Phase Separation of Fluids in Confined Geometry – Partial and Complete Wetting

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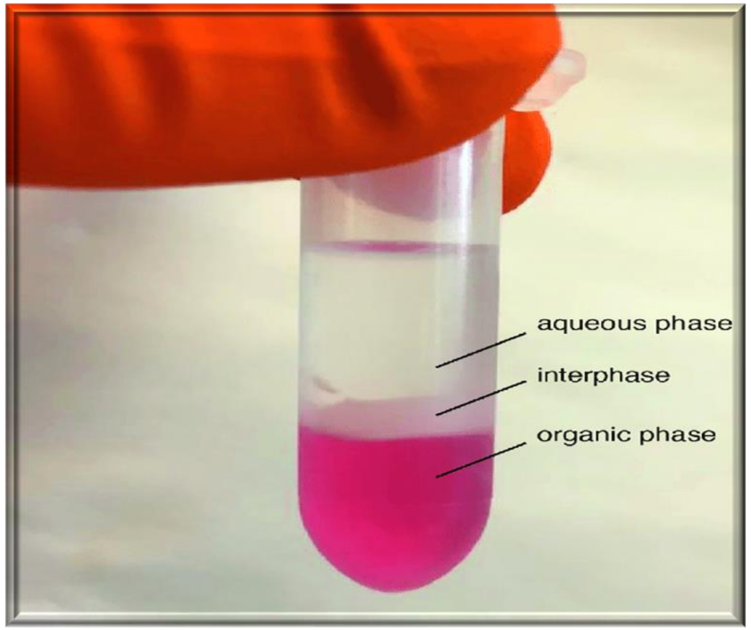
What is Phase Separation?

