Lattice Boltzmann simulation of droplet formation in T-junction geometries

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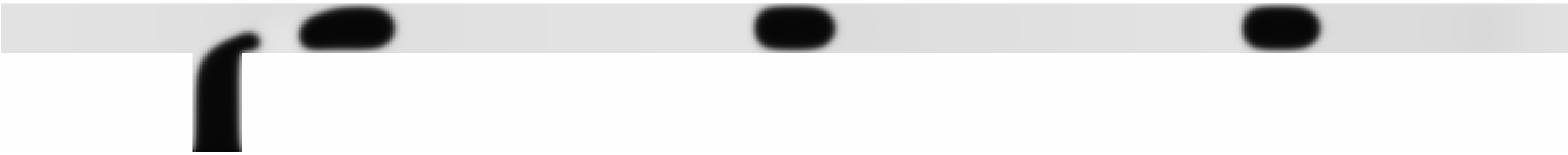
Outline

- Motivation and T-junction devices
- Moments of $f^{(\mathrm{eq})}$ and order of a LB model.
- Numerical scheme for off-lattice velocity sets: corner-transport upwind schemes.
- Application: T-junction droplet formation

Motivation



- Droplet generating microfluidic devices are getting a lot of attention due to their ability to control droplet sizes.
- Their potential applications range from control of chemical reactions[1], biotechnology[2], flow and heat transfer in micro-electromechanical systems[3] to food processing and personal health care products[4].
- The T-junction is one of the most used microfluidic devices.

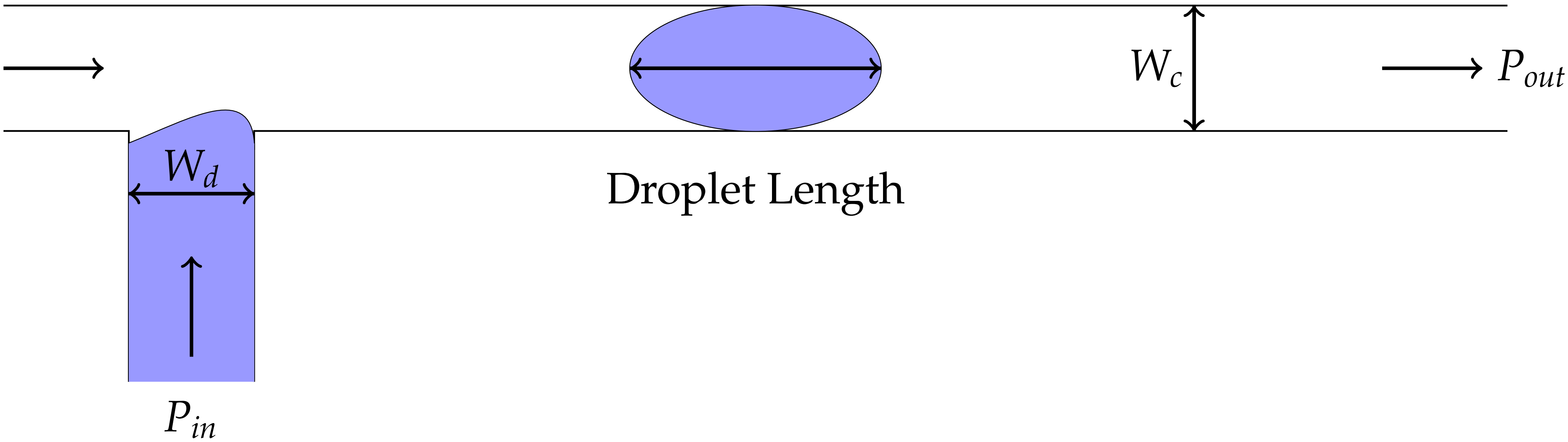
[1] A.Gunther, M. Jhunjhunwala, M.Thalmann, M.A. Schimdt, K.F.Jensen, Langmuir 21(4) 1547-1547 (2005)

