Lattice Boltzmann approach to liquid - vapour separation

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Flowing Matter 2016, Porto (Portugal)

The Boltzmann equation

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

$$\partial_t f + \frac{1}{m}\mathbf{p} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = J[f].$$

- The collision operator $J[f]$ is often approximated by:

$$J_{\mathrm{BGK}}[f] = -\frac{1}{\tau}(f - f^{(\mathrm{eq})}).$$

where $\tau \sim \mathrm{Kn}/n$ is the relaxation time and $f^{(\mathrm{eq})}$ is the equilibrium distribution (D is the number of space dimensions):

$$f^{(\mathrm{eq})}(\mathbf{x}, \mathbf{p}, t) = \frac{n}{(2\pi m K_B T)^{\frac{D}{2}}} \exp\left[-\frac{(\mathbf{p} - m\mathbf{u})^2}{2mK_B T}\right].$$

Moments of the distribution function f

- Macroscopic properties given as moments of order N of f:

$N = 0$: number density: $$n = \int d^D p f,$$

$N = 1$: velocity: $$\mathbf{u} = \frac{1}{nm} \int d^D p f \, \mathbf{p},$$

$N = 2$: temperature: $$T = \frac{2}{Dn} \int d^D p f \, \frac{\boldsymbol{\xi}^2}{2m}, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}),$$

viscous tensor: $$\sigma_{\alpha\beta} = \int d^D p \, \frac{\xi_\alpha \xi_\beta}{m} f - nT\delta_{\alpha\beta},$$

$N = 3$: heat flux: $$\mathbf{q} = \int d^D p f \, \frac{\boldsymbol{\xi}^2}{2m} \frac{\boldsymbol{\xi}}{m}.$$

Gauss-Hermite Lattice Boltzmann models (1)

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 $\boldsymbol{\mathcal{H}}^{(n)}(\boldsymbol{\xi})$:

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

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

- A similar projection is performed for the equilibrium distribution function

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

- ... and for the derivative $\nabla_{\xi} f$ in the force term:

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

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

Gauss-Hermite Lattice Boltzmann models (2)

- In practice, f and $f^{(eq)}$ are 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 2D, this procedure gives the *HLB* model of order N with $K = Q \times Q$ vectors $\boldsymbol{\xi}_k$ and the corresponding weights w_k

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

- The set of "distribution functions" $\{f_k\}$ evolve on a 2D square lattice:

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

- After solving these equations one can find the evolution of all 2D moments of f^N up to order $s_\alpha \le N$:

$$\mathcal{M}_{n_x,n_y} \equiv \int f^N \xi_x^{n_x} \xi_y^{n_y} d\xi_x d\xi_y = \sum_{k=1}^{N} f_k \, \xi_{k,x}^{n_x} \xi_{k,y}^{n_y}.$$

- 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

Gauss-Hermite Lattice Boltzmann models (3)

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

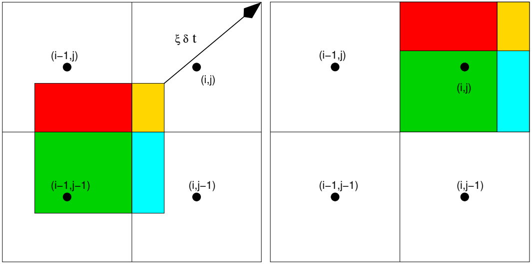
$$
\begin{aligned}
f_k^{(\mathrm{eq})} =& w_k \rho \left\{ 1 + \boldsymbol{\xi}_k \cdot \boldsymbol{u} + \frac{1}{2} \left[(\boldsymbol{\xi}_k \cdot \boldsymbol{u})^2 - u^2 + (T-1)(\xi_k^2 - 2) \right] \right. \\
& \left. + \frac{\boldsymbol{\xi}_k \cdot \boldsymbol{u}}{6} \left[(\boldsymbol{\xi}_k \cdot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

- 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 Corner Transport Upwind scheme



$$f_{k;(i,j)}^{t+\delta t} = \frac{1}{(\delta s)^2}\Big[f_{k;(i,j)}^{t}(\delta s - \xi_x \delta t)(\delta s - \xi_y \delta t) + f_{k;(i-1,j-1)}^{t}(\xi_x \delta t)(\xi_y \delta t) + f_{k;(i-1,j)}^{t}(\xi_x \delta t)(\delta s - \xi_y \delta t) + f_{k;(i,j-1)}^{t}(\delta s - \xi_x \delta t)(\xi_y \delta t)\Big]$$