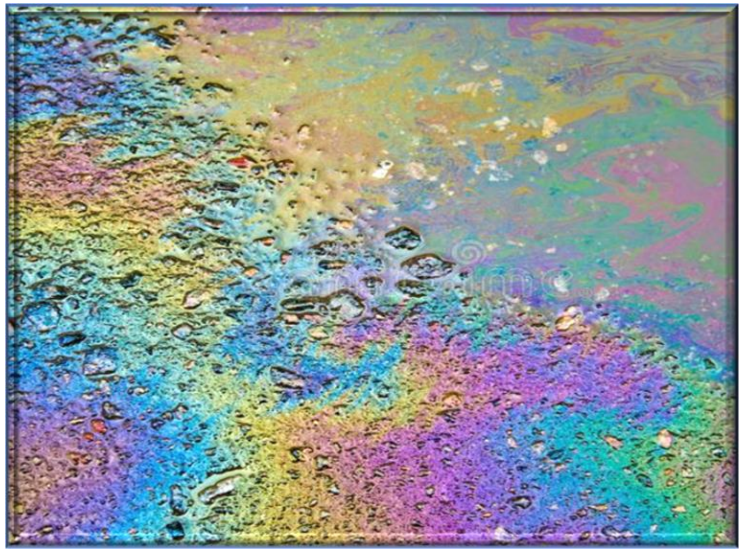
RBC and Plasma



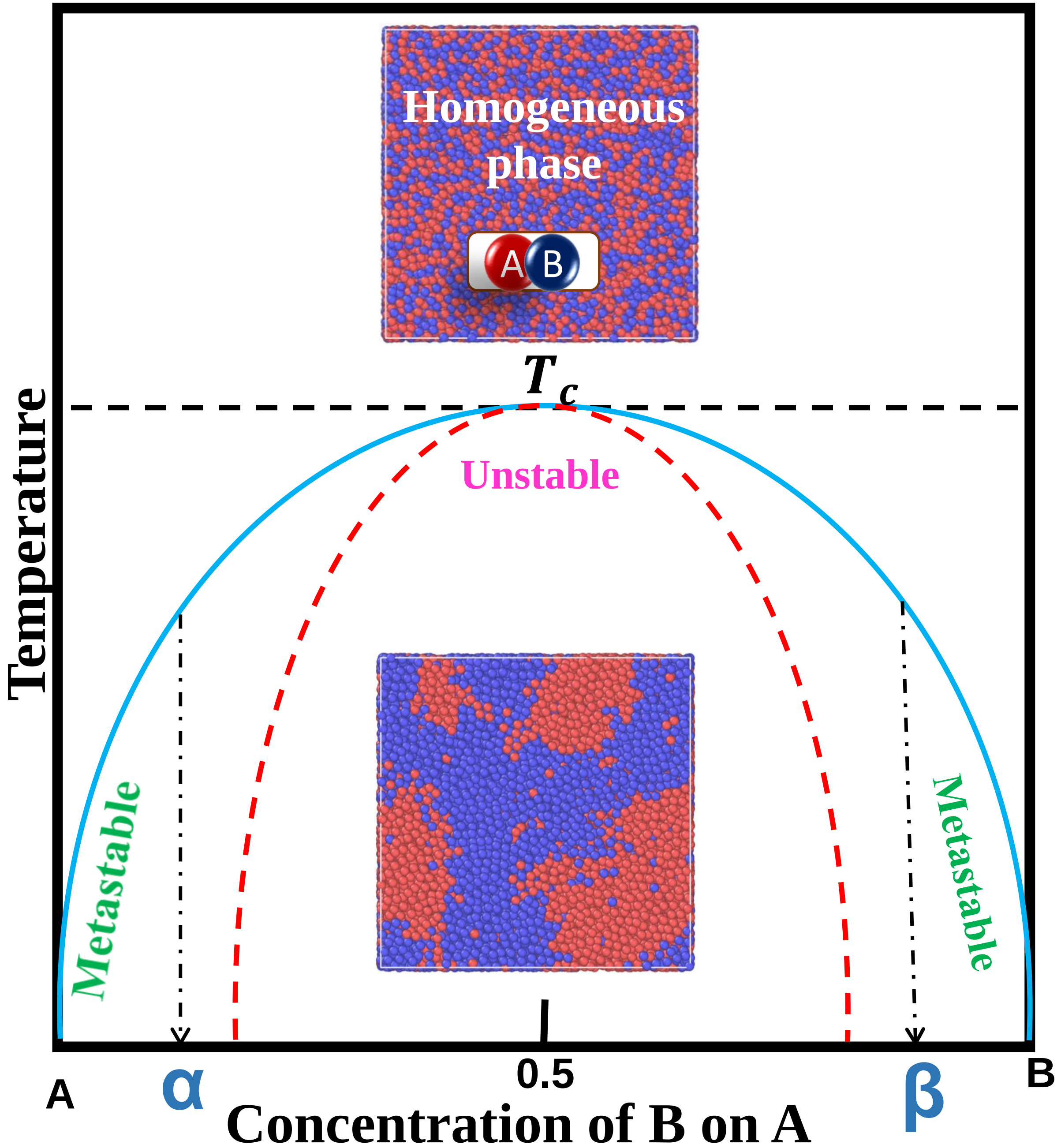
Oil and Vinegar

Water and Oil

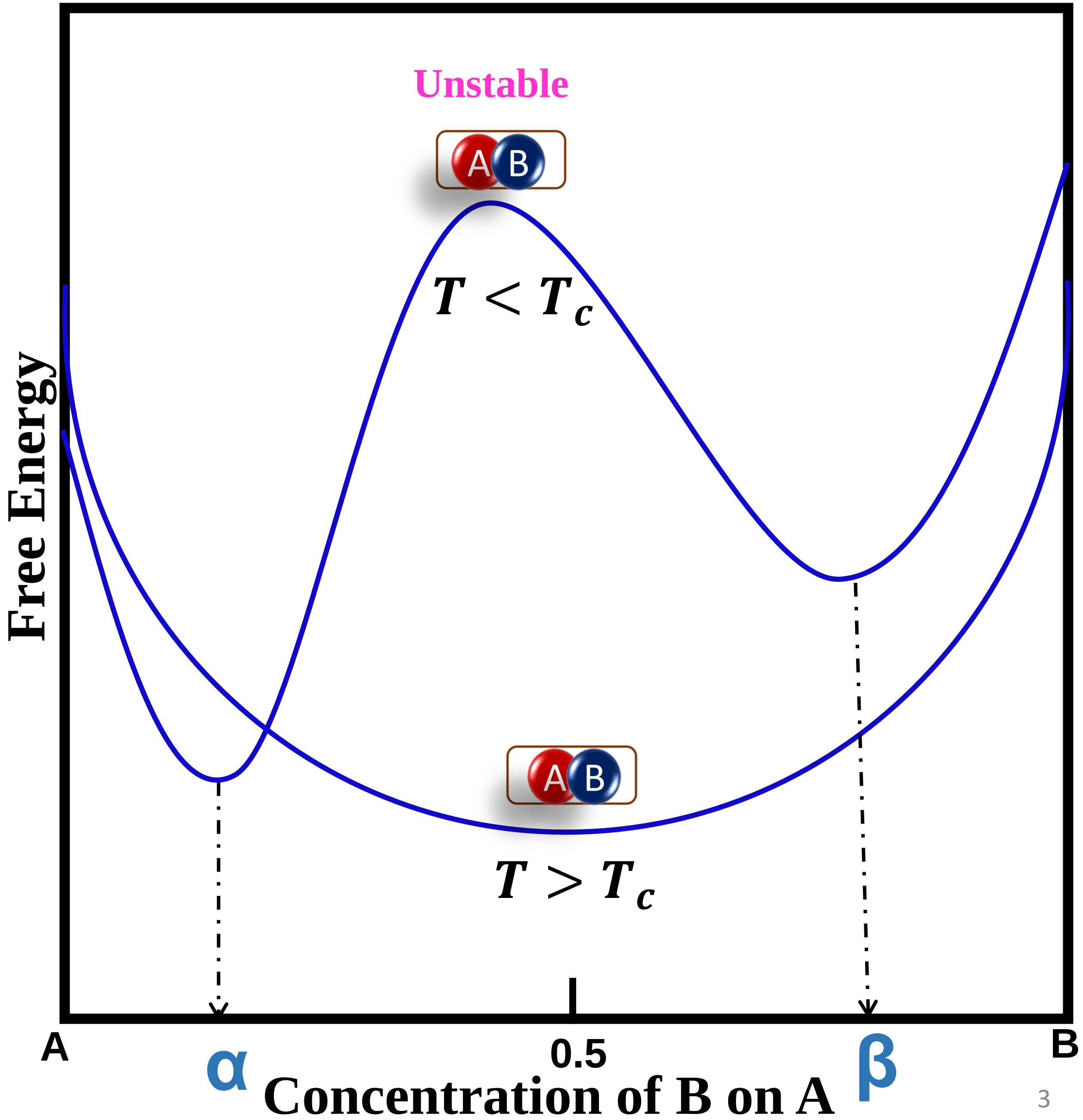
Petrol and Water



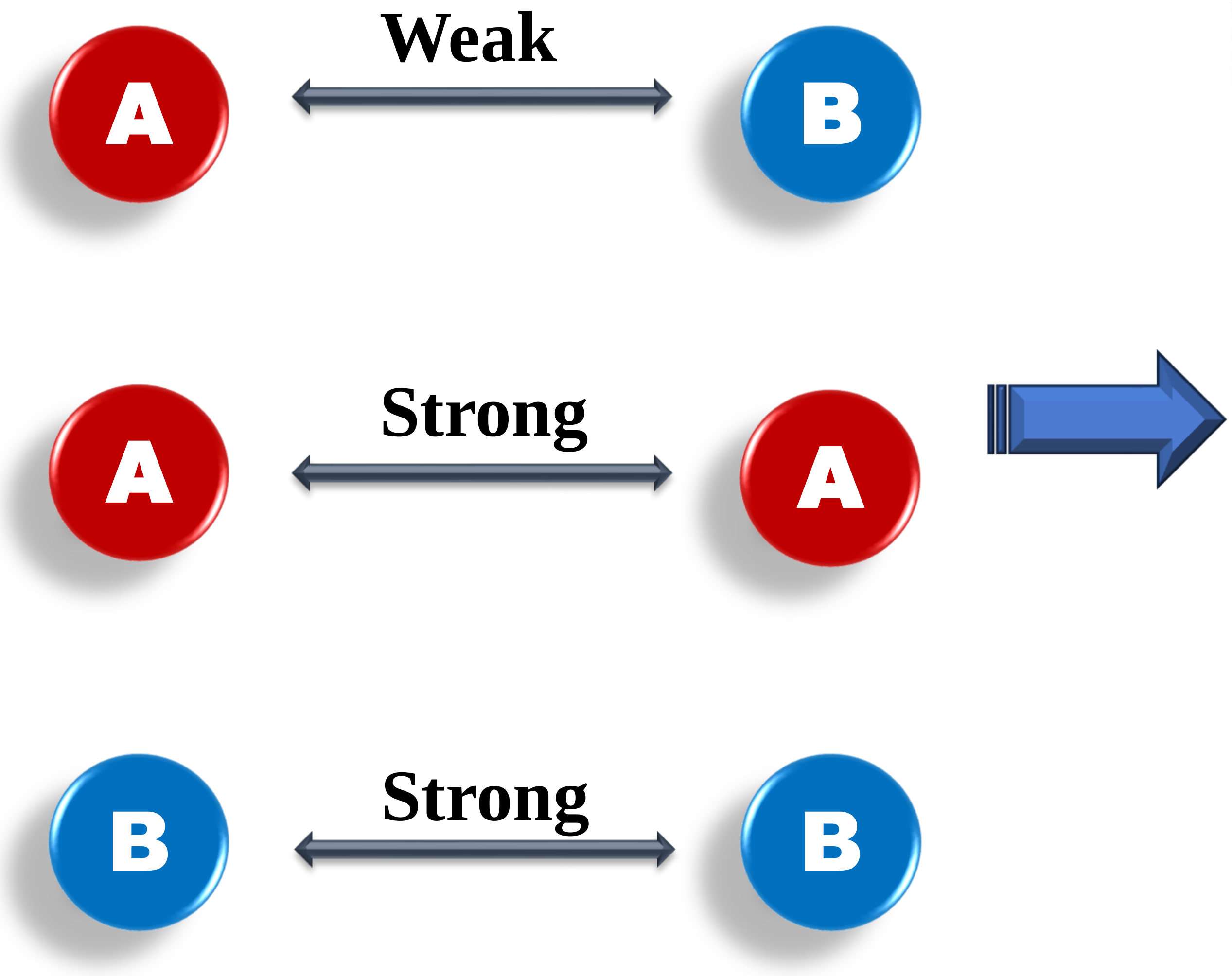
Phase Diagram

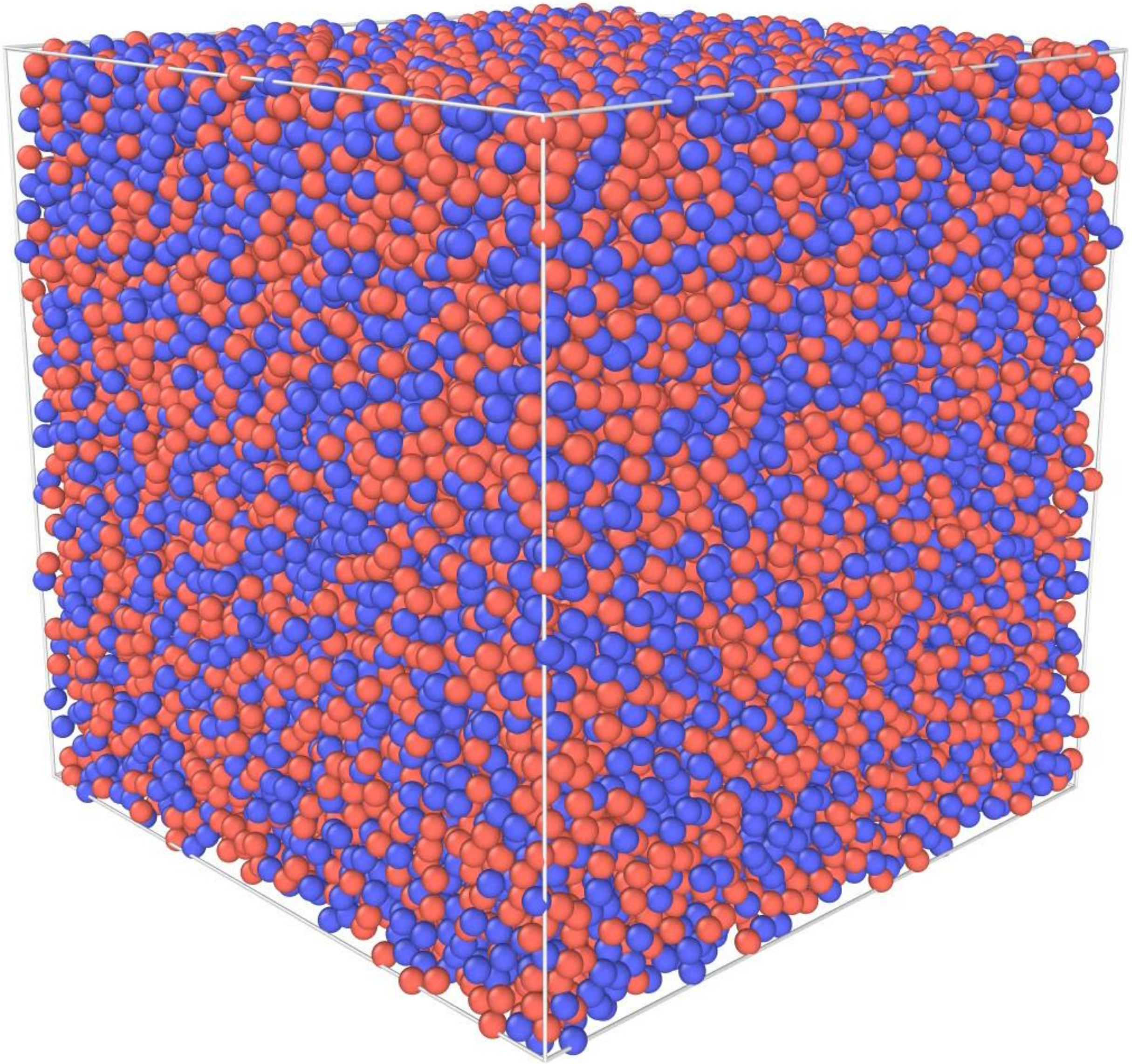


Free Energy profile



Phase Separation of Fluid Mixtures – Computer Simulation



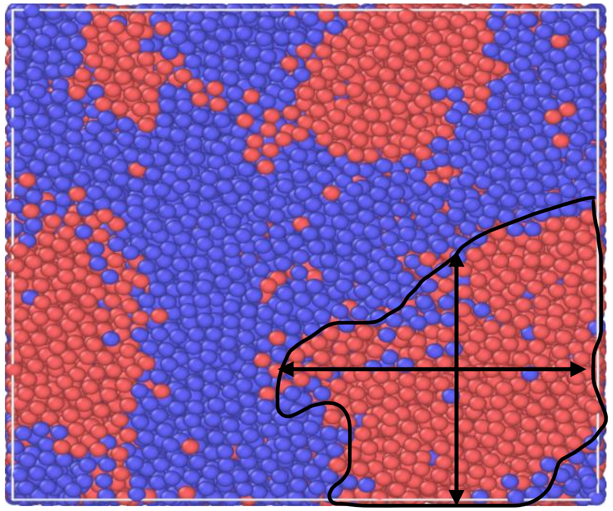


DOMAIN Size Estimation

- **Domain size** (Length scale) ~ $l(t)$

  $l(t) \sim A^{*} t^{\alpha}$

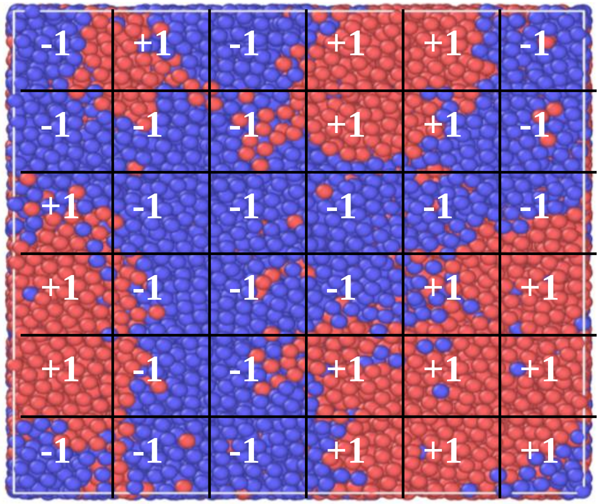
  α = growth exponent, A = Pre-factor



- **Order parameter**

  $$\varphi = \frac{N_A - N_B}{N_A + N_B} \qquad \varphi = \{+1, -1\}$$

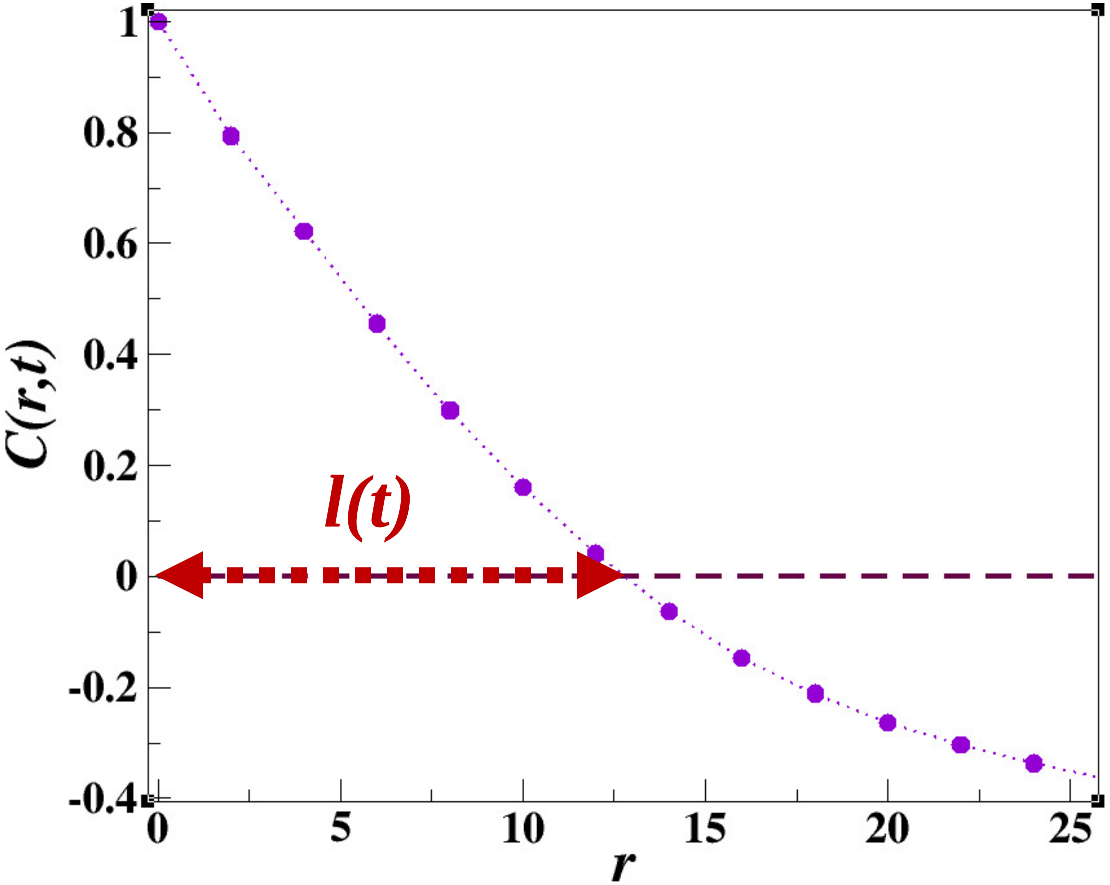
  N_A, N_B = No of A and B particles



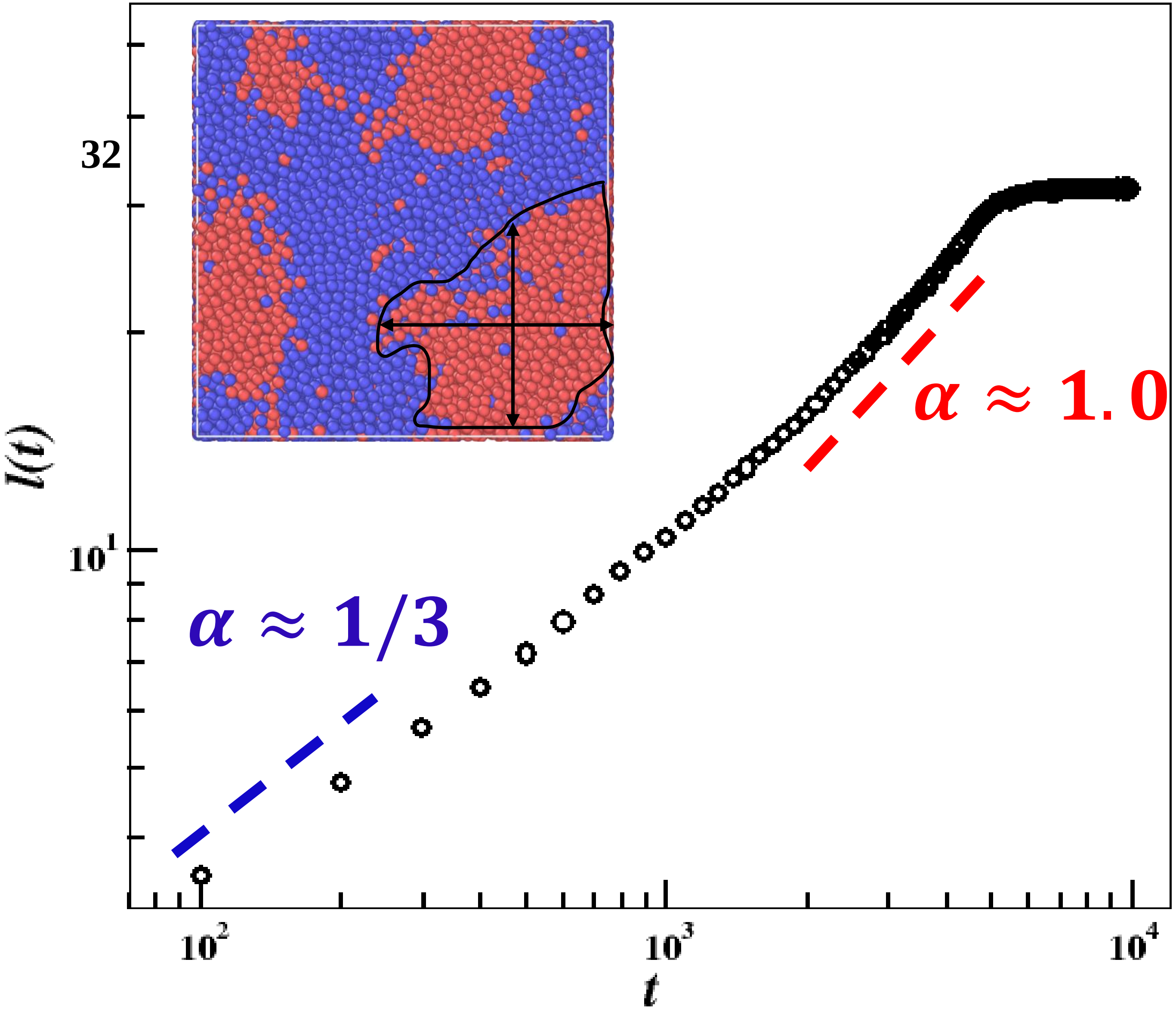
DOMAIN Size Estimation

