Thermal Lattice Boltzmann models on GPGPUs

Sergiu Busuioc[1,2], Victor E. Ambruș[1,2] and Victor Sofonea[1]

[1]Center for Fundamental and Advanced Technical Research, Romanian Academy
Bd. Mihai Viteazul 24, R – 300223 Timişoara, Romania

[2]Department of Physics, West University of Timisoara
Bvd. Vasile Parvan nr. 4, Timisoara, Romania

HPC LEAP Workshop, Rome, 11/10/2016

Motivation

- Thermal flow simulations usually employ multiple distributions or an external coupling to the temperature field obeying the Fourier law.
- Our goal is to construct a quadrature-based Lattice Boltzmann model with a single distribution function able to simulate a liquid-vapour thermal flow.

Boltzmann Equation

- Evolution equation of the one-particle distribution function $f \equiv f(\mathbf{x}, \mathbf{p})$

$$\partial_t f + \frac{1}{m}\mathbf{p} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = J[f] = -\frac{1}{\tau}(f - f^{eq})$$

- Hydrodynamic moments of order N give macroscopic quantities:

$$\begin{aligned}
N =0: &\quad \text{number density:} && n = \int d^3p\, f, \\
N =1: &\quad \text{velocity:} && \mathbf{u} = \frac{1}{nm}\int d^3p\, f\, \mathbf{p}, \\
N =2: &\quad \text{temperature:} && T = \frac{2}{3n}\int d^3p\, f\, \frac{\boldsymbol{\xi}^2}{2m}, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}), \\
N =3: &\quad \text{heat flux:} && \mathbf{q} = \frac{1}{2m^2}\int d^3p\, f\, \boldsymbol{\xi}^2\, \boldsymbol{\xi}.
\end{aligned}$$

Gauss-Hermite quadratures

- f and $f^{eq} = \frac{n}{(2\pi T)^{D/2}} e^{-\frac{(\mathbf{p}-\mathbf{u})^2}{2T}}$ are projected on the orthogonal Hermite polynomials, e.g.(2D case):

$$f^{eq}(\mathbf{x}, t) = \frac{e^{-\mathbf{p}^2/2}}{2\pi} \sum_{\ell,m=0}^{\infty} \frac{1}{\ell! m!} \mathbf{a}^{eq}_{(\ell,m)}(\mathbf{x}, t) \mathcal{H}^{(\ell)}(p_x) \mathcal{H}^{(m)}(p_y)$$

$$\mathbf{a}^{eq}_{(\ell,m)}(\mathbf{x}, t) = \iint f^{eq}(\mathbf{x}, \mathbf{p}, t) \mathcal{H}^{(\ell)}(p_x) \mathcal{H}^{(m)}(p_y) dp_x dp_y$$

- The moments up to order N of f and f^{eq} are recovered by replacing the integrals by quadrature sums:

$$\int d^2p\, f(\mathbf{x}, \mathbf{p}, t)\, P(\mathbf{p}) = \sum_{k=1}^{Q\times Q} f_k(\mathbf{x}, t) P(\mathbf{p}_k), \quad Q = N + 1$$

- After discretization, f and f^{eq} are expressed as:

