Effects of thermally induced capillary waves on nano-ligaments fragmentation

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DSFD conference

Worcester, USA, 26 June. 2018

Plateau-Rayleigh Instability

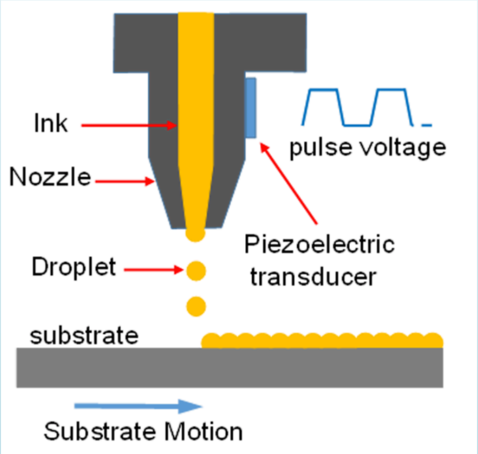
Ohnesorge number

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

Capillary time

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

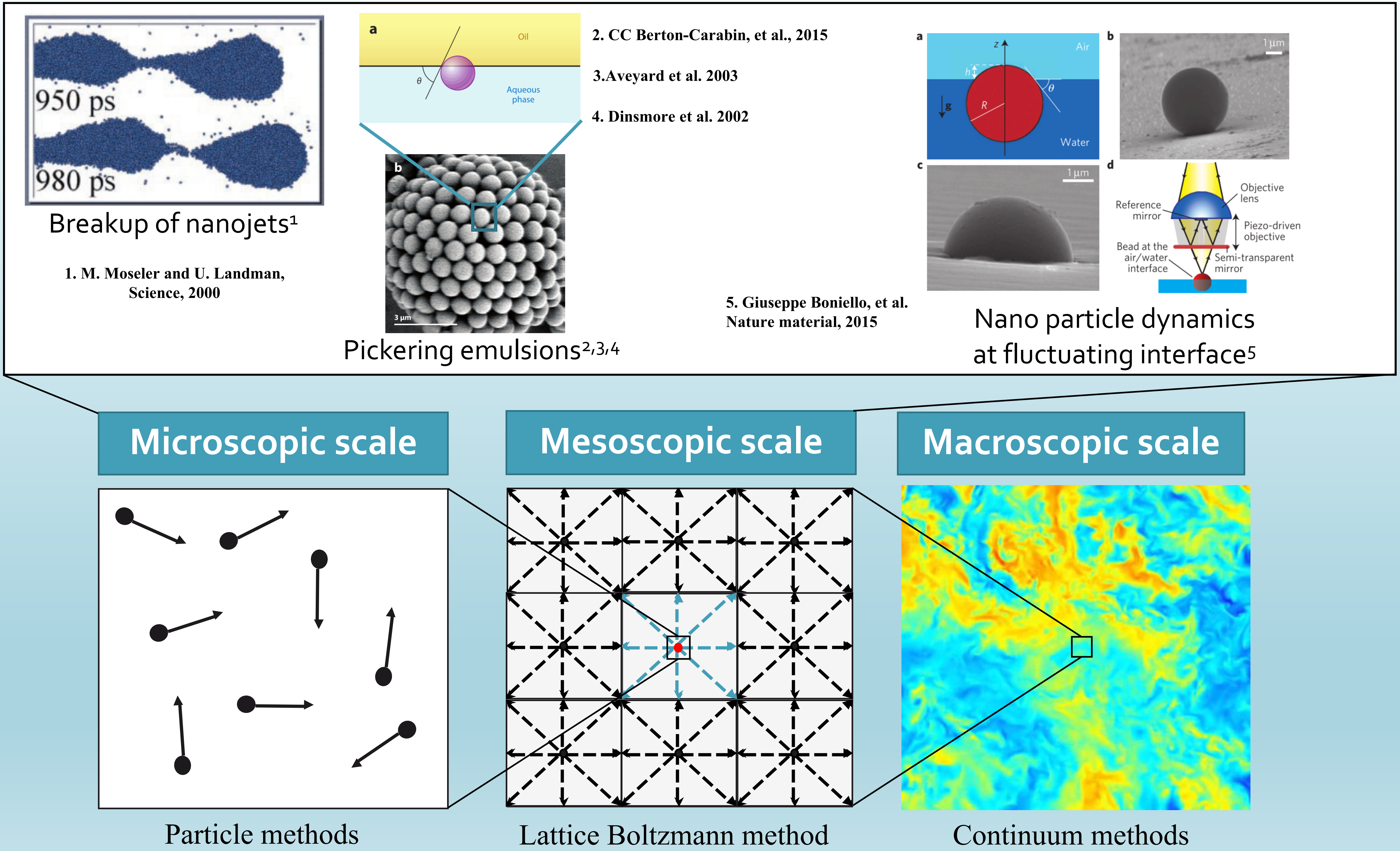
Droplet formation at faucet



Inkjet printing

Formation of soap bubble

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


950 ps
980 ps
Breakup of nanojets[1]
1. M. Moseler and U. Landman, Science, 2000
a
Oil
θ
Aqueous phase
b
3 μm
Pickering emulsions[2,3,4]
2. CC Berton-Carabin, et al., 2015
3.Aveyard et al. 2003
4. Dinsmore et al. 2002
5. Giuseppe Boniello, et al. Nature material, 2015
a
Air
z
h
θ
g
R
Water
b
1 μm
c
1 μm
d
Objective lens
Reference mirror
Piezo-driven objective
Bead at the air/water interface
Semi-transparent mirror
Nano particle dynamics at fluctuating interface[5]
Microscopic scale
Mesoscopic scale
Macroscopic scale
Particle methods
Lattice Boltzmann method
Continuum methods

Microscopic scale ← **Fluctuating multicomponent lattice Boltzmann model** — **Mesoscopic scale**

