzmann methods for fluid flow. The results show [3] that the proposed method for inlets and outlets is highly nonreflecting, and mass conserving.

References:

1. T. Colonius, Annu. Rev. Fluid Mech. 36, 315 (2004)
2. T. Poinsot and S. K. Lele, J. Comput. Phys. 101, 104 (1992)
3. S. Izquierdo and N. Fueyo, Phys. Rev. E. 78, 046707 (2008)

Denis Ricot

Renault - Research, Advanced Engineering and Materials Department, Guyancourt, France

Application of Lattice Boltzmann Method in automotive industry

The lattice Boltzmann Method, associated to a turbulence model, can be used for high Reynolds number flow simulations on complex geometry. In automotive industry, the LBM-based commercial code PowerFLOW is widely used in many application fields : aerodynamic optimization, computation of aeroacoustic sources, thermal management simulations. In this talk, the main features of PowerFLOW are presented (LBM model, turbulence model, immersed boundary condition approach,. . .). Some examples of aerodynamic drag simulations are given. The LBM allows the simulation of weakly compressible flows. Therefore, it is well suited for aeroacoustic computations. The example of the direct computation of the noise generated by an automotive ventilation outlet is presented. In aeroacoustic field, other applications such as sunroof buffeting simulation or the prediction of wall pressure fluctuations on side windows will be also discussed.

Lyazid Djenidi

School of Engineering University of Newcastle, NSW Australia

Lattice Boltzmann Method, Turbulence and Micromixing

Direct numerical simulation (DNS) using the lattice Boltzmann method have been carried out in various turbulent and laminar flows. The aim of the work is to show that the LBM can be an alternative DNS method to the classical procedure based on the resolution of the Navier-Stokes equations. The results which compare well with both experimental and DNS data indicate clearly that the LBM can be considered as a reliable DNS method for fluid flow simulation.

Valérie Pot (1), Nadia Elyeznasni (1), Irina Ginzburg (2) and Hassan Hammou (2)

1. UMR INRA-AgroParisTech, Environnement et Grandes Cultures, Equipe Sol, Grignon, France

2. CEMAGREF, Centre Régionale d'Antony, France

3. Faculté des Sciences, Université Mohammed Ier, Oujda, Maroc

Application of the TRT LB model to simulate pesticide transport in cultivated soils

We present preliminary results of transport of pesticide in 3D images of soil pore space of a cultivated soil obtained with the two-relaxation time Lattice-Boltzmann model. Motivations to use this technique were to be able to simulate the flow and transport of pesticide in the presence of the real physical, physico-chemical and biological soil heterogeneities. Indeed, transport of pesticides is controlled by the topology of soil pores (their size, spatial organization, and connectivity), nature and spatial localization of soil constituents (organo-minerale phase, organic matter) and microorganisms (bacteria, fungi). Soil structure was obtained by 3D computed X-Ray tomography (CT) images of intact clay-loam soil cores containing organic matter residues (wheat straws). Particulate organic matter was identified and spatially localised in the 3D soil pore space. Kinetic sorption was introduced in the TRT LB model and heterogeneity of reactivity of pesticides was was further modeled by using different reaction kinetic laws to the particulate organic matter and organo-minerale phase. Further development of the TRT LB model is to introduce biological reactivity of pesticides.

References:

1. V. Pot and A. Genty. *Dispersion Dependence on retardation in a real fracture geometry using lattice-gas cellular automaton,* Adv. Water Res., 30:273-283, 2007.

2. I. Ginzburg. *Lattice Boltzmann modeling with discontinuous collision components. Hydrodynamic and advection-diffusion equations.* J. Stat. Phys, 126:157–203, 2007.

Frédérik Kuznik

Departément Génie Civil & Urbanisme, Institut National des Sciences Appliquées de Lyon, Centre Thermique de Lyon, France

LBM based flow simulation using GPU

Nowadays, computational methods and hardware are really inseparable. In fact, the numerical method should fit the hardware architecture to gain benefits from computational possibilities. Of course, the relation reciprocity is also true: the hardware architecture progress lead the numerical methods that can be used with a reasonable computational cost. In the last two decades, the Lattice Boltzmann method (LBM) has proved its capability to simulate a large variety of fluid flows. However, it has been recognized that the LBM is both computationally expensive and memory demanding. But, because LBM is explicit and generally needs only nearest neighbor information, the method allows a highly efficient parallel implementation using GPU (Graphics Processing Units) architececture: that is the purpose of this presentation.

