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Simulating Heat Flux and Bubble Nucleation using Molecular Dynamics

APS 2016

3:49 PM–4:02PM

By

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In collaboration with,

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APS | DFD 16

Division of Fluid Dynamics

Portland, Oregon | November 20 -22

APS physics

EPSRC

Pioneering research and skills

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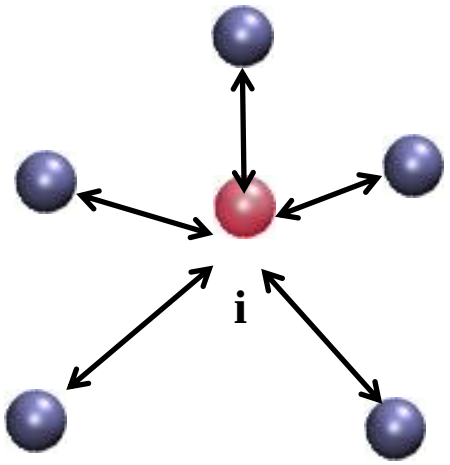
Molecular Dynamics

Discrete molecules in continuous space

- Molecular position evolves continuously in time
- Position and velocity from acceleration

$$\ddot{\boldsymbol{r}}_i \rightarrow \dot{\boldsymbol{r}}_i$$
$$\dot{\boldsymbol{r}}_i \rightarrow \boldsymbol{r}_i(t)$$



Acceleration obtained from forces

- Governed by Newton's law for an N-body system
- Point particles with pairwise interactions only

$$m_i \ddot{\boldsymbol{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^{N} \boldsymbol{f}_{ij}$$

$$\Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

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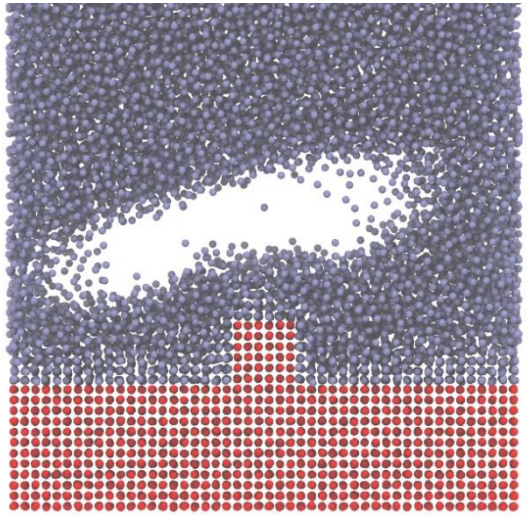
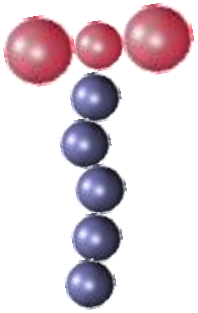
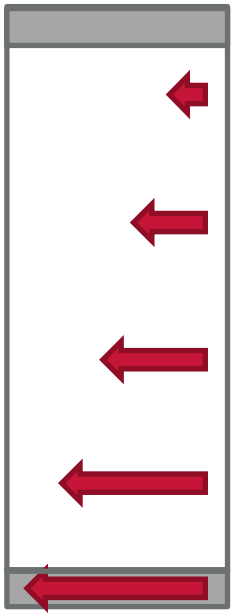
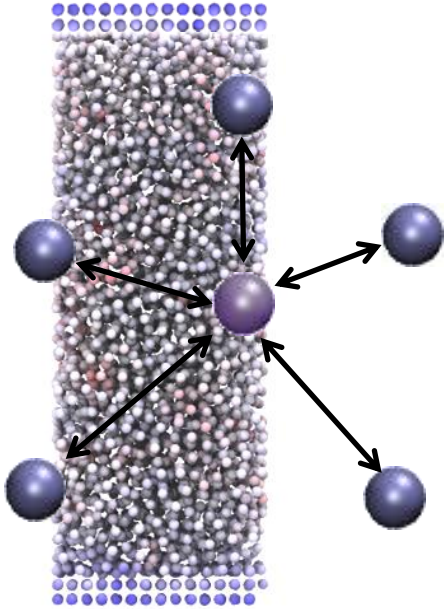
Molecular Dynamics

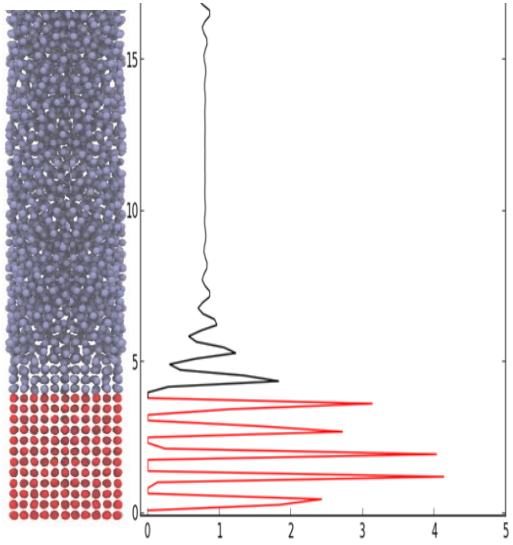


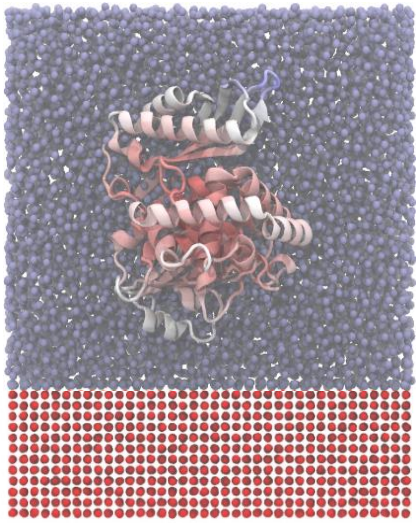
Superspreading Surfactant, e.g. Silwet-L77











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Pressure and viscosity from an MD Simulation

