Simulation of liquid-vapour phase separation on GPUs using Lattice Boltzmann models with off-lattice velocity sets

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construction of LB models: Shan, Yuan and Chen, J. Fluid Mechanics 550 (2006) 413

- projection of the distribution function $f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ on the orthogonal basis in the momentum space formed up by the tensor Hermite polynomials $\boldsymbol{\mathcal{H}}^{(n)}(\boldsymbol{\xi})$:

$$f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \boldsymbol{\mathcal{H}}^{(n)}(\boldsymbol{\xi})$$

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

- a similar projection is performed for the equilibrium distribution function

$$f^{eq} \equiv f^{eq}[\boldsymbol{\xi}; \rho(\boldsymbol{x}, t), \boldsymbol{u}(\boldsymbol{x}, t), T(\boldsymbol{x}, t)] = \rho / \sqrt{(2\pi T)^{D/2}} \exp\left[-(\boldsymbol{\xi} - \boldsymbol{u})^2 / 2T\right]$$

- the derivative $\nabla_{\xi} f$ that appears in the force term $F = -\boldsymbol{g} \cdot \nabla_{\xi} f$ of the Boltzmann equation is calculated using the derivatives of Hermite polynomials :

$$\nabla_{\xi} f = \sum_{n=0}^{\infty} \frac{1}{n} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \nabla_{\xi} \left[\omega(\boldsymbol{\xi}) \boldsymbol{\mathcal{H}}^{(n)}(\boldsymbol{\xi})\right] = -\omega(\boldsymbol{\xi}) \sum_{n=0}^{\infty} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x}, t) \boldsymbol{\mathcal{H}}^{(n+1)}(\boldsymbol{\xi})$$

instead of the widely used approximation $\nabla_{\xi} f \simeq \nabla_{\xi} f^{eq} = -\frac{1}{k_B T} (\boldsymbol{\xi} - \boldsymbol{u}) f^{eq}$

- the resulted Boltzmann equation containing f, feq and $\nabla_\xi f$ projected on the tensor Hermite polynomials is truncated up to order N
- the momentum space is discretized using the Gauss-Hermite quadrature of order $Q = N+1$ on each Cartesian axis; in the $2D$ space this procedure gives the *HLB model* of order N with $K = Q \times Q$ vectors $\boldsymbol{\xi}_k$ and the corresponding weights w_k

$$f^N(\boldsymbol{x},\boldsymbol{\xi},t) \simeq \omega(\boldsymbol{\xi}) \sum_{n=0}^{N} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x},t)\, \boldsymbol{\mathcal{H}}^{(n)}(\boldsymbol{\xi}) \quad , \quad f_k \equiv f_k^N(\boldsymbol{x},t) = \frac{w_k}{\omega(\boldsymbol{\xi}_k)} f^N(\boldsymbol{x},\boldsymbol{\xi}_k,t)$$

- the functions f_k evolve on a $2D$ square lattice according to ($\partial_t = \partial/\partial_t$, $\partial_\gamma = \partial/\partial_{x_\gamma}$)

$$\partial_t f_k + \xi_{k,\gamma}\partial_\gamma f_k = -\frac{1}{\tau}\left[f_k - f_k^{eq}\right] + F_k \qquad , \qquad 1 \le k \le K$$

- after solving these equations one can find the evolution of all $2D$ moments of f^N up to order $(s_x + s_y) \le N$:

$$\mathcal{M}_{\alpha_1\alpha_2....\alpha_s} \equiv \int f^N \xi_{\alpha_1}\xi_{\alpha_2}\ldots\xi_{\alpha_n} = \sum_{k=1}^{N} f_k\, \xi_{k,\alpha_1}\xi_{k,\alpha_2}\ldots\xi_{k,\alpha_n} = \sum_{k=1}^{N} f_k\, \xi_{k,x}^{s_x}\xi_{k,y}^{s_y}$$