- **First zero crossing of the Correlation function $C(\vec{r},t)$ gives *l(t)***

$$C(\vec{r},t) = \langle \varphi(\vec{R},t)\varphi(\vec{R}+\vec{r},t) \rangle - \langle \varphi(\vec{R},t) \rangle \langle \varphi(\vec{R}+\vec{r},t) \rangle$$



Domain Growth Laws



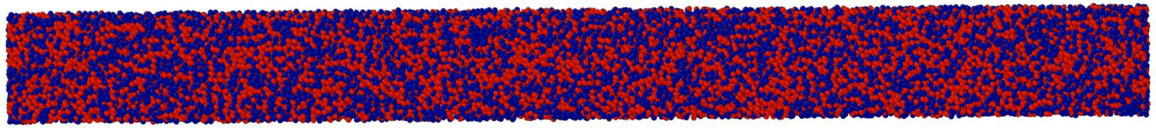
- **Initial time diffusive growth**
  Lifshitz-Slyozov law: $l(t) \sim t^{\frac{1}{3}}$
- **Intermediate hydrodynamic growth**
  Viscous hydrodynamics: $l(t) \sim t$
- **Late time growth**
  Inertial hydrodynamic: $l(t) \sim t^{\frac{2}{3}}$

What happens if the system is CONFINED instead of BULK

Phase Separation In Confined Geometry

Neutral Wall

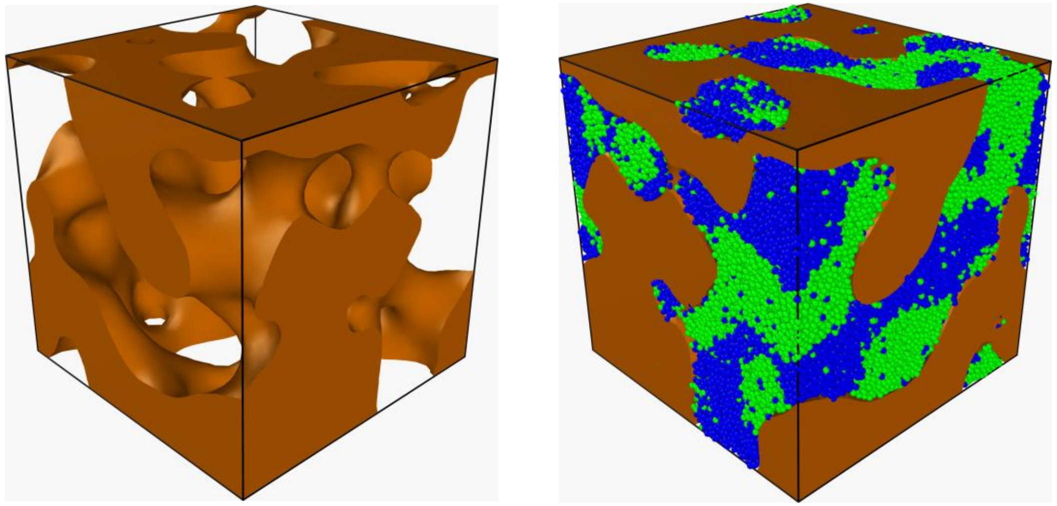
Simple Pore



- **Plug-like domains are formed**
- **Metastable state is obtained**
- **Full phase separation *not* possible**