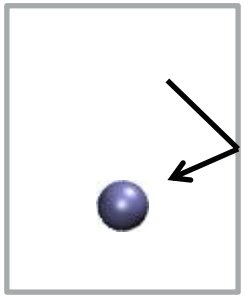
- Pressure includes kinetic and structural (configurational) component
  - Average over a control volume

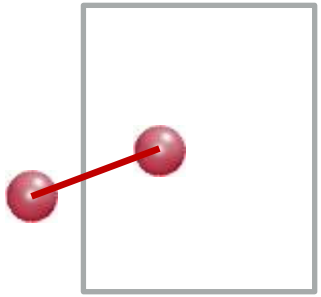
$$\oint_S \mathbf{\Pi} \cdot d\mathbf{S} = \underbrace{\sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i \boldsymbol{p}_i}{m_i} \cdot d\mathbf{S}_i \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij} \right\rangle}_{\text{Configurational}}$$

- Autocorrelation of the shear pressure is the viscosity

Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





Configurational part

Inter-molecular bonds act like the stress in a stretched spring

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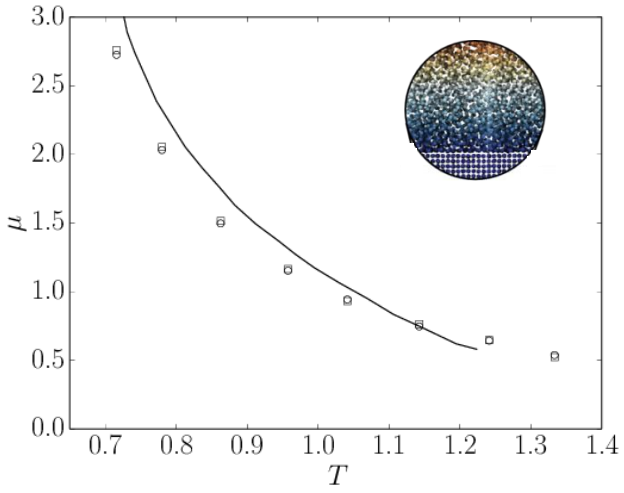
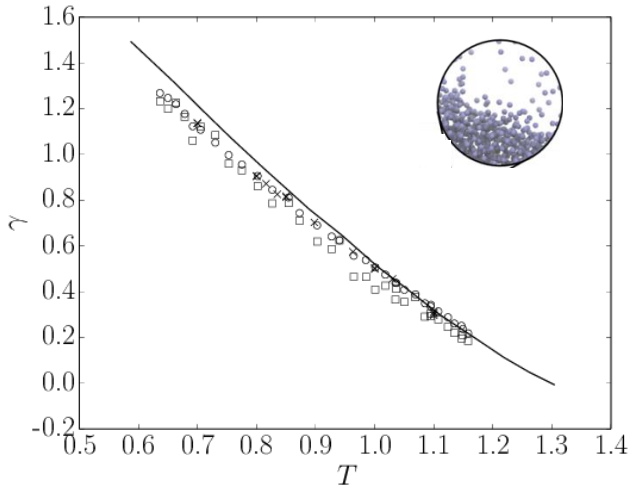
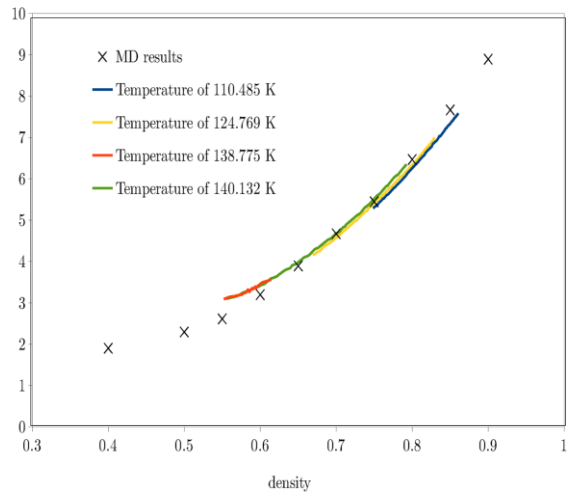
Viscosity, Surface Tension and Heat Flux