- for isothermal systems, the Navier-Stokes equations are recovered for $N = 3$
- the widely used value $N = 2$ is sufficient only in the incompressible limit

- according to Shan, Yuan and Chen, J. Fluid Mechanics 550 (2006) 413, the expressions of f^{eq} and F_k up to order $N = 3$ are:

$$
\begin{aligned}
f_k^{eq} &= w_k\rho\Big\{1 + \boldsymbol{\xi}_k\cdot\boldsymbol{u} + \frac{1}{2}\Big[(\boldsymbol{\xi}_k\cdot\boldsymbol{u})^2 - u^2 + (T-1)(\xi_k^2-2)\Big] \\
&+ \frac{\boldsymbol{\xi}_k\cdot\boldsymbol{u}}{6}\Big[(\boldsymbol{\xi}_k\cdot\boldsymbol{u})^2 - 3u^2 + 3(T-1)(\xi_k^2-4)\Big]\Big\} \\
F_k &= w_k\rho\Big\{\boldsymbol{\xi}_k\cdot\boldsymbol{g} + (\boldsymbol{\xi}_k\cdot\boldsymbol{u})(\boldsymbol{\xi}_k\cdot\boldsymbol{u}) - \boldsymbol{g}\cdot\boldsymbol{u} + \frac{1}{2\rho}\boldsymbol{a}^2\Big[(\boldsymbol{\xi}_k\cdot\boldsymbol{g})\boldsymbol{\mathcal{H}}^{(2)}(\boldsymbol{\xi}_k) - 2\boldsymbol{g}\boldsymbol{\xi}_k\Big]\Big\}
\end{aligned}
$$

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

$$
\boldsymbol{g} = \frac{1}{\rho}\boldsymbol{\nabla}(p^i - p^w) + \kappa\boldsymbol{\nabla}(\Delta\rho) \qquad p^i = \rho T \qquad p^w = \frac{3\rho T}{3-\rho} - \frac{9}{8}\rho^2
$$

a 25 point stencil is used to compute $\boldsymbol{\nabla}(p^i - p^w)$ and $\boldsymbol{\nabla}(\Delta\rho)$ in $2D$:

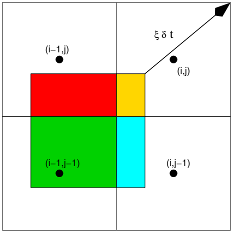
M.Patra and M.Karttunen, Numer. Methods. Partial Differ. Eqs. **22** (2006) 936

S.Leclaire, M. El-Hachem, J.Y.Trepanier, M.Reggio, J. Sci. Comput. **59** (2014) 545

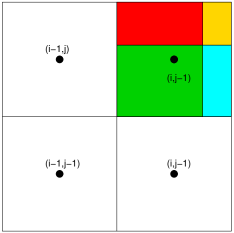
- the roots of the Hermite polynomials of order $Q \geq 4$ are irrational
  $\Rightarrow$ *HLB* models of order $N \geq 3$ ($Q \geq 4$) in 2*D* or 3*D* are off-lattice
- other (recently developed) LB models based on Gauss quadratures based on off-lattice momentum sets:
  - *SLB* (DSFD 2012 Bangalore) – Laguerre and Legendre polynomials (these models use the spherical coordinate system in the momentum space)
  - *LLB* (DSFD 2013, Yerevan) – Laguerre polynomials (Cartesian system)
  - *HHLB* (DSFD 2014, Paris) – half-range Hermite polynomials
- the widely-used collision streaming scheme is designed for on-lattice LB models – specific treatment of the momentum set, abscissas, weights and the boundary conditions is required (results reported by Philippi et al., Karlin et al., Ansumali et al., as well as many other groups)
- other schemes (ISLB - Interpolation Supplemented LB), FDLB (Finite Difference LB), projection schemes involving Flux Limiters, etc., frequently exhibit stability problems when applied to 2*D* or 3*D* problems
- $\Rightarrow$ exploration of the literature related to hyperbolic equations in 2*D* or 3*D*