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

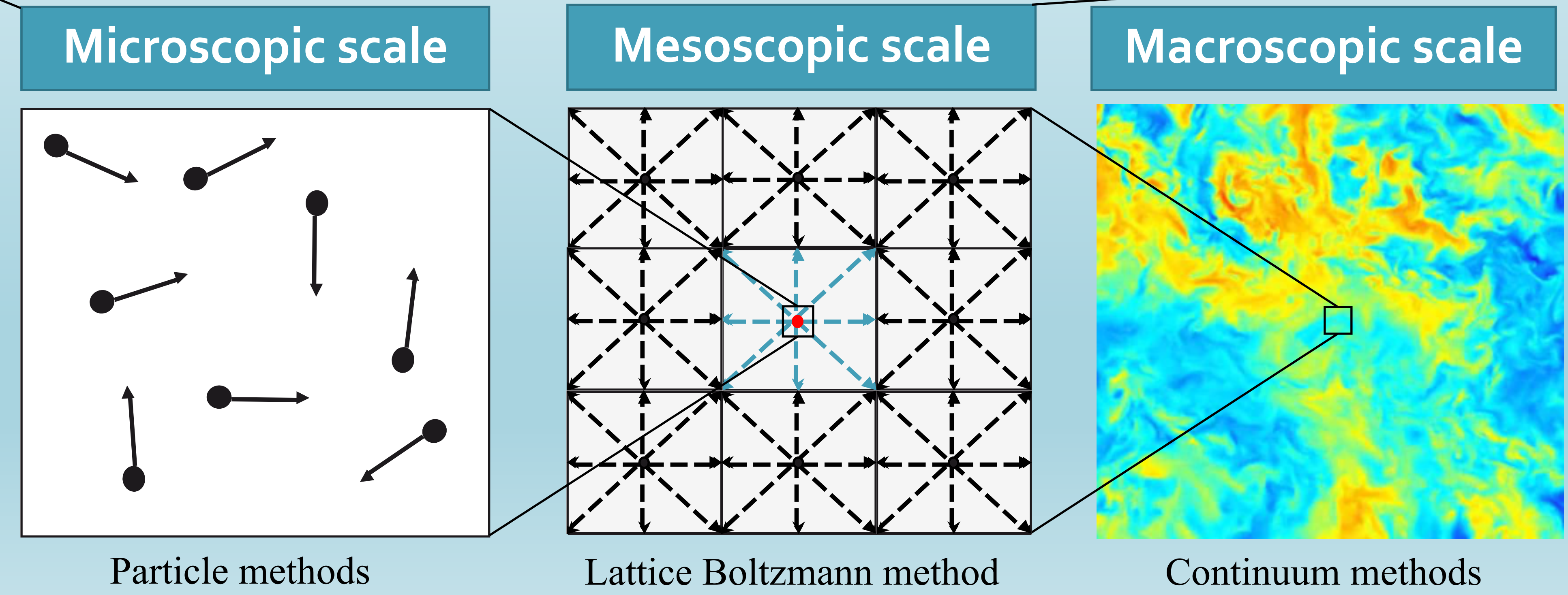
Noise term

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

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

Gaussian noise

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



Objective:

Understanding thermal fluctuations on nano-ligaments break-up

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

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

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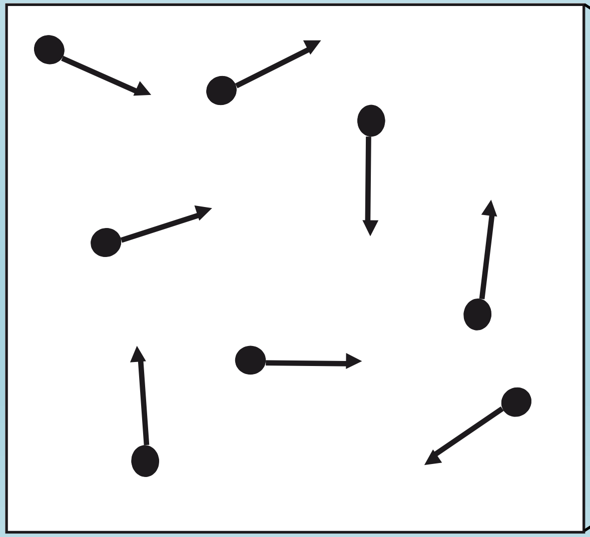
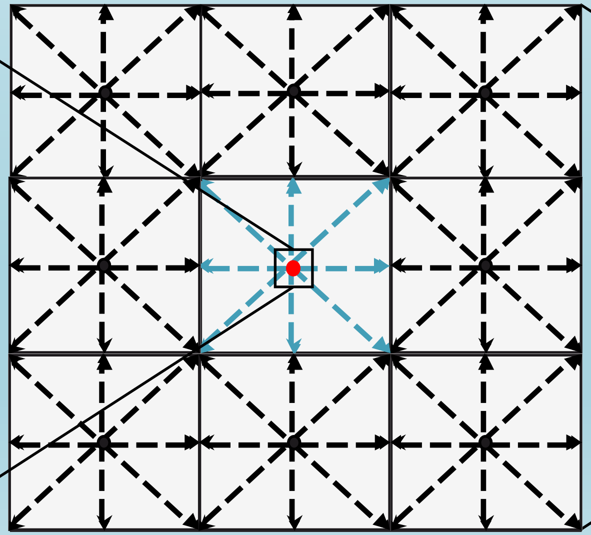
$$\rho_{tot} = \rho_r + \rho_b \quad \mathbf{v}_{tot} = \frac{\rho_r \mathbf{v}_r + \rho_b \mathbf{v}_b}{\rho_r + \rho_b}$$

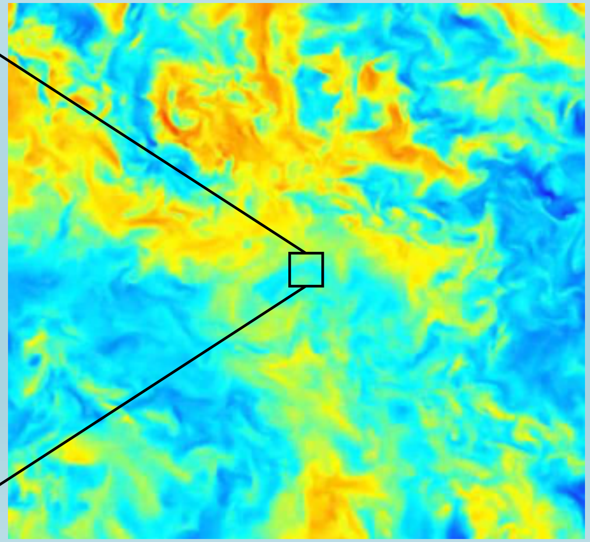
Microscopic scale	Mesoscopic scale	Macroscopic scale



Particle methods



Lattice Boltzmann method



Continuum methods

Basic lattice multicomponent Boltzmann model

Streaming

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

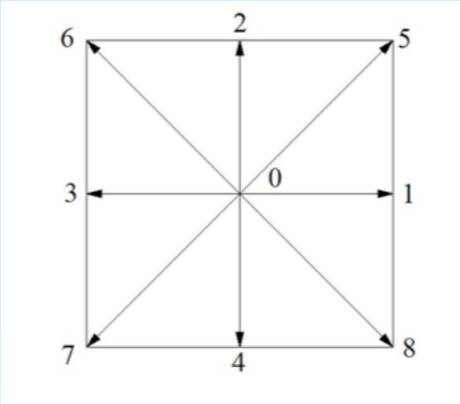
Collision

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

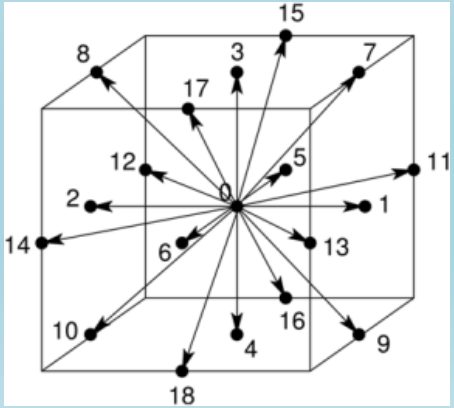
Hydrodynamics quantities

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

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



D2Q9 model



D3Q19 model

Basic lattice multicomponent Boltzmann model

Streaming

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

Collision

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

Hydrodynamics quantities

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

Shan-Chen forcing

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

Basic lattice multicomponent Boltzmann model

Streaming

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

Collision

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

Hydrodynamics quantities

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

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

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Streaming

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Champman-Enskog expansion

Navier-Stoke

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

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

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

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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

