Effects of thermal fluctuations on a nanoligament fragmentation

Xiao Xue[1,2], Mauro Sbragaglia[1], Luca Biferale[1], Federico Toschi[2]

1. Department of Physics, University of Rome “Tor Vergata”

2 Department of Physics, Eindhoven University of Technology

Cambridge, U.K., 12.07.2018

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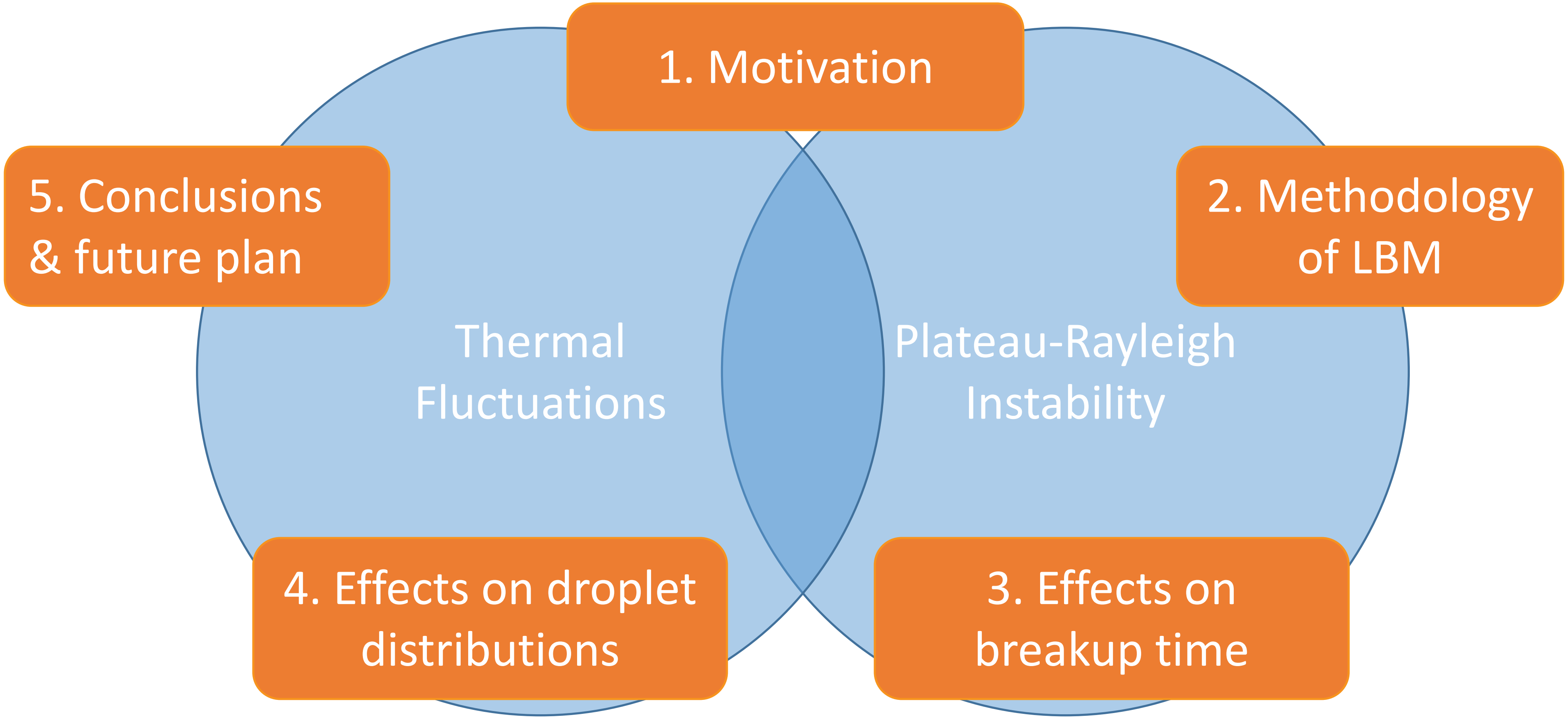
Content



1. Motivation

2. Methodology of LBM

3. Effects on breakup time

4. Effects on droplet distributions

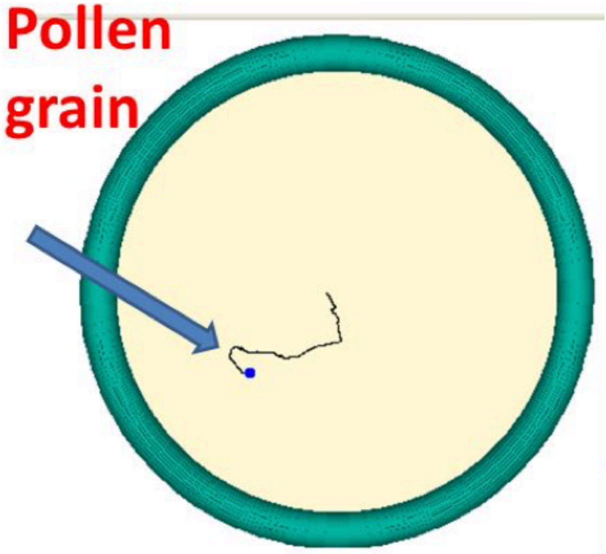
5. Conclusions & future plan

Thermal Fluctuations

Plateau-Rayleigh Instability

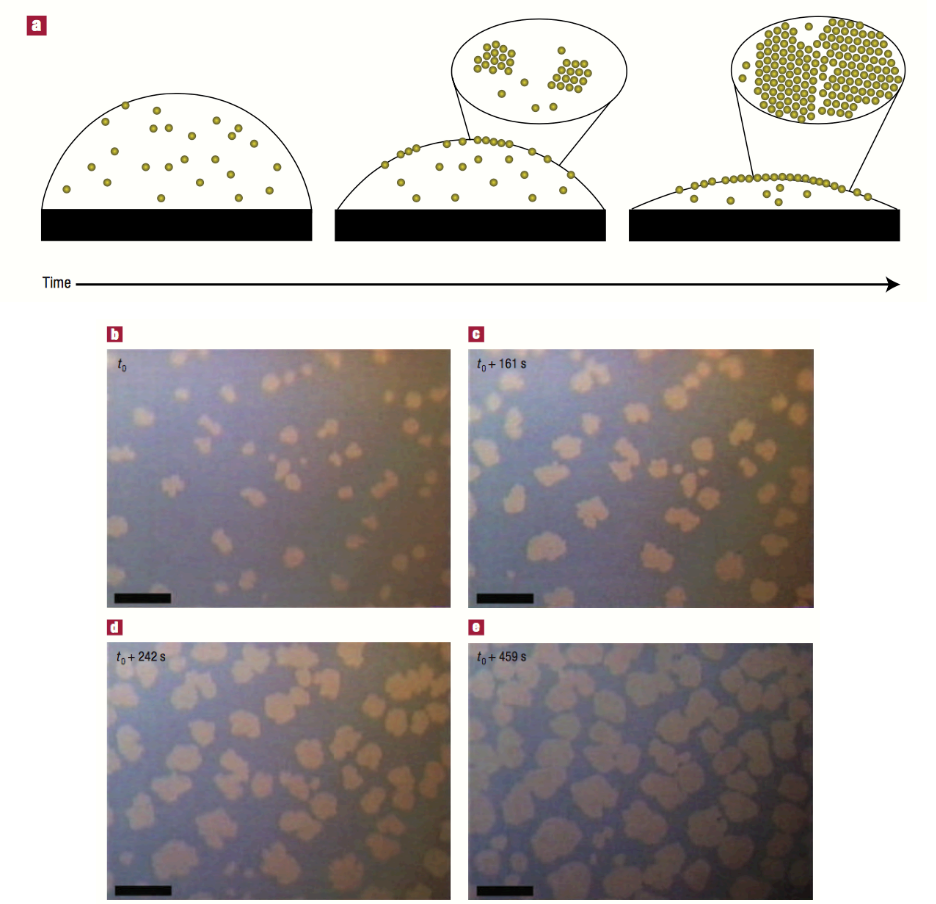
Motivation

1827 Robert Brown

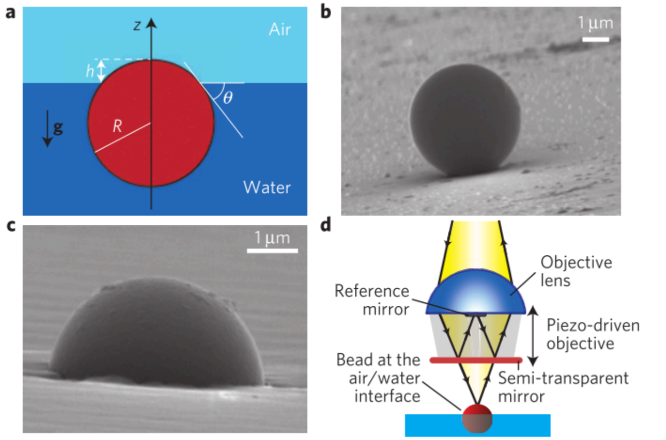


Pollen of the plant suspended in water under a microscope

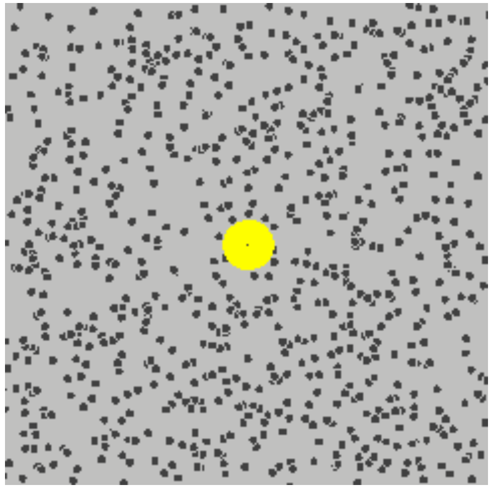
TP Bigioni et. al. Nature materials, 2006