[2] A.D. Griffiths, D.S. Tawfik, Trends Biotechnol. 24(9) 395-402 (2006)

[3] R.N. Dean, A.Luque, IEEE Trans. Ind. Electron. 56(4) 913-925 (2009)

[4] G.F.Christopher, S.L.Anna, J. Phys. D, Appl. Phys. 40 (19) R319-336 (2007)

T-junction device



- Two inlets(liquid and vapour) and one outlet flow.
- $Z = \frac{W_c}{W_d}$ is used to characterise the geometry.
- $\Delta P = P_{in} - P_{out}$

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:

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

Gauss-Hermite quadratures

- Replace integrals by quadrature sums:

$$\int d^3p f\, P(\mathbf{p}) = \sum_k f_k P(\mathbf{p}_k)$$

- f and $f^{(\mathrm{eq})}$ are expanded with respect to the orthogonal Hermite polynomials, e.g.:

$$f_k^{eq}(\mathbf{x},t) = w_k \sum_{\ell=0}^{N} \frac{1}{\ell!} \mathbf{a}^{eq,(\ell)}(\mathbf{x},t)\mathcal{H}^{(\ell)}(\mathbf{p}_k)$$

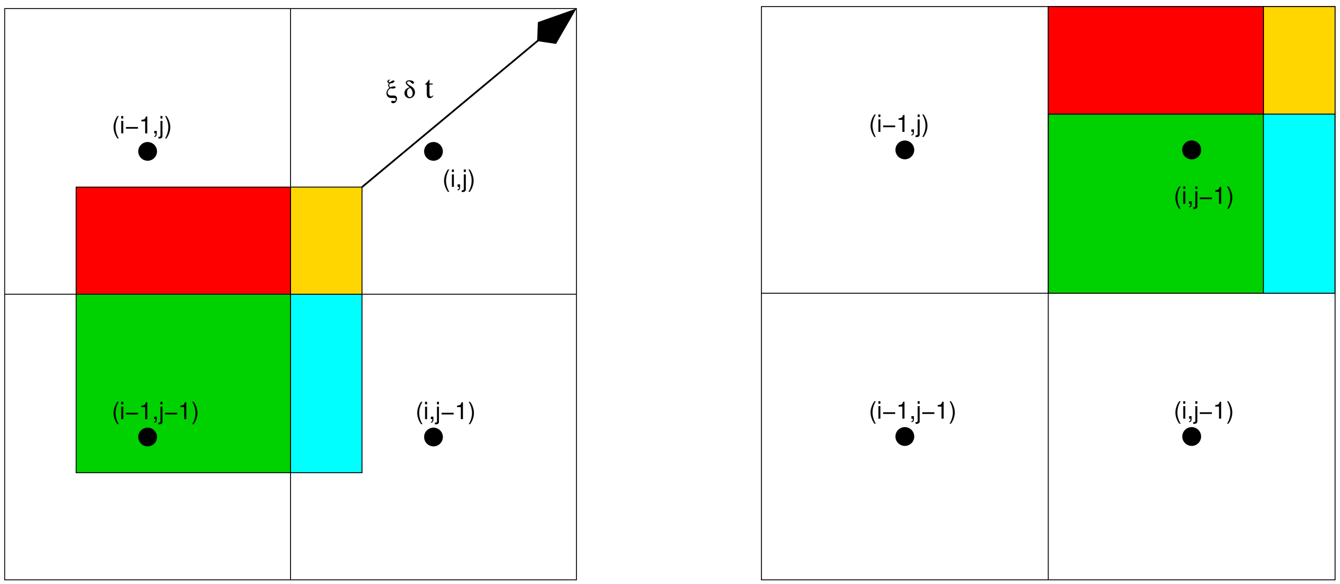
$$\mathbf{a}^{eq,(\ell)}(\mathbf{x},t) = \int f^{eq}(\mathbf{x},\mathbf{p},t)\mathcal{H}^{(\ell)}(\mathbf{p})d\mathbf{p}$$

where $f^{eq}(\mathbf{x},\mathbf{p},t) = \frac{n}{(2\pi T)^{D/2}} e^{-\frac{(\mathbf{p}-\mathbf{u})^2}{2T}}$.