- Outputs of the simulation, shown here for liquid Argon







- Viscosity

$$\mu = \frac{V}{k_B T} \langle \Pi_{xy}(t) \Pi_{xy}(0) \rangle$$

- Green-Kubo

- Surface tension

$$\gamma = \int (\Pi_N - \Pi_T)\, dx$$

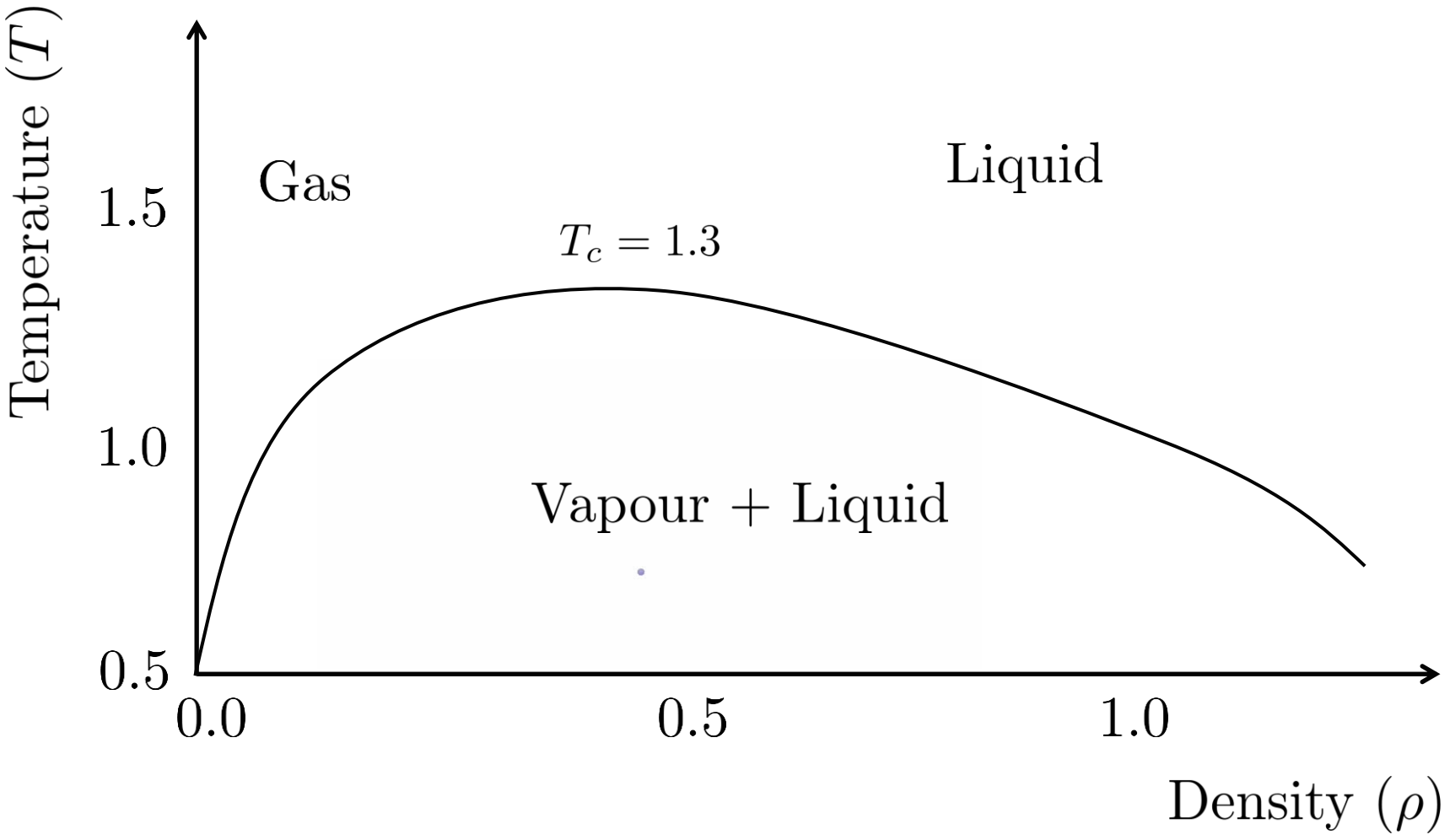
Kirkwood Buff

- Heat Flux

$$\kappa = \frac{V}{k_B T} \langle q_y(t) q_y(0) \rangle$$

Green-Kubo

Phase Diagram



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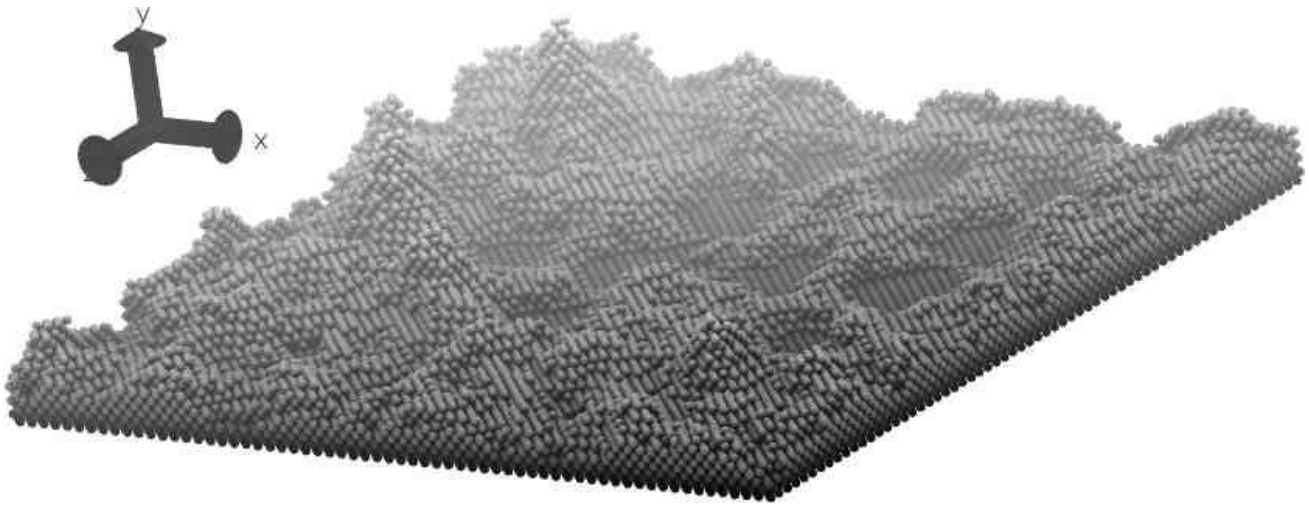
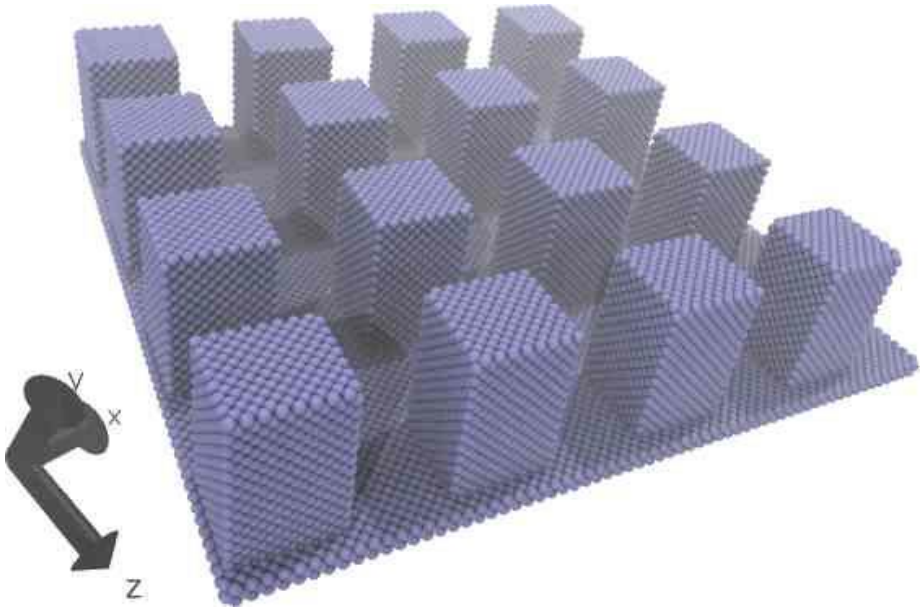
Surfaces