Self assembly particle in industry application & medical application

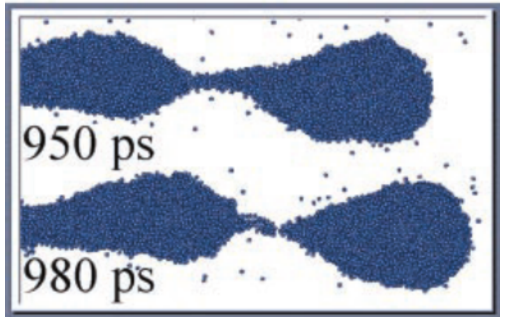


Giuseppe Boniello, et al. ,Nature material, 2015



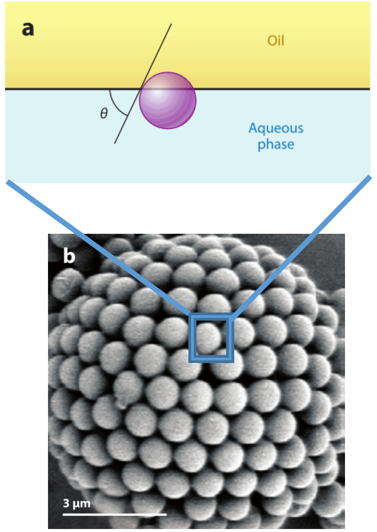
https://en.wikipedia.org/wiki/Brownian_motion

Motivation



Breakup of nanojets[1]

M. Moseler and U. Landman, Science, 2000



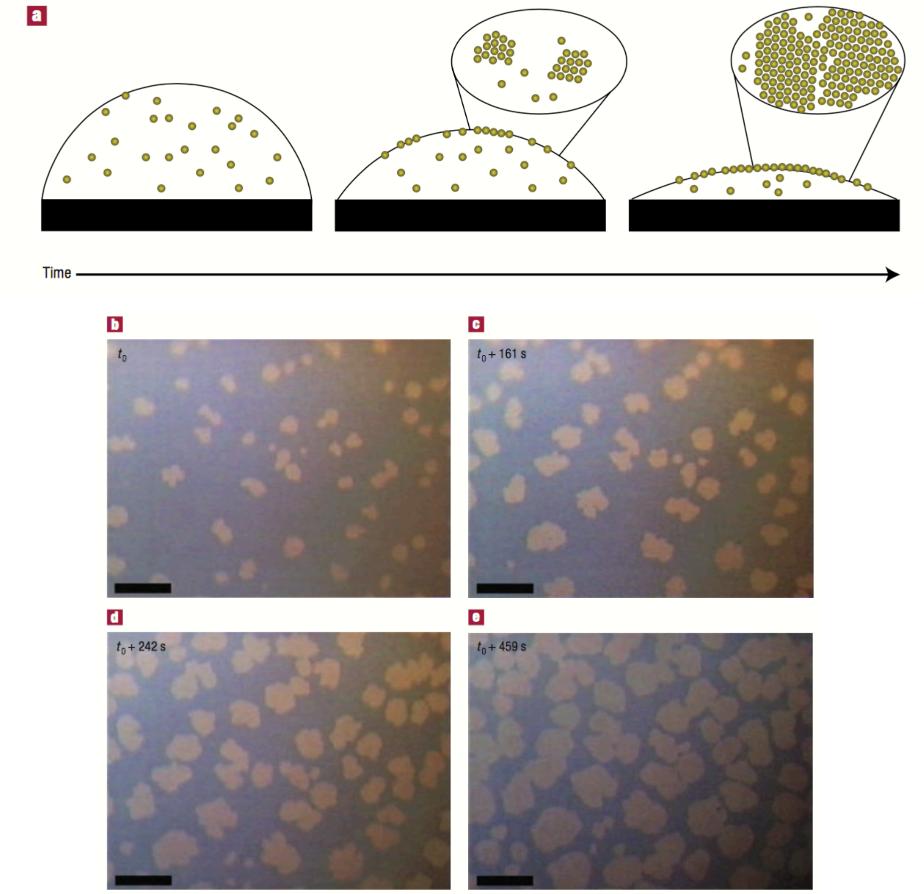
Dinsmore et al. 2002

CC Berton-Carabin, et al., 2015·

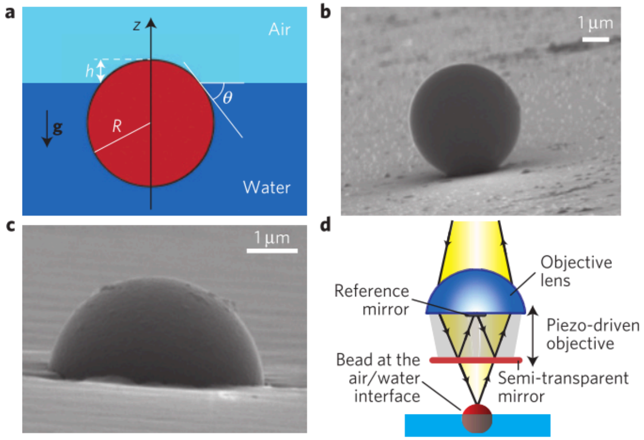
Aveyard et al. 2003

Pickering emulsions

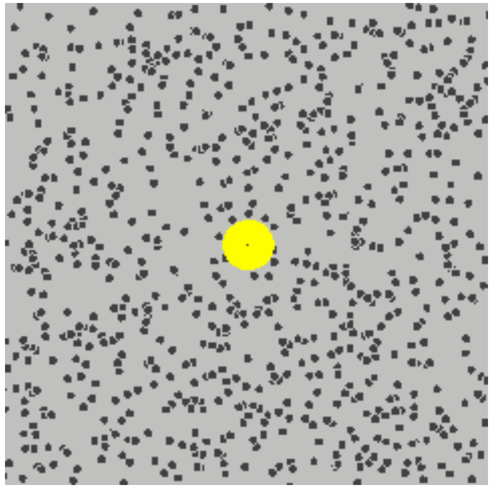
TP Bigioni et. al. Nature materials, 2006



Self assembly particle in industry application & medical application



Giuseppe Boniello, et al. ,Nature material, 2015



https://en.wikipedia.org/wiki/Brownian_motion

Plateau-Rayleigh Instability

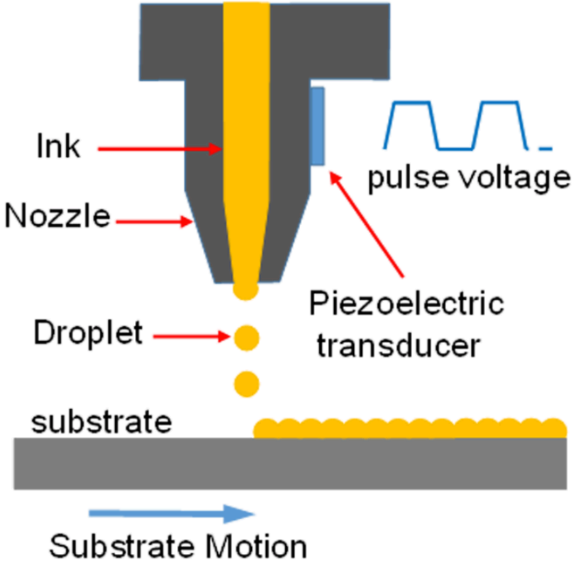
Ohnesorge number

$$Oh = \mu_l \sqrt{\rho_l / (\sigma R_0)}$$

Capillary time

$$T_{cap} = \sqrt{\rho_l R_0^3 / \sigma}$$

Droplet formation at faucet



Inkjet printing

Microscopic scale

Fluctuating multicomponent lattice Boltzmann model

Mesoscopic scale

$$\partial_t \rho_{tot} + \nabla\cdot(\rho_{tot}\mathbf{v}_{tot}) = 0 \qquad \partial_t\rho_{r,b} + \nabla\cdot(\rho_{r,b}\mathbf{v}_{tot}) = \nabla\cdot(D\nabla\mu + \boldsymbol{\Phi})$$

