LATTICE BOLTZMANN MODELS FOR MULTIPHASE SYSTEMS

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Thesis structure

1. General theory of Lattice Boltzmann Models

- General aspects related to lattice Boltzmann theory

2. Numerical algorithms for Lattice Boltzmann Models

- Overview on numerical schemes used in this thesis
- Programming tools

3. Computing results

- Minkowski functionals
- Presentation of the computer results related to 2D and 3D phase separation

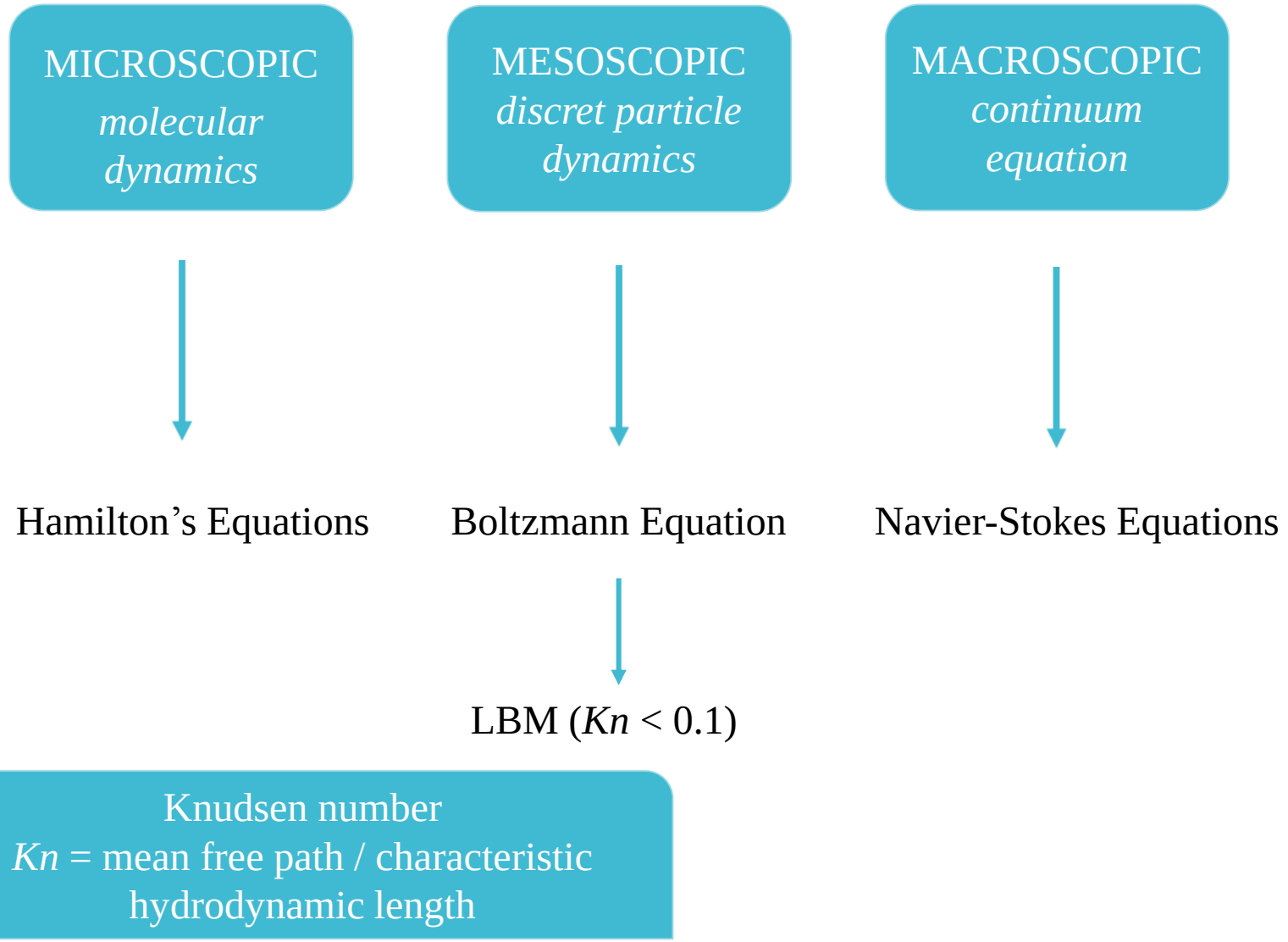
4. Conclusion

Overview

Lattice Boltzmann method (LBM) was introduced by McNamara and Zanetti in 1988, to overcome the disadvantages of the lattice gas cellular automata. This method established itself as a powerful tool for simulation of a wide range of physical phenomena and one of its main applications is in the field of computational fluid dynamics. Computational fluid dynamics is the science of modeling various phenomena related to fluid mechanics.