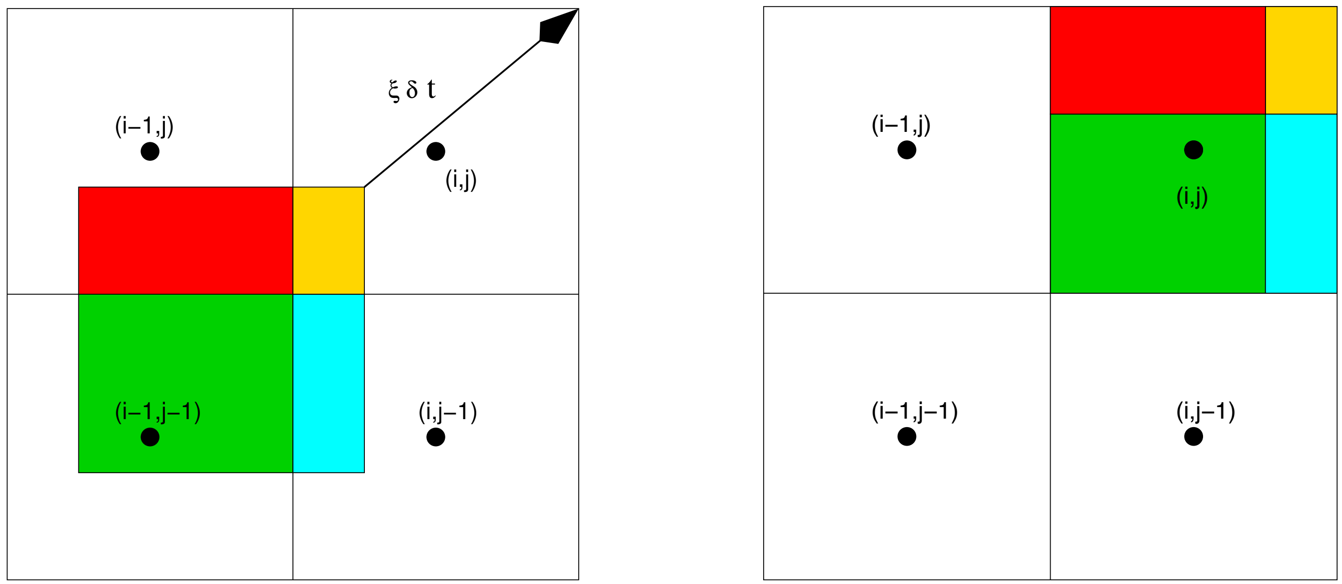
$$f^{eq}_k(\mathbf{x}, t) = w_k \sum_{\ell,m=0}^{N} \frac{1}{\ell! m!} \mathbf{a}^{eq}_{(\ell,m)}(\mathbf{x}, t) \mathcal{H}^{(\ell)}(p_{k,x}) \mathcal{H}^{(m)}(p_{k,y})$$

X. Shan, X. Yuan, H. Chen, J. Fluid. Mech 550 (2006) 413.

Off-lattice LB models: numerical scheme

$$\partial_t f_k + \frac{1}{m}\mathbf{p}_k \cdot \nabla f_k + \mathbf{F} \cdot \nabla_{\mathbf{p}_k} f_k = -\frac{1}{\tau}(f_k - f_k^{eq})$$

- Corner transport upwind*: information moves according to the direction of $\mathbf{p}$ from all surrounding cells (i.e. including diagonally, as below).
- Stability condition(CFL condition): $\frac{\delta t}{\delta s} \max_{k,\alpha}\{\frac{|p_{k,\alpha}|}{m}\} \leq 1$.

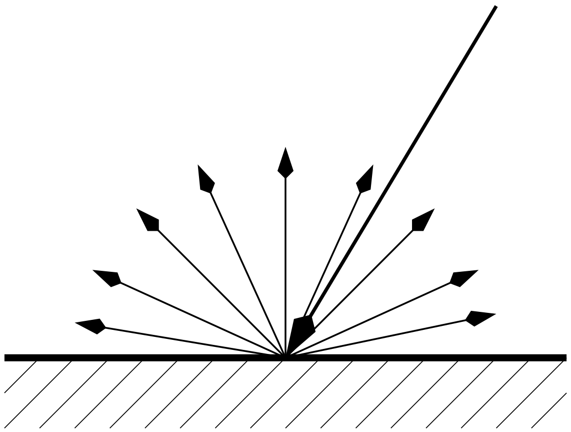


Images from T. Biciușcă, A. Horga, V. Sofonea, COMPTES RENDUS MECANIQUE 343 (10-11) 580-588 (2015)

* R. J. Leveque, SIAM J. Numer. Anal. **33** (2), 627 (1996)

Diffuse reflection boundary conditions

Reflected particles carry some information that belongs to the wall.



diffuse reflection

- The diffuse reflection boundary conditions require:

$$f(\mathbf{x}_{\mathrm{w}}, \mathbf{p}, t) = f^{(\mathrm{eq})}(n_{\mathrm{w}}, \mathbf{u}_{\mathrm{w}}, T_{\mathrm{w}}) \qquad (\mathbf{p} \cdot \chi < 0),$$

  where χ is the outwards-directed normal to the boundary.
- The density n_{w} is fixed by imposing zero flux through the boundary:

$$\int_{\mathbf{p}\cdot\chi>0} d^2p\, f\, (\mathbf{p} \cdot \chi) = -\int_{\mathbf{p}\cdot\chi<0} d^2p\, f^{(\mathrm{eq})}\, (\mathbf{p} \cdot \chi).$$