Corner Transport Upwind (CTU) schemes for hyperbolic equations in $2D$ and $3D$

- the CTU schemes belong to the family of Finite volume schemes (FV)
- these schemes extend the $1D$ upwind scheme (S.K.Godunov, 1959) to $2D$ and $3D$
- introduced in :
  - P. Colella, Multidimensional Upwind Methods for Hyperbolic Conservation Laws
    J. Comput. Phys. **87** (1990) 171
  - R.J. Leveque, High-Resolution conservative algorithms for advection in incompressible flow
    SIAM J. Numer. Anal. **33** (1996) 627
- 1^{st} and 2^{nd} order versions of the CTU scheme (the second one involves flux limiters)
- textbooks at Cambridge University Press :
  - R.J. Leveque, Finite Volume Methods for Hyperbolic Problems (2002)
  - J.A. Trangenstein, Numerical Solution of Hyperbolic Partial Differential Equations (2007)
- the 1^{st} order CTU scheme - already used in the Volumetric LB models, especially for non-uniform meshes
  - F. Nannelli and S.Succi, J.Stat.Phys. **68** (1992) 401
  - H. Chen, Phys. Rev. E **58** (1998) 3955
  - R. Zhang, H. Chen, Y. Qian and S. Chen, Phys. Rev. E **63** (2001) 056705
  - M. Sbragaglia and K. Sugiyama, Phys. Rev. E **82** (2010) 046709
  - D.M. Bond, W. Wheatley, M.N. Macrossan, M. Goldsworthy, J. Comput. Phys **259** (2014) 175



time = t



time = $t + \delta t$

P. Colella

Multidimensional Upwind Methods for Hyperbolic Conservation Laws

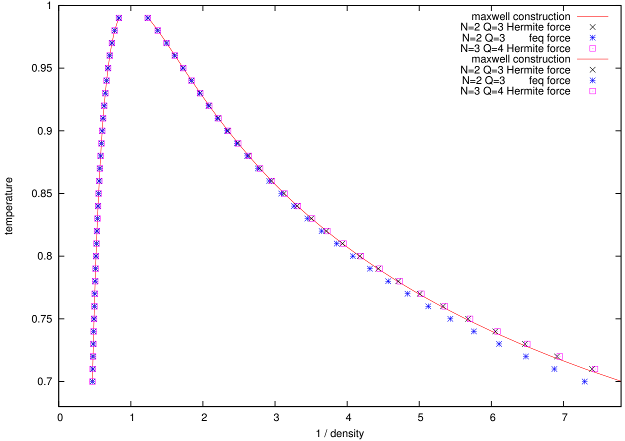
J. Comput. Phys. **87** (1990) 171

- the CTU scheme allows one to solve $\partial_t f + \xi_\gamma \partial_\gamma f = 0$
- when $\xi_x > 0$ and $\xi_y > 0$, the information is transported across the lower left corner of the cell (i, j)
- the distribution function $f \equiv f(\xi)$ in cell (i, j) at $t + \delta t$ results from partial contributions from the four cells that share the corner, i.e., (i, j), $(i-1, j)$, $(i-1, j-1)$, $(i, j-1)$
- each contribution is proportional to the colored area transported through the corner during the interval δt :

$$f_{i,j}^{t+\delta t} (\delta s)^2 = f_{i,j}^{t}(\delta s - \xi_x \delta t)(\delta s - \xi_y \delta t) + f_{i-1,j-1}^{t}(\xi_x \delta t)(\xi_y \delta t) + f_{i-1,j}^{t}(\xi_x \delta t)(\delta s - \xi_y \delta t) + f_{i,j-1}^{t}(\delta s - \xi_x \delta t)(\xi_y \delta t)$$

- the CFL condition $\max \left\{ |\xi_x| \delta t \, , \, |\xi_y| \delta t \right\} \leq \delta s$ ensures that only the nearest neighbours of cell (i, j) contribute to $f^{t+\delta t}$