Noise term

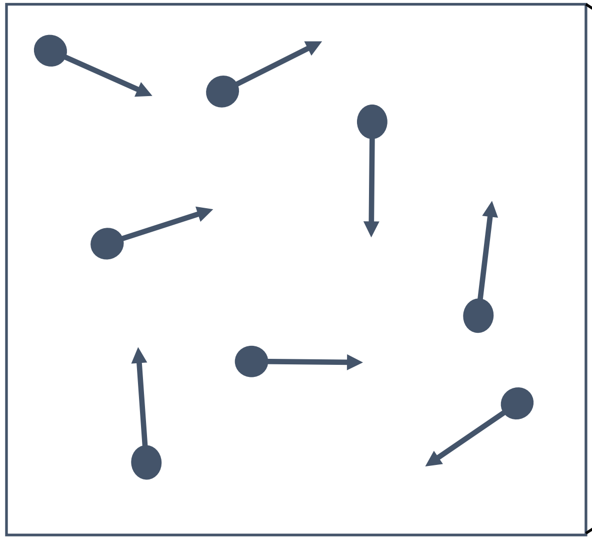
$$\partial_t(\rho_{tot}\mathbf{v}_{tot}) + \nabla\cdot(\rho_{tot}\mathbf{v}_{tot}\mathbf{v}_{tot}) = -\nabla\mathbf{P} + \nabla\cdot\{\eta\left[\nabla\mathbf{v}_{tot} + (\nabla\mathbf{v}_{tot})^T\right] + \boldsymbol{\Sigma}\}$$

$$\Phi = \sqrt{2k_BTD}\,\hat{\mathbf{W}}, \boldsymbol{\Sigma} = \sqrt{\eta k_B T}(\mathbf{W} + \mathbf{W}^T)$$

Gaussian noise

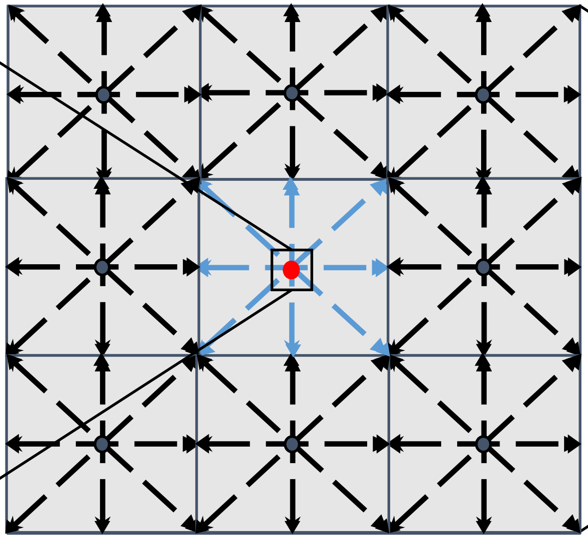
$$\rho_{tot} = \rho_r + \rho_b \quad \mathbf{v}_{tot} = \frac{\rho_r\mathbf{v}_r + \rho_b\mathbf{v}_b}{\rho_r + \rho_b}$$

Microscopic scale



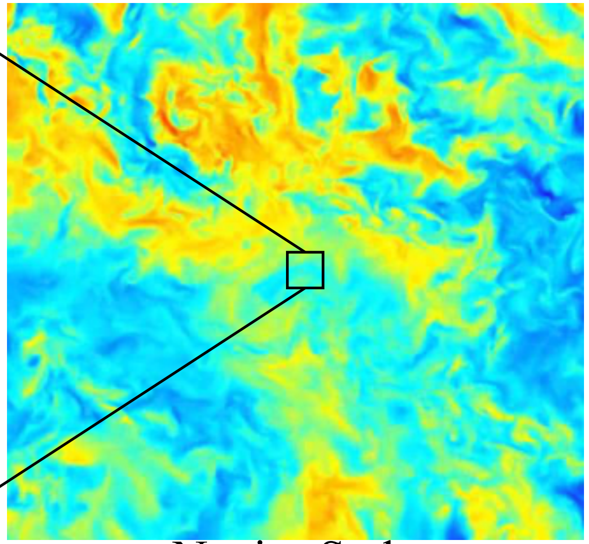
Particle methods

Mesoscopic scale



Lattice Boltzmann method

Macroscopic scale



Navier-Stokes

Objective:

Understanding thermal fluctuations on nano-ligaments break-up

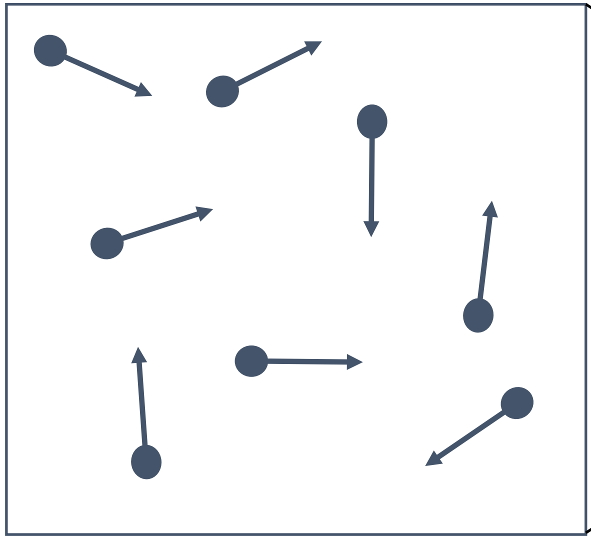
$$\partial_t \rho_{tot} + \nabla \cdot (\rho_{tot}\mathbf{v}_{tot}) = 0 \qquad \partial_t \rho_{r,b} + \nabla \cdot (\rho_{r,b}\mathbf{v}_{tot}) = \nabla \cdot (D\nabla\mu + \mathbf{\Phi})$$

$$\partial_t(\rho_{tot}\mathbf{v}_{tot}) + \nabla \cdot (\rho_{tot}\mathbf{v}_{tot}\mathbf{v}_{tot}) = -\nabla\mathbf{P} + \nabla \cdot \left\{\eta\left[\nabla\mathbf{v}_{tot} + (\nabla\mathbf{v}_{tot})^T\right] + \mathbf{\Sigma}\right\}$$

$$\Phi = \sqrt{2k_BTD}\hat{\mathbf{W}}, \mathbf{\Sigma} = \sqrt{\eta k_BT}(\mathbf{W} + \mathbf{W}^T)$$

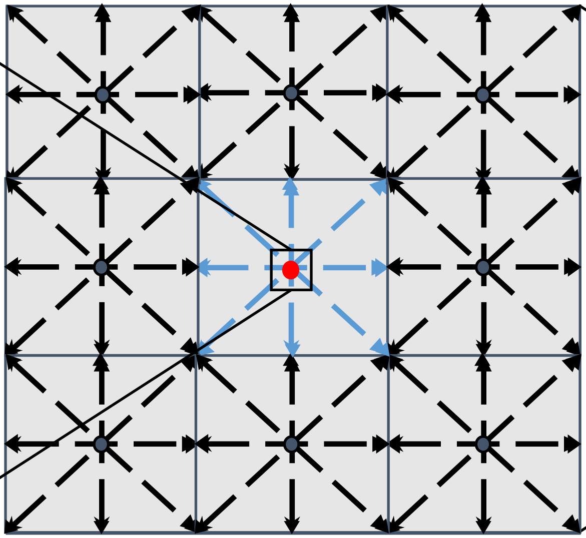
$$\rho_{tot} = \rho_r + \rho_b \quad \mathbf{v}_{tot} = \frac{\rho_r\mathbf{v}_r + \rho_b\mathbf{v}_b}{\rho_r + \rho_b}$$

Microscopic scale



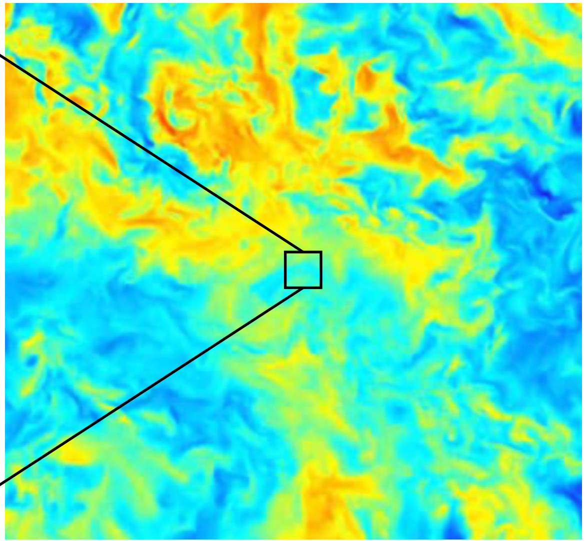
Particle methods

Mesoscopic scale



Lattice Boltzmann method

Macroscopic scale



Navier-Stokes

Streaming

$$f_i^{r,b} = f_i^{r,b}(x - c_i\Delta t, t - \Delta t)$$

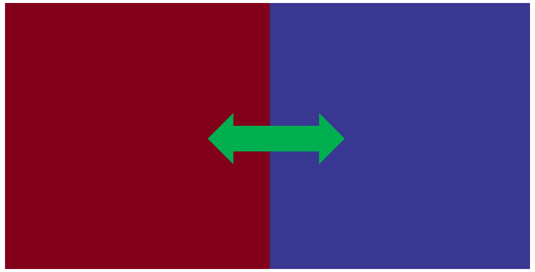
Collision

$$f_i^{r,b}(x + c_i\Delta t, t + \Delta t) = f_i^{r,b}(\mathbf{x}, t) + \mathfrak{L}^{r,b}(f_i(\mathbf{x}, t)) + \underline{F_{sc}^{r,b}} + \xi_{noise}^{r,b}$$