Force term $\mathbf{F} \cdot \nabla_\xi f$

- To get the van der Waals equation of state and the surface tension, one sets

$$\mathbf{F} = \frac{1}{\rho}\nabla(p^i - p^w) + k\nabla(\Delta\rho), \qquad p^i = \rho T \qquad p^w = \frac{3\rho T}{3-\rho} - \frac{9}{8}\rho^2$$

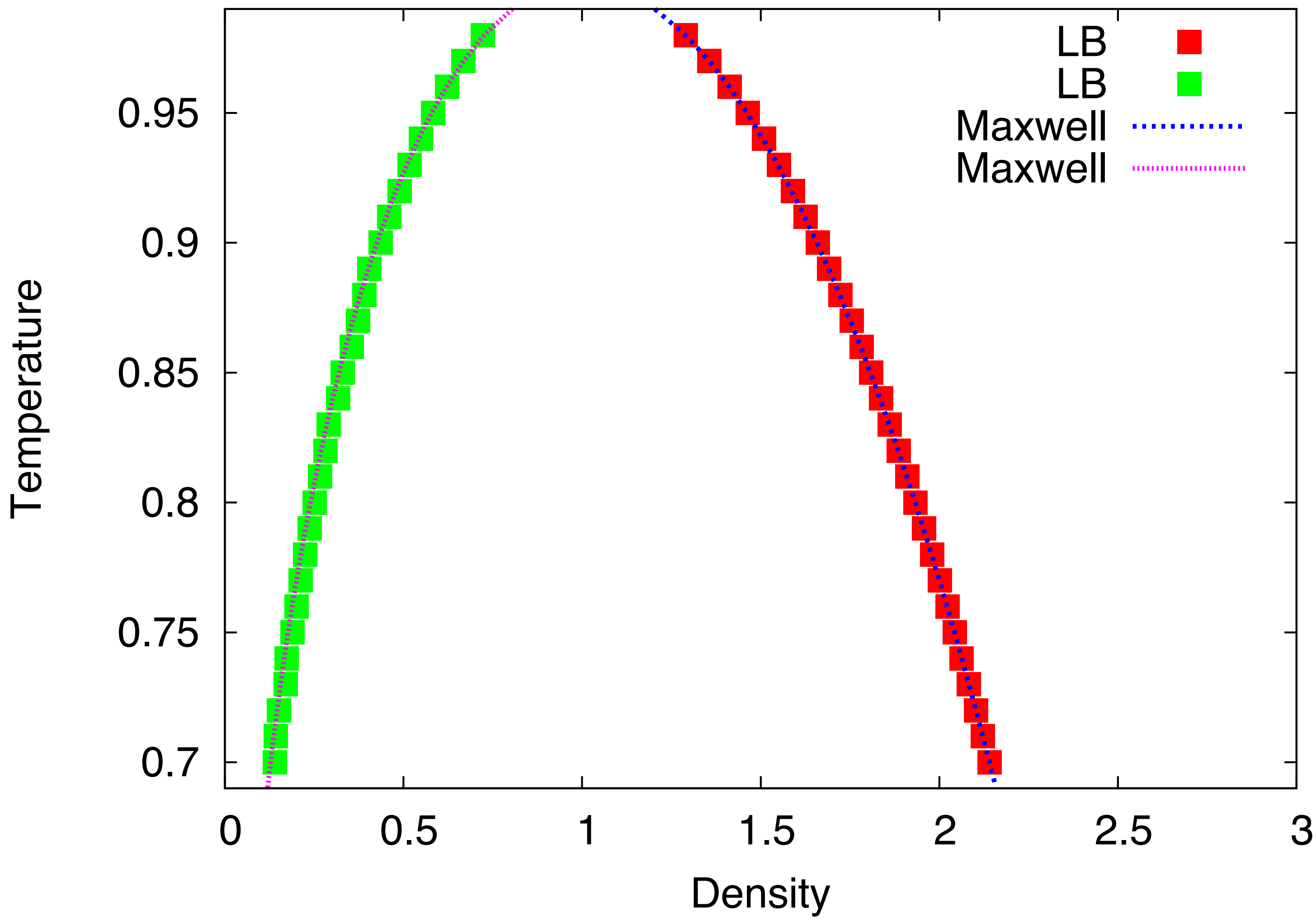
  with $\rho_c = 1$, $T_c = 1$. We used a 25-point stencil to evaluate $\nabla(\Delta\rho)$ and $\nabla(p^i - p^w)$.
- The components of the vector $\nabla_\xi f$ are calculated using the recurrence relation of the Hermite polynomials $\mathcal{H}^{(\ell+1)}(\xi) = \mathcal{H}^{(\ell)}(\xi) - \ell\mathcal{H}^{(\ell-1)}(\xi)$:

$$\frac{\partial f}{\partial p_\gamma} = -\frac{e^{-\mathbf{p}^2/2}}{2\pi}\sum_{\ell,m=0}^{\infty}\frac{1}{\ell!m!}\,\boldsymbol{a}_{(\ell,m)}(\boldsymbol{x},t)\left[\delta_{\gamma x}\mathcal{H}^{(\ell+1)}(p_x)\mathcal{H}^{(m)}(p_y)+\delta_{\gamma y}\mathcal{H}^{(\ell)}(p_x)\mathcal{H}^{(m+1)}(p_y)\right]$$

$$\frac{\partial f_k}{\partial p_{k,\gamma}} = -w_k\sum_{\ell,m=0}^{N}\frac{1}{\ell!m!}\,\boldsymbol{a}_{(\ell,m)}(\boldsymbol{x},t)\left[\delta_{\gamma x}\mathcal{H}^{(\ell+1)}(p_{k,x})\mathcal{H}^{(m)}(p_{k,y})+\delta_{\gamma y}\mathcal{H}^{(\ell)}(p_{k,x})\mathcal{H}^{(m+1)}(p_{k,y})\right]$$

$$\boldsymbol{a}_{(\ell,m)}(\boldsymbol{x},t) = \sum_{k=1}^{Q\times Q} f_k(\boldsymbol{x},t)\mathcal{H}^{(\ell)}(p_{k,x})\mathcal{H}^{(m)}(p_{k,y})$$

Phase diagram



Application

Phase separation between parallel plates.