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

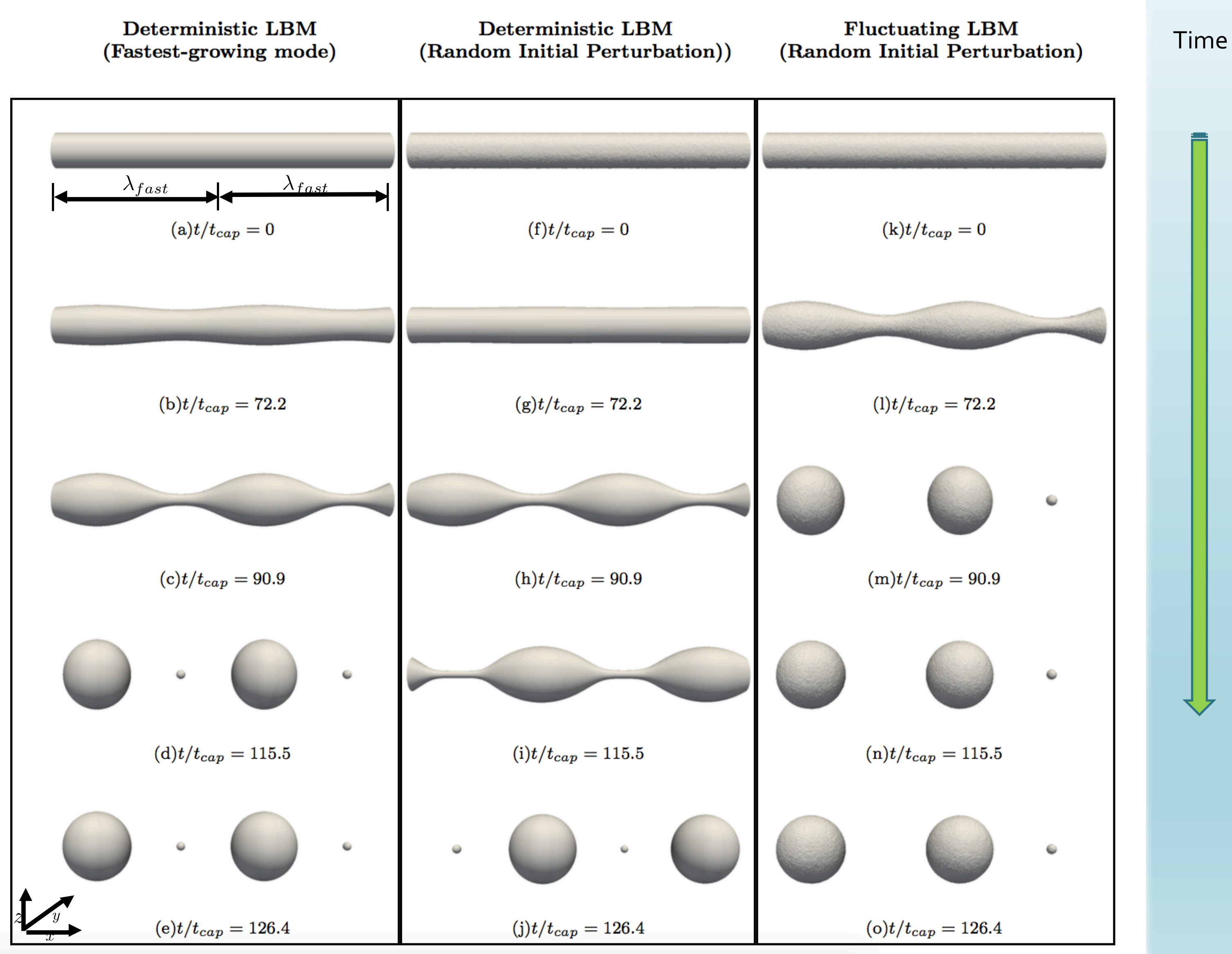
Capillary time

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

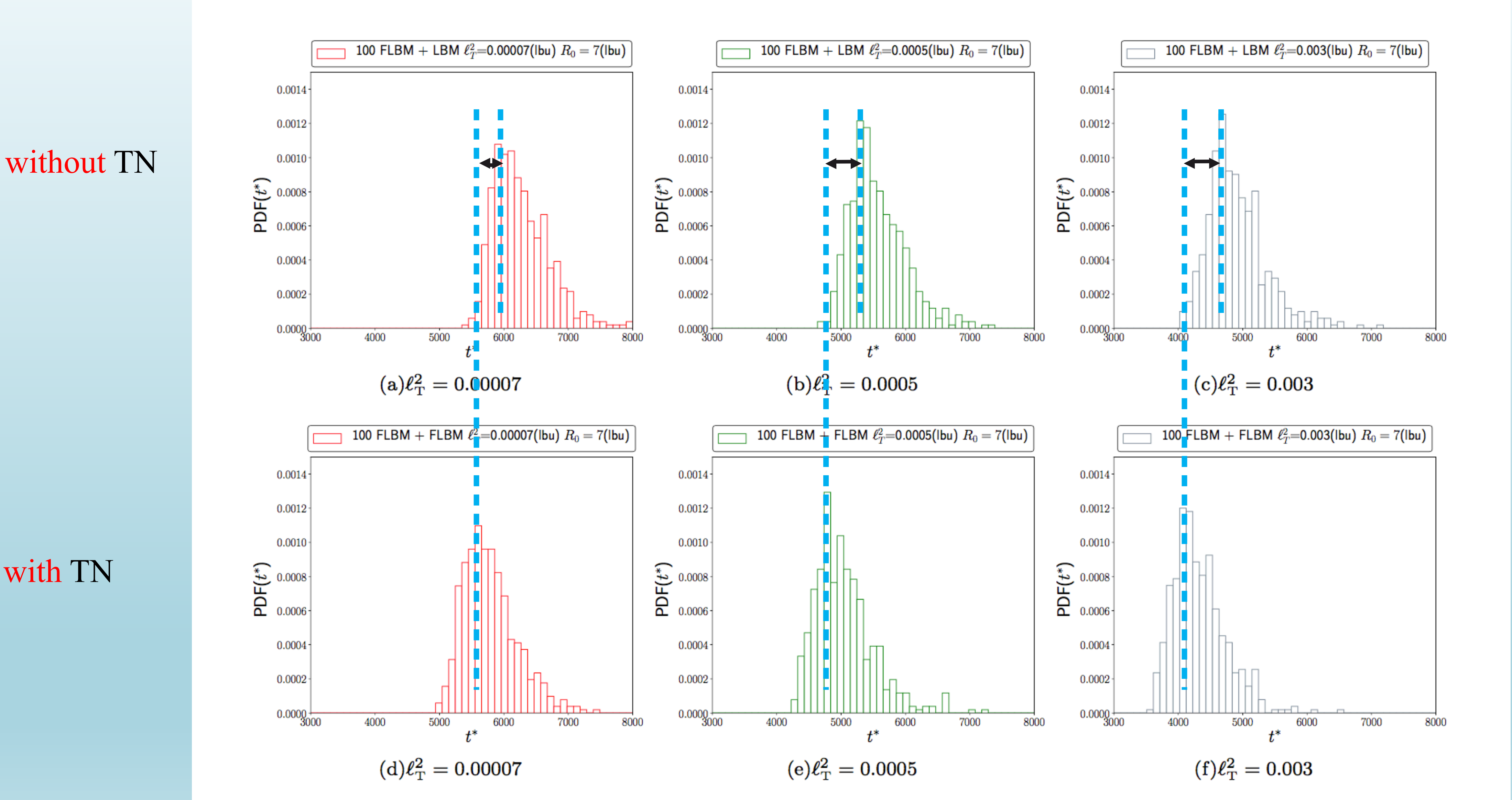
Domain size: 192X192X512

Thermal length: $\ell_T = 0.1$

X.Xue et al. arXiv preprint arXiv:1804.09520