LBM represents the statistical description of equlibrium distribution function on the computational grid named lattice. These description mimic the fluid flow and yield excellent results for many difficult problems.

General theory of Lattice Boltzmann Models



General theory of Lattice Boltzmann Models

The Boltzmann equation represents the time evolution of the distribution function $f(x, \xi, t)$:

$$\left(\partial_t + \boldsymbol{\xi} \cdot \nabla_x + \frac{\boldsymbol{F}}{m} \cdot \nabla_\xi\right) f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \Omega$$

collision operator

Boltzmann – BGK (*Bhatnagar – Gross – Krook*) equation:

$$\left(\partial_t + \boldsymbol{\xi} \cdot \nabla_x + \frac{\boldsymbol{F}}{m} \cdot \nabla_\xi\right) f(\boldsymbol{x}, \boldsymbol{\xi}, t) = -\frac{1}{\tau}[f(x, \xi, t) - f^{eq}(x, \xi, t)]$$

f^{eq} is the equlibrium distribution

$$f^{eq} = \rho \left(\frac{m}{2\pi k_B \theta}\right)^{\frac{3}{2}} \exp\{-\frac{m}{2k_B\theta}[\xi - u(x,t)]^2\}$$

function (the Maxwell –Boltzmann distribution function)

General theory of Lattice Boltzmann Models

Because the equilibrium distribution function is a Gaussian and the computation of macroscopic variables (mass, velocity, temperature) involve calculation of integrals that can be performed efficiently using the Gauss – Hermite quadrature method → f^{eq} is projected on the orthogonal basis formed by Hermite polynomials:

$$f^{eq}(\boldsymbol{x},\boldsymbol{\xi},t) \cong f^{N}(\boldsymbol{x},\boldsymbol{\xi},t) = \omega(\boldsymbol{\xi}) \cdot \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}_{\alpha}^{(n)}(\boldsymbol{x},t)\, \boldsymbol{\mathcal{H}}_{\alpha}^{(n)}(\boldsymbol{\xi})$$

weight function

Hermite polynomial

$$\boldsymbol{a}_{\alpha}^{(n)}(\boldsymbol{x},t) = \int f(\boldsymbol{x},\boldsymbol{\xi},t)\boldsymbol{\mathcal{H}}_{\alpha}^{(n)}(\boldsymbol{\xi})d\,\xi$$

$$= \sum_{i=1}^{d} \frac{w_i}{\omega(\xi_i)} f^{N}(\boldsymbol{x},\boldsymbol{\xi},t)\boldsymbol{\mathcal{H}}_{\alpha}^{(n)}(\xi_i)$$

expansion coefficients $a_{\alpha}^{(n)}$ → thermohydrodynamic variables

General theory of Lattice Boltzmann Models

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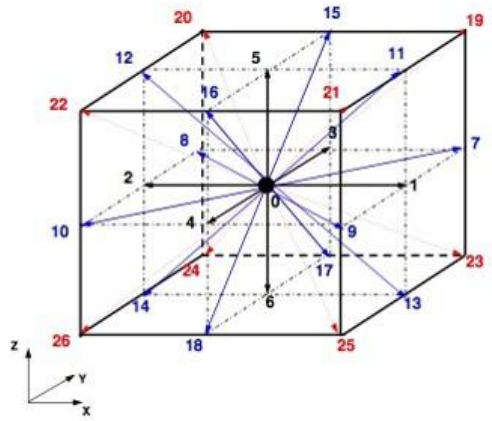
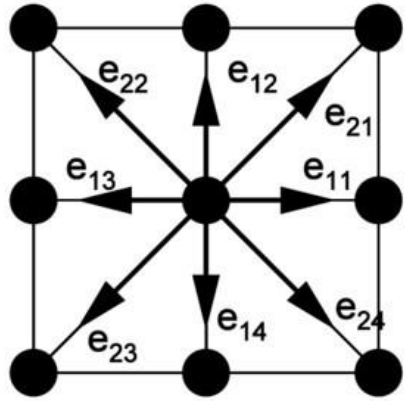


