Pinning and facetting in lattice Boltzmann simulations

Tim Reis

Oxford Centre for Collaborative Applied Mathematics
Mathematical Institute
University of Oxford

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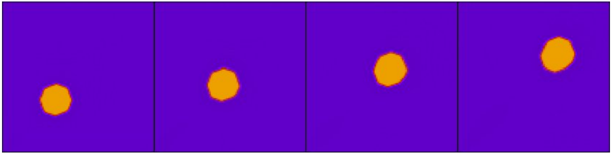
Recolouring in multiphase lattice Boltzmann models

Lattice Boltzmann models for continuum multiphase flows use a “colour field" to represent different phases.

A recolouring algorithm is needed to encourage phase segregation and maintain narrow boundaries between fluids.

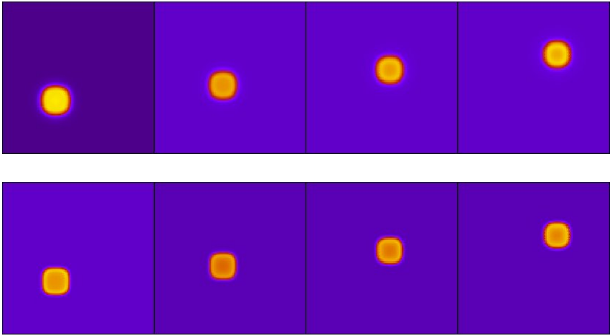
Maximising the work done against the colour gradient predicts sharp interfaces but causes spurious behaviour:



Other recolouring algorithms

Latva-Kokko and Rothman (2005) offer an alternative redistribution:

$$f_i^k = \frac{\rho^k}{\rho} f_i' \pm \beta \frac{\rho^r \rho^b}{\rho^2} f_i^{(0)} \cos\alpha$$



See also D'Ortona *et al.* (1995), Tölke *et al.* (2002)

Motivation

- Multiphase LBEs are prone to lattice pinning and facetting (Latva-Kokko & Rothman (2005), Halliday *et al.* (2006)).
- Similar difficulties arise in combustion (Colella (1986), Pember (1993)).
- Spurious phenomena associated with stiff source terms investigated by LeVeque & Yee (1990).
- Unphysical behaviour can be corrected with a random projection method (Bao & Jin (2000)).
- LB formulation of these models can shed light on pinning and facetting.

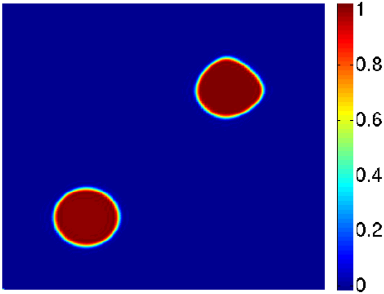
Phase fields, pinning and facetting

Two types of particles: red & blue.

Scalar field ϕ, the “colour”
$\phi \approx 1$ in red phase (oil)
$\phi \approx 0$ in blue phase (water)

Diffuse interfaces marked by transitions from $\phi \approx 1$ to $\phi \approx 0$.

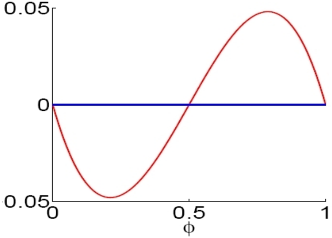
$\partial_t \phi + \mathbf{u} \cdot \nabla \phi = S(\phi)$.



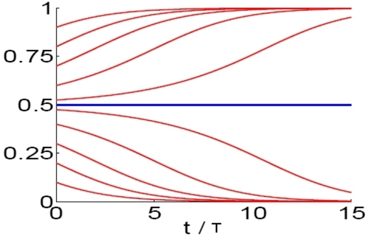
Model problem for propagating sharp interfaces

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = S(\phi) = -\frac{1}{T}\,\phi\,(1-\phi)\,\left(\tfrac{1}{2}-\phi\right)$$

$TS(\phi) = -\,\phi\,(1-\phi)\,\left(\tfrac{1}{2}-\phi\right)$



$\frac{d\phi}{dt} = S(\phi)$



" The numerical results presented above indicate a disturbing feature of this problem – it is possible to compute perfectly reasonable results that are stable and free from oscillations and yet are completely incorrect. Needless to say, this can be misleading."