CFL condition: $\max_k \{ |\xi_{k,x}|\delta t\,,\, |\xi_{k,y}|\delta t \} \le \delta s$

collision - streaming scheme: $\xi_x \delta t = \xi_y \delta t = \delta s$

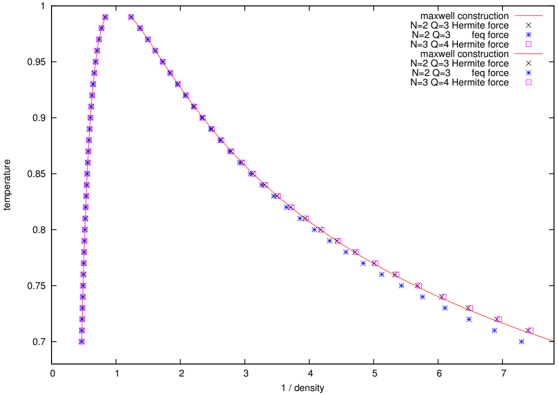
P. Colella, J. Comput. Phys. 87 (1990) 171 , T. Biciuşcă, A. Horga, V. Sofonea, Comptes Rendus Mech. 343 (2015) 580

Phase separation - implementation on GPU systems

- 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 256,000,000 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, Physics Reports **347** (2001) 461

Liquid - vapour phase diagram



Navier Stokes
Kn negligible

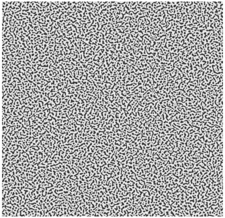
relaxation time $\tau = 0.001$

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

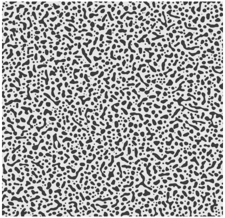
⇒ The "Hermite" force term gives smaller errors in the phase diagram than the "$f^{(\mathrm{eq})}$" force term $\nabla_\xi f \simeq \nabla_\xi f^{(\mathrm{eq})}$ even for small values of Kn (or τ) !

T. Biciuşcă, A. Horga, V. Sofonea, Comptes Rendus Mech. 343 (2015) 580

Phase separation $\rho_{mean} = 0.90$



iter = 20000



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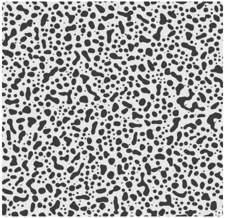

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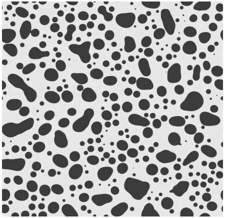

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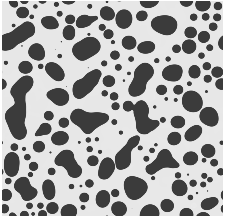

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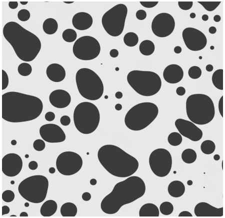
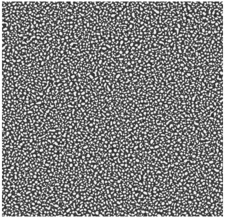


iter = 2000000

Phase separation $\rho_{mean} = 1.30$



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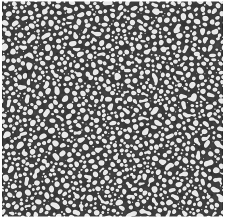
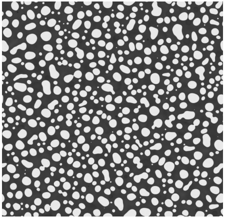
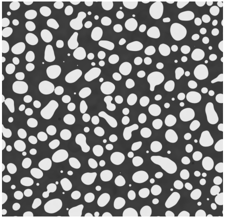