Thermal fluctuations accelerate the fragmentation process

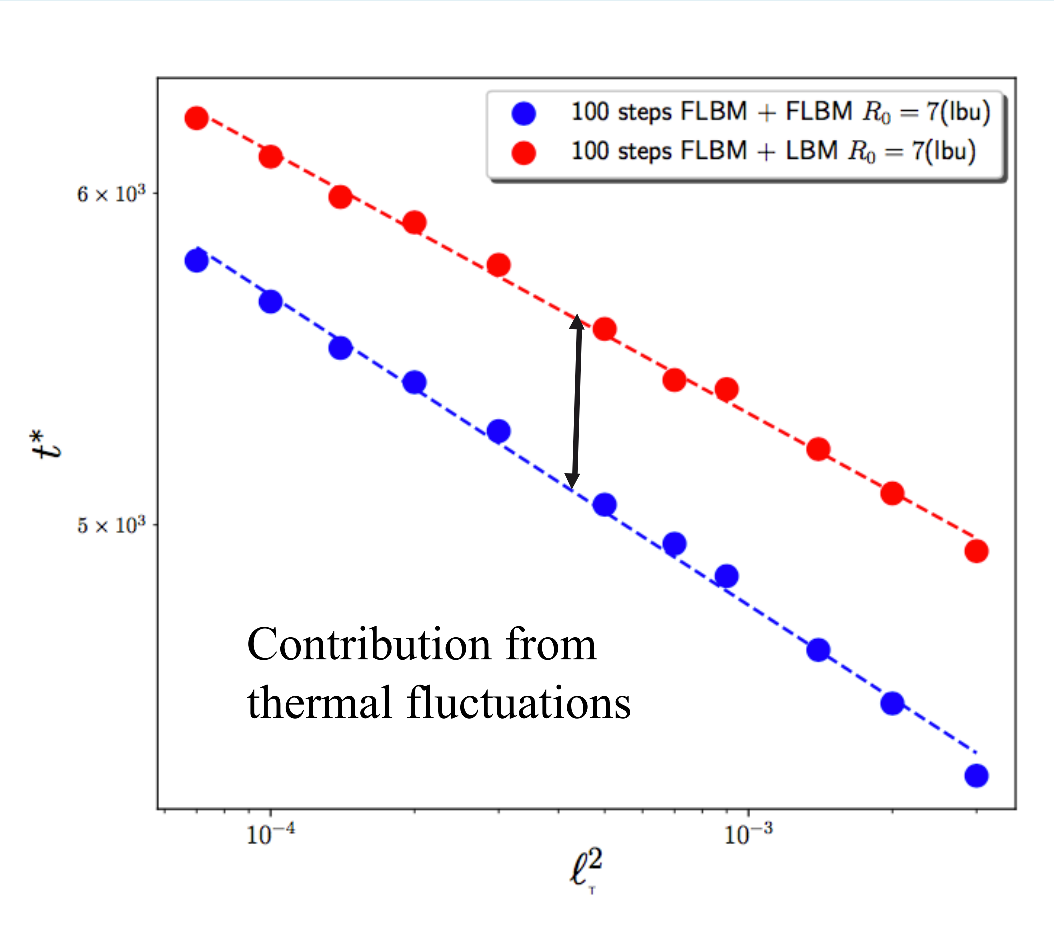


Break up time PDF for LBM and FLBM at fixed $R_0 = 7$

Thermal fluctuations accelerate the fragmentation 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 ℓ_T^2 LBM and FLBM at fixed $R_0 = 7$