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)

Chapman-Enskog expansion and moments of $f^{(\mathrm{eq})}$

- Close to the equilibrium state, the Chapman-Enskog expansion gives f as a series in powers of $\mathrm{Kn} = \lambda/L$:

$$f = f^{(0)} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \ldots$$
$$\partial_t = \partial_{t_0} + \mathrm{Kn}\, \partial_{t_1} + \mathrm{Kn}^2 \partial_{t_2} + \ldots$$

- Navier-Stokes equations are recovered at $O(\mathrm{Kn})$:

$$\partial_t \rho + \nabla(\rho \mathbf{u}) = 0$$
$$\rho(\partial_t \mathbf{u} + \mathbf{u}\nabla\mathbf{u}) = -\nabla p^i + \nabla(\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)) + \nabla(\lambda\nabla\mathbf{u}) + \rho\mathbf{F}$$

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

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

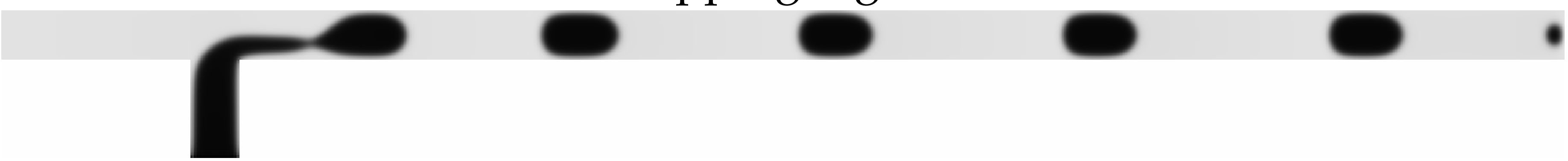
with $\rho_c = 1$, $T_c = 1$.

T-junction droplet formation regimes

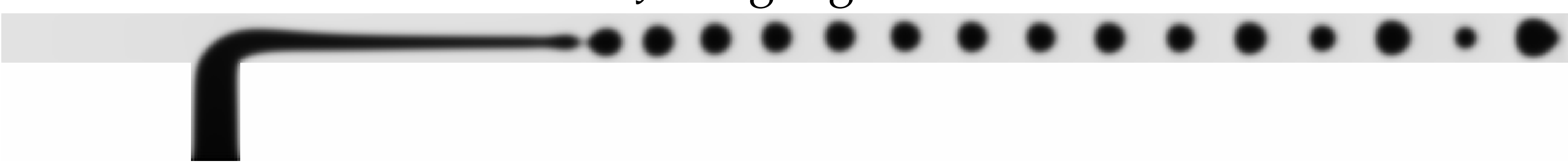
Isothermal flows at $T = 0.8$ with hydrophobic surfaces.