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Nucleation at the molecular level

Wall w
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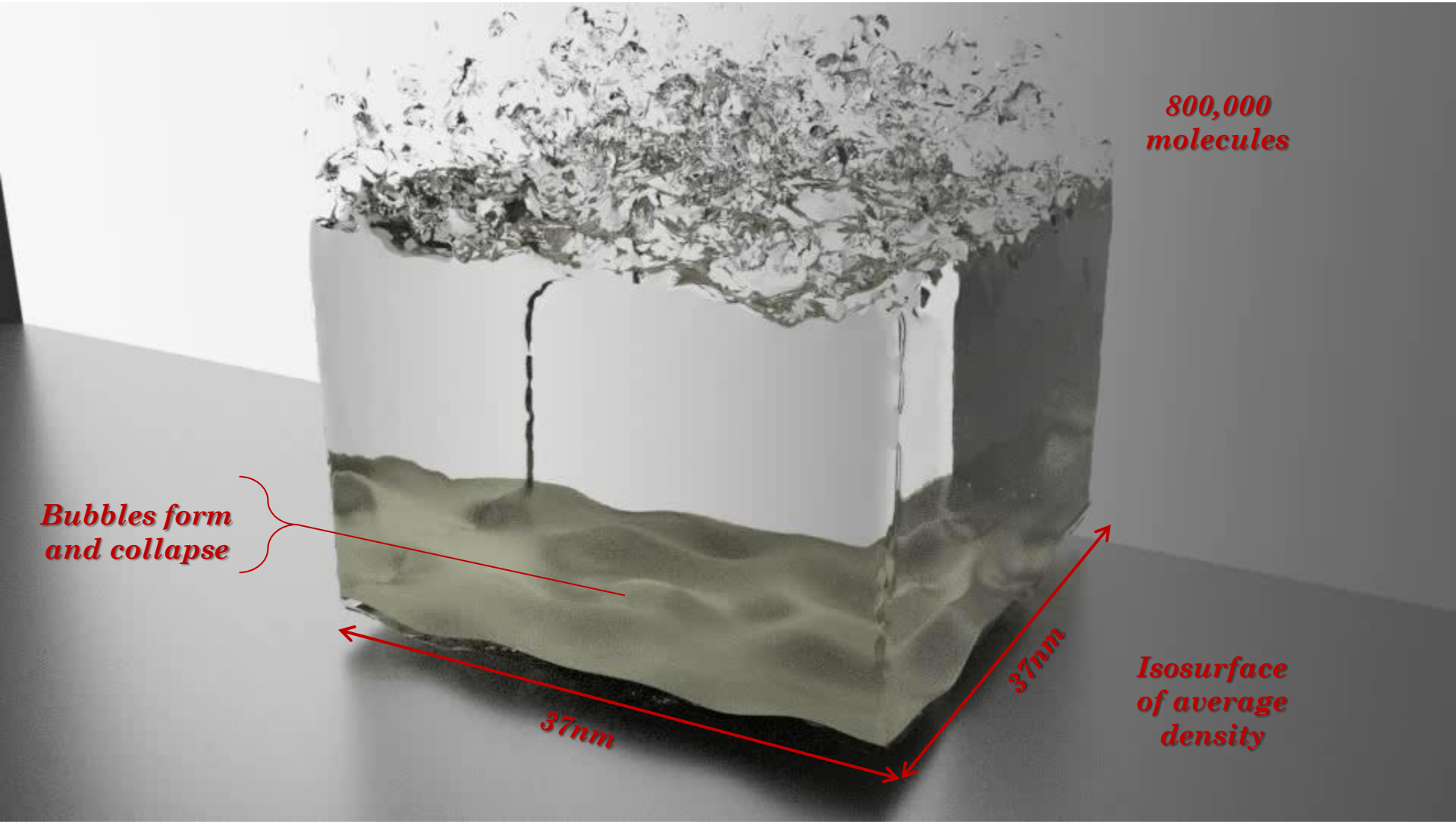
Low Heating T_{wall}=1.0 (T_c = 1.3)



