MDPD Simulation of liquid thread break-up and formation of droplets

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Introduction

Key Concept: The formation of droplets from a liquid jet is infuenced by fluid properties and thermal fluctuations.
Aim: Understand the mechanism of break-up that leads to the formation of droplets at the molecular scale.
Applications: Inkjet printing, microfluidic devices

Model and Methodology

Method: Molecular dynamics simulation of a cylindrical liquid geometry to reproduce the Rayleigh-Plateau instability

Model: Many-body dissipative particle dynamics was chosen for this problem due to its lower computational cost when compared to traditional MD.

Analysis: To obtain the characteristic wavelength that leads to the break-up, the following density correlation function was used:

$$G(r,\delta z) = \frac{\langle \rho(r,\phi,z)\rho(r,\phi,z+\delta z)\rangle_{z,\phi}}{\langle [\rho(r)]^2\rangle_{z,\phi}}$$

Results

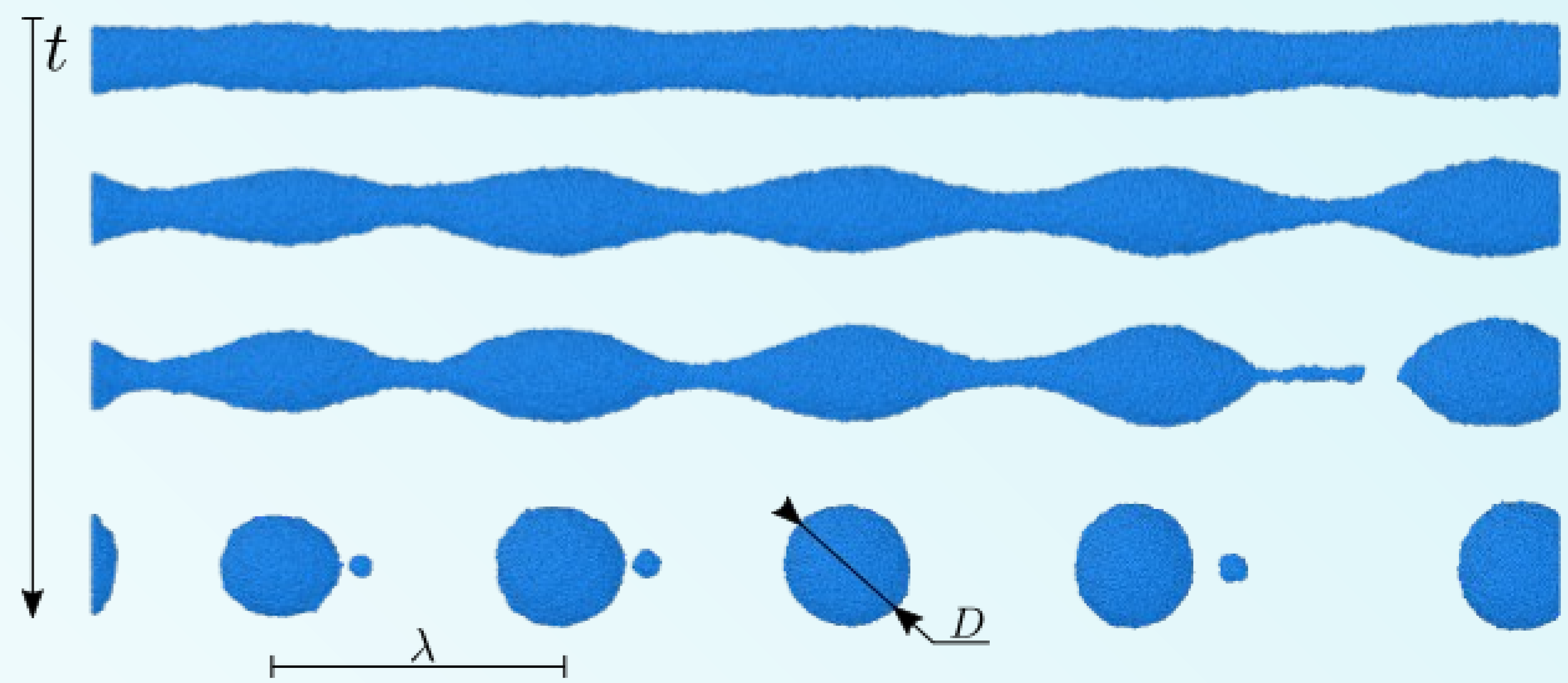


Figure: Time evolution of a liquid thread breaking into main droplets with the presence of satellite droplets.