*PRL **65** (1990) 1897
*PRL **69** (1992) 1548
*EPL **116** (2016) 56003

Complex Topology



- **Domain growth slows down**
- **Domain size depended on pore size**

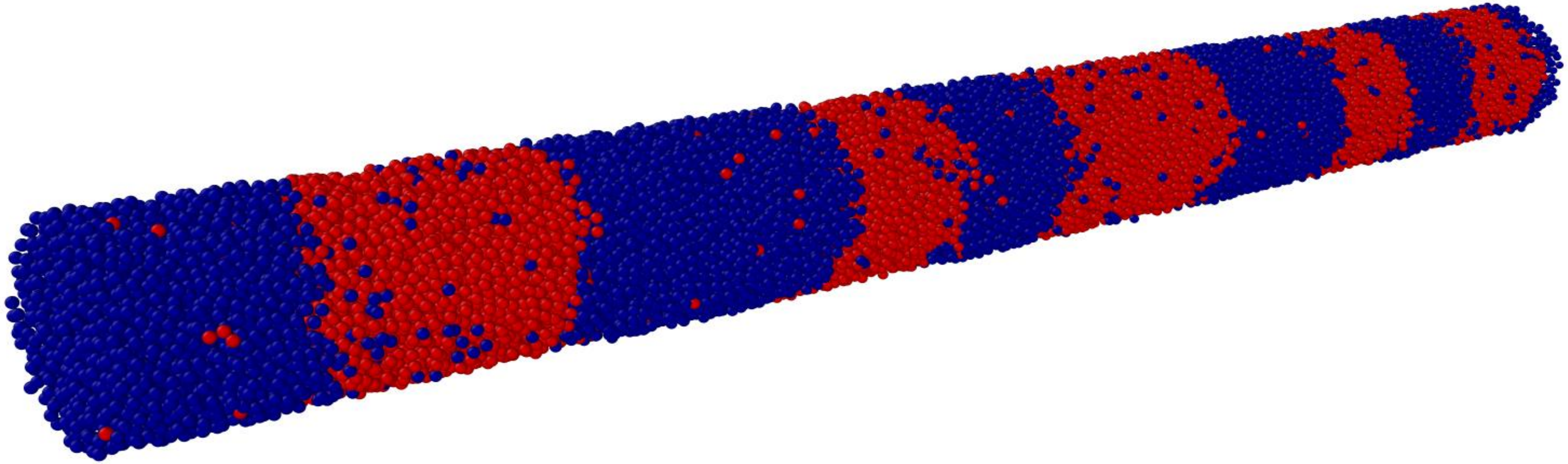
*EPL **140** (2022) 47002

MOTIVATION FOR THE WORK

What happens in a real system where the fluids interact with the container?

PARTIAL or COMPLETE WETTING

Phase Separation in Cylindrical Pore



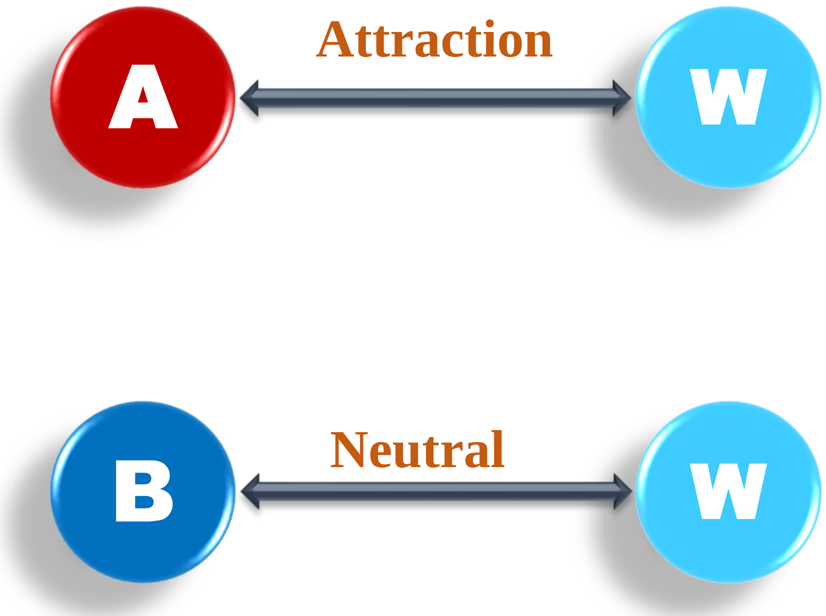
Whether it is POSSIBLE to –

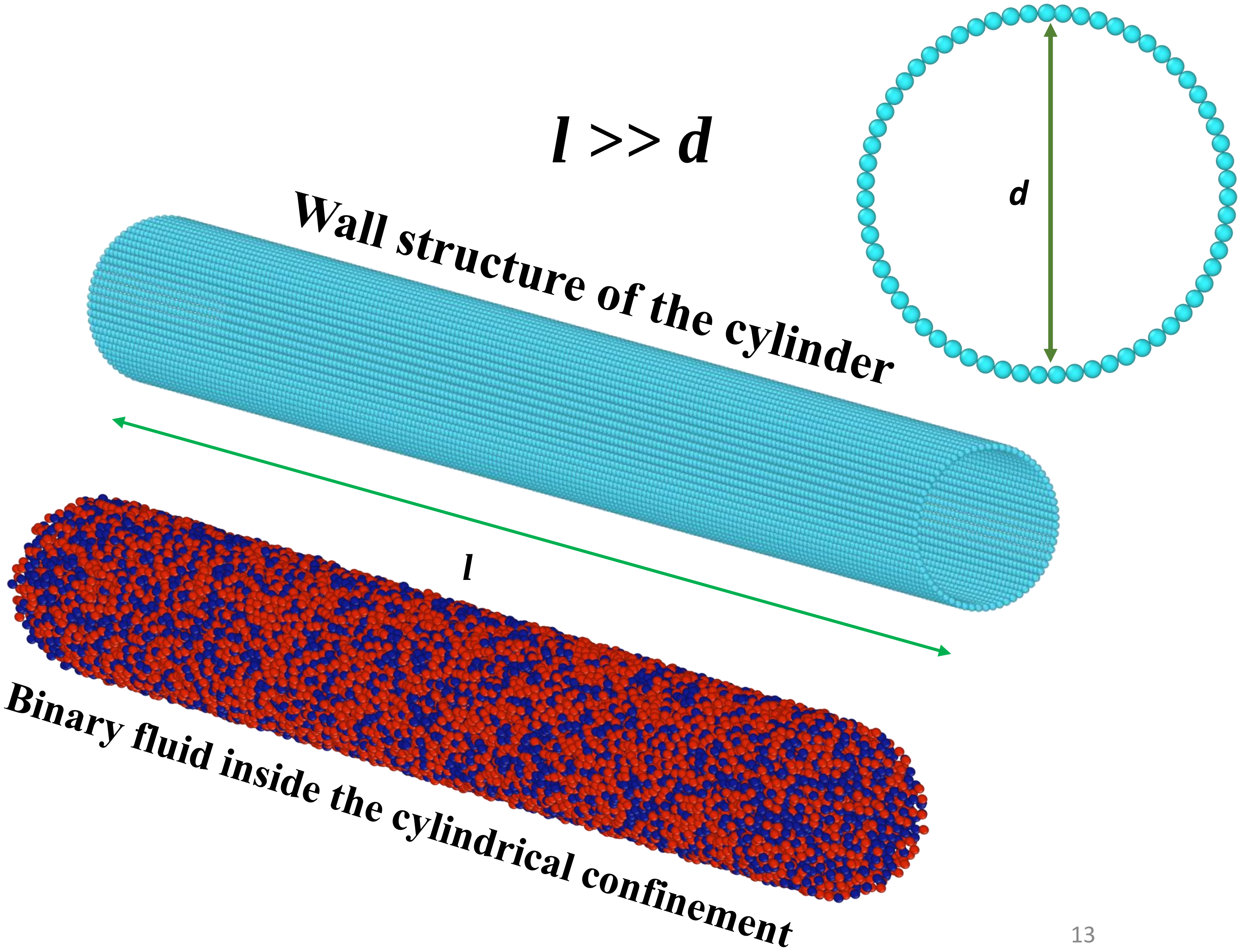
Break the Metastable State?

Achieve the Full Phase Separation?