LeVeque & Yee (1990)

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Lattice Boltzmann Implementation

Suppose $\phi = \sum_i f_i$ and postulate the discrete Boltzmann equation:

$$\partial_t f_i + c_i \, \partial_x f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right) + R_i.$$

With the following equilibrium function and discrete source term :

$$\begin{aligned} f_i^{(0)} &= W_i \phi (1 + \lambda c_i u), \\ R_i &= -\tfrac{1}{2} S(\phi)(1 + \lambda c_i u); \end{aligned}$$

the Chapman-Enskog expansion yields the
advection-reaction-diffusion equation:

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = S(\phi) + \tau(1 - u^2)\frac{\partial^2 \phi}{\partial x^2}$$

.

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Reduction to Fully Discrete Form

The previous discrete Boltzmann equation can be written as

$$\partial_t f_i + c_i \, \partial_x f_i = \Omega_i$$

Integrate along a characteristic for time Δt:

$$f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = \int_0^{\Delta t} \Omega_i(x + c_i s, t + s) \, ds,$$

and approximate the integral by the trapezium rule:

$$\begin{aligned} f_i(x+c_i\Delta t, t+\Delta t) - f_i(x, t) &= \frac{\Delta t}{2}\Big(\Omega_i(x+c_i\Delta t, t+\Delta t) \\ &+ \Omega_i(x, t)\Big) + O\left(\Delta t^3\right). \end{aligned}$$

This is an implicit system.

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Change of Variables

To obtain a second order explicit LBE at time $t + \Delta t$ define

$$\bar{f}_i(x', t') = f_i(x', t') - \frac{\Delta t}{2\tau}\left(f_i(x', t) - f_i^{(0)}(x', t)\right) - \frac{\Delta t}{2} R_i(x', t)$$

The new algorithm is

$$\begin{aligned}\bar{f}_i(x + c_i\Delta t\ ,\ t + \Delta t) - \bar{f}_i(x, t) \\ = \quad -\frac{\Delta t}{\tau + \Delta t/2}\ \left(\bar{f}_i(x, t) - f_i^{(0)}(x, t)\right) + \frac{\tau \Delta t}{\tau + \Delta t/2} R_i(x, t),\end{aligned}$$

However, we need to find ϕ in order to compute $f_i^{(0)}$ and R_i.

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Reconstruction of ϕ

The source term does not conserve ϕ:

$$\bar{\phi} = \sum_i \bar{f}_i = \sum_i \left[f_i - \frac{\Delta t}{2\tau}\left(f_i - f_i^{(0)}\right) - \frac{\Delta t}{2} R_i \right]$$

$$= \phi + \frac{\Delta t}{2T}\,\phi\,(1-\phi)\,\left(\tfrac{1}{2} - \phi\right) = N(\phi).$$

We can reconstruct ϕ by solving the nonlinear equation $N(\phi) = \bar{\phi}$ using Newton's method:

$$\phi \to \phi - \frac{N(\phi) - \bar{\phi}}{N'(\phi)},$$

Note that $N(\phi) = \phi + O(\Delta t / T)$.

Lengthscale of Transition

The diffusive extension of LeVeque and Yee's model is

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = S(\phi) + \kappa\frac{\partial^2 \phi}{\partial x^2}$$

Solving the ODE

$$0 = S(\phi) + \kappa\frac{\partial^2 \phi}{\partial x^2}$$

gives us the interface profile

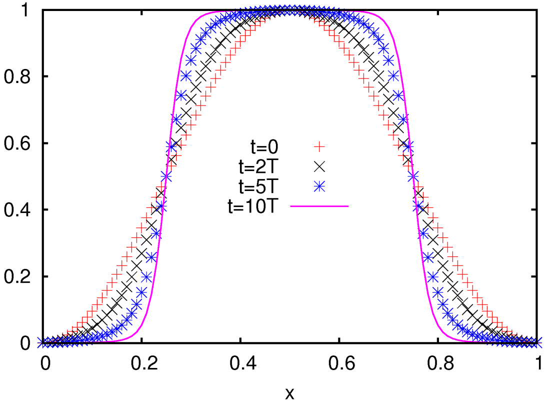
$$\phi(x) = (1 + \exp x/L)^{-1},$$

where $L = \sqrt{2\tau T}\Delta x$ is the lengthscale of transition

Sharpening without Advection

Initial condition: $\phi = \sin^2(\pi x)$

$T = \tau = 0.01$



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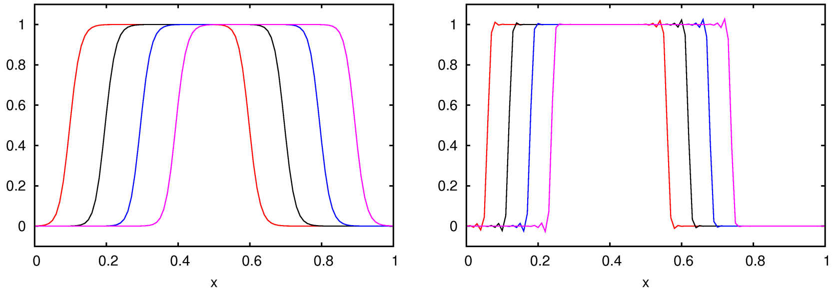
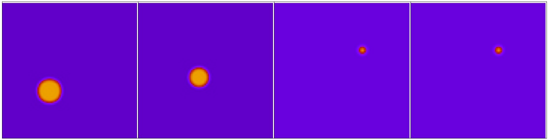
Pinning as a result of sharpening