X.Xue et al. arXiv preprint arXiv:1804.09520

Thermal fluctuation impact on the break-up process

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

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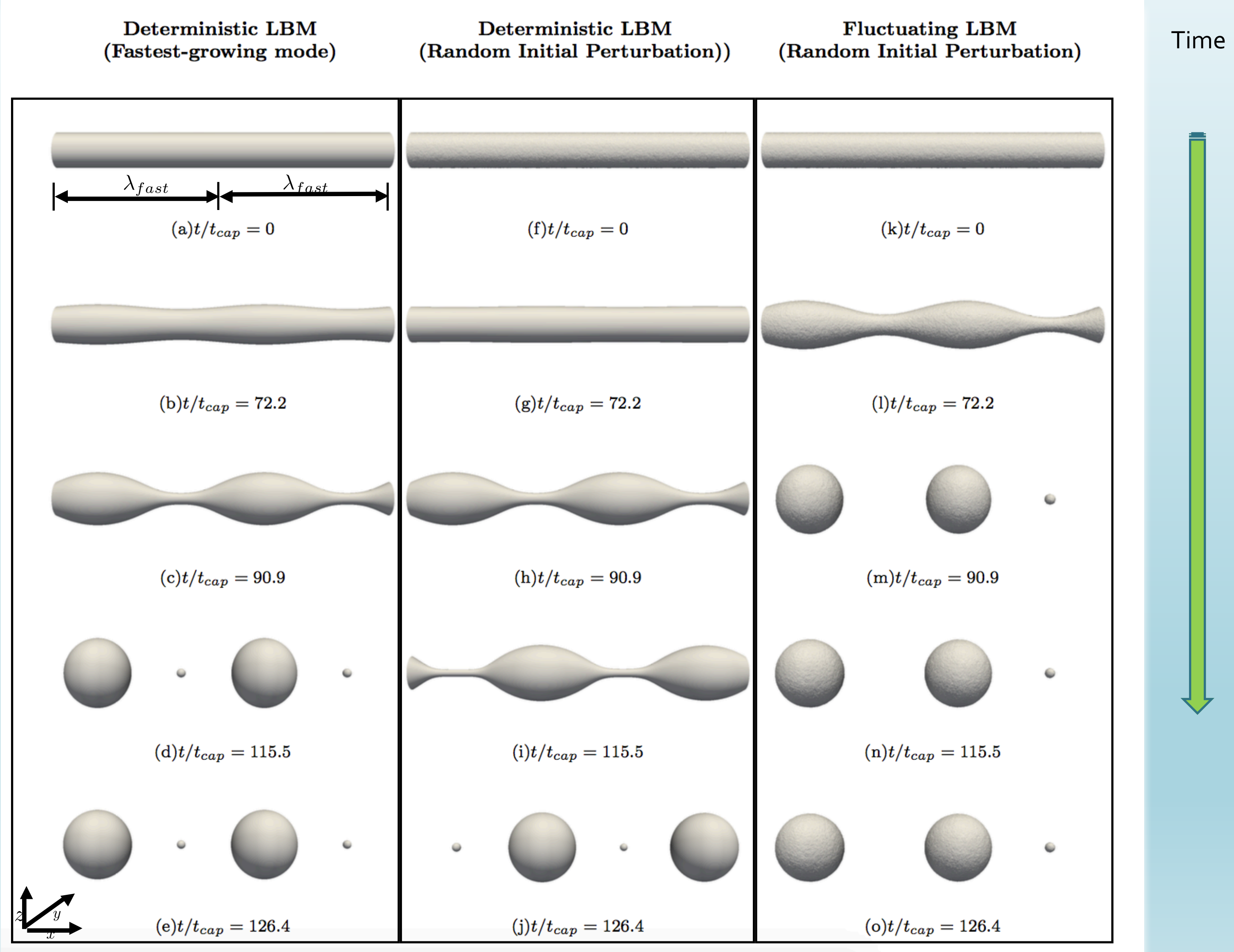
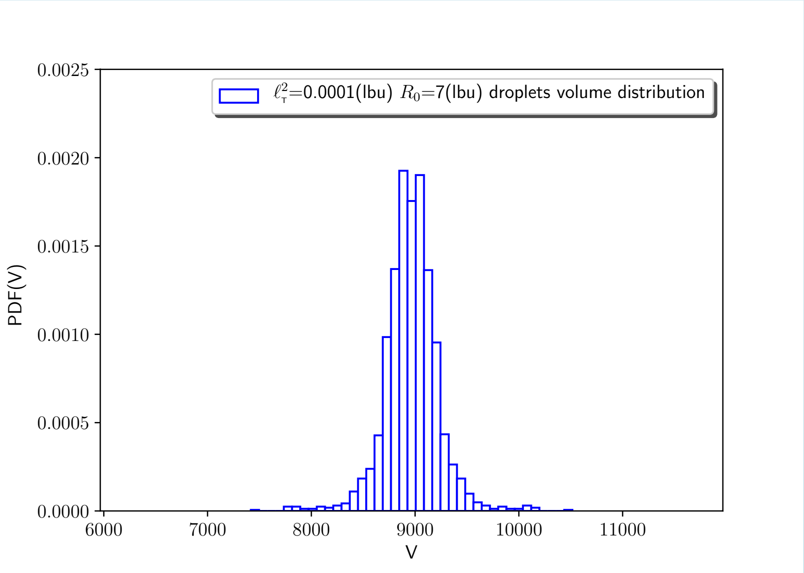
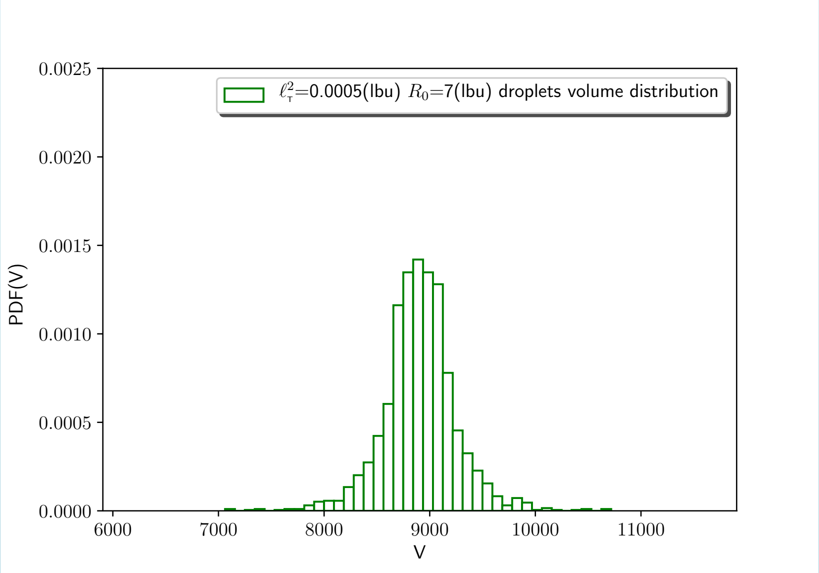


Thermal fluctuations enhanced droplets' polydispersity

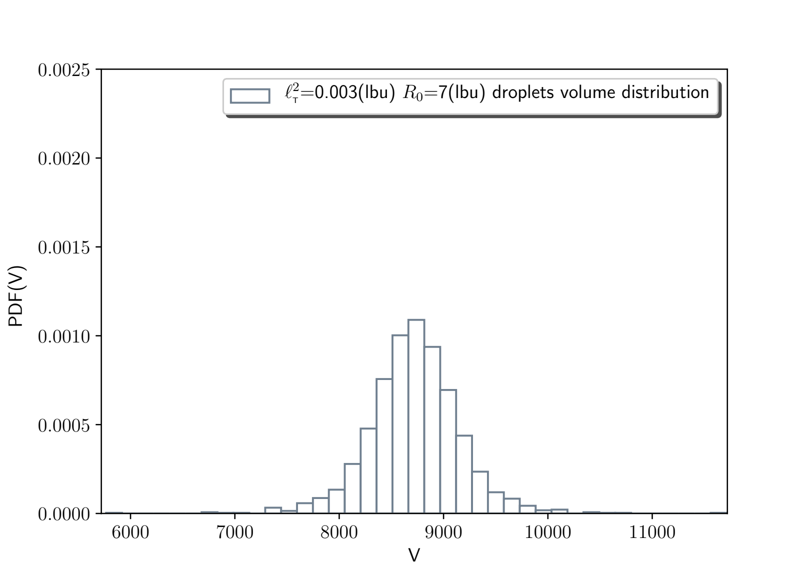
- Standard deviation of the droplet volumes are increasing with increasing of ℓ_T^2
- What is shape of the distribution?