Partial and Complete Wetting Scenario

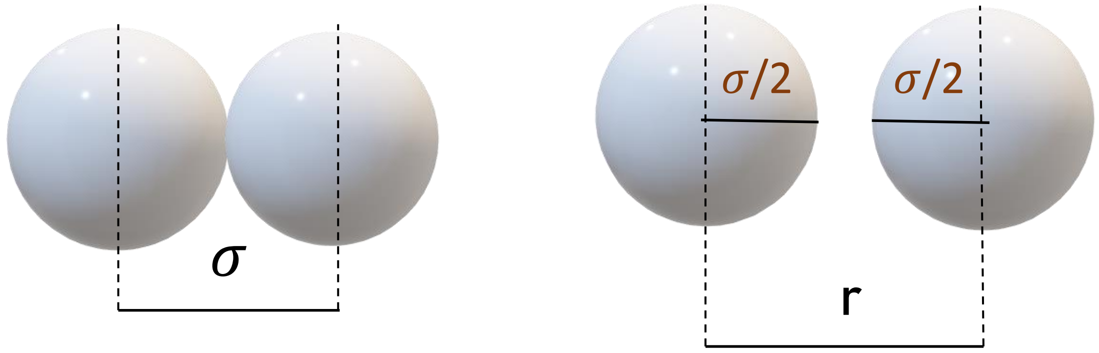
Wetting – Interaction with the Wall

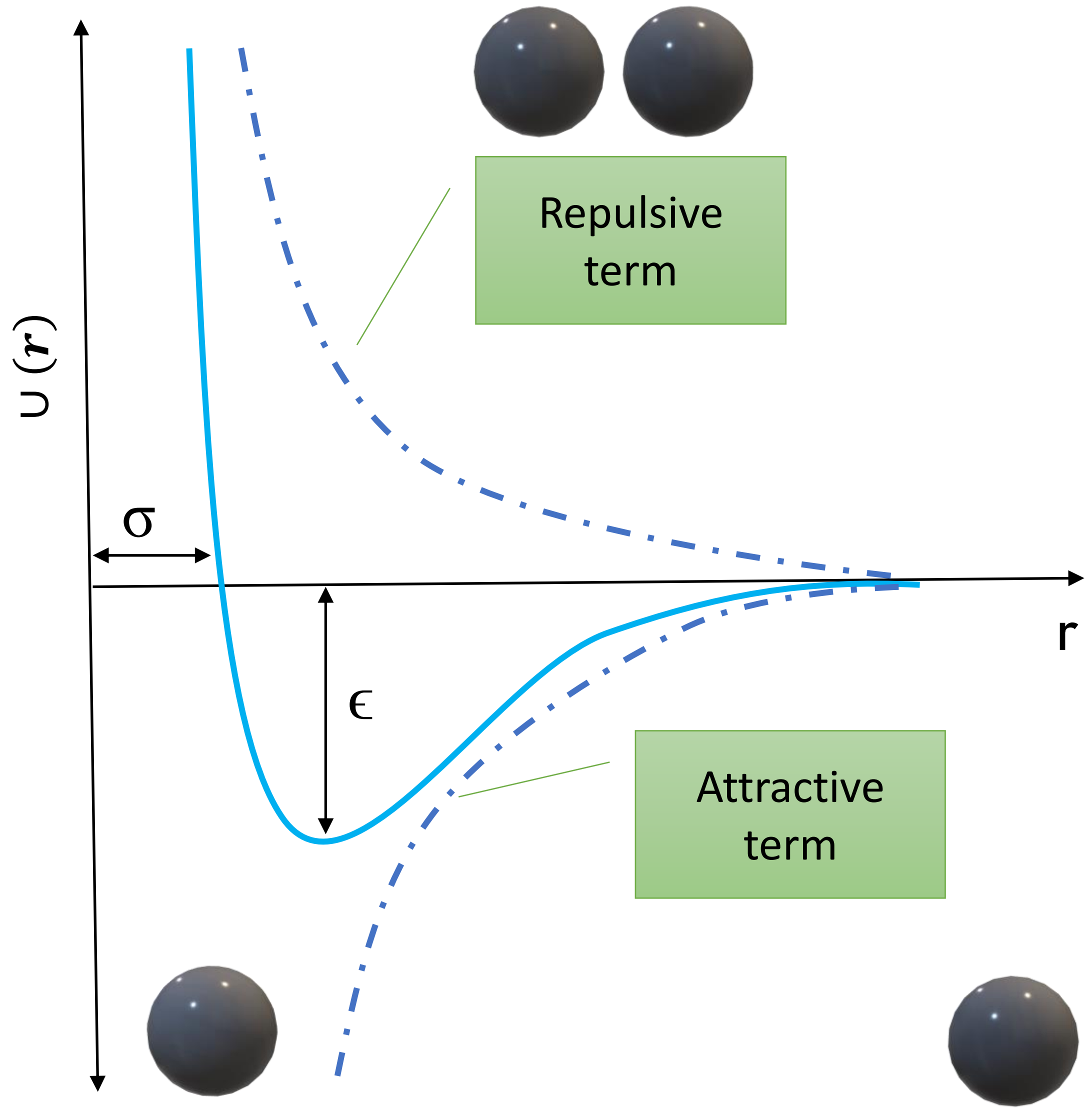




Interaction Potential : LENNARD JONES

$$U(\boldsymbol{r}) = 4\epsilon\left[\left(\frac{\boldsymbol{\sigma}}{\boldsymbol{r}}\right)^{12} - \left(\frac{\boldsymbol{\sigma}}{\boldsymbol{r}}\right)^{6}\right]$$

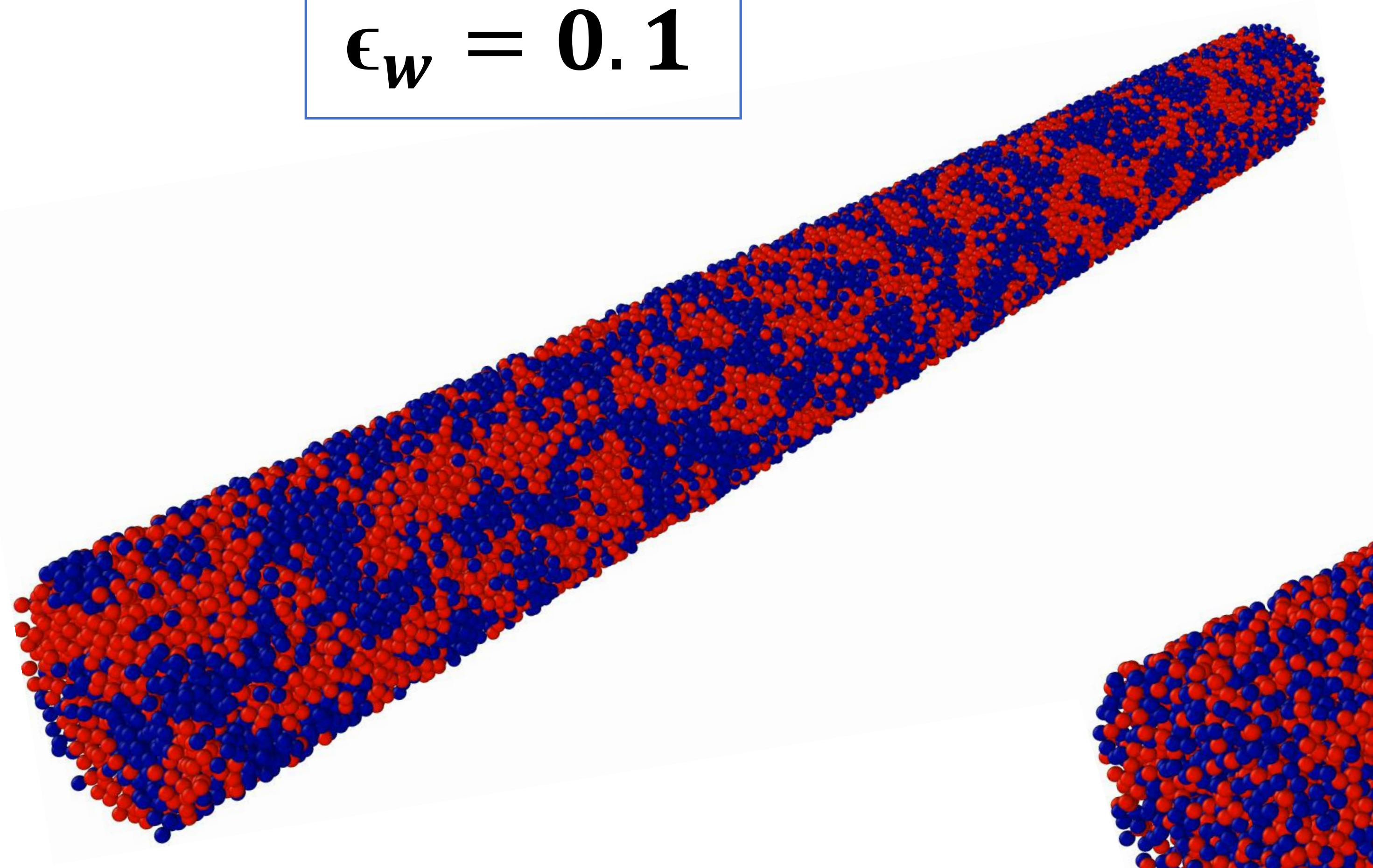




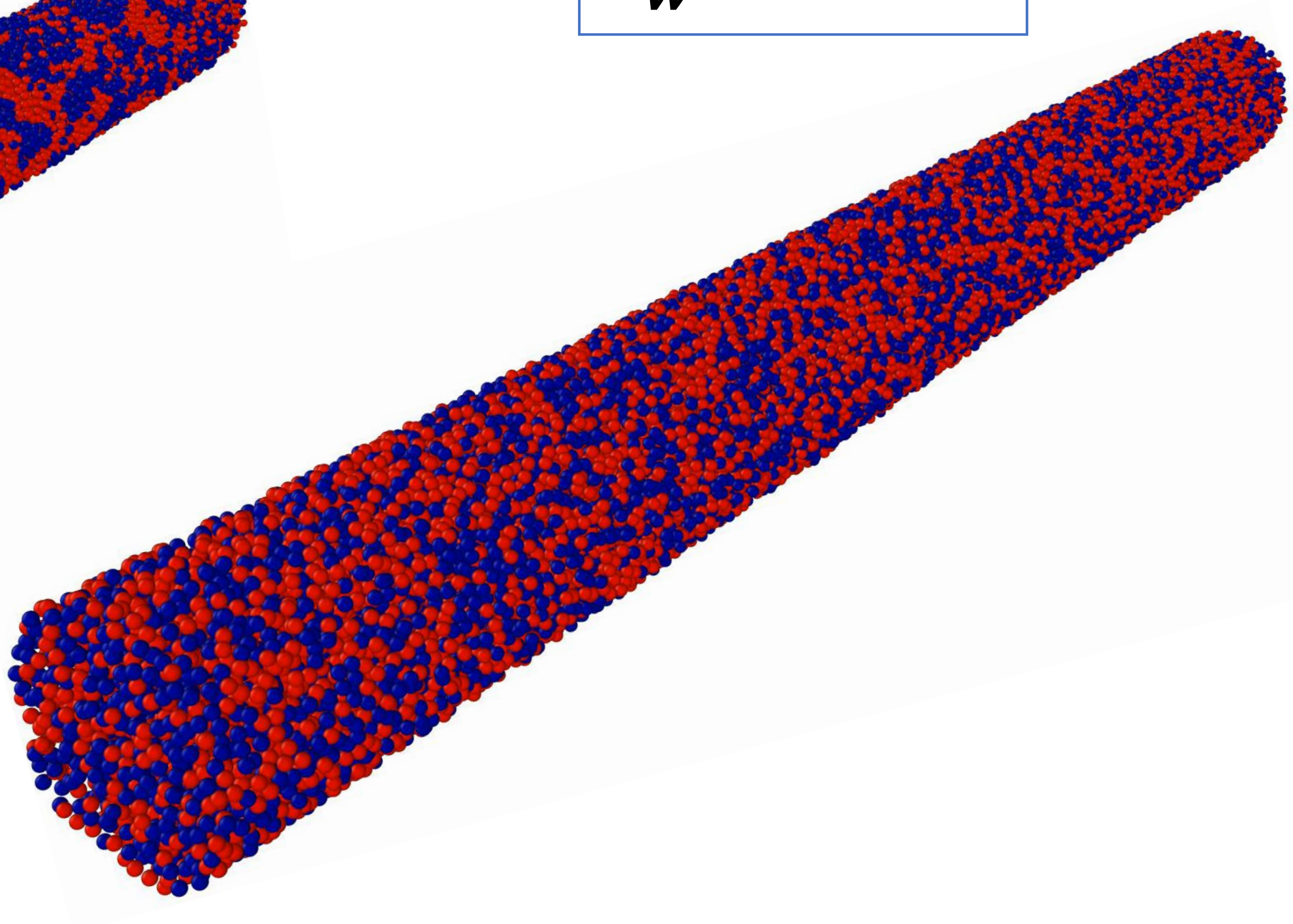
σ = Interparticle diameter
ϵ = Depth of the potential well
r = Distance between the center of the particles