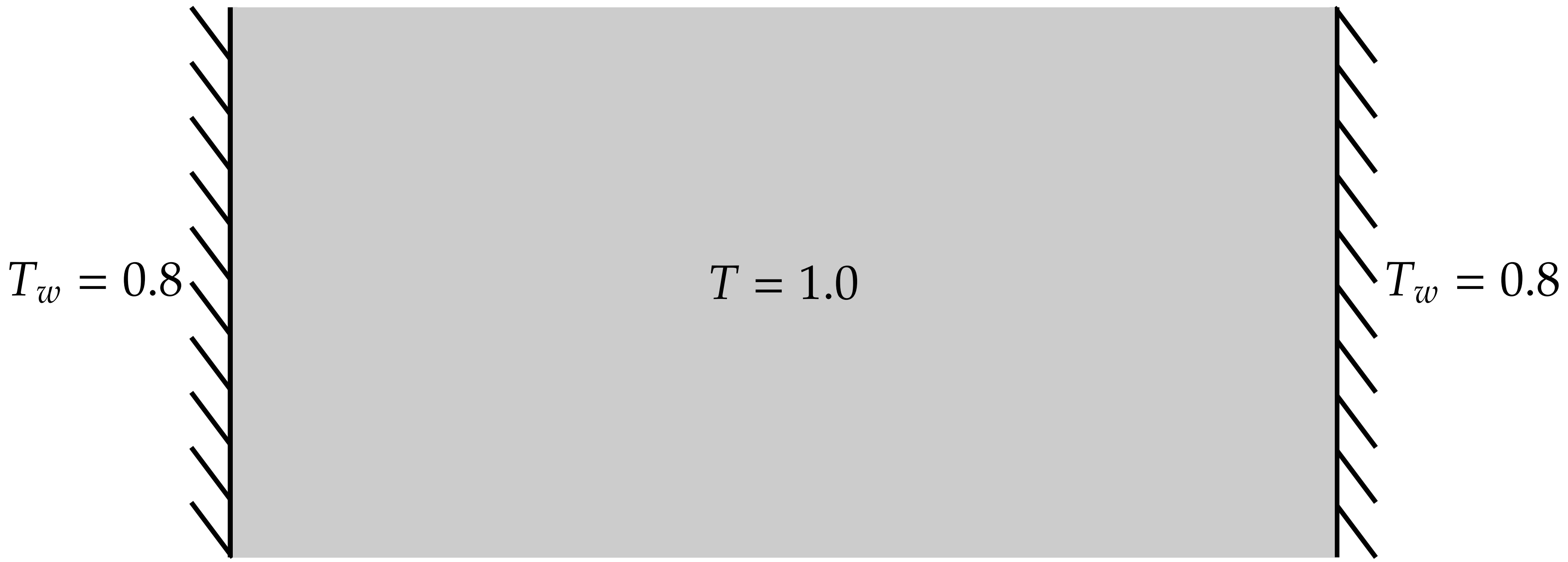


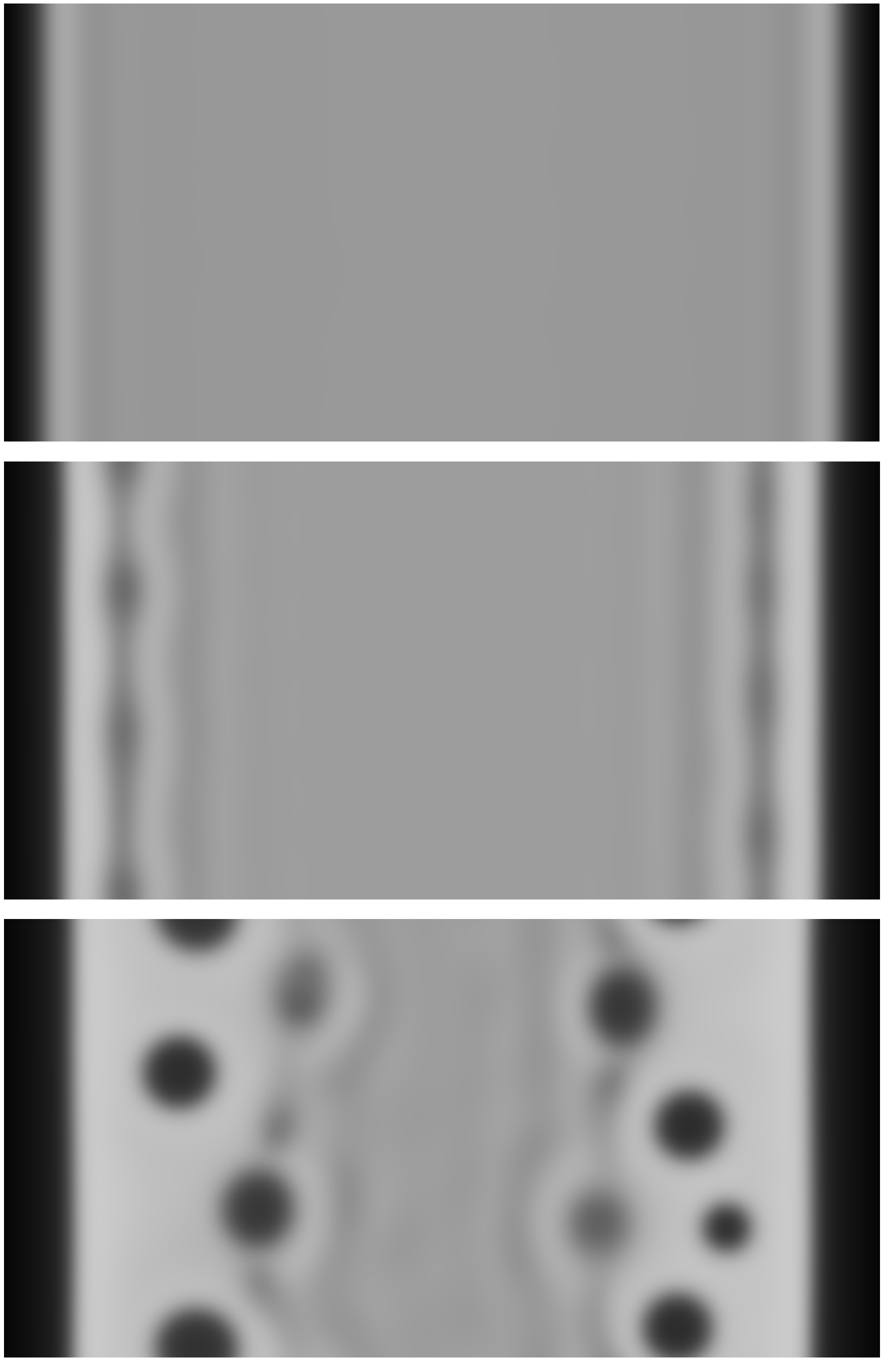
Figure : Initial setup.