$\ell_T^2 = 0.0001$



$\ell_T^2 = 0.0005$

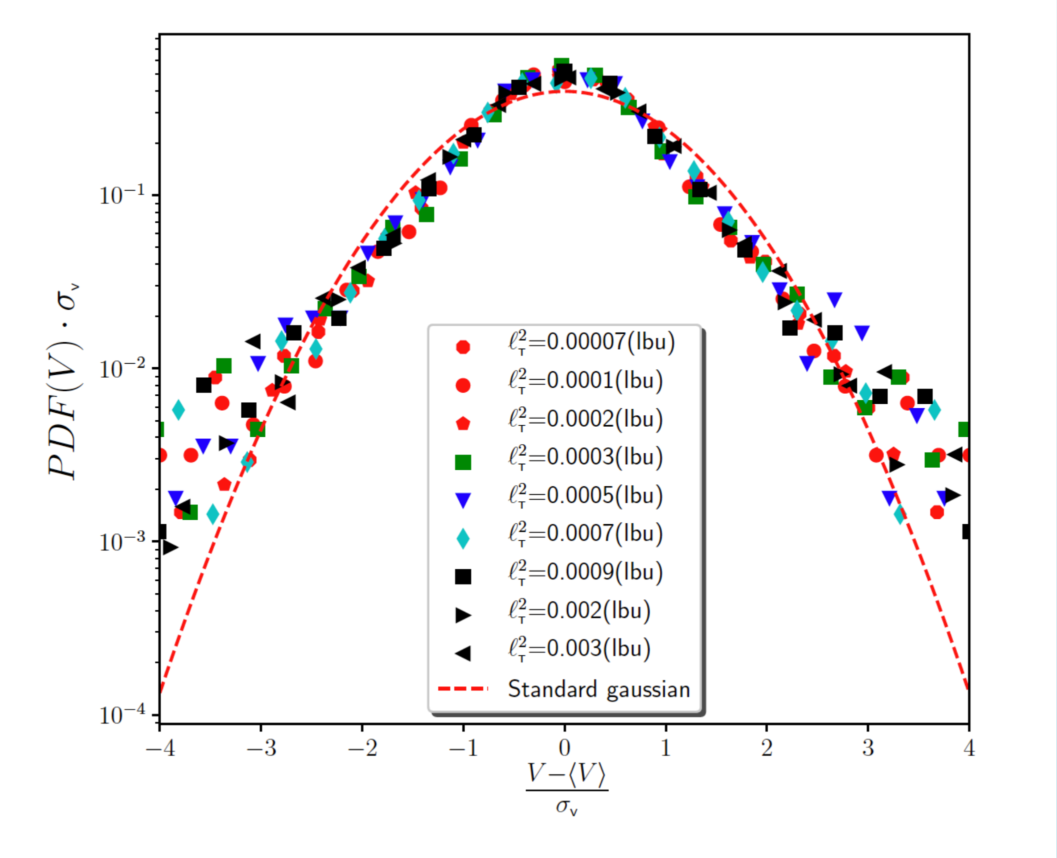


$\ell_T^2 = 0.003$

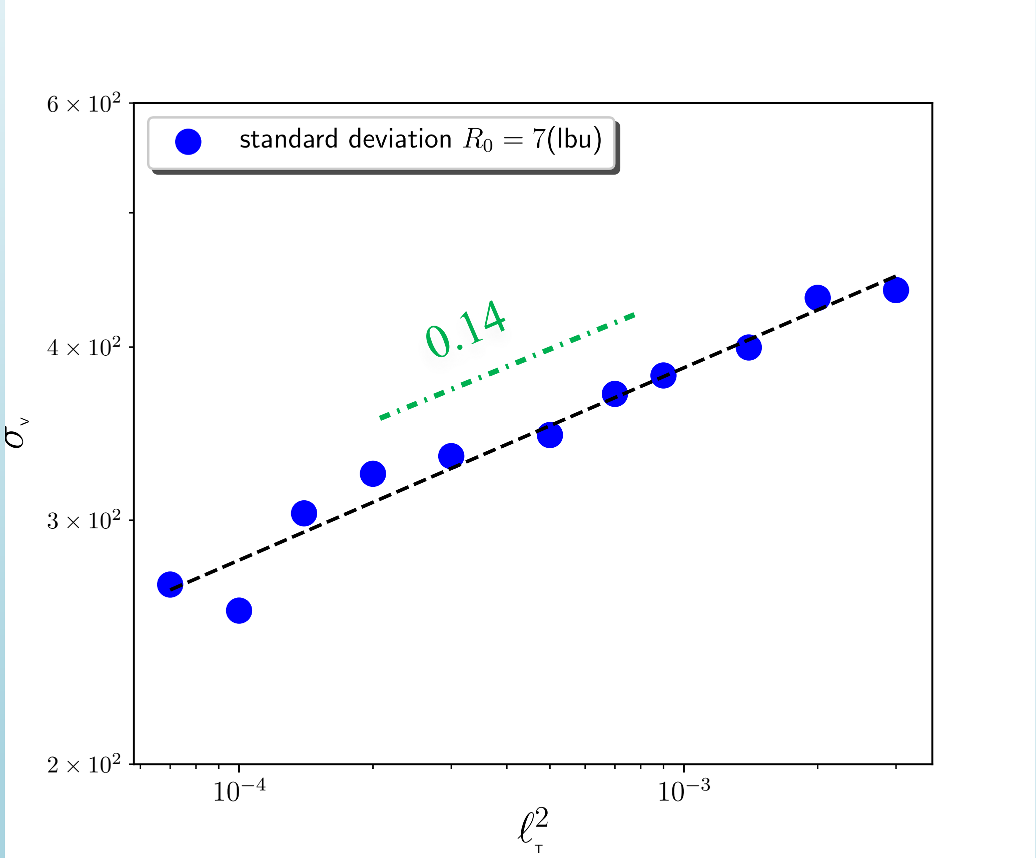
Distributions of droplets volumes at different values of ℓ_T^2 at fixed $R_0 = 7$

X.Xue et al. arXiv preprint arXiv:1804.09520

Droplet volumes distributions have small deviation from Gaussian distribution



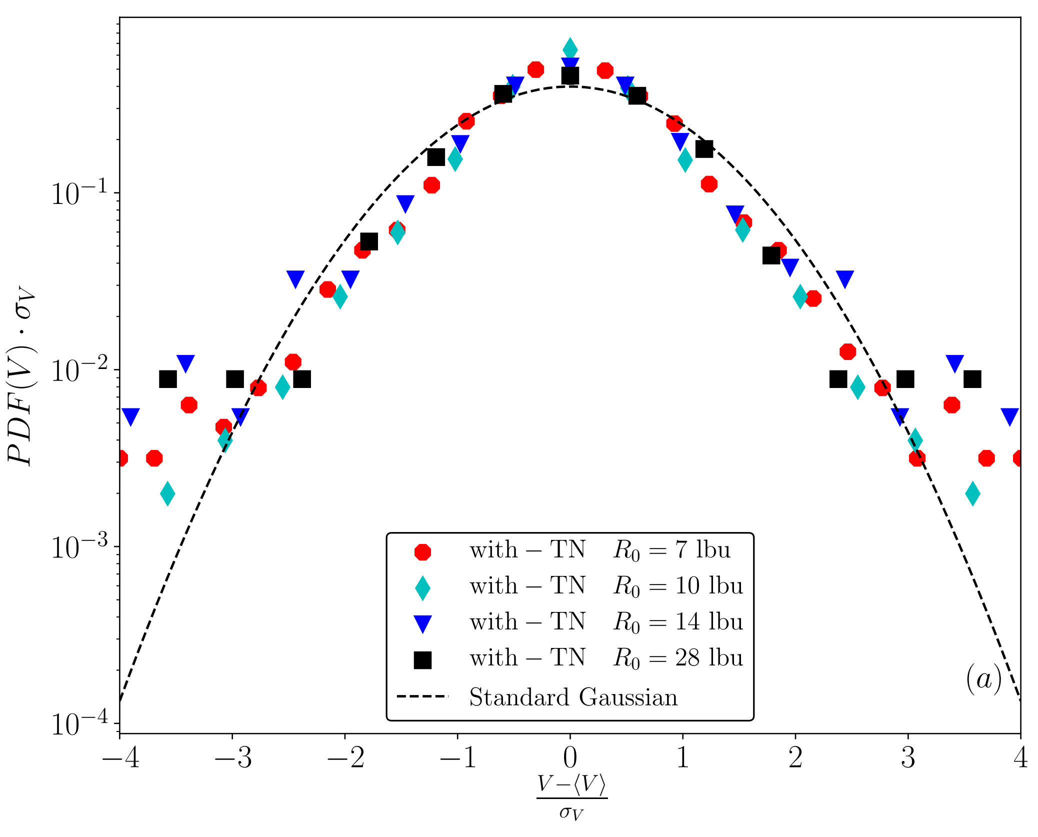
Normalized PDF for fixed $R_0 = 7$ vs Gaussian distributions