D2Q9



General Hermite expansion of the Maxwellian:

$$f^{eq}(\boldsymbol{x},t) = w\sum_{n=0}^{N}\frac{1}{c_s^{2n}n!}\boldsymbol{a}_{\alpha}^{(n)}(\boldsymbol{x},t)\boldsymbol{H}_{\alpha}^{(n)}(\boldsymbol{\xi})$$

Force term :

$$F(\boldsymbol{x},t) = w\sum_{n=1}^{N-1}\frac{1}{n!\,c_s^{2n}}\boldsymbol{H}_{\alpha}^{(n)}(\boldsymbol{\xi})\boldsymbol{a}_{0}^{(n)}(\boldsymbol{x},t)$$

$c_s = \sqrt{k_B T/m}$, c_s sound speed;

Numerical algorithms for LBM

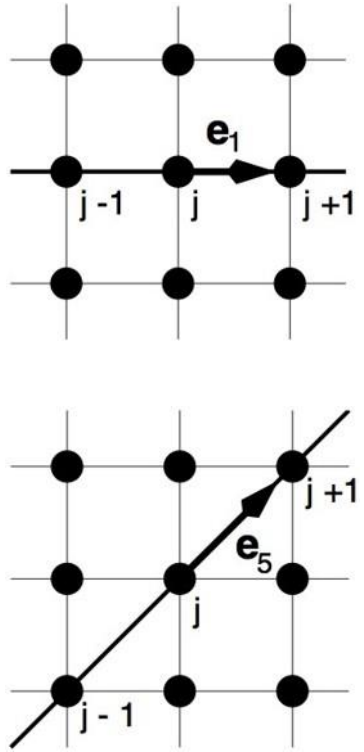
- *First order upwind scheme*

$$f_i(x, t+\delta t) = f_i(x,t) - \frac{c\delta t}{\delta s}\left[f_i(x,t) - f_i\left(x - \frac{\delta s e_i}{c}, t\right)\right] + \delta t Q_i(x,t)$$

- *Flux limiter techniques*

$$f_{i,j}^{k+1} = f_{i,j}^{k} - \frac{c\delta t}{\delta s}\left[F_{i,j+\frac{1}{2}}^{k} - F_{i,j-\frac{1}{2}}^{k}\right] + \delta t Q_{i,j}^{k}$$

$$F_{i.j+1/2}^{k} = f_{i,j}^{k} + \frac{1}{2}\left(1 - \frac{c\delta t}{\delta s}\right)\left(f_{i,j+1}^{k} - f_{i,j}^{k}\right)\Psi\left(\Theta_{i,j}^{k}\right)$$



Numerical algorithms for LBM

First order upwind can be interpreted as wave propagation method (shown in Fig. 2.4. a) and we have:

$$F_{i-1/2,j} = u\, Q_{i-1,j}$$
$$G_{i,j-1/2} = v\, Q_{i,j-1}$$

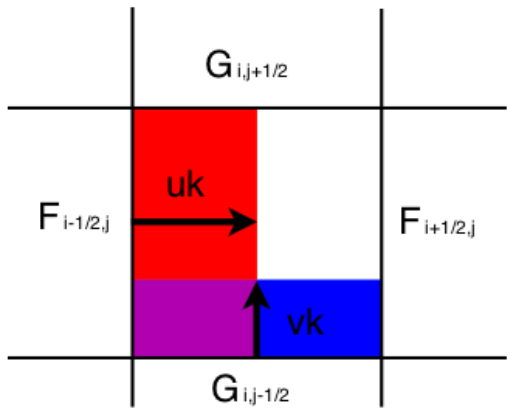
First order corner transport upwind. a. Transverse propagation affecting the fluxes $\tilde{F}_{i+1/2,j}$ and $\tilde{G}_{i,j+1/2}$. b. Transverse propagation affecting the fluxes $\tilde{F}_{i-1/2,j}$ and $\tilde{G}_{i,j-1/2}$.