Hydrodynamics quantities

$$\rho^{r,b} = \sum_i f_i^{r,b}$$

$$\rho^{r,b}\mathbf{u}^{r,b} = \sum_i f_i^{r,b}\mathbf{c}_i$$



Shan-Chen forcing

$$F_{sc}^{r,b}(\mathbf{x}, t) = -\sum_{\mu} G_{12} \sum_i \omega_i \varphi_\mu(\mathbf{x}, t)\varphi_\mu(\mathbf{x} + c_i\Delta t, t)$$

D. Belardinelli, et al. Fluctuating multicomponent lattice Boltzmann model, Phys. Rev. E, Vol 91, Iss.2, 2015

Streaming

$$f_i^{r,b} = f_i^{r,b}(x - c_i\Delta t, t - \Delta t)$$

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Hydrodynamics quantities

$$\rho^{r,b} = \sum_i f_i^{r,b}$$

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Noise correlations

$$\langle \xi_\rho^b \xi_\rho^b \rangle = \langle \xi_\rho^b \xi_\rho^r \rangle = 0$$

$$\langle \xi_{\mathbf{j}}^b \xi_{\mathbf{j}}^b \rangle = -\langle \xi_{\mathbf{j}}^b \xi_{\mathbf{j}}^r \rangle = 2\lambda k_B T \frac{\rho^b \rho^r}{\rho^b + \rho^r}\mathbf{1}$$

D. Belardinelli, et al. Fluctuating multicomponent lattice Boltzmann model, Phys. Rev. E, Vol 91, Iss.2, 2015

Streaming

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Champman-Enskog expansion

Navier-Stoke

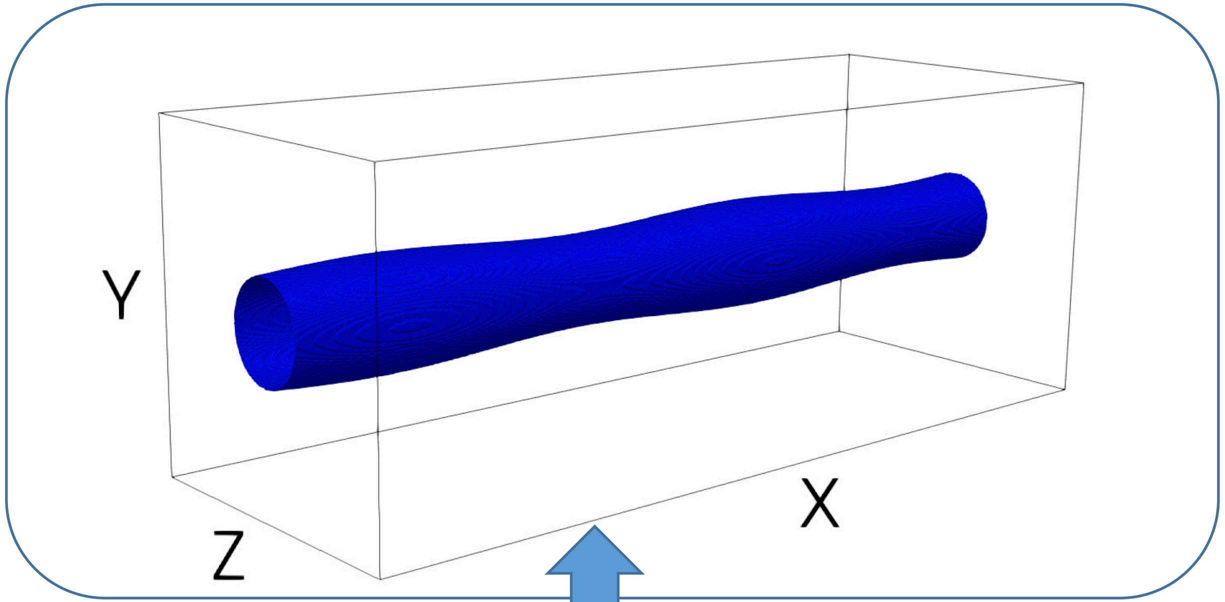
$$\partial_t \rho_{tot} + \nabla \cdot (\rho_{tot}\mathbf{v}_{tot}) = 0$$

$$\partial_t \rho_{r,b} + \nabla \cdot (\rho_{r,b}\mathbf{v}_{tot}) = \nabla \cdot (D\nabla\mu + \mathbf{\Phi})$$

$$\partial_t(\rho_{tot}\mathbf{v}_{tot}) + \nabla \cdot (\rho_{tot}\mathbf{v}_{tot}\mathbf{v}_{tot}) = -\nabla\mathbf{P} + \nabla \cdot \left\{\eta\left[\nabla\mathbf{v}_{tot} + (\nabla\mathbf{v}_{tot})^T\right] + \mathbf{\Sigma}\right\}$$

D. Belardinelli, et al. Fluctuating multicomponent lattice Boltzmann model, Phys. Rev. E, Vol 91, Iss.2, 2015

Simulation set up



Protocol 1

LBM + Fastest Growing mode

Protocol 2

LBM + Gaussian initial interface

Protocol 3

Protocol 2 + Thermal Noise(TN)