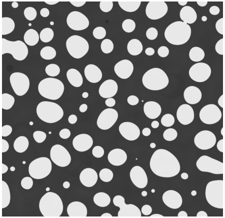
iter = 50000



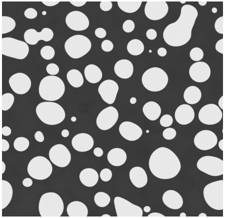
iter = 100000



iter = 200000

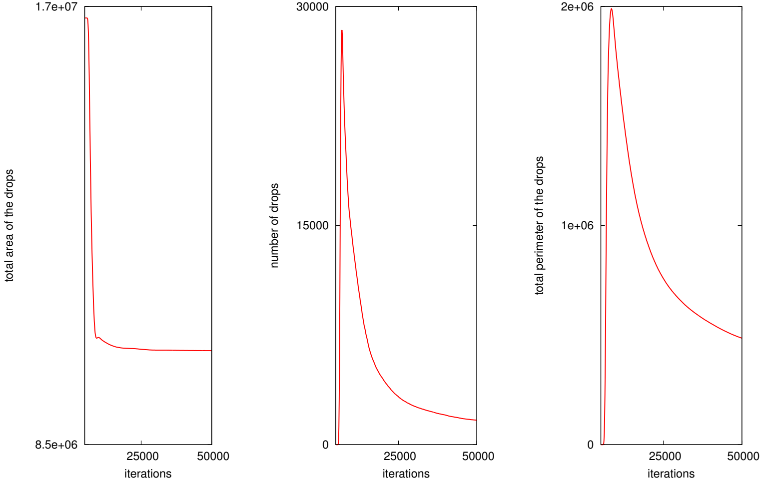


iter = 500000

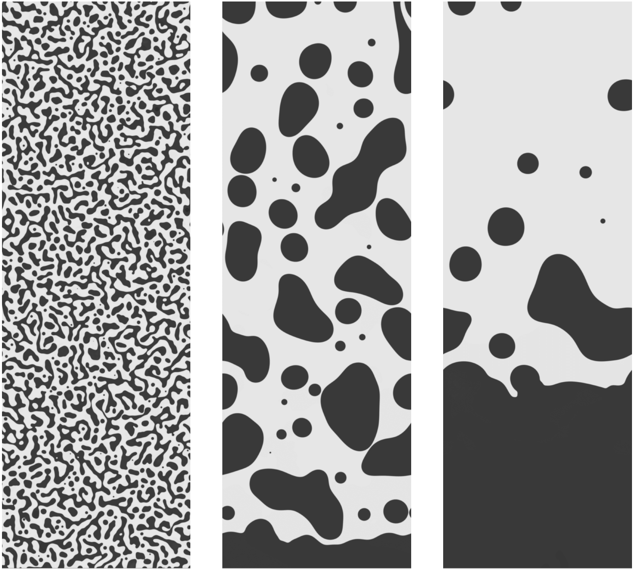


iter = 600000

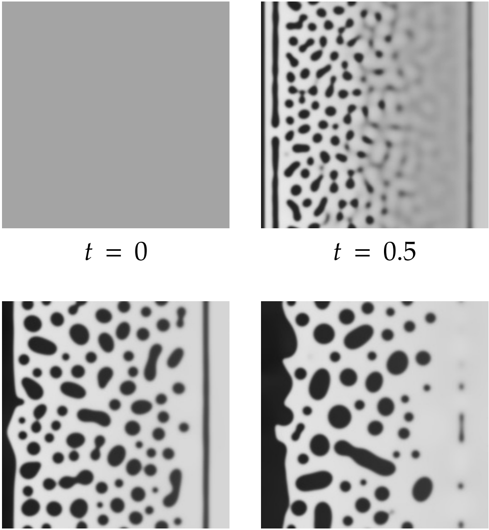
$\rho_{mean} = 0.90$: Evolution of Minkowski functionals