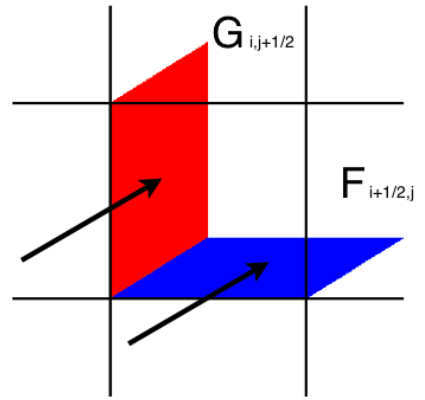
$$\tilde{F}_{i-1/2,j} = -\frac{1}{2}\frac{\Delta t}{h} uv(Q_{i-1,j} - Q_{i-1,j-1})$$

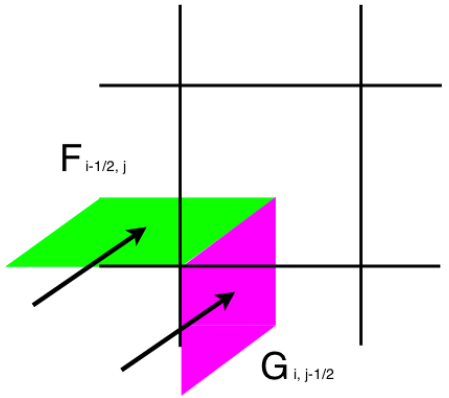
$$\tilde{F}_{i+1/2,j} = -\frac{1}{2}\frac{\Delta t}{h} uv(Q_{i,j} - Q_{i,j-1})$$

$$\tilde{G}_{i,j-1/2} = -\frac{1}{2}\frac{\Delta t}{h} uv(Q_{i,j-1} - Q_{i-1,j-1})$$

$$\tilde{G}_{i,j+1/2} = -\frac{1}{2}\frac{\Delta t}{h} uv(Q_{i,j} - Q_{i-1,j})$$







Numerical algorithms for LBM

- **PETSc** (Portable, Extensible Toolkit for Scientific Computation) is a suite of open source software libraries for parallel solution of linear and nonlinear equations.

CPU

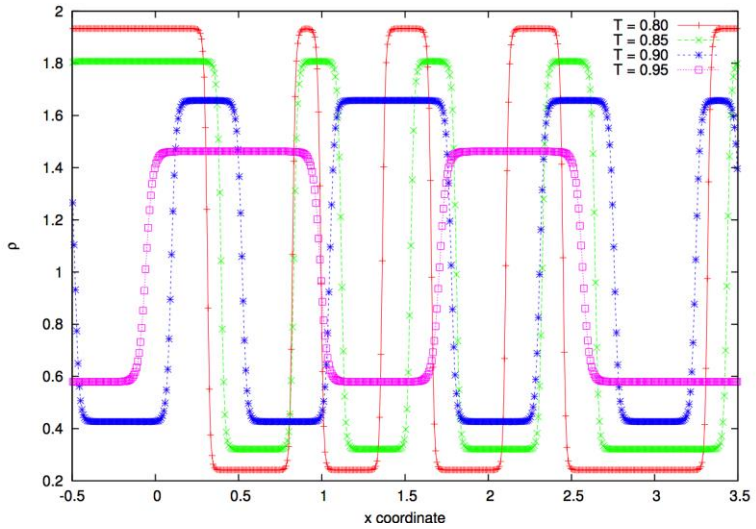
- **CUDA** (Computing Unified Device Architecture) is an extension to the C programming language, that allows GPU code to be written in regular C.

GPU

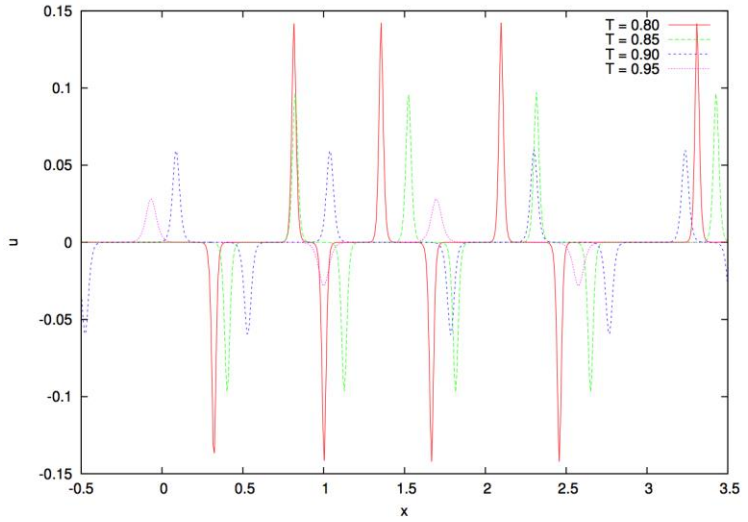
IBM Blue Gene / P System

Computing results

Simulation of phase separation in two – dimensional systems at constant temperature



a.