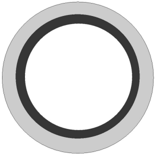
Numerical solutions for $\tau/T = 1$ (*left*) and $\tau/T = 50$ (*right*).

Conservation Trouble

In the 2D case the circular region shrinks and eventually disappears:



This is due to the curvature of the interface:

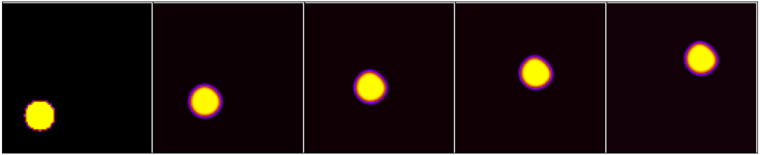


We find ϕ_c that satisfies

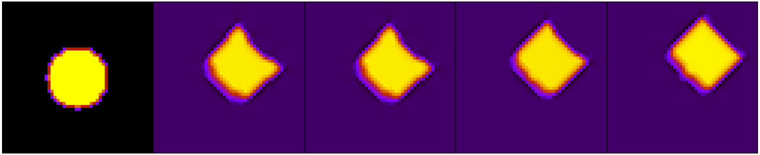
$$M = \int_{\Omega} S(\phi, \phi_c) d\Omega.$$

Facetting with a D2Q9 Model

Propagating circular patch when $\tau / T = 10$. Notice the beginnings of a facet on the leading edge . . .



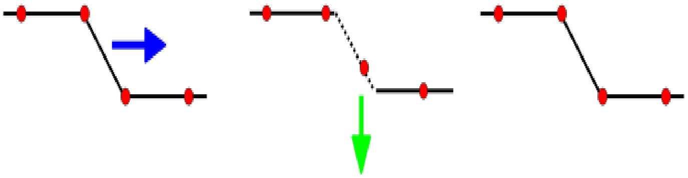
When $\tau / T = 50$ the facetting is severe . . .



Recap: Model problem for propagating sharp interfaces (LeVeque & Yee 1990)

$$\frac{\partial \phi}{\partial t} + u\,\frac{\partial \phi}{\partial x} = S(\phi) = -\,\frac{1}{T}\,\phi\,(1-\phi)\,\left(\tfrac{1}{2}-\phi\right)$$

Usually implemented as separate advection and sharpening steps.



$\frac{\partial \phi}{\partial t} + u\,\frac{\partial \phi}{\partial x} = 0$

$$\frac{\partial \phi}{\partial t} = S(\phi)$$

The Random Projection Method

The LeVeque & Yee source term is effectively the deterministic projection

$$S_D(\phi): \quad \phi(x, t + \Delta t) = \begin{cases} 1 & \textit{if} \quad \phi'(x,t) > 1/2, \\ 0 & \textit{if} \quad \phi'(x,t) \leq 1/2. \end{cases}$$

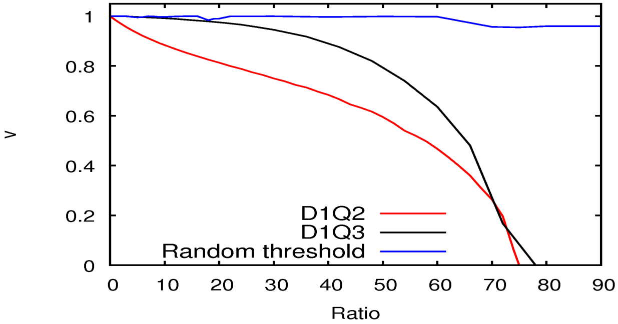
Bao & Jin (2000) replace the critical $\phi_c = 1/2$ with a uniformly distributed random variable $\phi_c^{(n)}$:

$$S_R(\phi): \quad \phi(x, t + \Delta t) = \begin{cases} 1 & \textit{if} \quad \phi'(x,t) > \phi_c^{(n)}, \\ 0 & \textit{if} \quad \phi'(x,t) \leq \phi_c^{(n)}. \end{cases}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = -\frac{1}{T}\, \phi \left(1 - \phi\right) \left(\phi_c^{(n)} - \phi \right).$$

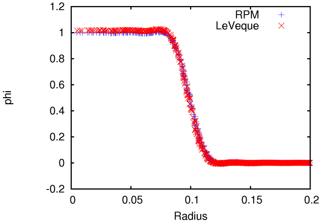
Comparison of Propagation Speed (1D)

The speed of the interface is dictated by the ratio of timescales, $\frac{\tau}{T}$.