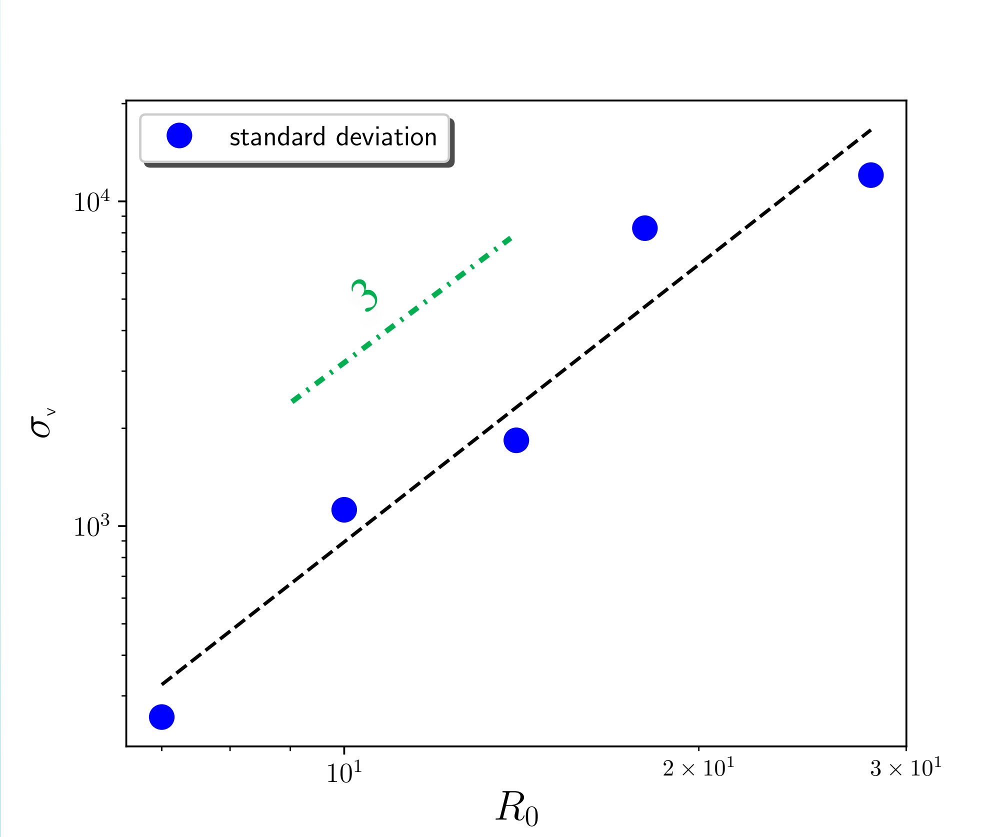


Standard deviation as function of ℓ_T^2 for fixed $R_0 = 7$

X.Xue et al. arXiv preprint arXiv:1804.09520

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 $\ell_T^2 = 0.0001$

X.Xue et al. arXiv preprint arXiv:1804.09520

Comparison with lubrication theory?

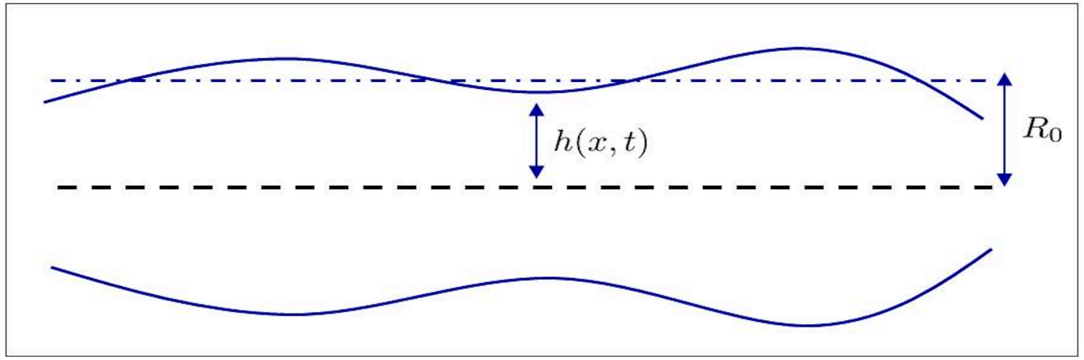
Initial Gaussian disturbance → Hydrodynamics → Shape of droplets volume PDF

Axisymmetric Lubrication theory (high viscosity ratio)