Squeezing regime

Dripping regime



Jetting regime



Case I: Z=1

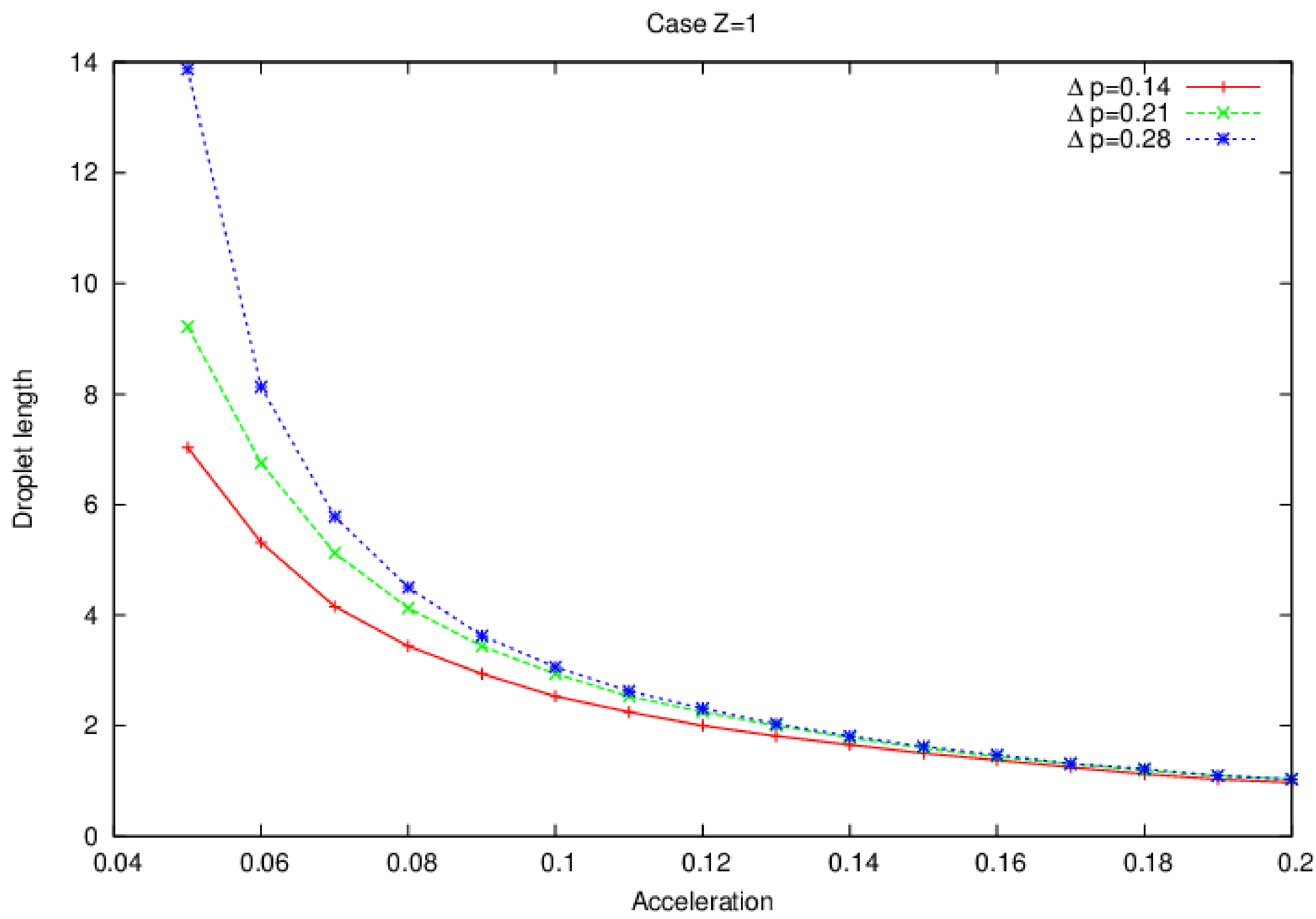
$a_x = 0.06$

$a_x = 0.1$

$a_x = 0.14$

Mesh: (1024x32) & (32x64).