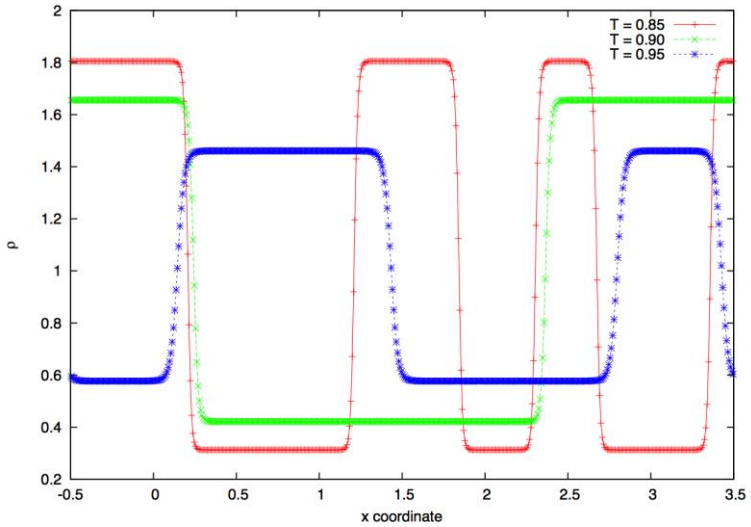


b.

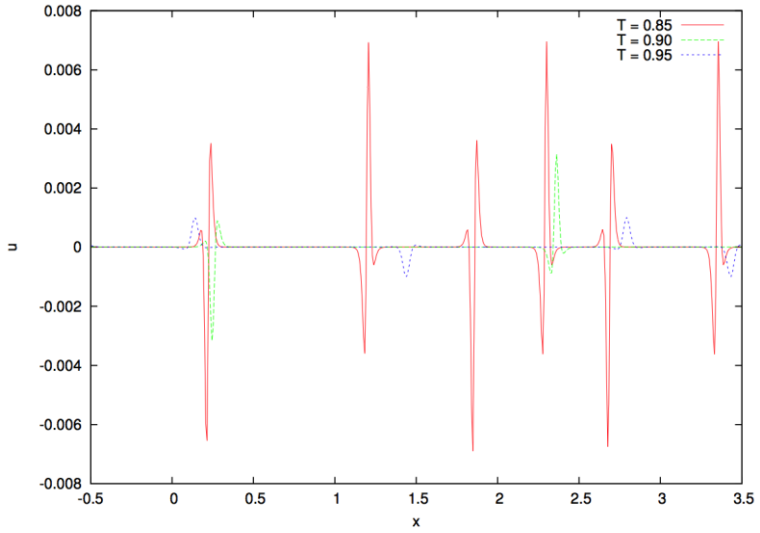
a. Equilibrium density profiles. b. Equilibrium velocity profiles. In both cases, it is key_enabla $= 2$, k$ey_tau = 0$ and T = 0.80.

Computing results

Simulation of phase separation in two – dimensional systems at constant temperature



a.

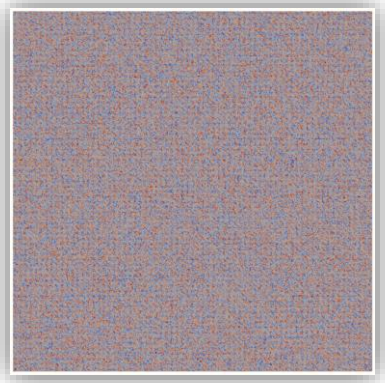


b.

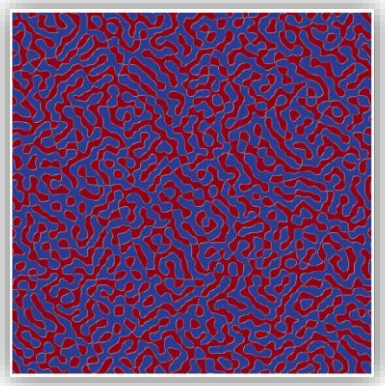
a. Equilibrium density profiles. b. Equilibrium velocity profiles. In both cases, it is key_enabla $= 4$, k$ey_tau = 0$ and T = 0.80.