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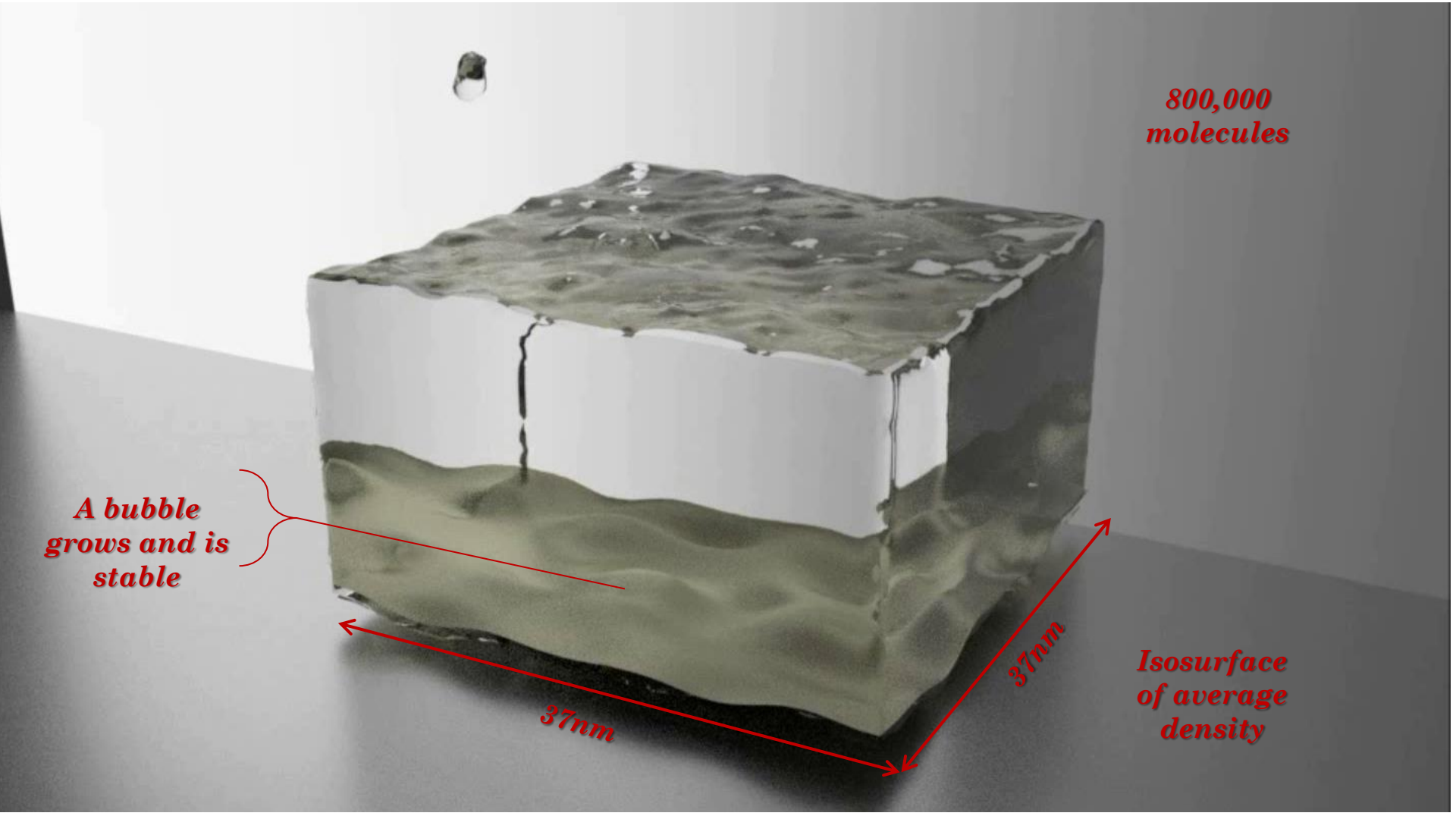
Medium Heating T_{wall}=1.1 (T_c = 1.3)



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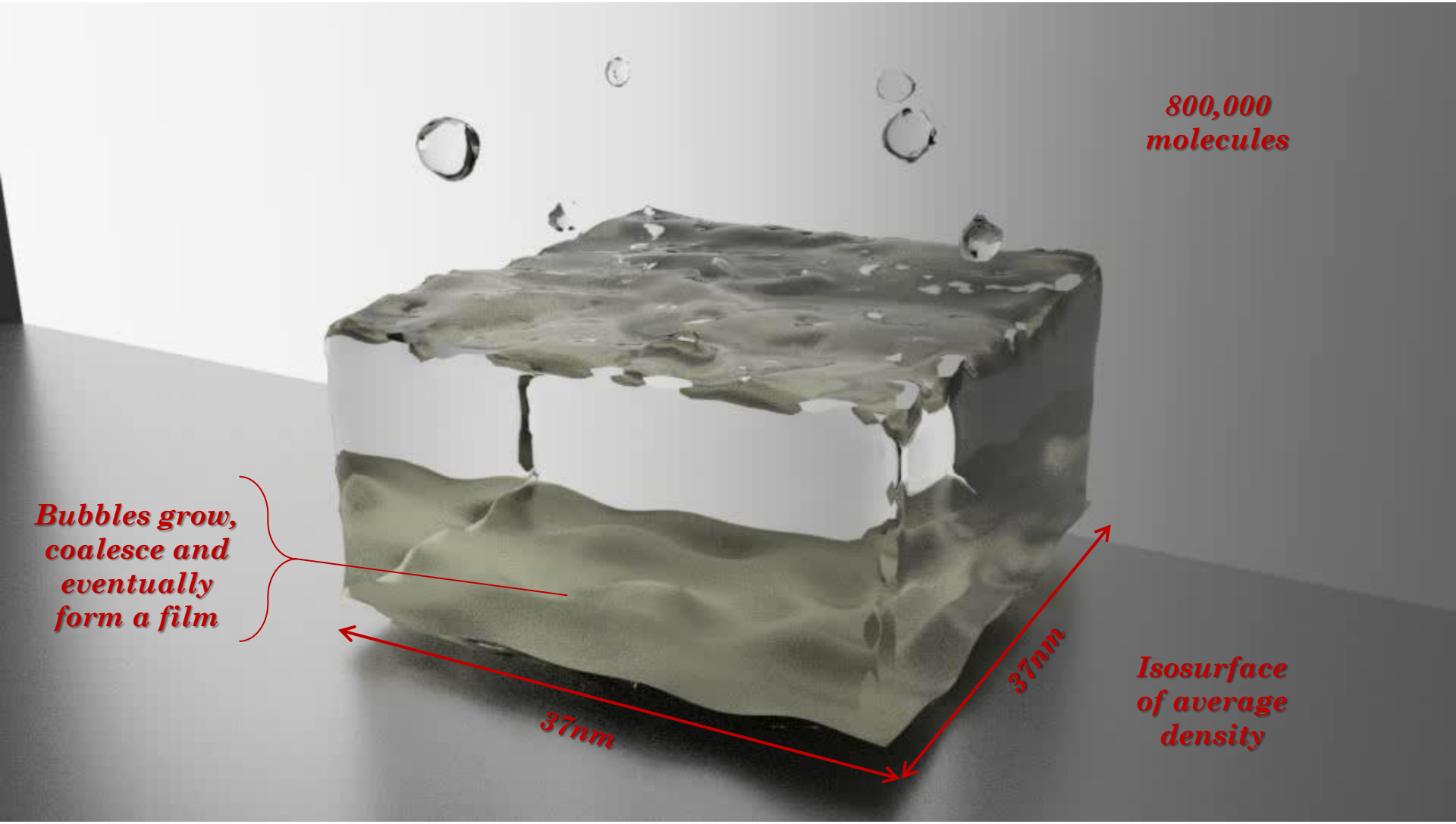
High Heating T_{wall}=1.3 (T_c = 1.3)