2D phase separation under gravity



Phase separation in 2D : linear temperature gradient



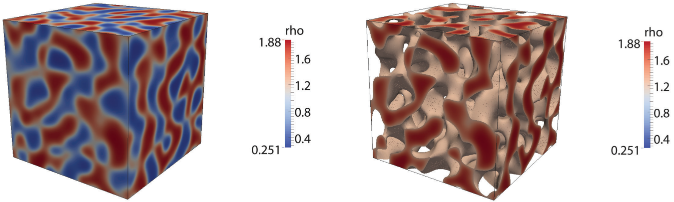
$t = 0$ $t = 0.5$ $t = 1.0$ $t = 1.5$

Lattice size:
256×256 nodes

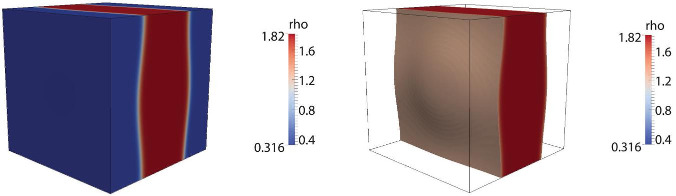
$T_{left\_wall} = 0.80$
$T_{right\_wall} = 0.90$
$\rho_{mean} = 0.80$

The liquid phase heads towards the cold wall

$T = 0.85$: Liquid - vapour separation on a 3D lattice with 128 x 128 x 128 nodes



iter = 10000

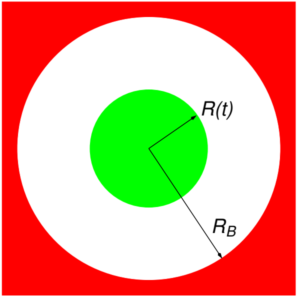


iter = 160000

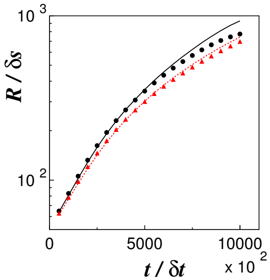
2D cavitation – Rayleigh Plesset equation

Rayleigh-Plesset equation in 2D : $r_\infty = R_B$ (boundary radius)

$$\ln\left(\frac{r_\infty}{R}\right)\left[\left(\frac{dR}{dt}\right)^2 + R\frac{d^2R}{dt^2}\right] - \frac{1}{2}\left[1 - \frac{R^2}{r_\infty^2}\right]\left(\frac{dR}{dt}\right)^2 + \frac{\sigma}{\rho_L R} + \frac{2\mu_L}{\rho_L R}\frac{dR}{dt} = \frac{p_R(t) - p_\infty(t)}{\rho_L}.$$



$t = 0$



$t = 5.0$

square lattice

$L \times L$ nodes

L = 2048

L = 4096

$T = 0.80$

$\rho_L = 1.932703$

$\rho_V = 0.244658$

$\rho_{r>R_B} = 1.923$

lines: RP solution

LB results : dots

T. Biciuşcă, V. Sofonea, G. Gonnella, A. Lamura, submitted to Physical Review E (2015)

2D cavitation – shear flow

Capillary number

$Ca = \frac{\mu_L \dot{\gamma} \hat{R}}{\sigma}$

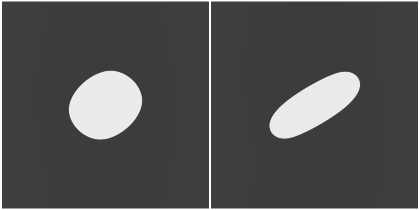
average bubble radius

$\hat{R} = (a + b)/2$

liquid viscosity μ_L

shear rate $\dot{\gamma}$

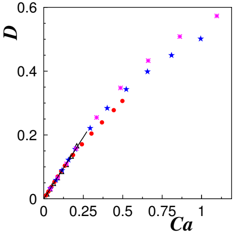
surface tension σ

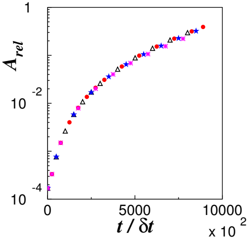


bubble deformation

$D = (a - b)/(a + b)$

$D(Ca)$ = linear for $Ca < 0.2$





bubble area

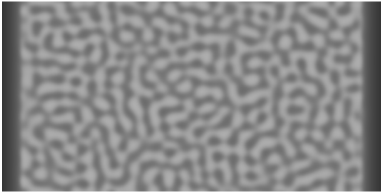
$A_{rel} = A/L^2$

$L = 4096$

Phase separation in a thermal liquid – vapour system (1)