Computing results

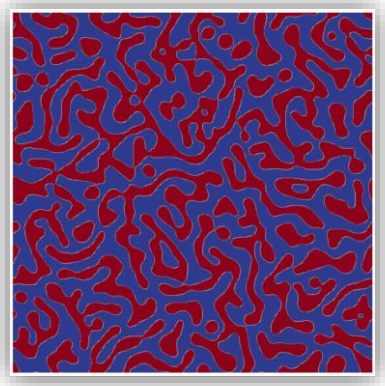
Dynamics of phase separation on a 2D lattice with 512 x 512 nodes



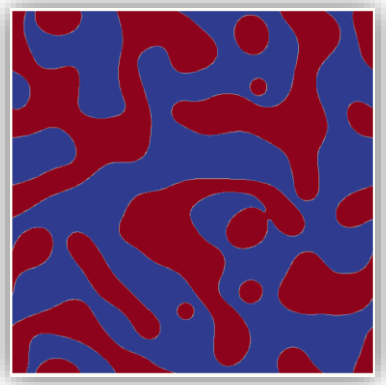
0 iter.



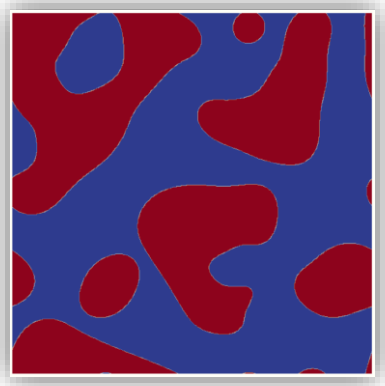
5000 iter.



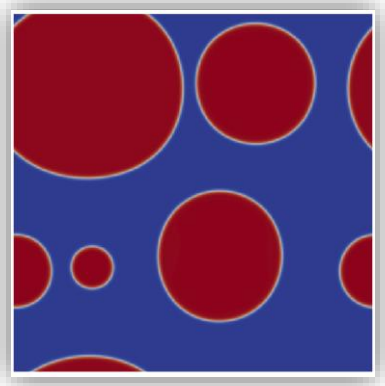
10000 iter.



40000 iter.