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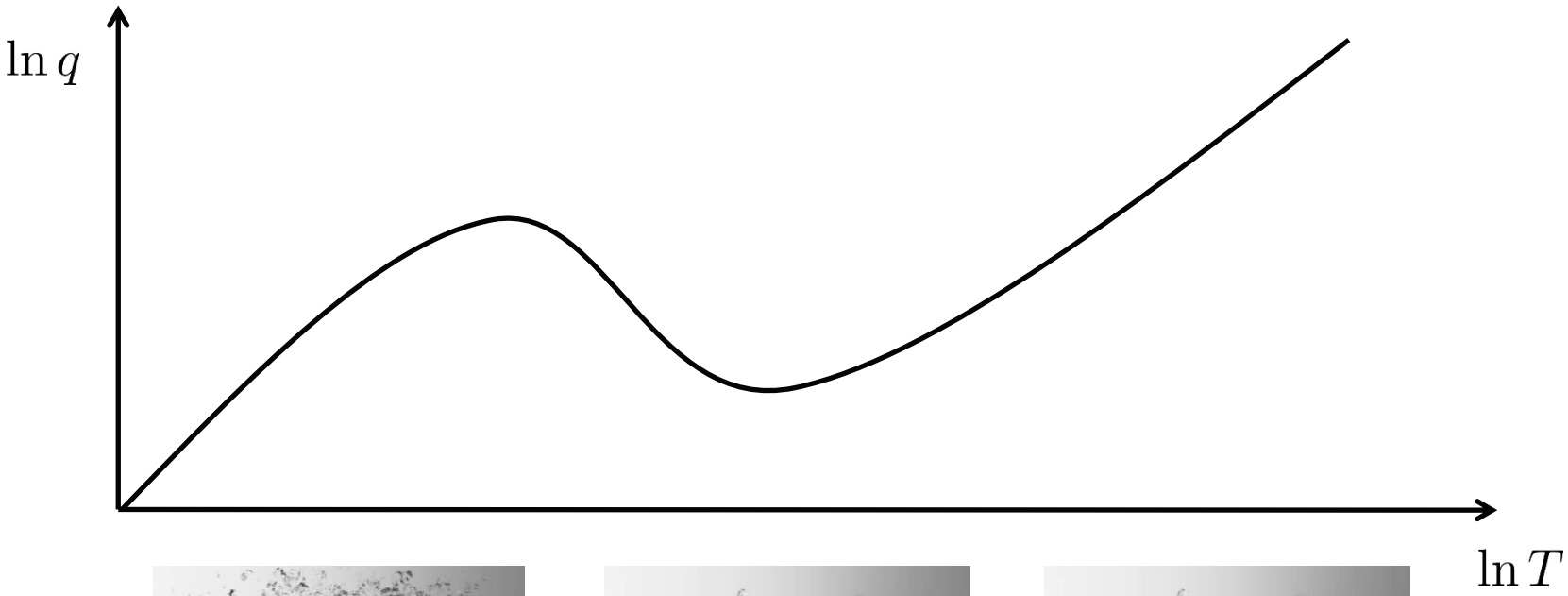
Pool Boiling Curve



No nucleation and convection

Nucleate Boiling

Film Boiling

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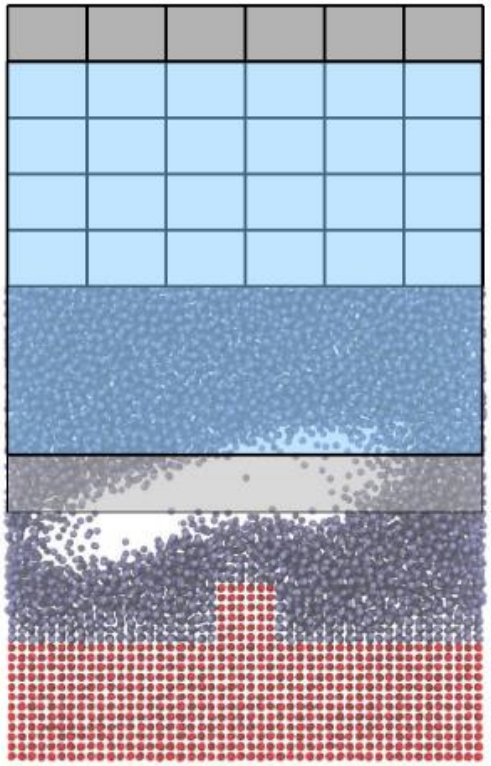
Coupled Simulation



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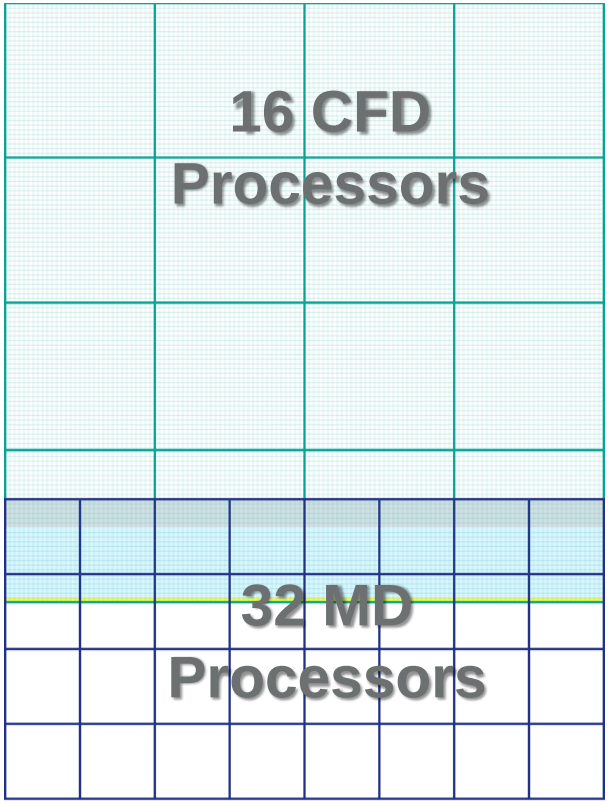
CFD Region