Thermal fluctuation impact on the break-up process

1. Ligament breaks up faster under the influence of thermal fluctuations?

2. What is the impact of thermal fluctuations on Droplet distributions?

Thermal length

$$\ell_T = \sqrt{k_B T/\sigma}$$

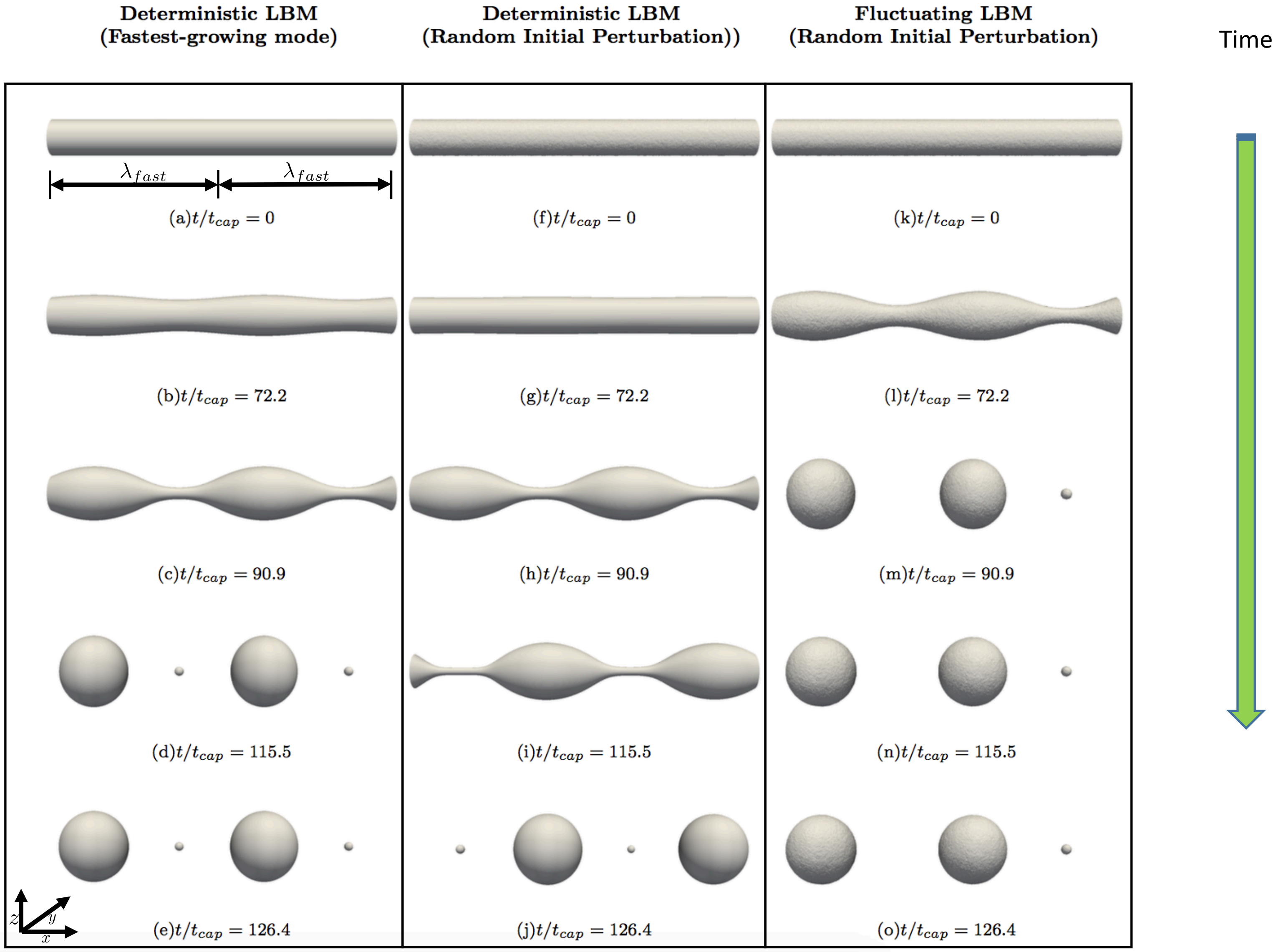
Capillary time

$$T_{cap} = \sqrt{\rho_l R_0^3/\sigma}$$

Domain size: 192X192X512

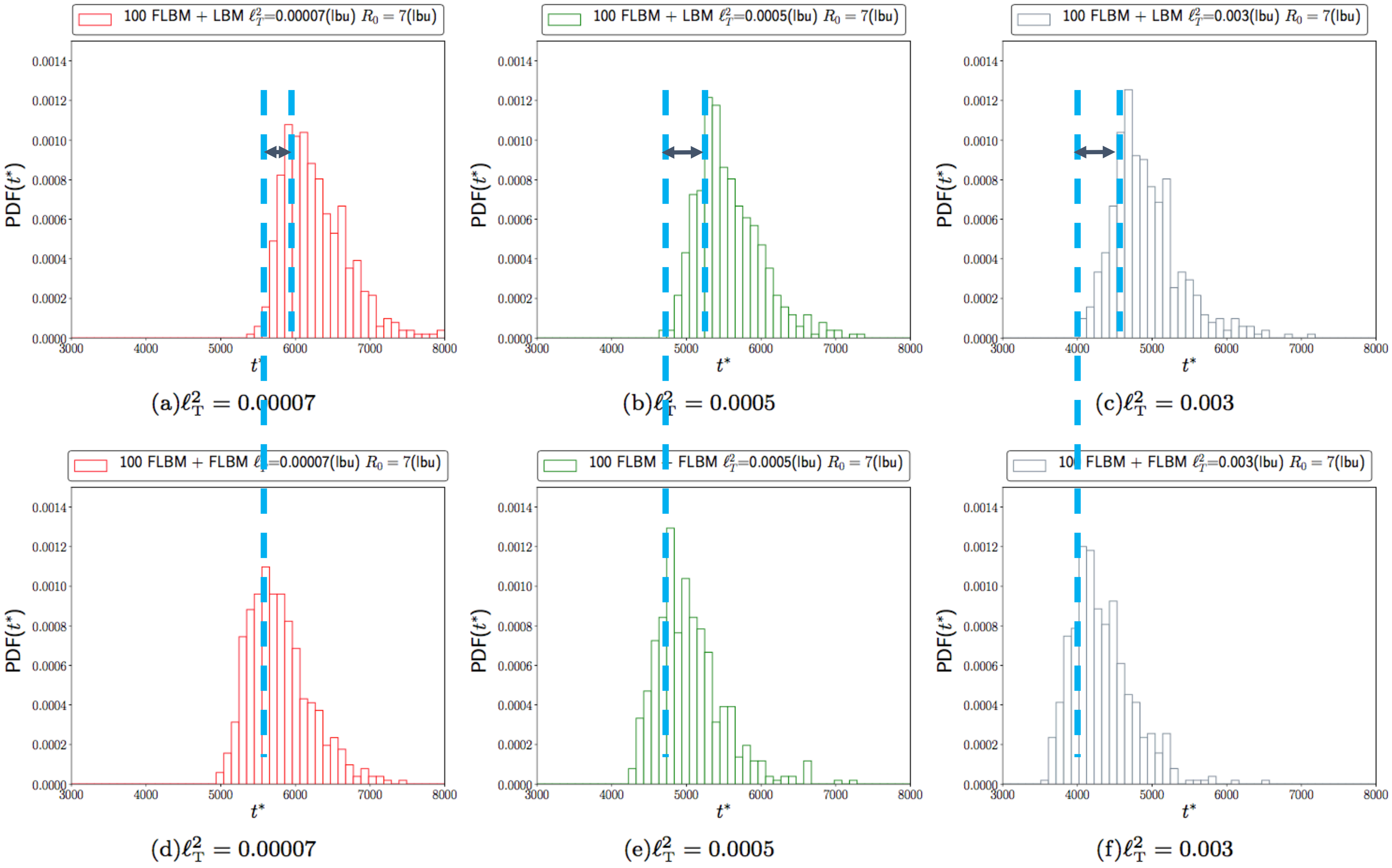
Thermal length: $\ell_T = 0.1$

X.Xue et al. accepted at PRE, arXiv:1804.09520



without TN

with TN



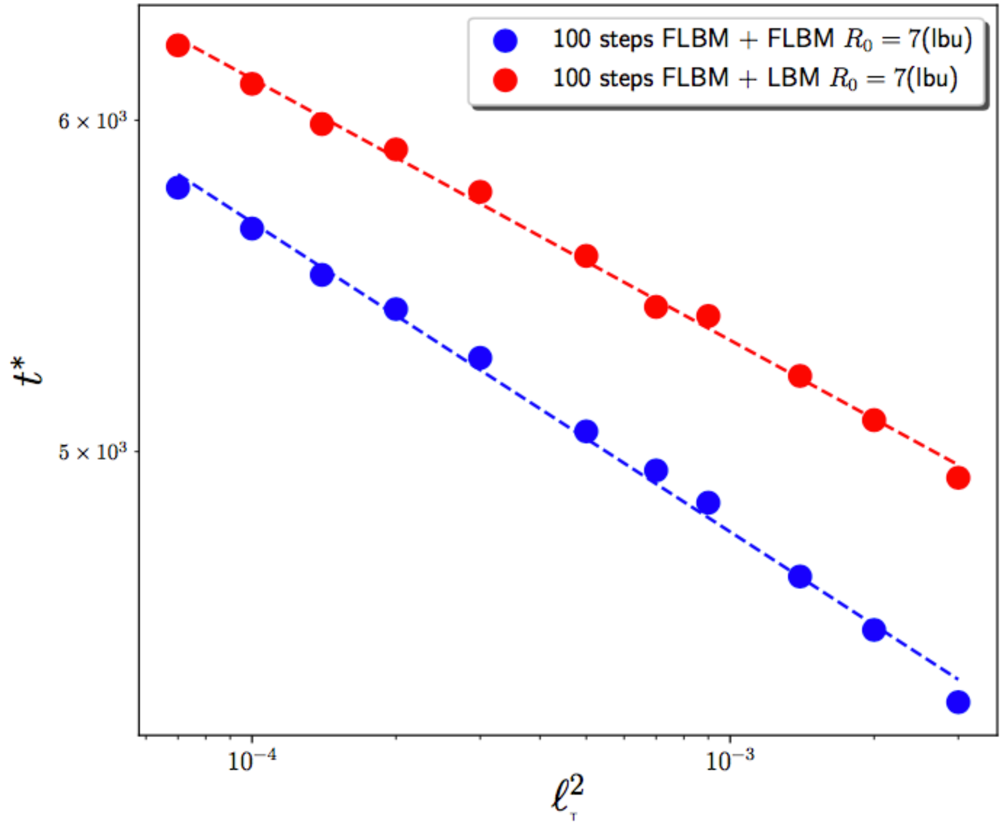
(a)$\ell_{\mathrm{T}}^2 = 0.00007$ (b)$\ell_{\mathrm{T}}^2 = 0.0005$ (c)$\ell_{\mathrm{T}}^2 = 0.003$

(d)$\ell_{\mathrm{T}}^2 = 0.00007$ (e)$\ell_{\mathrm{T}}^2 = 0.0005$ (f)$\ell_{\mathrm{T}}^2 = 0.003$

Break up time PDF for LBM and FLBM at fixed $R_0 = 7$

Thermal fluctuation impact on the break-up process

- Initial condition of the hydrodynamics can the decrease the breakup time
- Thermal fluctuations enhance the effect of acceleration