Application

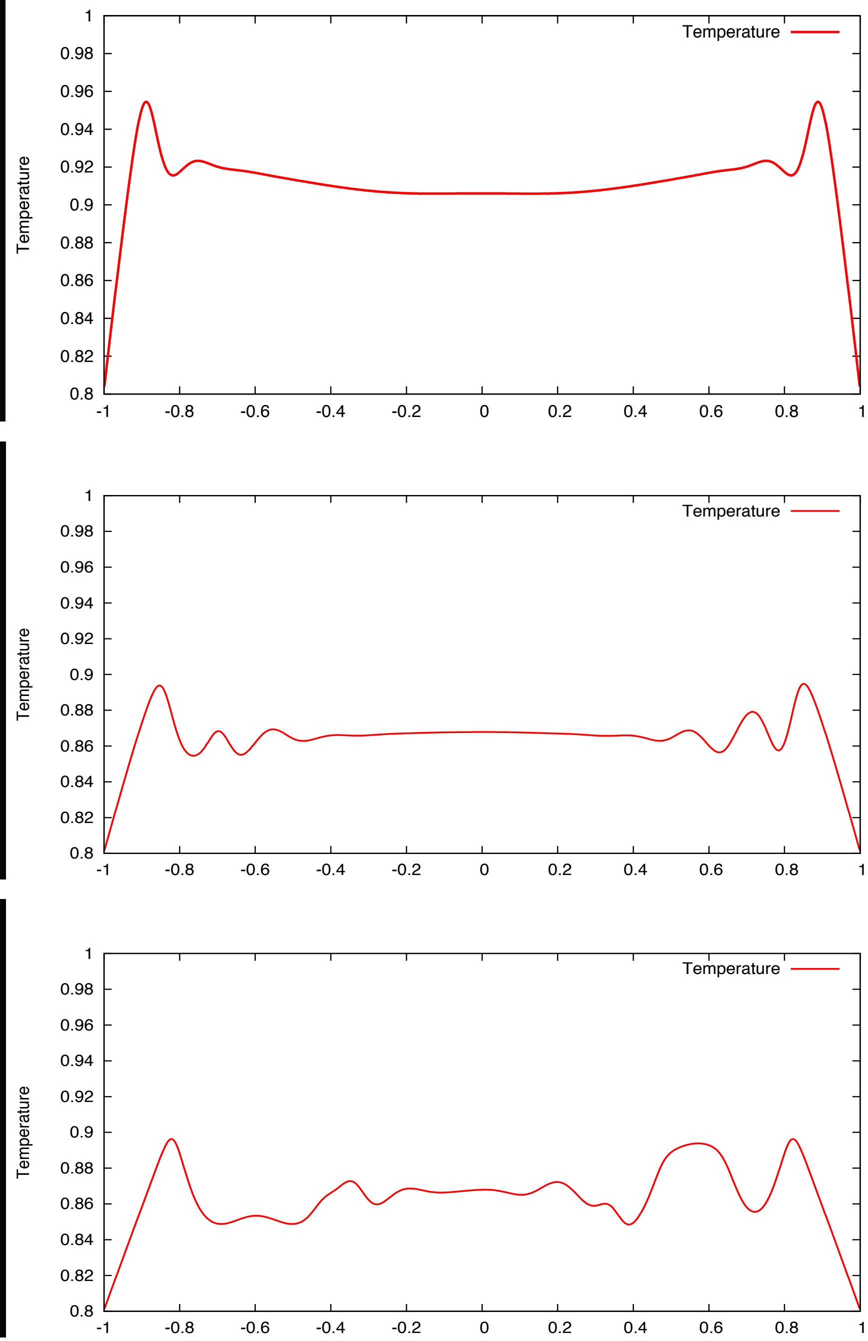
Phase separation between parallel plates.

Figure : Initial setup.

Density profile



Temperature



Application

Heat pump.