Overlap Region

MD Region

mpiexec –n 32./md.exe : -n 16 ./cfd.exe



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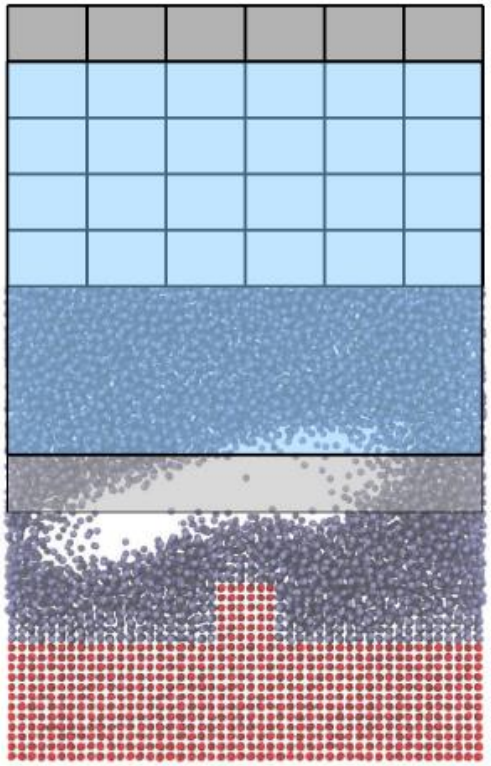
Coupled Simulation



CFD Region

Overlap Region

MD Region

CFD→MD Boundary condition

MD→CFD Boundary condition

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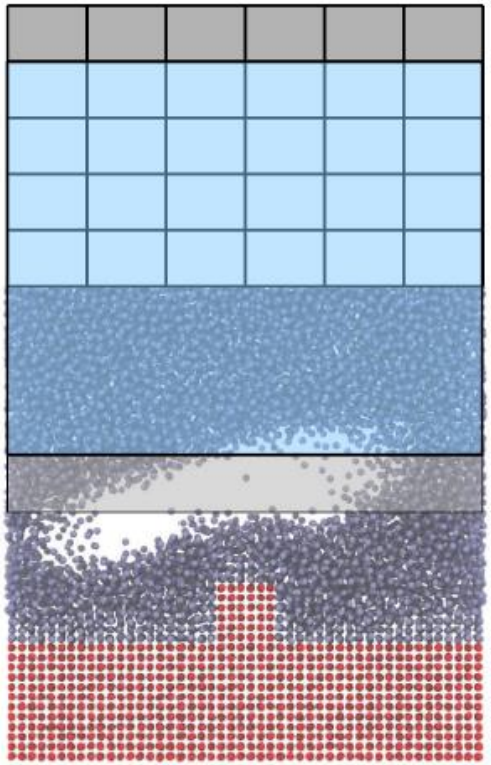
Coupled Simulation



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Energy minimisation constraint

$$\frac{\partial}{\partial \boldsymbol{r}_{ij}} \sum_{i=1}^{N} \left[\boldsymbol{F}_i - \boldsymbol{r}_{ij}\right]^2 - \boldsymbol{\lambda} \cdot \boldsymbol{g} = 0$$

CFD→MD Boundary condition

MD→CFD Boundary condition

Control Volume Form

$$\oint_S \boldsymbol{\Pi} \cdot d\mathbf{S} = \underbrace{\sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i \boldsymbol{p}_i}{m_i} \cdot d\mathbf{S}_i \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij} \right\rangle}_{\text{Configurational}}$$

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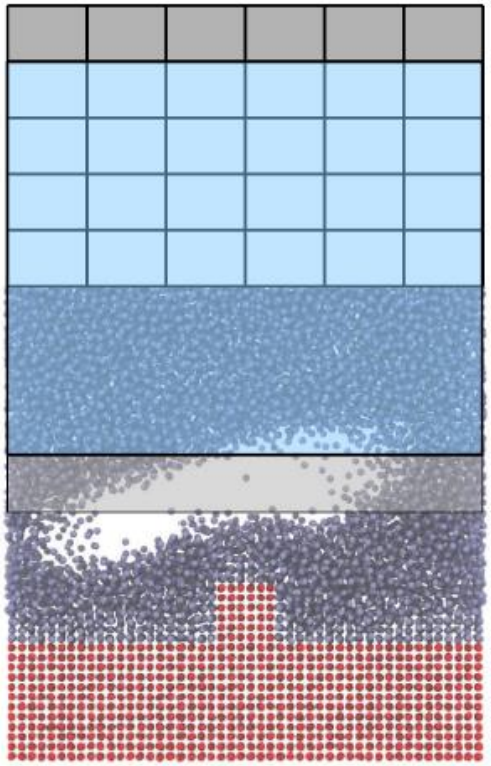
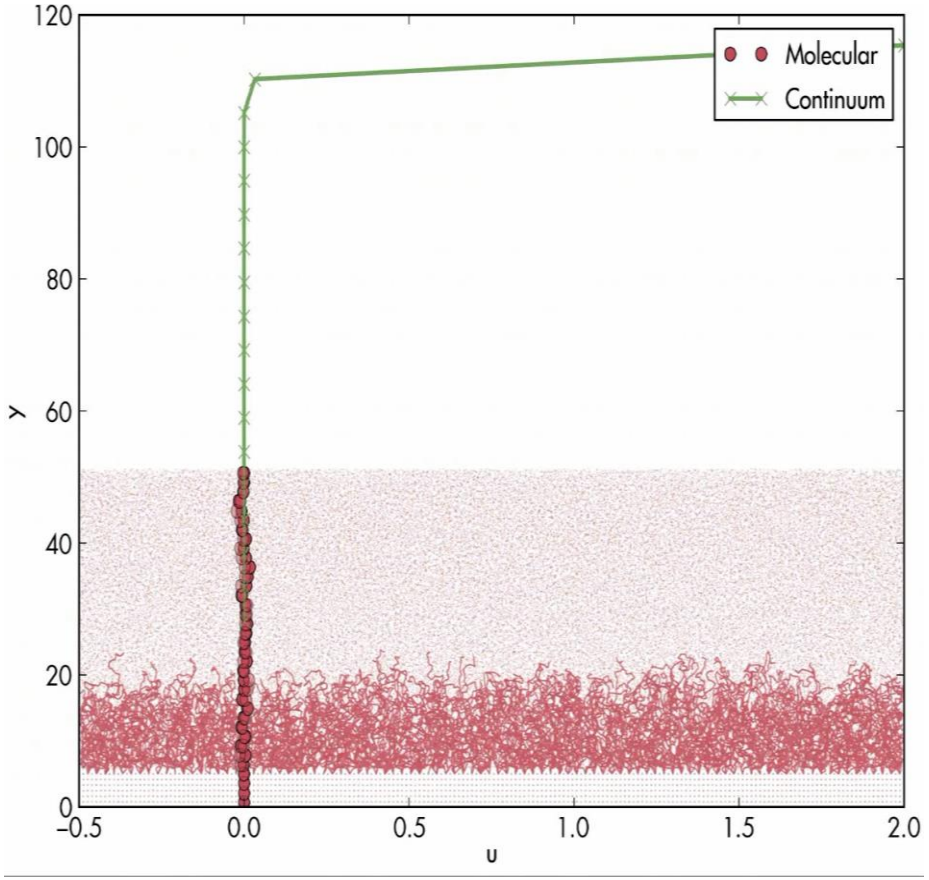
Coupled Simulation