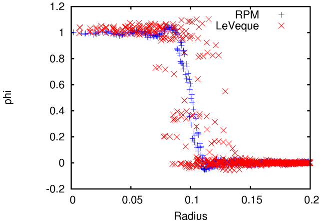


Comparing the Radii of the Patches at $t = 0.4$

The Random Projection model preserves the circular shape at $\tau/T = 10$

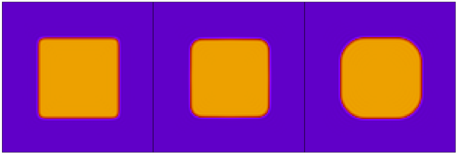


and is clearly superior to the LeVeque model when $\tau/T = 30$

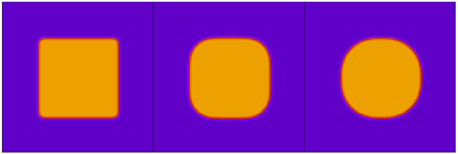


A non-smooth problem: $\frac{\tau}{T} = 30$

An initial square patch fails to collapse to a circle when using a deterministice volume preserving threshold ...

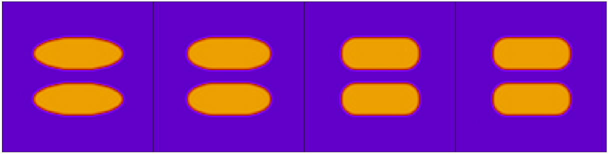


...but behaves correctly when we introduce the van der Corput sequence:



Topological changes: $\frac{\tau}{T} = 30$

An initial square patch fails to collapse to a circle when using a deterministice volume preserving threshold . . .



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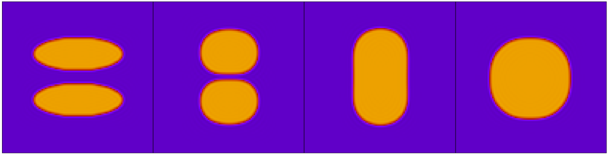


A conservative scheme

If we assume $L = \sqrt{2\tau T}\Delta x$ then

$$
\begin{aligned}
\frac{\partial \phi}{\partial n} &= \nabla\phi \cdot \mathbf{n} = -|\nabla\phi| = \frac{-\phi(1-\phi)}{L}, \\
\frac{\partial^2 \phi}{\partial n^2} &= \frac{(\nabla\phi\cdot\nabla)|\nabla\phi|}{|\nabla\phi|} = -\frac{\phi(1-\phi)(\frac{1}{2}-\phi)}{L^2}.
\end{aligned}
$$

We can now show that a DBE of the form

$$
\frac{\partial f_i}{\partial t} + c_i \frac{\partial f_i}{\partial x} = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right) + W_i \frac{\phi(1-\phi)}{L} c_i \cdot n
$$

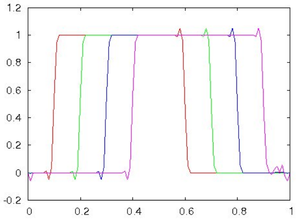
furnishes

$$
\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = \tau(1-u^2)\nabla^2\phi + \tau\nabla^2\phi - \frac{\phi(1-\phi)(\frac{1}{2}-\phi)}{T}
$$

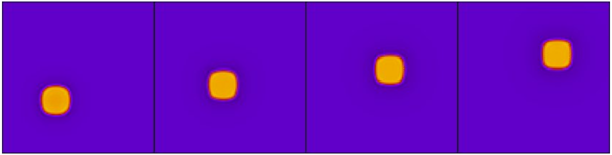
in the macroscopic limit.

Some preliminary results

First in one dimension. . .



. . . and also in two dimensions. . .



Conclusion

- We have studied the combination of advection and sharpening of the phase field that commonly arises in lattice Boltzmann models for multiphase flows.
- Overly sharp phase boundaries can become pinned to the lattice. This has been shown to be a purely kinematic effect.
- Replacing the threshold with a uniformly distributed pseudo-random variable allows us to predict the correct propagation speed at very sharp boundaries ($\tau/T > 100$).
- The onset of facetting is signifficanly delayed if we introduce a random term into the volume-preserving multi-dimensional extension.