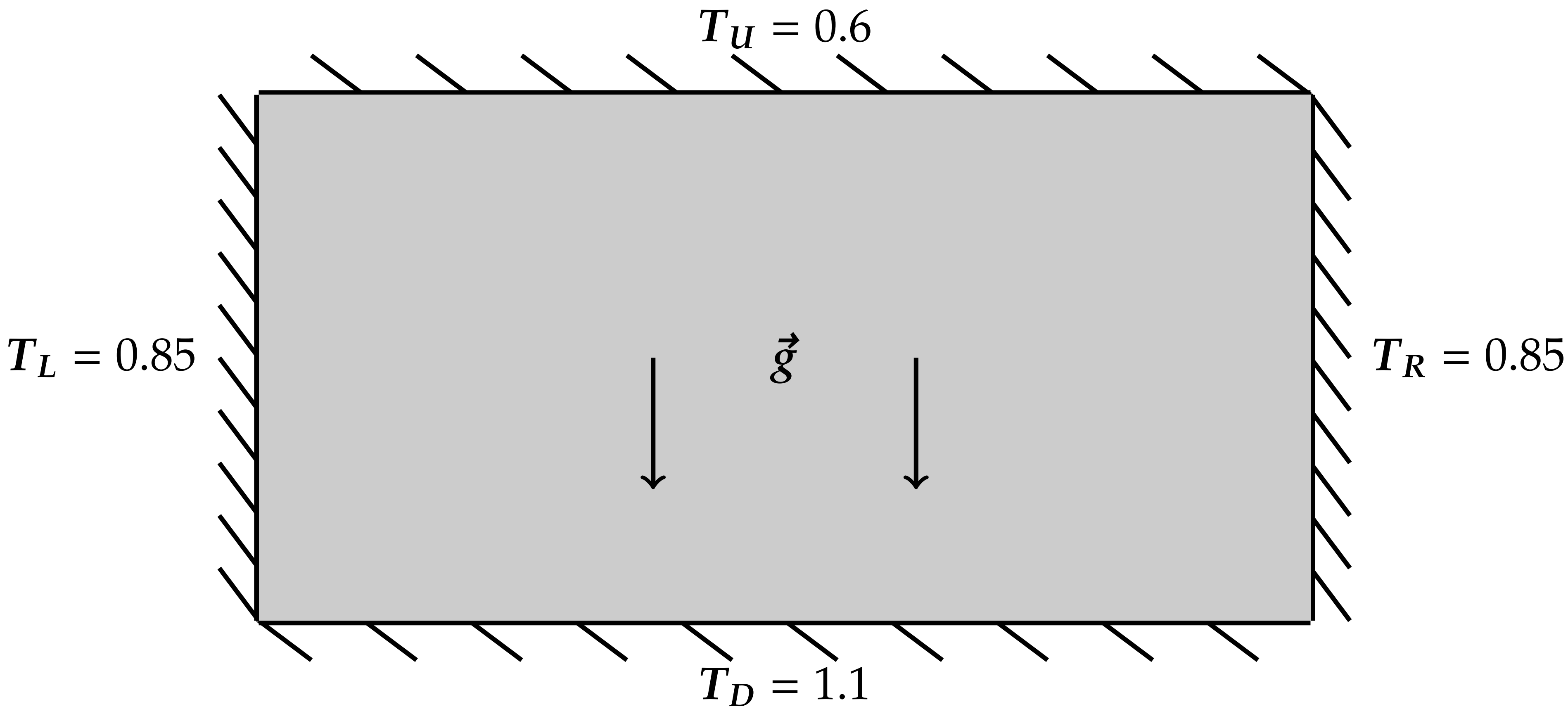


Figure : Initial setup.

Nvidia K40c

Conclusion

- Lattice Boltzmann (LB) simulations provide a convenient tool for the investigation of interface phenomena in liquid-vapour systems.
- The single distribution function of order $N = 4$ is able to tackle liquid-vapour thermal flow.
- Temperature fluctuations due to spurious currents are below 1% in the stationary state.
- The simulations were performed using CUDA C programming library on a desktop computer with an NVIDIA Tesla K40 Graphics Processing Unit (2880 Cores, 12 GB memory).

- This work is supported by the grants from the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, projects PN-II-RU-TE-2014-4-2910, PN-II-ID-PCE-2011-3-0516 and PN-II-ID-JRP-2011-2-0060.