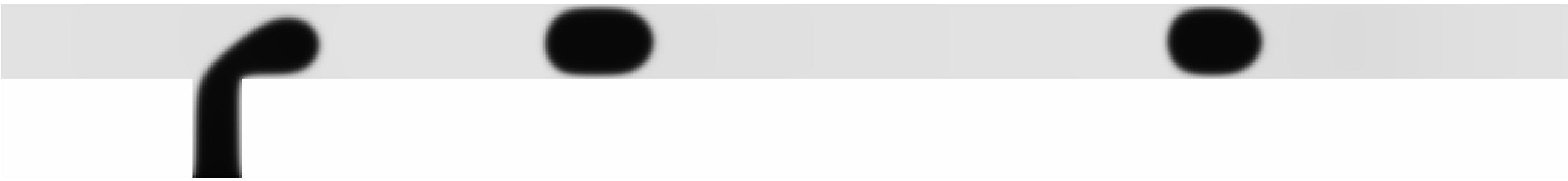
Case I: Z=1



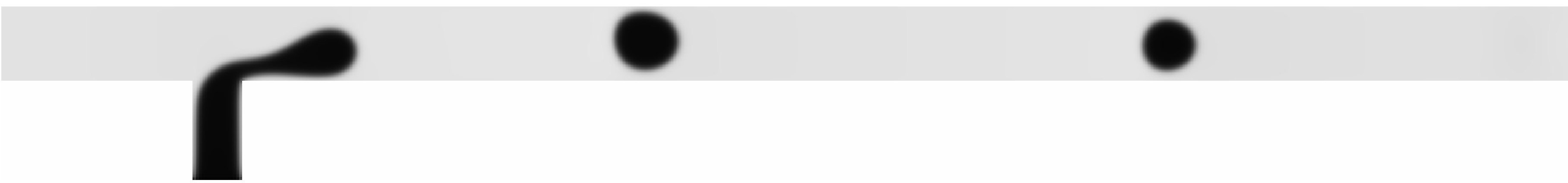
Case Z=1
Δ p=0.14
Δ p=0.21
Δ p=0.28
Droplet length
Acceleration
0
2
4
6
8
10
12
14
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2