PARTIAL WETTING (PW) $0.1 \leq \epsilon_w \leq 0.5$

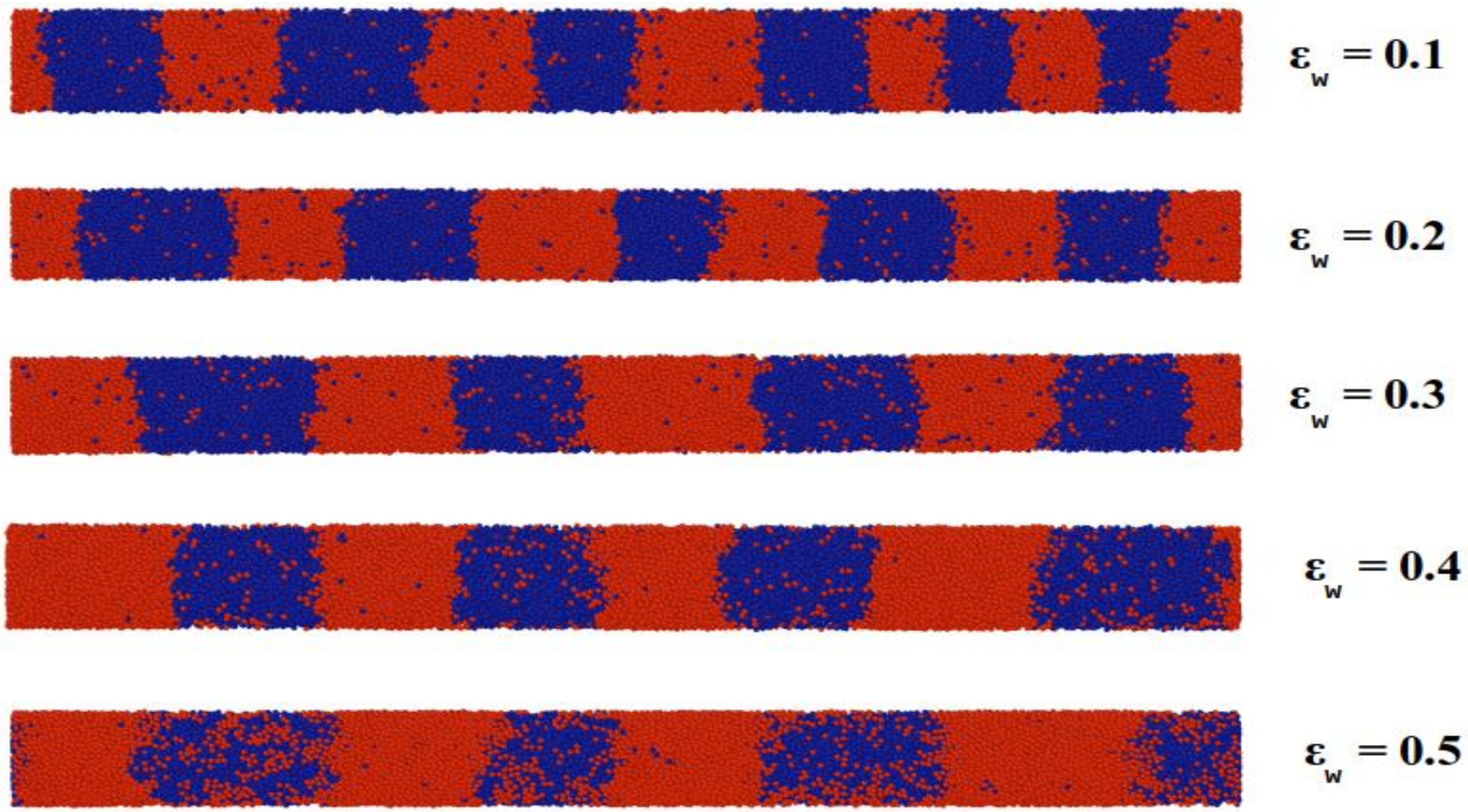
$\epsilon_w = 0.1$



$\epsilon_w = 0.5$

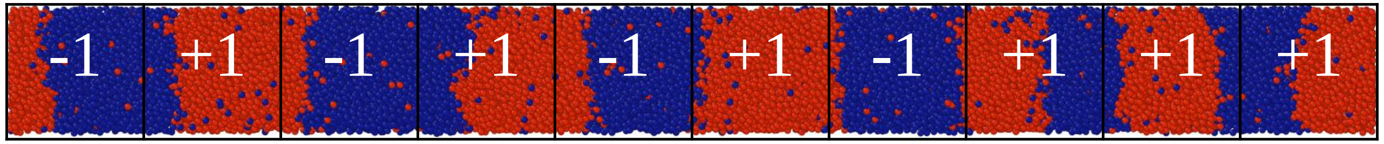


PW: Different Wetting Strength

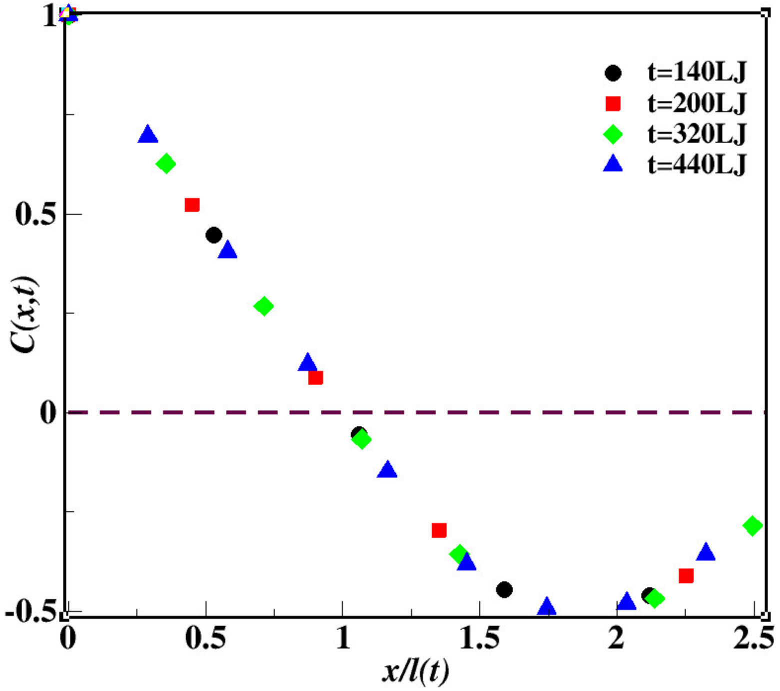


PW: CORRELATION

Order Parameter and Correlation functions are calculated along the axis of the cylinder.

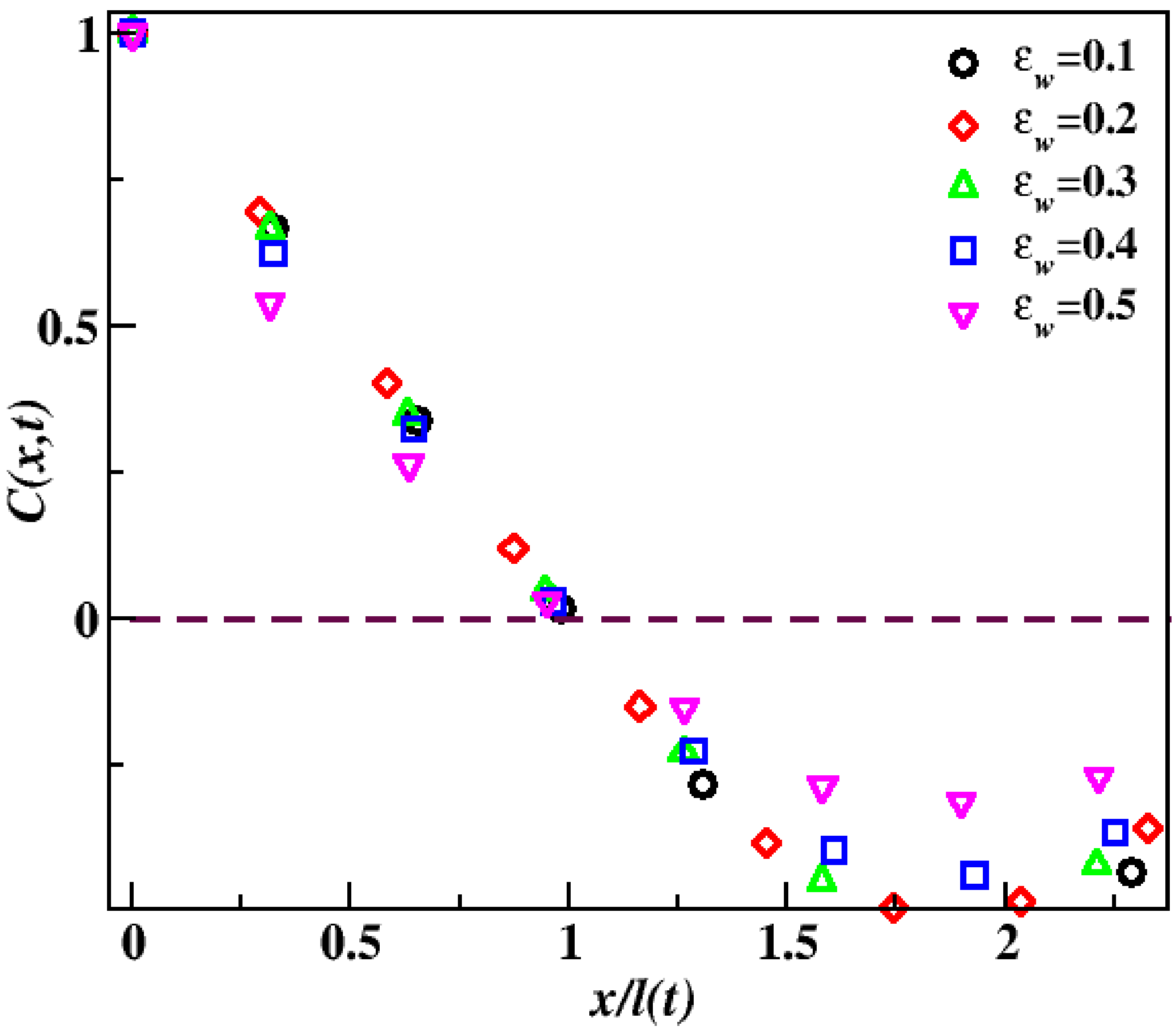


$$C(x,t) = \langle \varphi(0,t)\varphi(x,t) \rangle - \langle \varphi(0,t) \rangle \langle \varphi(x,t) \rangle$$