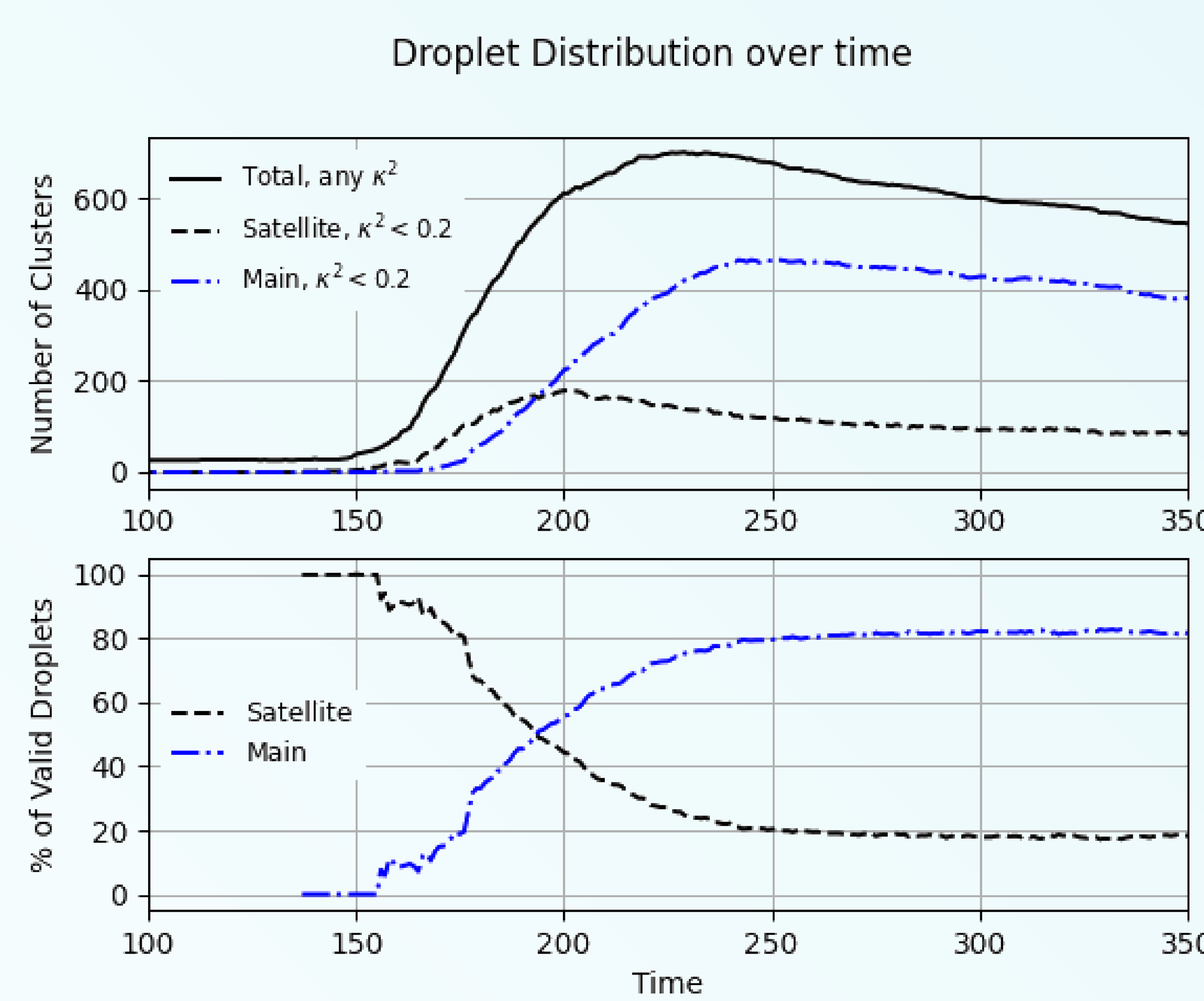


Figure: Variation on the number of droplets (clusters with small shape anisotropy κ²) through the whole simulation.