Case I: Z=1.5

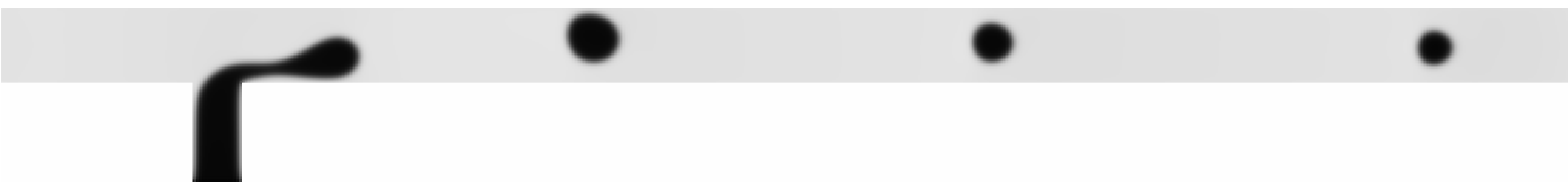
$a_x = 0.06$



$a_x = 0.1$

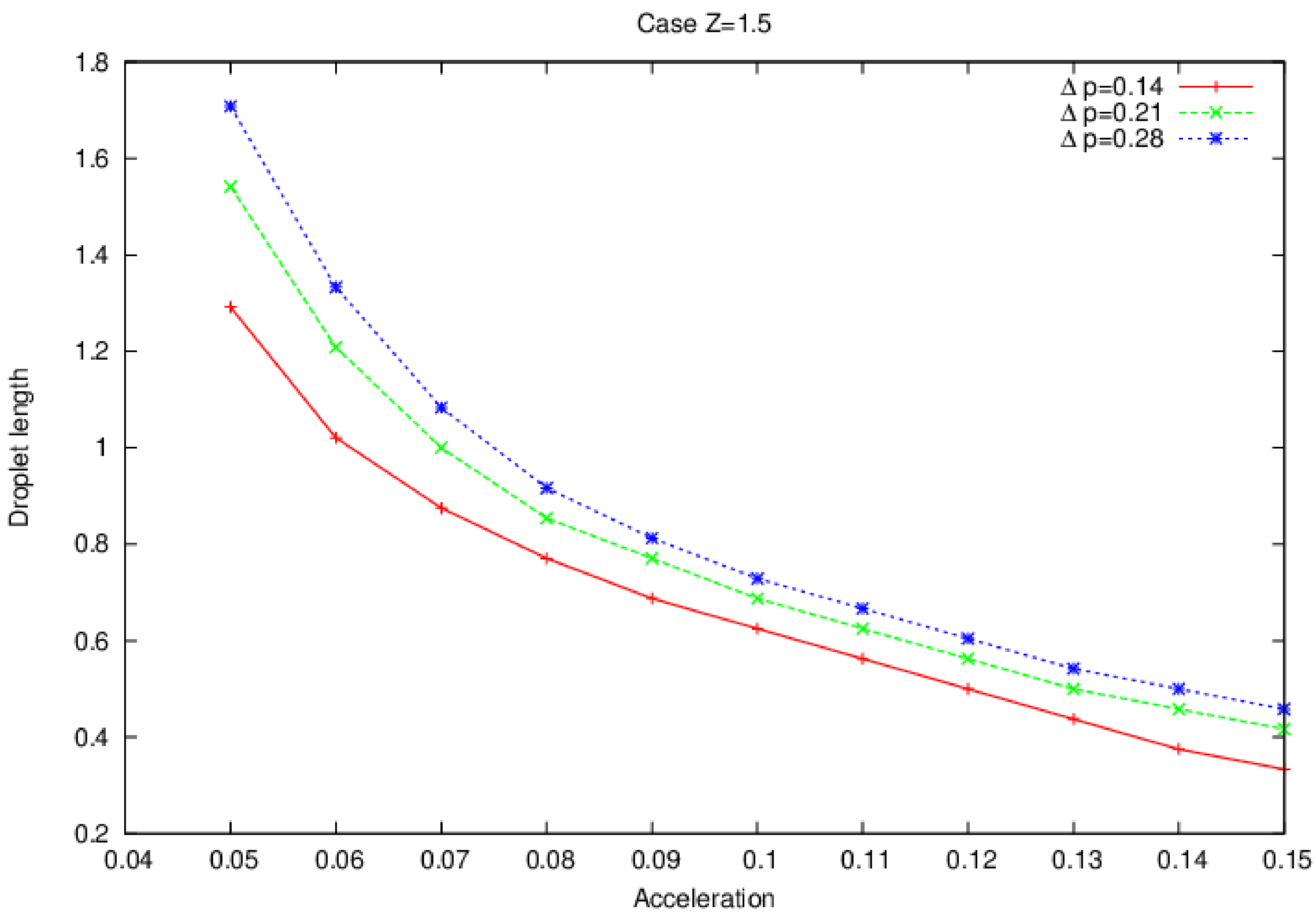


$a_x = 0.14$



Mesh: (1024x48) & (32x64).

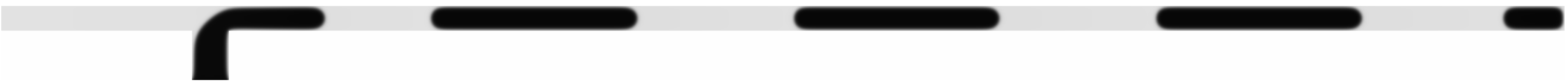
Case I: Z=1.5



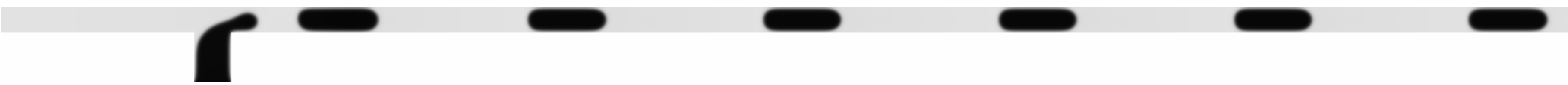
Case Z=1.5
Δ p=0.14
Δ p=0.21
Δ p=0.28
Droplet length
Acceleration
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15