List of participants, LBE Workshop, 5.12.08

1. Jean-Luc Aider ESPCI Paris aider@pmmh.espci.fr
2. Raed Arab UNI Limoges m.raed.arab@etu.unilim.fr
3. Pietro Asinari POLITECNICO di TORINO pietro.asinari@polito.it
4. Alain Bélanger EXA alain@exa.com
5. Hayat Benkhelifa CEMAGREF Hayat.Benkhelifa@cemagref.fr
6. Mohamed Bouzidi CNAM mh_bouzidi@yahoo.fr
7. Rachid Bennacer, UNI Cergy-Pontoise rachid.bennacer@u-cergy.fr
8. Alain Cartalade CEA Saclay alain.cartalade@cea.fr
9. Stephane Dellacherie CEA Saclay stephane.dellacherie@cea.fr
10. Lyazid Djenidi UNI Newcastle lyazid.djenidi@newcastle.edu.au
11. Francois Dubois CNAM fdubois@cnam.fr
12. Martin Geier UNI Freiburg martin.geier@imtek.uni-freiburg.de
13. Irina Ginzburg CEMAGREF irina.ginzburg@cemagref.fr
14. Benjamin Graille UNI Orsay benjamin.graille@math.u-psud.fr
15. Illy Herve RENAULT herve.illy@renault.com
16. Dominique D'Humières l'ENS Paris dominique.dhumieres@lps.ens.fr
17. Salvador Izquierdo UNI Zaragoza salvador.izquierdo@unizar.es
18. Christian Janssen TU Braunschweig janssen@irmb.tu-bs.de
19. Nolwenn Jarrige, FAST Orsay jarrige@fast.u-psud.fr
20. Carlier Johan CEMAGREF Carlier.Johan@cemagref.fr
21. Frederic Kuznik INSA, LYON frederic.kuznik@insa-lyon.fr
22. Pierre Lallemand CNRS pierre.lal@free.fr
23. Emmanuel Leveque l'ENS LYON eleveque@ens-lyon.fr
24. Brigitte Licquin UNI Paris 6 lucquin@ann.jussieu.fr
25. Bouchaib Mabchour CEMAGREF Bouchaib.Mabchour@cemagref.fr
26. Simon Marié Heclectic's Pictures Production simon@heclectics-pictures.com
27. Jean-François Maitre CNRS jean.maitre@noos.fr

28. Moureh Jean CEMAGREF Jean.Moureh@cemagref.fr
29. Yves Nédélec, CEMAGREF Yves.Nédélec@cemagref.fr
30. Bernard Peyron UNI Limoges pateyron@unilim.fr
31. Valerie Pot l'INRA Grignon vpot@grignon.inra.fr
32. Christophe Le Potier CEA Sacla clepotier@cea.fr
33. Patrick Le Quéré LIMSI Patrick Le Quéré LIMSI
34. Nicole Rakotomalala FAST Orsay rako@fast.u-psud.fr
35. Martin Rheinlaender UNI Konztanz martin.rheinlaender@uni-konstanz.de
36. Denis Ricot RENAULT denis.ricot@renault.com
37. Eric Savin ONERA Eric.Savin@onera.fr
38. Jonathan Summers UNI Leeds j.l.summers@leeds.ac.uk
39. Laurent Talon FAST Orsay talon@fast.u-psud.fr
40. Jonas Tölke TU Braunschweig toelke@cab.bau.tu-bs.de

J'ai le plaisir de vous convier à ma soutenance d'HDR, prévue le 16 Janvier 2009 à 15 h 30 au Cemagref d'Antony, Salle H6, et au pot qui suivra.
A bientôt. Irina Ginzburg

Une variation sur les propriétés magiques de modèles de Boltzmann pour l'écoulement microscopique et macroscopique

Résumé: Ce manuscrit est consacré à l'étude de divers aspects de la modélisation par la méthode de Boltzmann sur réseau – les équations hydrodynamiques et d'advection diffusion anisotrope, les équations des différences-finies de récurrence (équivalentes au schéma de Boltzmann) et les liens entre leurs solutions exactes et la série infinie de Chapman-Enskog, les modèles cohérents pour un écoulement microscopique et macroscopique et leur couplage dans un milieux poreux, les fluides immiscibles à deux phases et à l'interface libre, l'écoulement d'eau dans un sol variablement saturé, en combinant approches analytiques et simulations numériques. Guidé par un argument simple de symétrie, notre analyse a pu être poursuivie au delà du second ordre requis pour l'obtention des équations macroscopiques. Cela nous a permis de découvrir que certaines combinaisons magiques de paramètres "hydrodynamiques" et "cinétiques" (libres) non seulement contrôlent la localisation des parois et des interfaces, mais influencent également la stabilité du modèle LBE et ses erreurs de troncature et, plus généralement, déterminent la paramétrisation exacte des équations modélisées par les nombres physiques sans dimension, au moins dans en régime stationnaire. Le modèle à deux temps de relaxation, un pour tous les modes symétriques de l'opérateur de collision et un autre pour tous ces modes antisymétriques, joue un rôle central dans nos études et permet de trouver des éléments de réponse à ces questions et à d'autres semblables.

It's my pleasure to invite you for the sustaining of my HDR thesis, which is scheduled the 16th January 2009, at Room H6 of Cemagref d'Antony, and for a small celebration after it. Looking forward to meet you. Irina Ginzburg

Magic recipes for Lattice Boltzmann modeling of micro and macro flow

Abstract: This manuscript is devoted to an investigation of various aspects of modelization with the approach of Lattice Boltzmann Equation - hydrodynamic and anisotropic advection-diffusion equations, directional finite-difference recurrence equations (equivalents to LBE schemes) and the links between their solutions and infinite Chapman-Enskog expansion, consistent models for microscopic and macroscopic flow and their coupling in porous media, two phase immiscible fluids and free interface flow, water behaviour in variably saturated soil – combining theoretical and numerical tools. Argument of symmetry with respect to underlying velocity set guides our analysis beyond the second order. We find that certain magic combinations of relaxation parameters, related to "hydrodynamic" and "kinetic" collision modes, take a control over the localisation of boundaries and interfaces, impact the stability and truncation errors of the model, and, more generally, determine the exact parametrization of the modelled equations by the governing non-dimensional physical numbers, at least in stationary regime. Two-relaxations-time model, with one relaxation parameter for all symmetric and another one for all anti-symmetric collision modes, play a distinctive role in our study and gives some elements of reply to these questions and other similar ones.