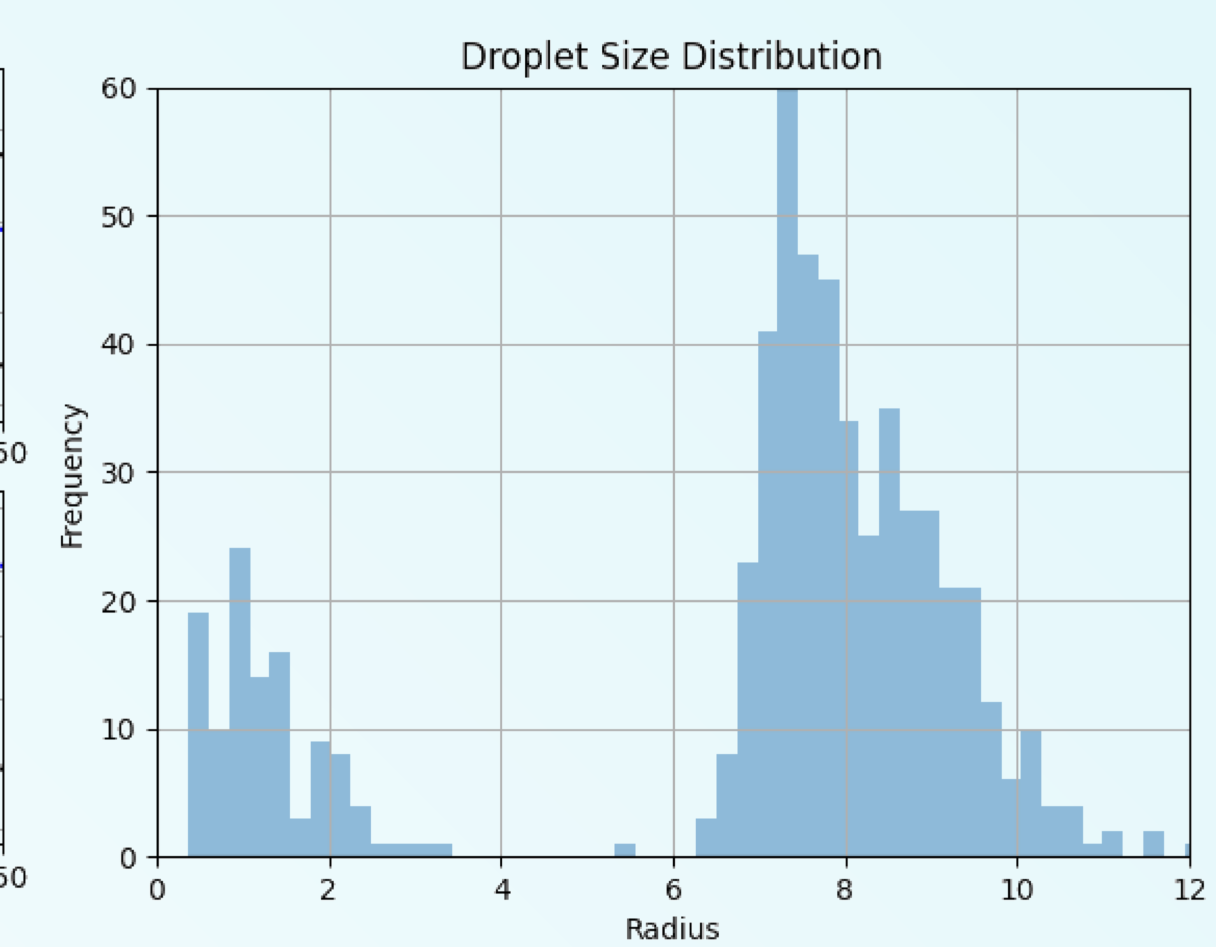
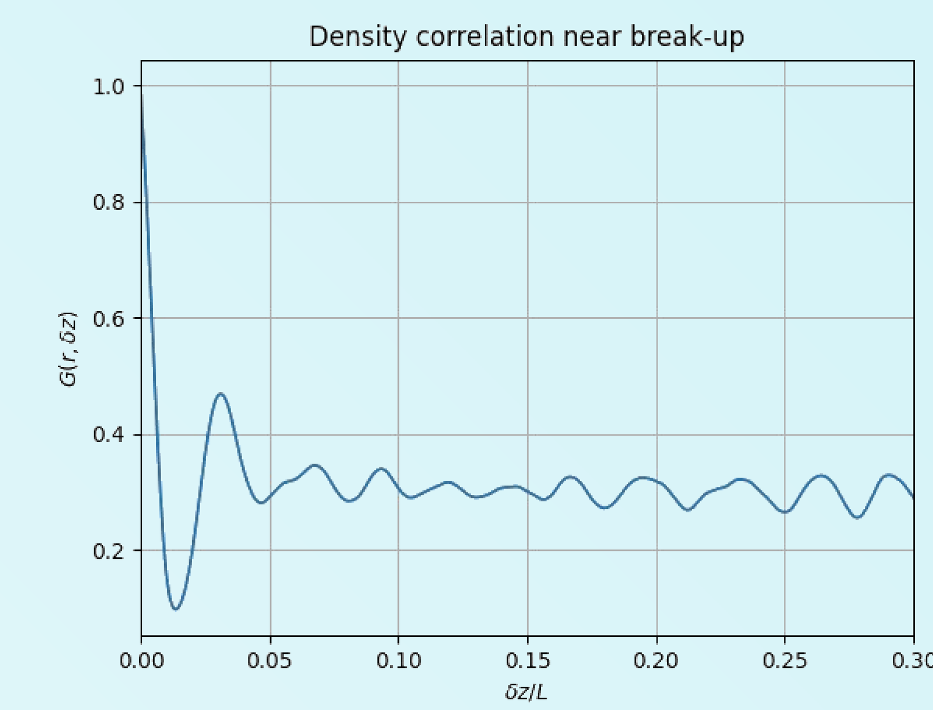