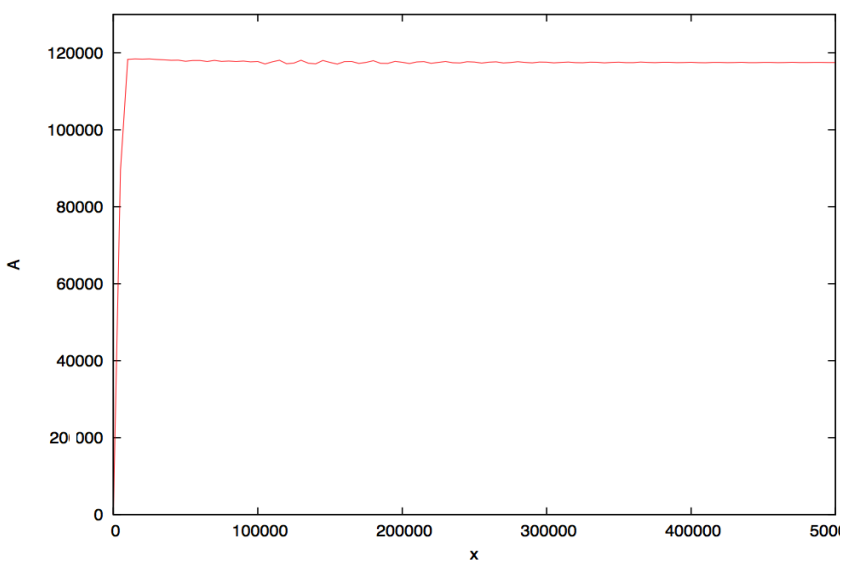


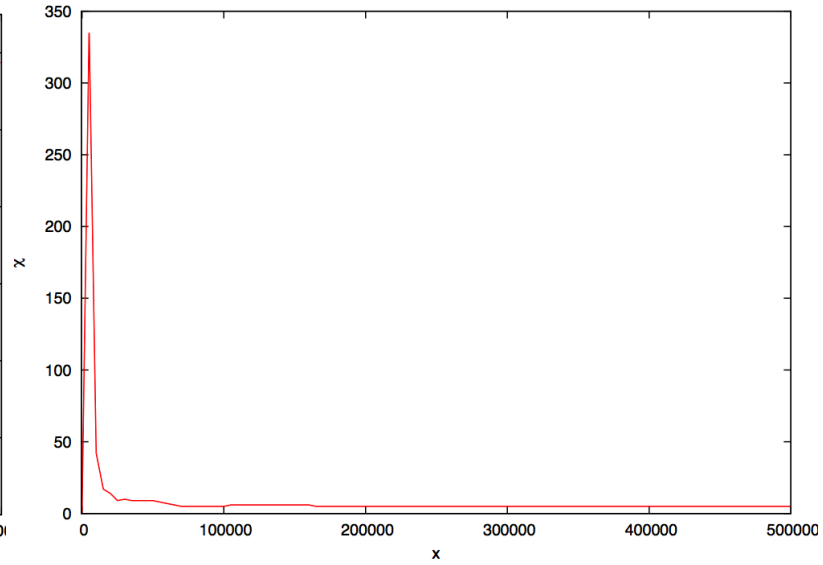
75000 iter.



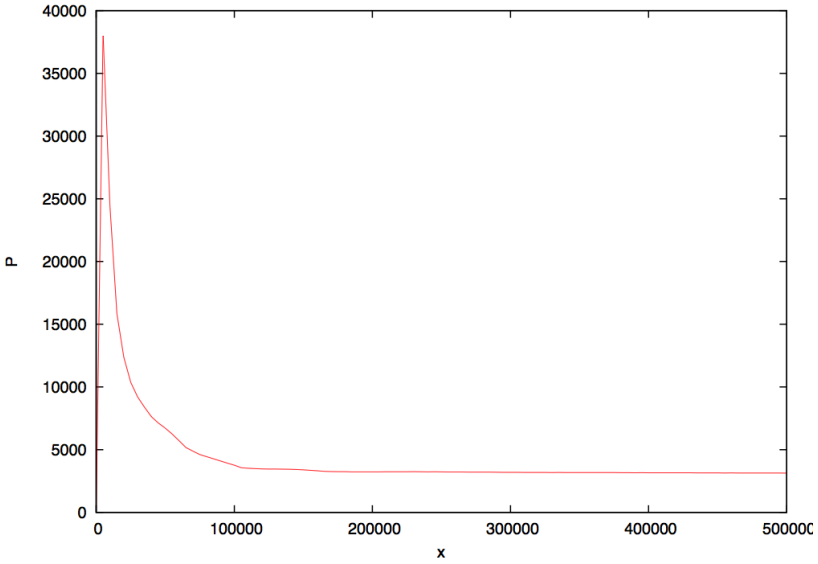
300000 iter.

Computing results



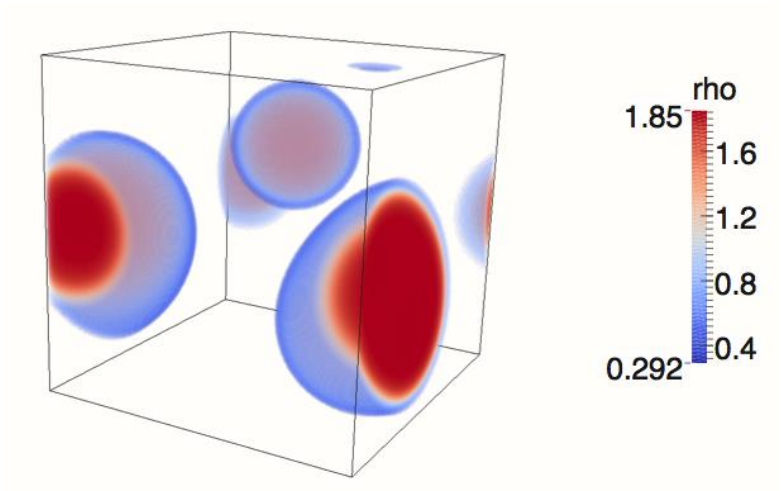


Minkowski functionals (area, perimeter and Euler characteristic) at T = 0.80.