Break up time as function of LBM and FLBM at fixed $R_0 = 7$

X.Xue et al. accepted at PRE, arXiv:1804.09520

Thermal fluctuation impact on the break-up process

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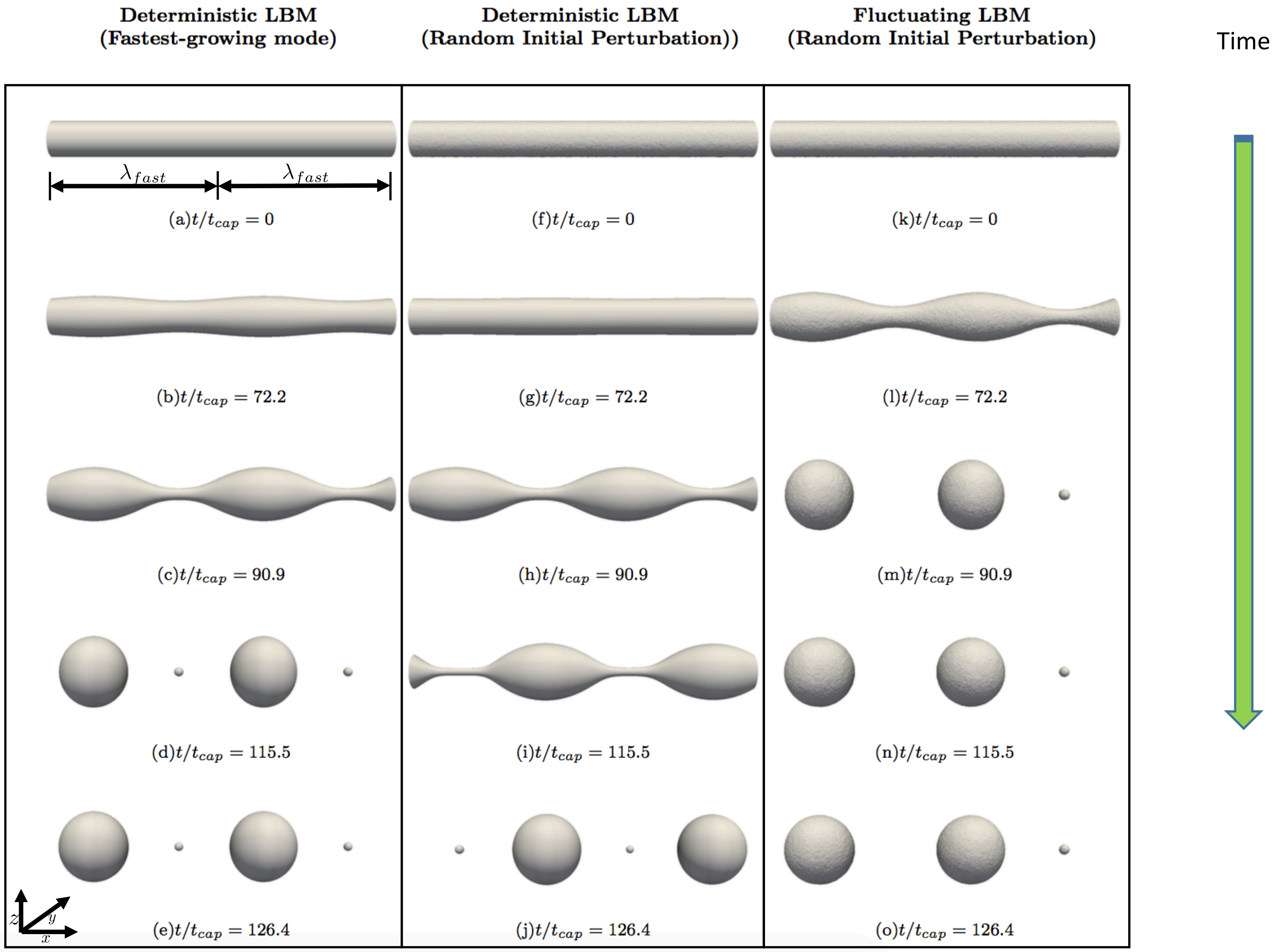


(a)$t/t_{cap} = 0$ (f)$t/t_{cap} = 0$ (k)$t/t_{cap} = 0$

(b)$t/t_{cap} = 72.2$ (g)$t/t_{cap} = 72.2$ (l)$t/t_{cap} = 72.2$

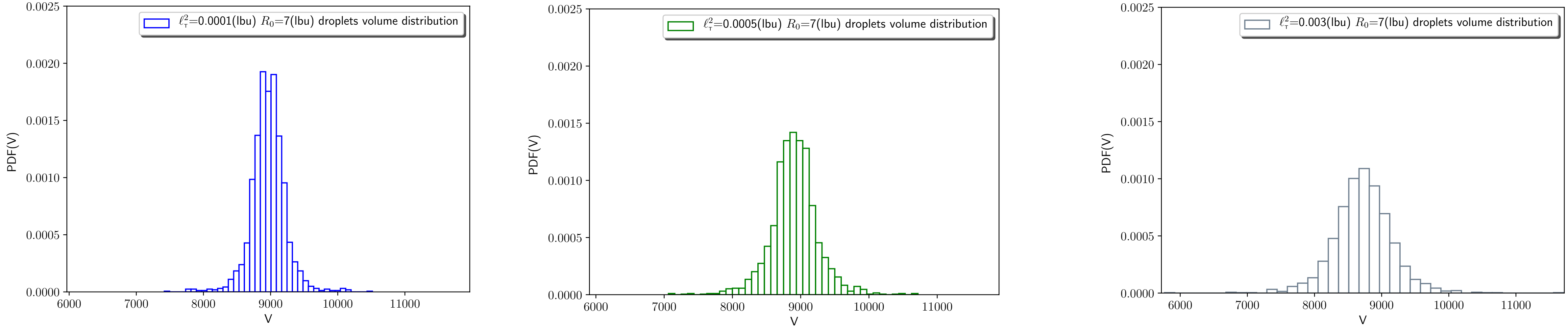
(c)$t/t_{cap} = 90.9$ (h)$t/t_{cap} = 90.9$ (m)$t/t_{cap} = 90.9$

(d)$t/t_{cap} = 115.5$ (i)$t/t_{cap} = 115.5$ (n)$t/t_{cap} = 115.5$

(e)$t/t_{cap} = 126.4$ (j)$t/t_{cap} = 126.4$ (o)$t/t_{cap} = 126.4$

Thermal fluctuations enhanced droplets' polydispersity

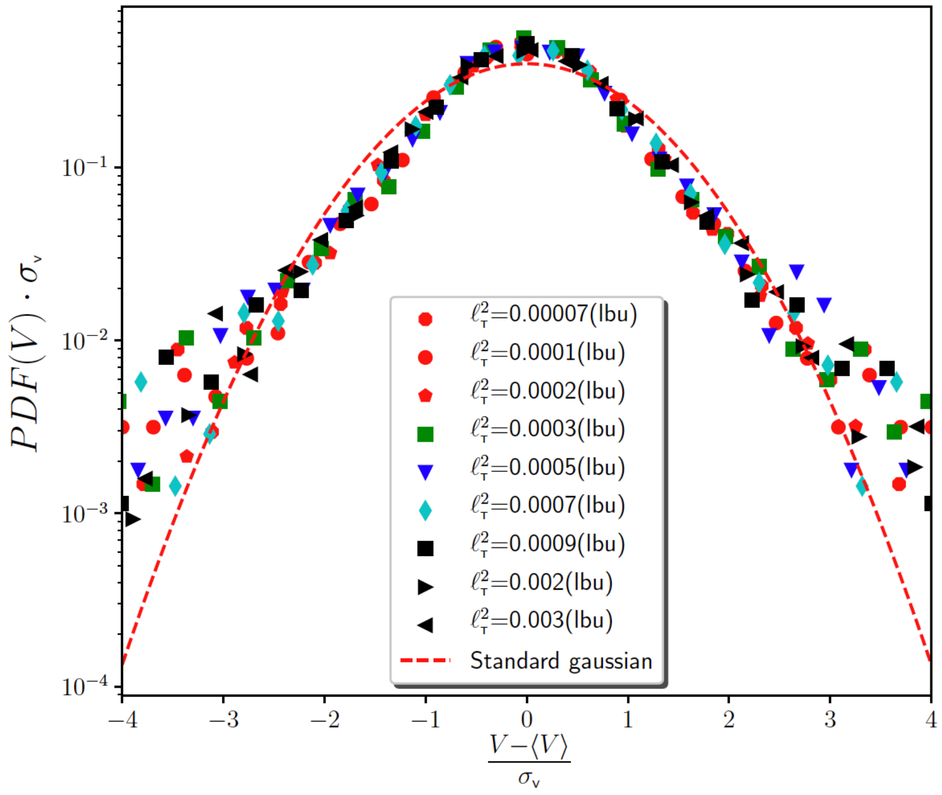
- ➢ Standard deviation of the droplet volumes are increasing with increasing of
- ➢ What is shape of the distribution?