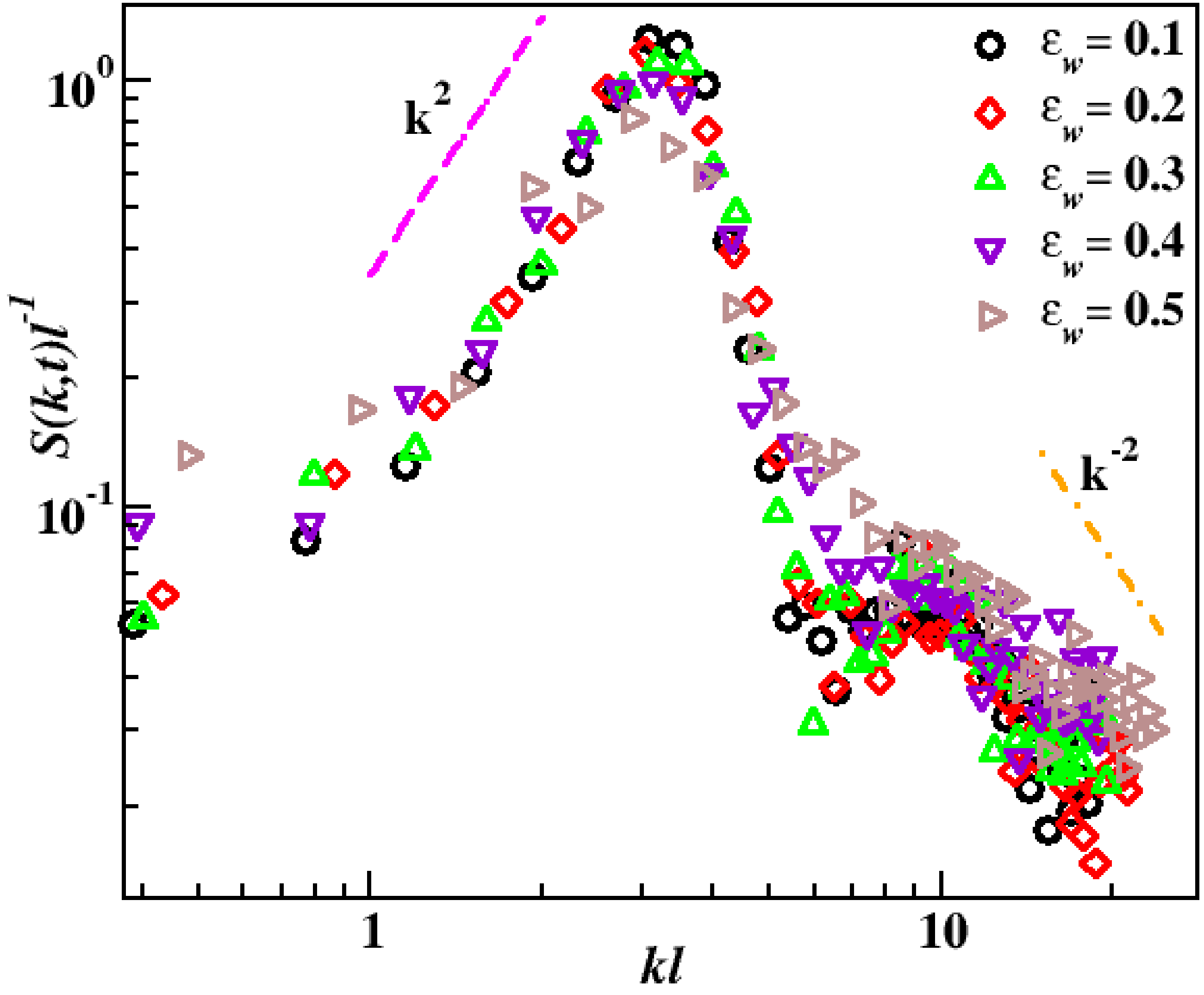
- ✓ **Perfect data Collapse**
- ✓ **Self-similar nature of domains**

PW: C(x,t) for different $\in_w$



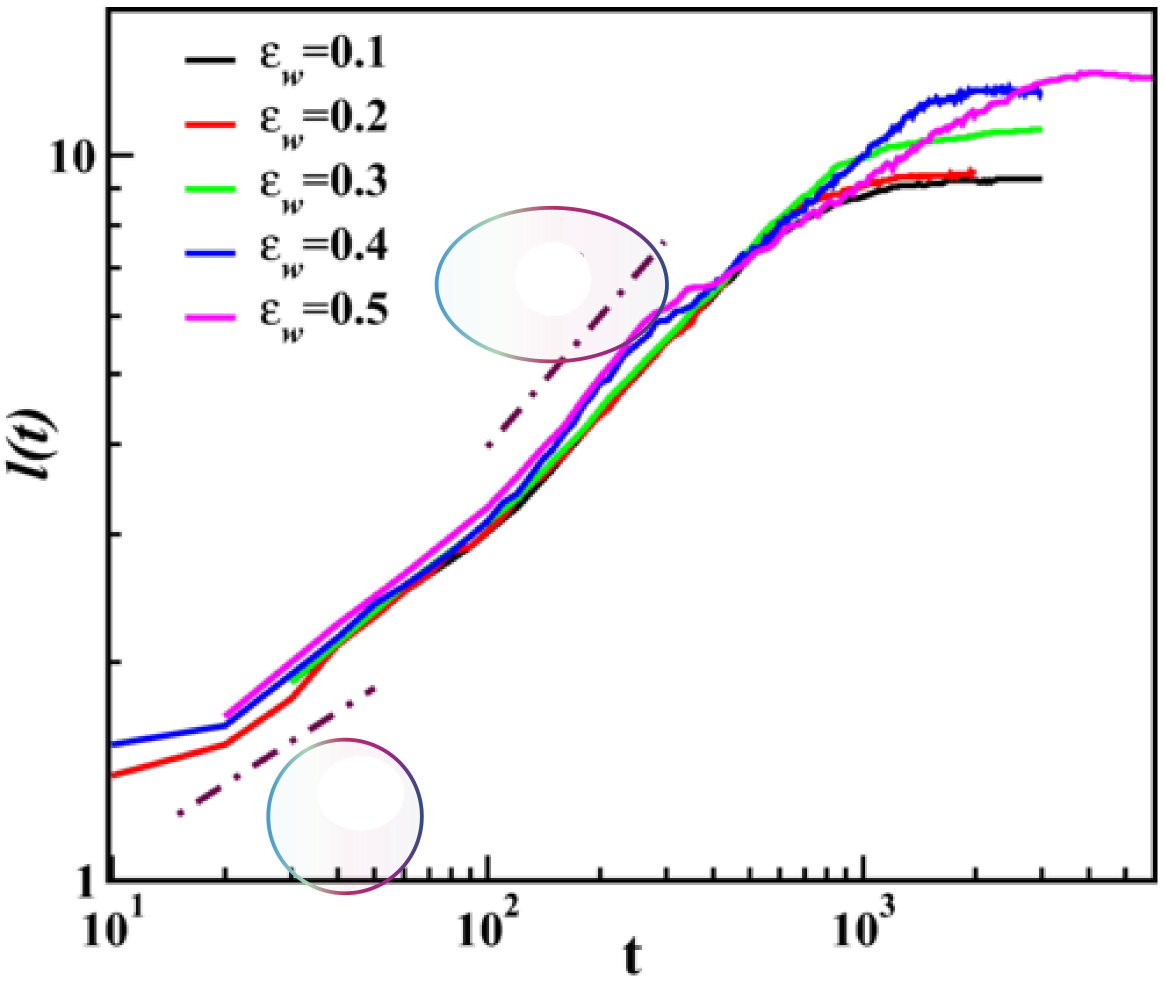
- Scaling behavior violated for higher values of $\in_w$.
- Self similarity nature broken once zero crossed shows the change in domain behavior for different $\in_w$

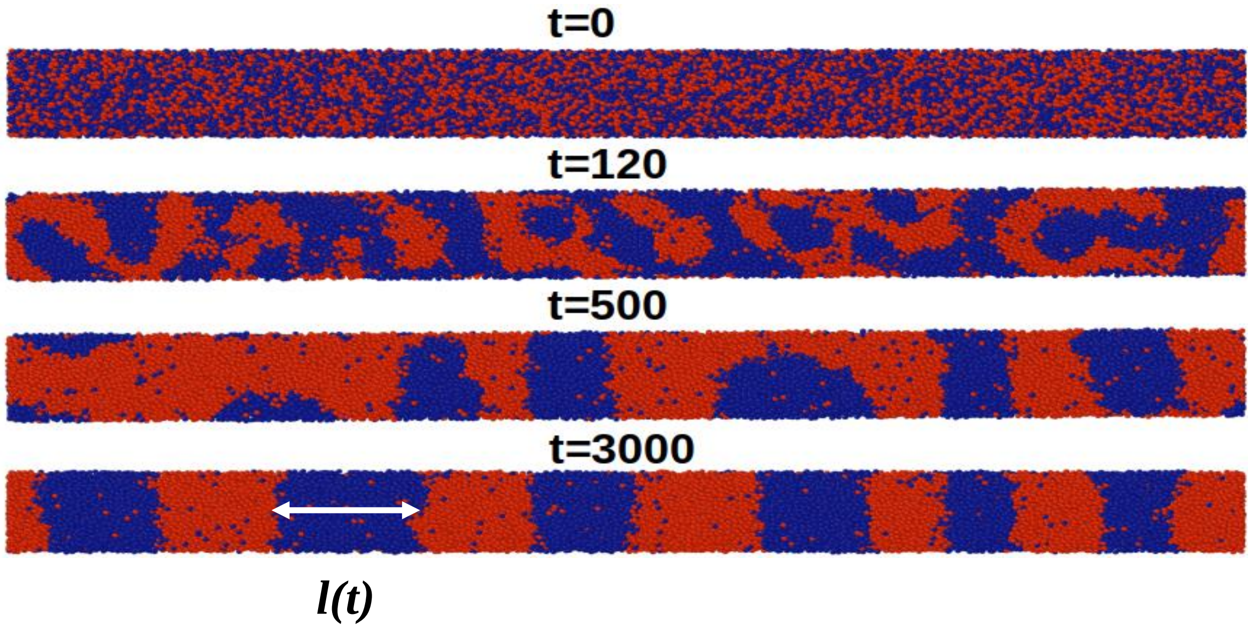
PW: Structure Factor



- $S(k,t) \approx k^{-(d+1)}$, here d=1
- Porod law violated for higher values of $\in_w$.
- Second peak at $kl \approx 10$ implies sharp domain boundaries.
- Peak almost vanishes for higher $\in_w$ ($\in_w = 0.5$) .