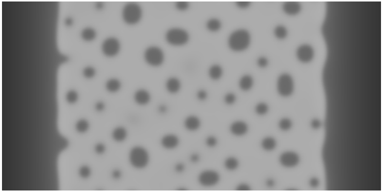
Initial temperature = critical value $T_c = 1.0$, lattice size: 512×256 nodes
Walls temperature $T_{wall} = 0.90 \Longrightarrow$ heat extraction and phase separation
2D LB model with variable temperature (Watari and Tsutahara, 2003)

$t = 1.0$



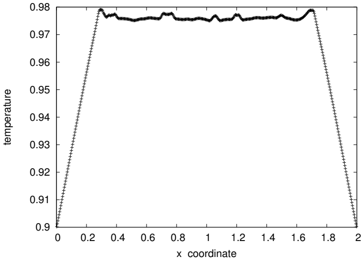
$t = 5.0$

$t = 20.0$

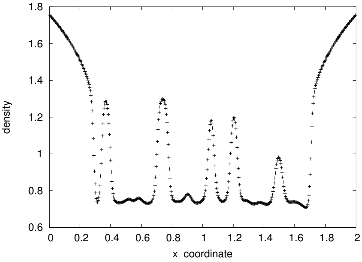


$t = 50.0$

Phase separation in a thermal liquid – vapour system (2)



Temperature



Density

Temperature and density profiles at $t = 50.0$

G.Gonnella, A.Lamura, V.Sofonea
Lattice Boltzmann simulation of thermal non-ideal fluids
Physical Review **E** 76 (2007) 036703

Two-component lattice Boltzmann model

- Consider a 2D two-component fluid ($\sigma = 0, 1$):

$$\partial_t f^\sigma + \frac{\mathbf{p}}{m} \nabla f^\sigma - \mathbf{F}^\sigma \nabla_{\mathbf{p}} f = -\frac{1}{\tau^\sigma} \left[f^\sigma - f^{\sigma,\text{eq}} \right].$$

- EQ method used for the momentum gradient:

$$\mathbf{F}^\sigma \nabla_{\mathbf{p}} f \rightarrow \mathbf{F} \cdot \frac{\mathbf{p} - m\mathbf{u}}{mT} f^{\sigma,\text{eq}}.$$

- The inter-particle interaction of strength ω and the surface tension described by κ is modelled as:

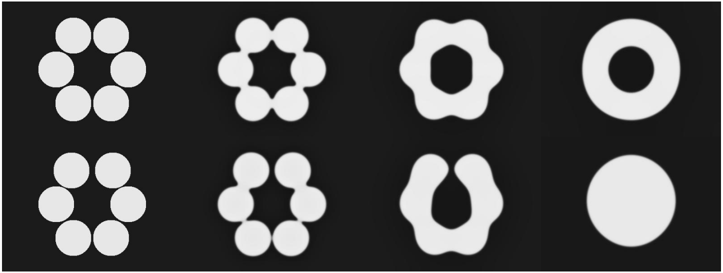
$$\mathbf{F}^\sigma = -\omega \nabla X^{1-\sigma} + \kappa \nabla (\nabla^2 X^\sigma),$$

where $X^\sigma = n^\sigma / (n^0 + n^1)$ is the mole fraction of species σ.

A. Cristea, A. Neagu, Biofabrication, under revision.

Fusion of multicellular cylinders in a hexagonal arrangement

3D organ printing technology



First row: cylindrical fusion.
Second row: Printing defect - structural collapse.

A. Cristea, A. Neagu, Biofabrication (in press).

Conclusion

- Full-range Lattice Boltzmann models based on the Gauss-Hermite quadrature provide a convenient tool for the simulation of multiphase fluids
- appropriate force terms need to be considered for single- or multi-component fluids in order to achieve the phase separation
- Finite difference and finite volume schemes can be used to evolve the values of the distribution function on a square lattice
- isothermal systems : models of order $N = 3$ ($Q = 4$) are required
  number of velocities: 4 (1D) , 16 (2D) and 64 (3D)
- thermal systems : models of order $N = 4$ ($Q = 5$) are required
  number of velocities: 5 (1D) , 25 (2D) and 125 (3D)

Acknowledgments
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