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

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

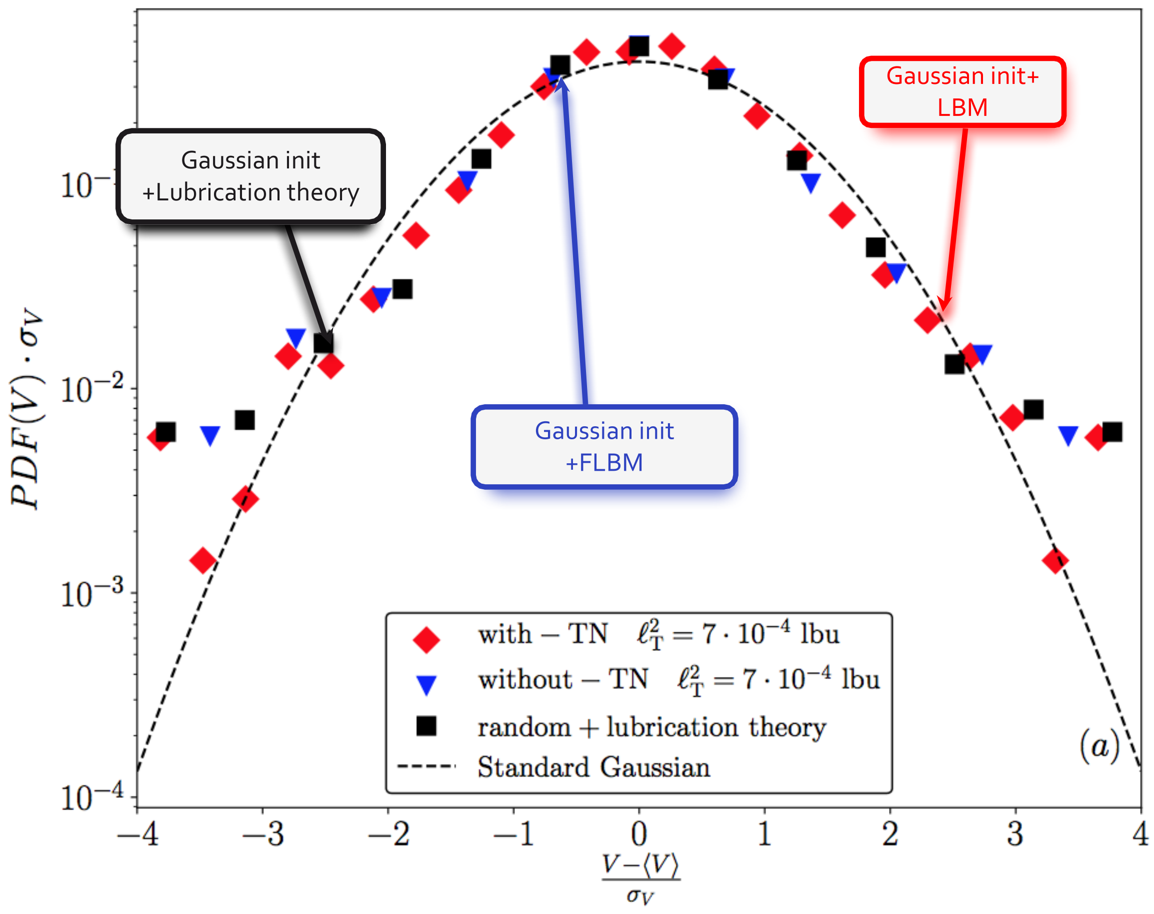
$$P = \sigma \left[\frac{1}{h(1+(h')^2)^{\frac{1}{2}}} - \frac{h''}{(1+(h')^2)^{\frac{3}{2}}} \right]$$

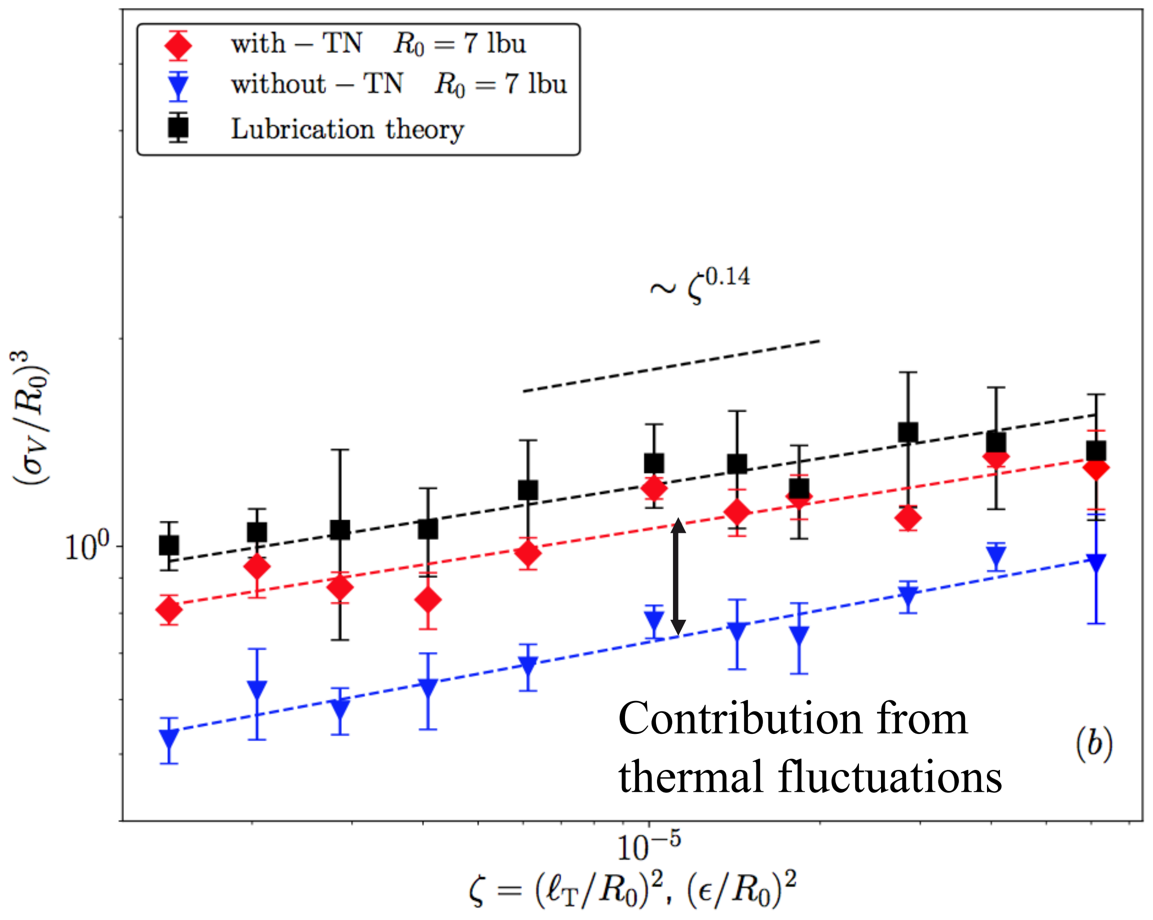


1. T. Driessen, R. Jeurissen, International Journal of Computational Fluid Dynamics, 2011

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

Future work:

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

Thank you for your attention. Questions?

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MARIE CURIE ACTIONS

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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.

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[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

Does initial configuration of the disturbance contribute to the shape of the PDF?

Initial Gaussian disturbance → Hydrodynamics → Shape of droplets volume PDF

Axisymmetric Lubrication theory (high viscosity ratio)

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

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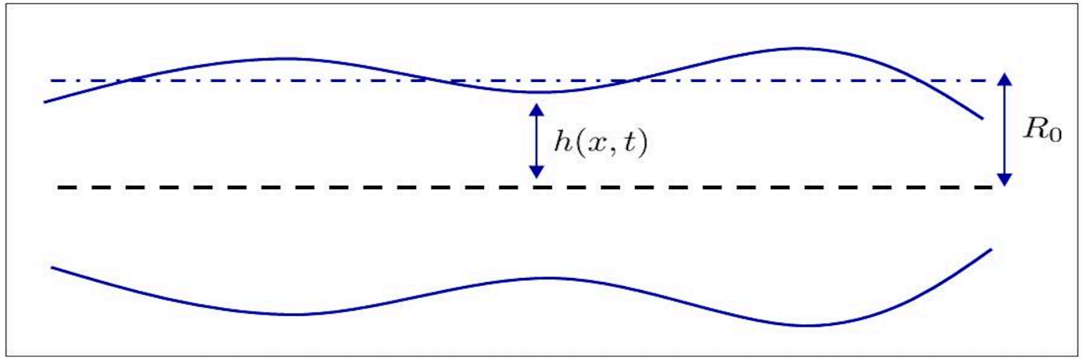

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