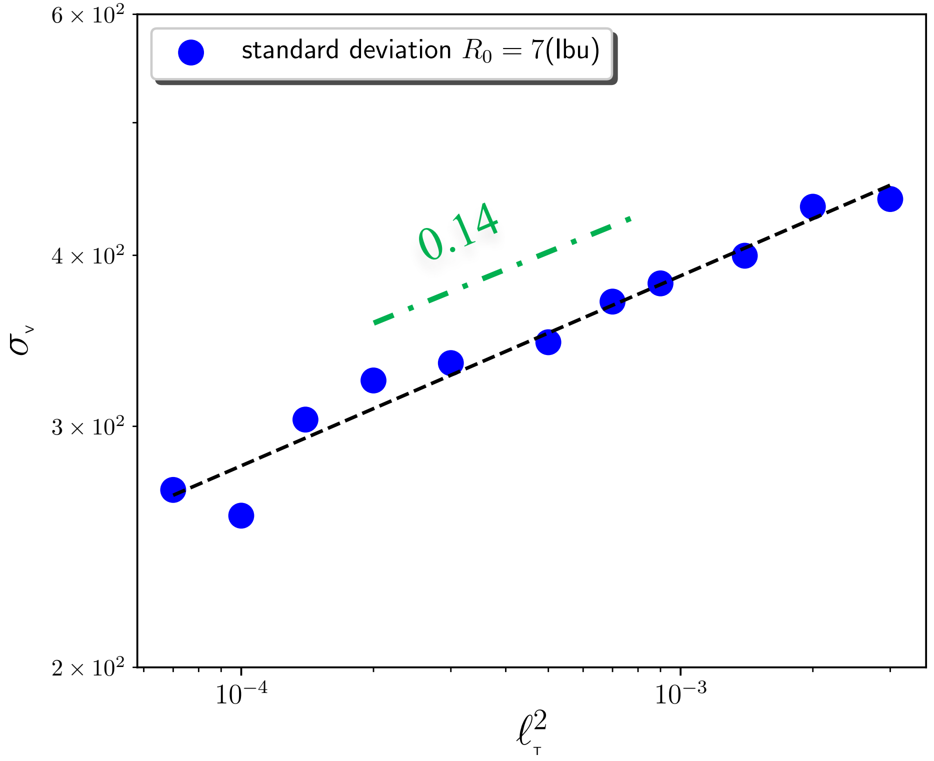
$\ell_T^2 = 0.0001$ $\ell_T^2 = 0.0005$ $\ell_T^2 = 0.003$

Distributions of droplets volumes at different values of ℓ_T^2 at fixed $R_0 = 7$

Droplet volumes distributions have small deviation from Gaussian distribution

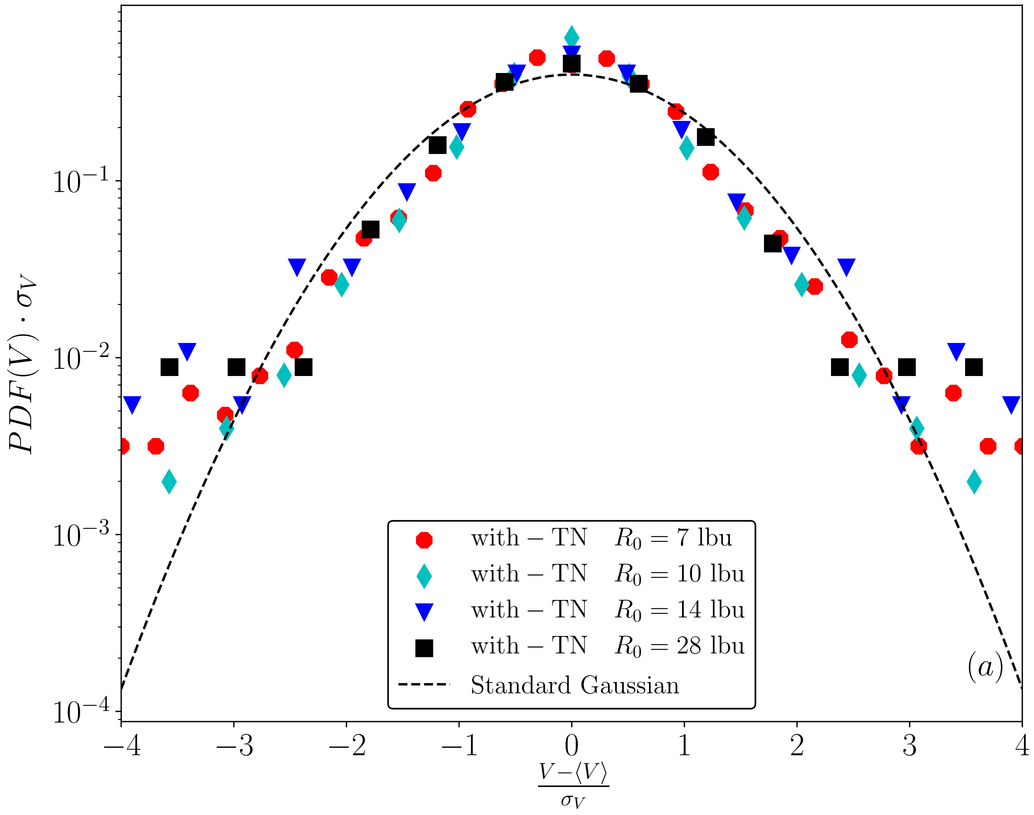


Normalized PDF for fixed $R_0 = 7$
vs Gaussian distributions

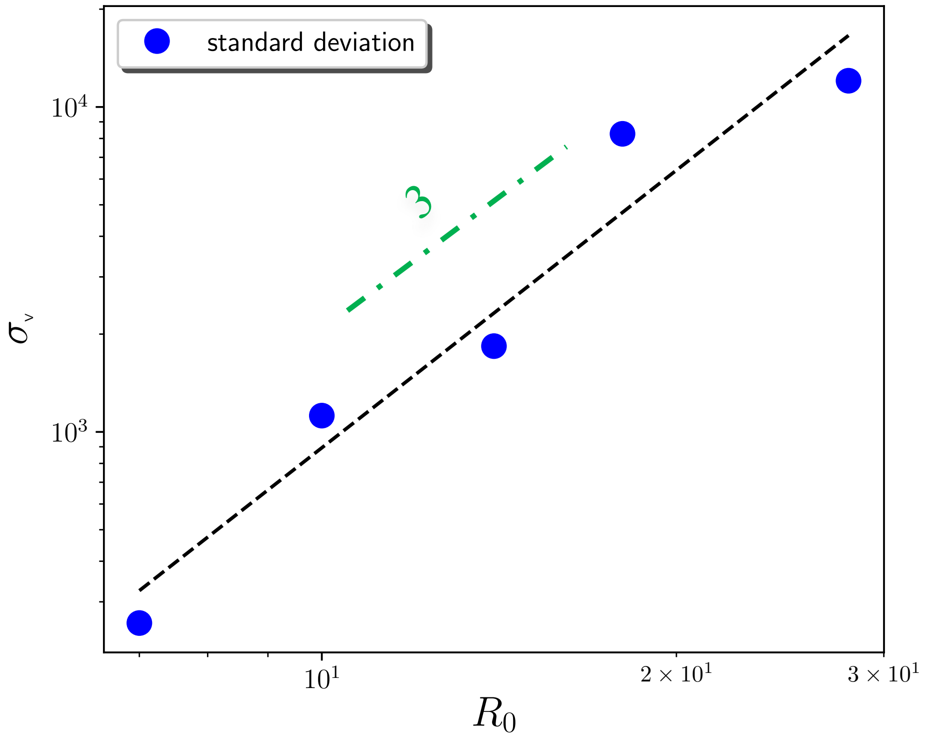


Standard deviation as function of ℓ_T^2 for
fixed $R_0 = 7$

What about different resolutions?



Normalized PDF for fixed $\ell_T^2 = 0.0001$ at different R$_0$ vs Gaussian distributions



Standard deviation of initial radius as a function of R$_0$ for fixed $\ell_T^2 = 0.0001$

Comparison with lubrication theory?