Case I: Z=$\frac{2}{3}$

$a_x = 0.06$



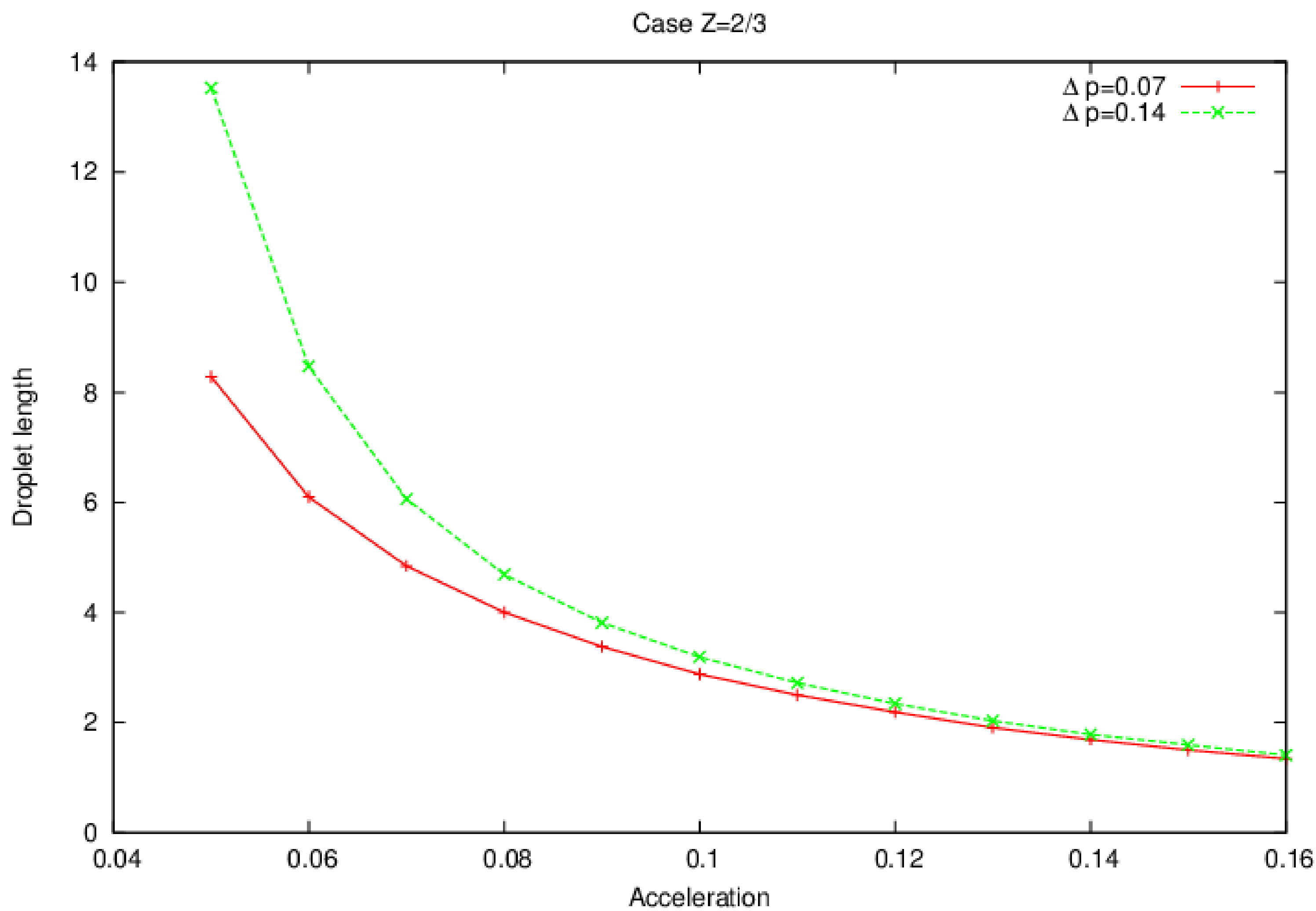
$a_x = 0.1$



$a_x = 0.14$

Mesh: (1024x32) & (48x64).

Case I: $Z=\frac{2}{3}$



Conclusion

- Lattice Boltzmann (LB) simulations provide a convenient tool for the investigation of interface phenomena in liquid-vapour systems.
- 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).
- The LB simulations allows one to capture the 3 droplet formation regimes in a T-junction device.
- The droplet shape and its dimension is determined by the inlet flow rates, as well as the geometry ($Z = \frac{W_c}{W_d}$).

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