- Tesla M2090 card from NVIDIA : 6 GB memory, 512 CUDA cores
- use of the shared memory to calculate the force term
- size of the $2D$ liquid - vapour system simulated on a single M2090 card: 4096×4096 nodes
- the HLB model of order $N = 3$ has 16 distribution functions in each node
  $\Rightarrow$ more than 16,000,000 values to be updated at each time step
- lattice spacing $\delta s = 1/128$, time step $\delta t = 10^{-4}$
- relaxation time $\tau = 10^{-3} \Rightarrow$ Navier-Stokes level
- the values of Minkowski functionals (total area $\mathcal{A}$ of the drops, total perimeter $\mathcal{P}$ and number of drops $\mathcal{N}$) calculated using the algorithm described in K. Michielsen and H. De Raedt, Phys. Reports **347** (2001) 461

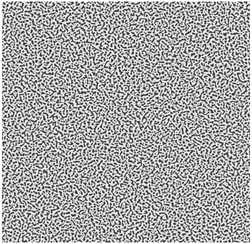


Navier Stokes
Kn negligible

relaxation time	$\tau = 0.001$
force term	relative error %
liquid phase	T=0.70
N2-Hermite	0.01140
N2-feq	0.05303
N3-Hermite	0.01593
gas phase	T=0.70
N2-Hermite	1.46506
N2-feq	7.06494
N3-Hermite	2.04941

$\Rightarrow$ the "Hermite" force term $\boldsymbol{\nabla}_{\xi} f \simeq -\omega(\boldsymbol{\xi}) \sum_{n=0}^{N-1} \frac{1}{n!} \boldsymbol{a}^{(n)}(\boldsymbol{x},t) \boldsymbol{\mathcal{H}}^{(n+1)}(\boldsymbol{\xi})$ gives smaller errors in the phase diagram than the "feq" force term $\boldsymbol{\nabla}_{\xi} f \simeq -\frac{1}{k_B T} (\boldsymbol{\xi} - \boldsymbol{u}) f^{eq}$ even for small values of Kn (or τ) !
– this was observed also in the case of Poiseuille flow – presentation of V.Ambruş at DSFD 2014

Phase separation $\rho_{mean} = 0.90$



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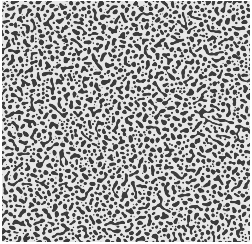

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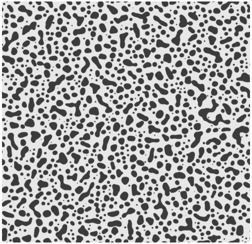

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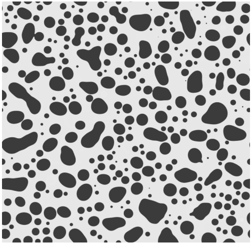

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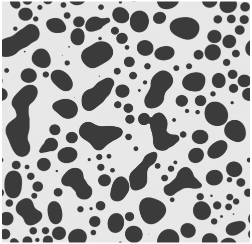

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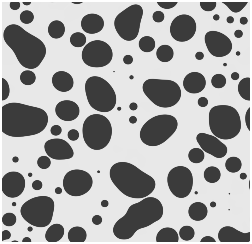
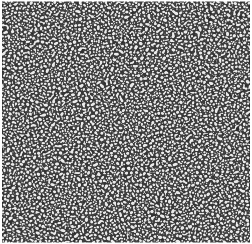


iter = 2000000

Phase separation $\rho_{mean} = 1.30$



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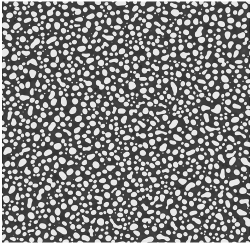

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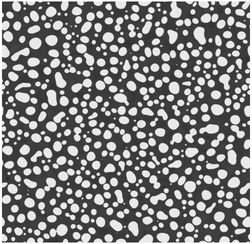