Initial Gaussian disturbance

Hydrodynamics

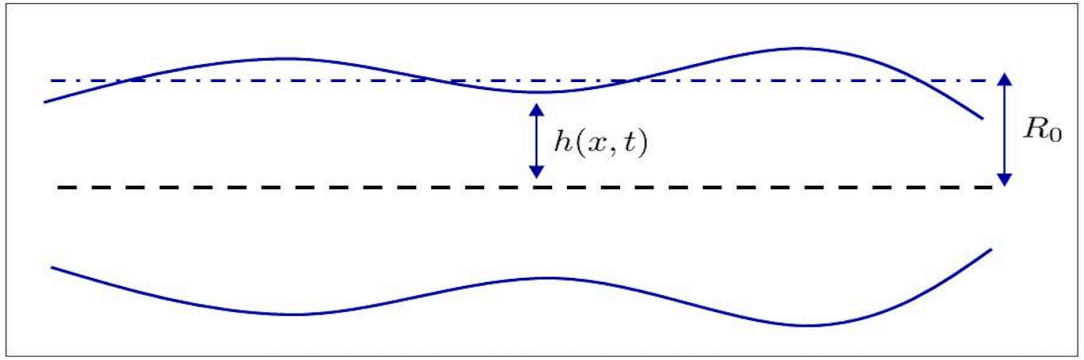
Shape of droplets volume PDF

Axisymmetric Lubrication theory (high viscosity ratio)

$$\partial_t h + vh' + \frac{1}{2}v'h = 0$$

$$\partial_t v + vv' = -P'/\rho_l + 3\mu_l/\rho_l (h^2 v')'/h^2$$

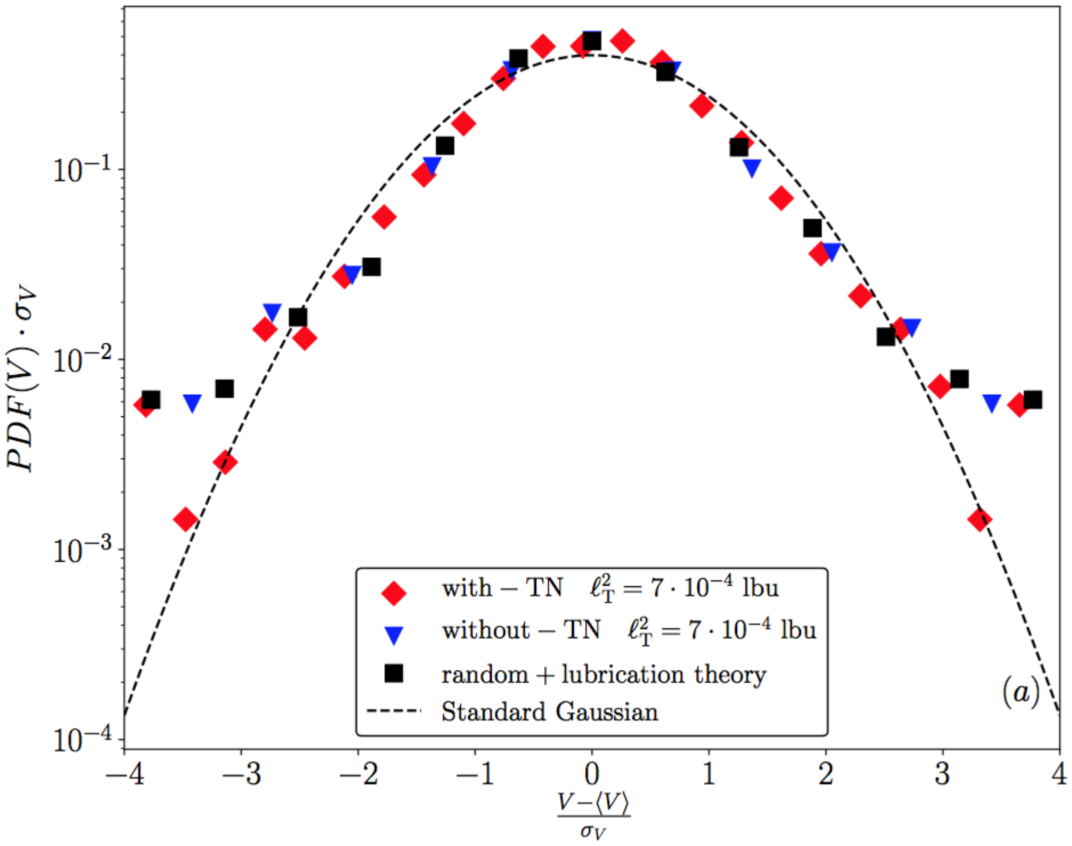
$$P = \sigma\left[\frac{1}{h(1+(h')^2)^{\frac{1}{2}}} - \frac{h''}{(1+(h')^2)^{\frac{3}{2}}}\right]$$



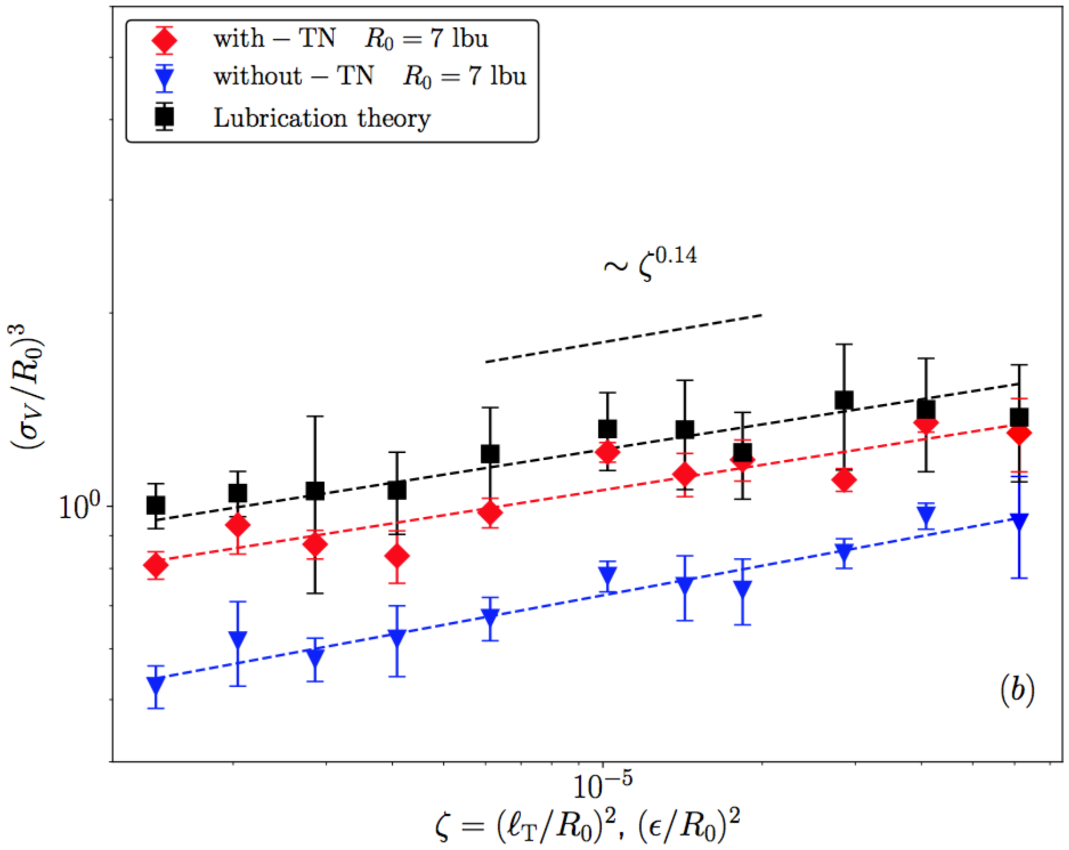
1. T. Driessen, R. Jeurissen, International Journal of Computational Fluid Dynamics, 2011

2. J Eggers, TF Dupont - Journal of fluid mechanics, 1994

Thermal fluctuations amplified the droplet polydispersity



Normalized PDF for lubrication theory, LBM, FLBM



Comparison of with-TN and without-TN at different ℓ_T^2

Summary and future plan

Summary:

- ✓ We investigated the nano-ligament the by using fluctuating lattice Boltzmann method
- ✓ Thermal fluctuations can speed up the ligament break-up process
- ✓ Thermal fluctuations can amplify the droplets polydispersity

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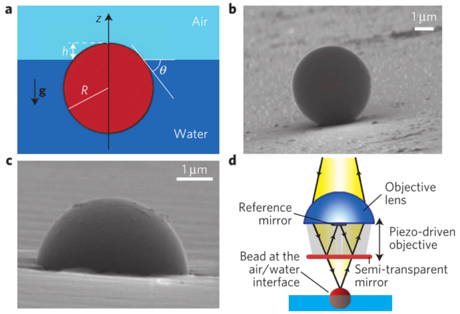
Future work:

- ➢ Exploring nano-scale simulation with fluid-particle interaction



Giuseppe Boniello, et al. ,Nature material, 2015

Thank you for your attention. Questions?

Funded by the Horizon 2020 Framework Programme of the European Union

MARIE CURIE ACTIONS

References

[1] D Belardinelli, M Sbragaglia, L Biferale, M Gross, and F Varnik. Fluctuating multicomponent lattice boltzmann model. *Physical Review E*, 91(2):023313, 2015.

[2] Sudhir Srivastava, JHM ten Thije Boonkkamp, and Federico Toschi. The lattice boltz- mann method for contact line dynamics. 2011.

[3] Sauro Succi. *The lattice Boltzmann equation: for fluid dynamics and beyond*. Oxford university press, 2001.

[4] S Van der Graaf, T Nisisako, C Schroen, RGM Van Der Sman, RM Boom. Lattice Boltzmann simulations of droplet formation in a T-shaped microchannel, Langmuir 22 (9), 4144-4152, 2006

[5] K van Dijke, G Veldhuis, K Schroën, R Boom, Parallelized edge-based droplet generation (EDGE) devices, Lab on a Chip 9 (19), 2824-2830, 2009