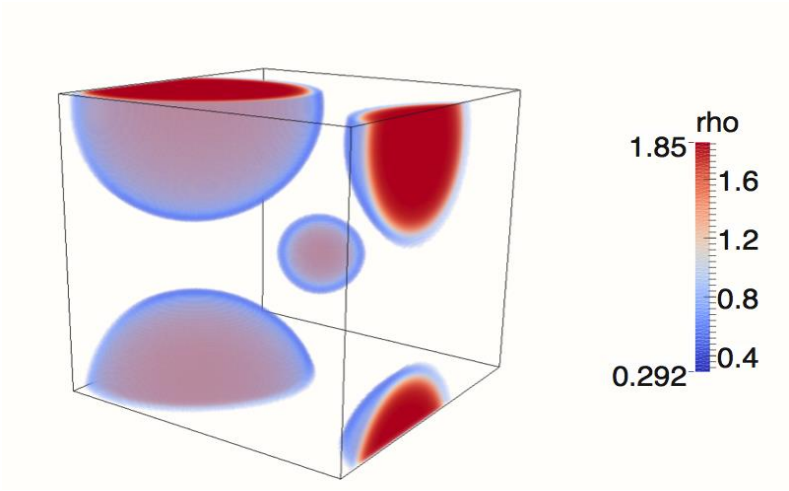


Computing results

Dynamics of phase separation on a 3D lattice with 128 x 128 x 128 nodes



150000 iterations

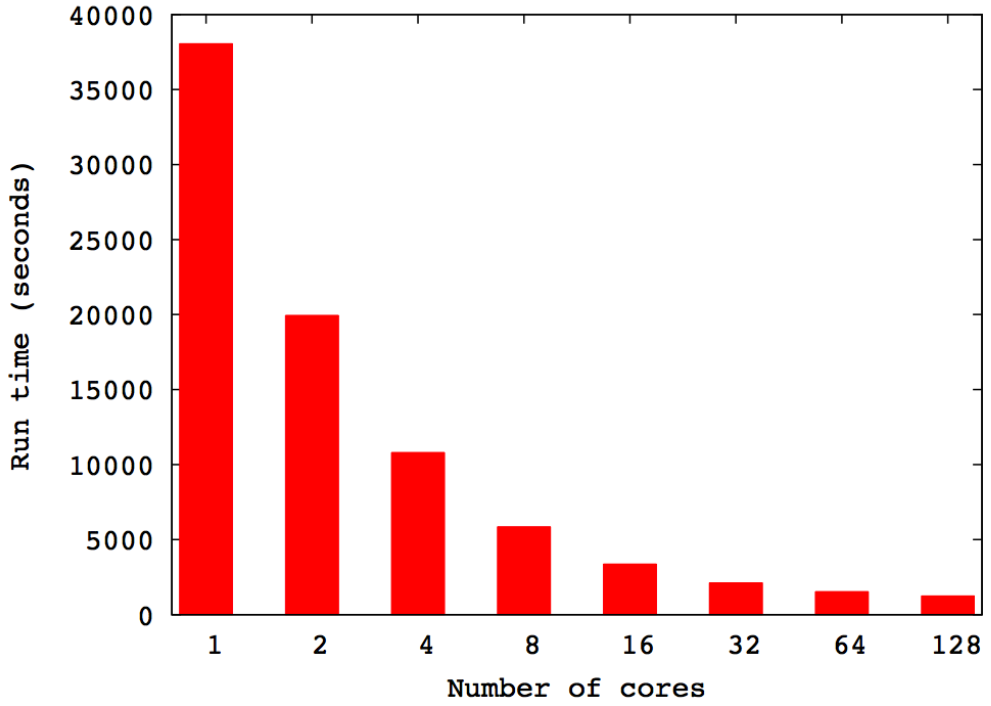


250000 iterations

Liquid drops separated at temperature T = 0.85.

Computing results

Performance studies



Typical dependence of the total run time vs. The number of cores used on the IBM Blue Gene / P system, when running the 2D lattice Boltzmann code for liquid – vapour system.

Conclusion

- Lattice Boltzmann models are based on the physics at the mesoscopic scale and provide an alternative to current computational fluid dynamics methods.
- LBM with Hermite polynomials can be used to study the dynamics of van der Waals fluids and phase separation of a isothermal system at various values of the temperature.
- Density profiles are not affected by the particular numerical scheme and interfaces are smooth. The interface width can be controlled by the surface tension
- The Minkowski functionals are appropriate for the description of morphology when we want to describe the domains that are formed during phase separation.

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Thank you !