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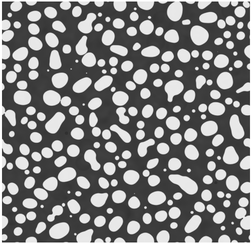

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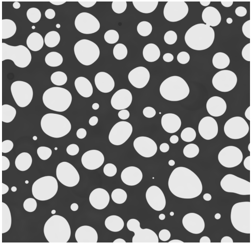

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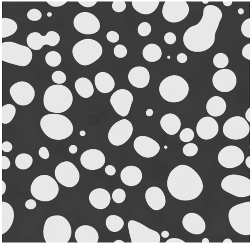
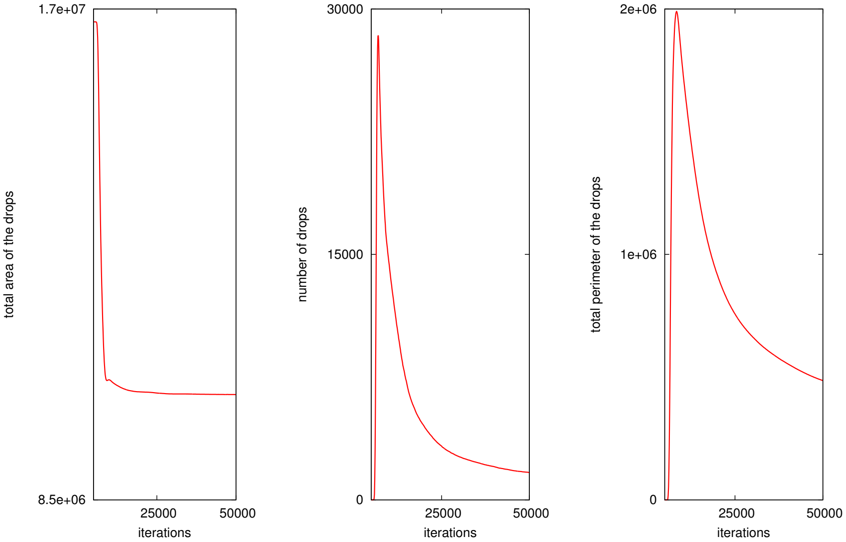
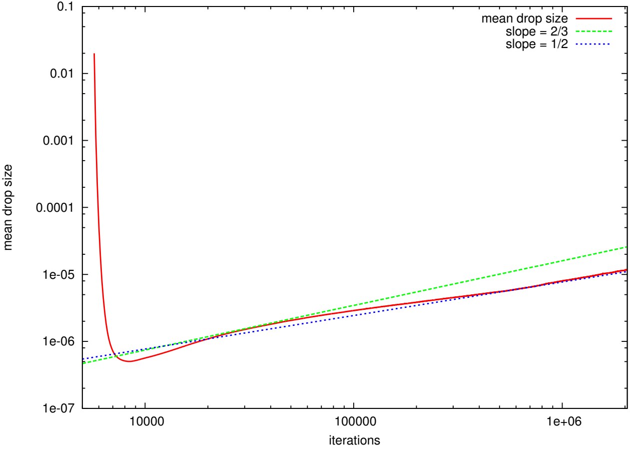


iter = 600000

$\rho_{mean} = 0.90$: Evolution of Minkowski functionals



$\rho_{mean} = 0.90$: Evolution of the mean drop size $1/\mathcal{P}$



crossover from the exponent 2/3 to 1/2

Conclusion

- the liquid-vapour phase separation was investigated using the HLB model of order $N = 3$, with 16 off-lattice velocity vectors
- the Corner Transport Upwind Scheme works well for off-lattice LB models
- use of the "Hermite" force term gives smaller errors in the phase diagram than the "feq" force term
- evidence of the growth exponents 2/3 and 1/2 during the liquid-vapour phase separation on a simulation domain with 4096×4096 nodes
- a $3D$ code that will run on a multi-GPU system is under development

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