CFD Region

Overlap Region

MD Region



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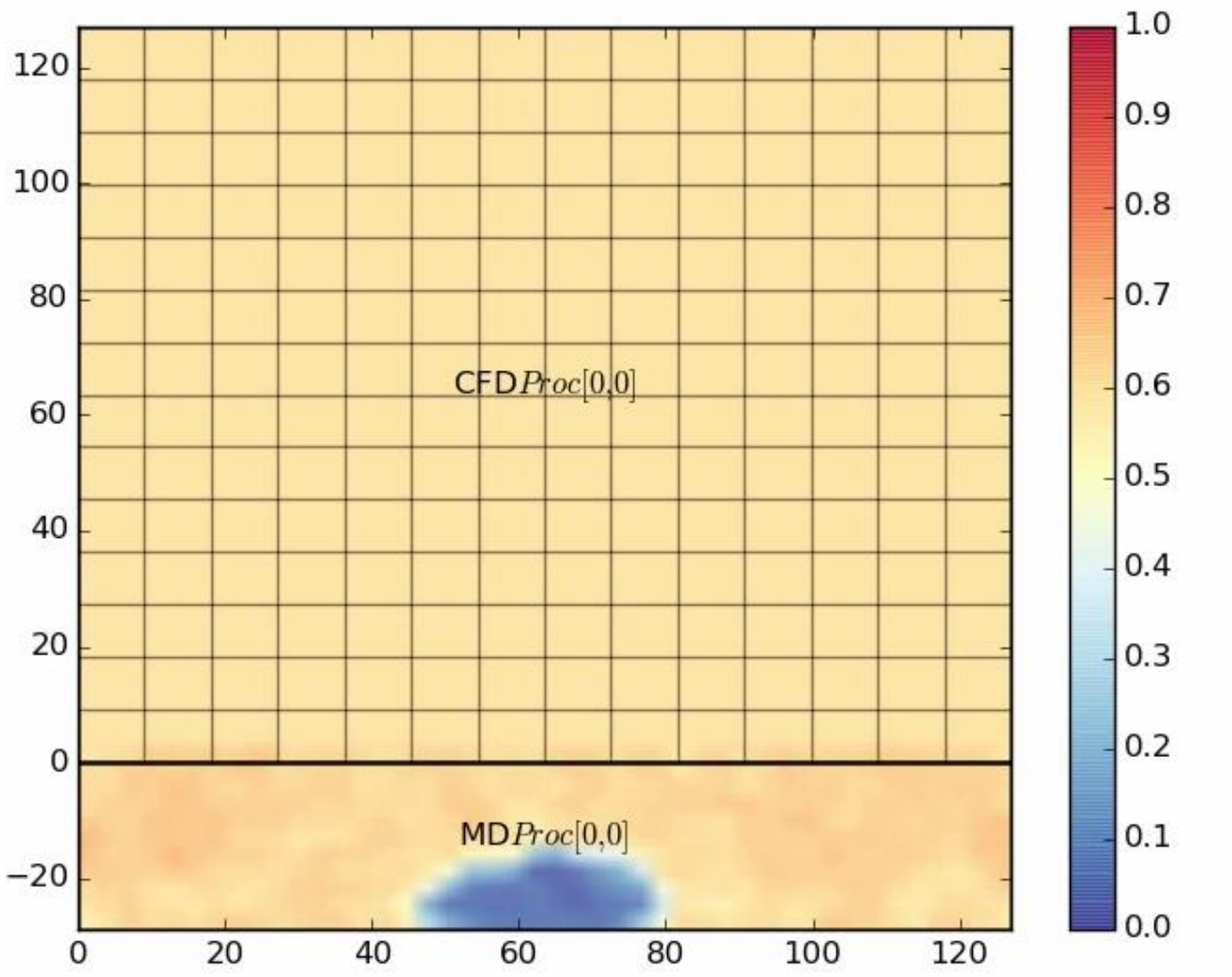
Coupled Simulation of Boiling



Summary and Outlook

- Molecular Dynamics (MD) can model the nucleation events on rough surfaces
- MD is limited to very small systems
- Coupled simulation extends the spatial and temporal scale accessible with MD
- MD could provide a-priori estimates of nucleation and insight into the dynamics of a nascent bubble