Figure: Distribution of different droplet sizes after all the break-up events have occurred in the simulation (when the number of clusters is at its maximum).

Results



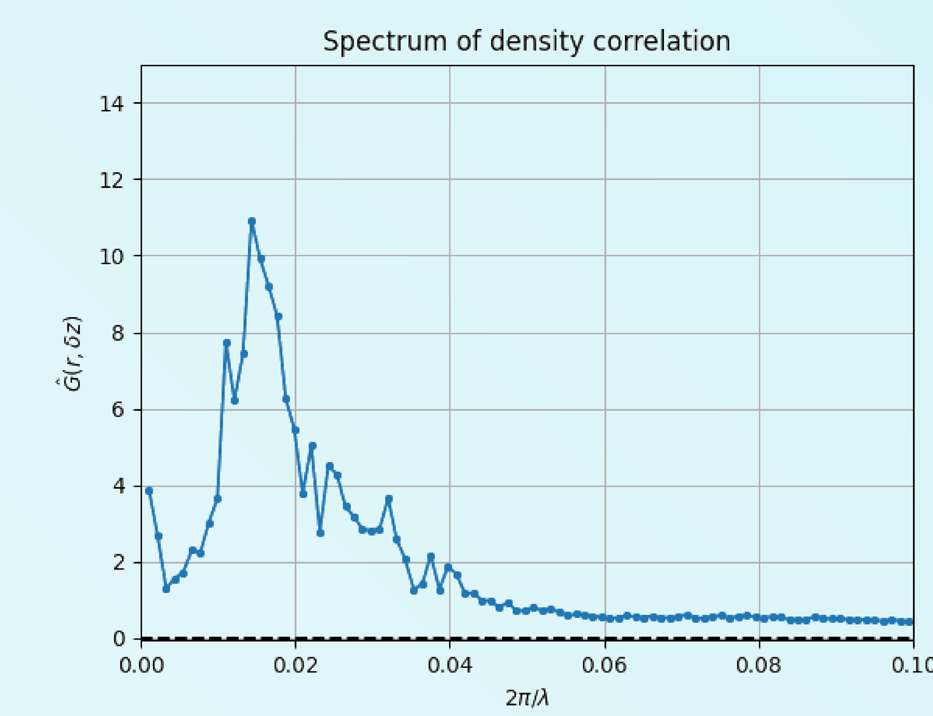


Figure: Density correlation and its Fourier transform near the moment of the first break-up.

Conclusion

- Density correlation is able to capture the characteristic wavelength λ;
- The number of droplets in a simulation decreases due to coalescence;
- Possible relation between λ and droplet sizes.

References:

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2. Jiayi Zhao, Nan Zhou, Kaixuan Zhang, Shuo Chen, Yang Liu, and Yuxiang Wang Phys. Rev. E 102, 023116 (2020)

Acknowledgment:

This research has been supported by the National Science Centre, Poland, under grant No. 2019/34/E/ST3/00232. This research was supported in part by PLGrid Infrastructure.