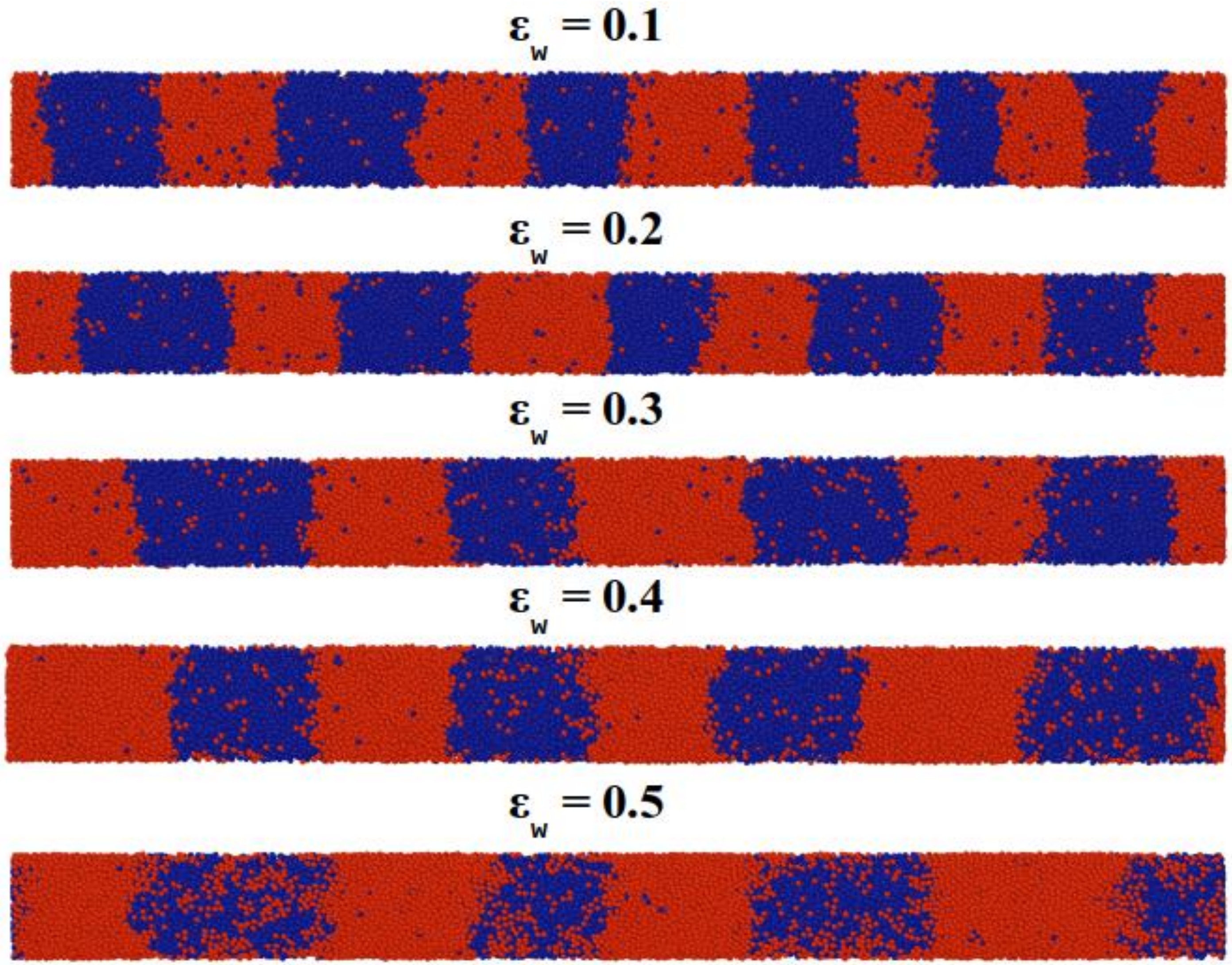
PW: Growth Dynamics





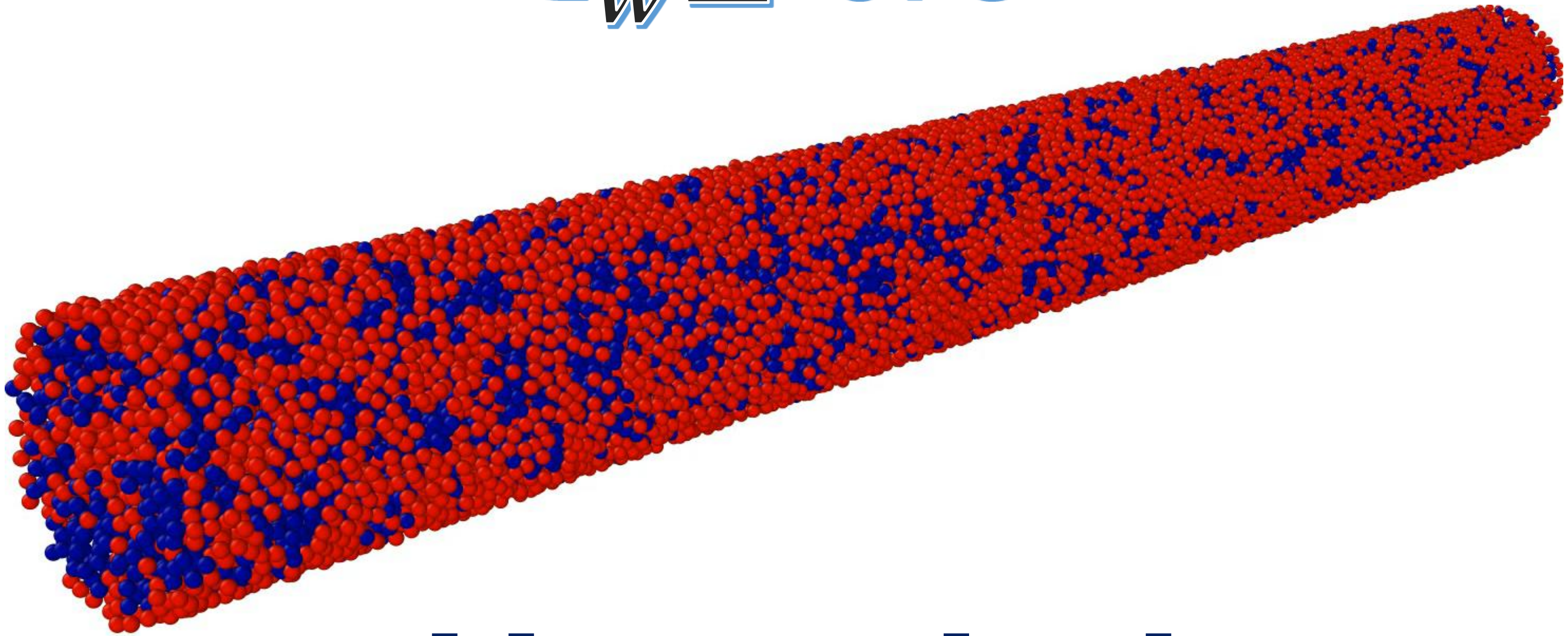
- Domain growth with time is represented using the lengthscale *l(t)*
- With increasing strength of interaction with wall, the size of domains increases.

PW: Final Configuration



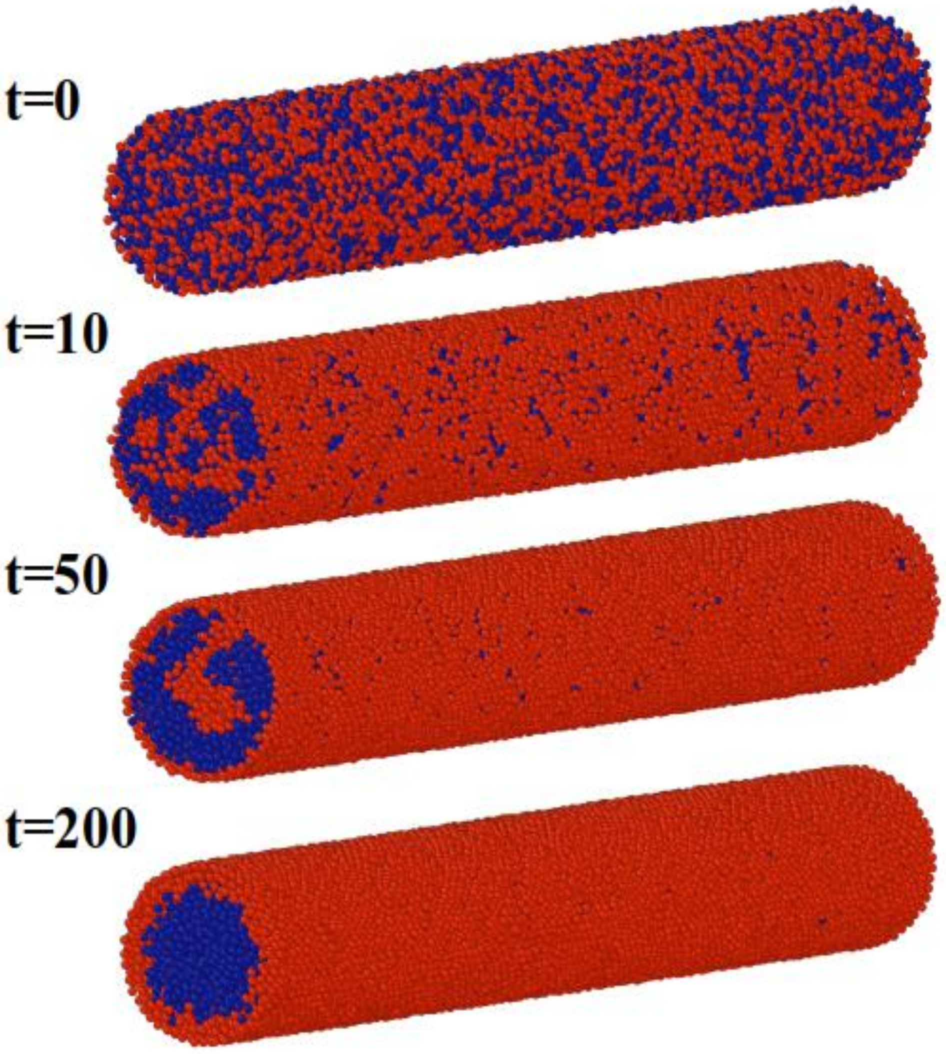
COMPLETE WETTING (CW)

$$\epsilon_w \geq 0.6$$

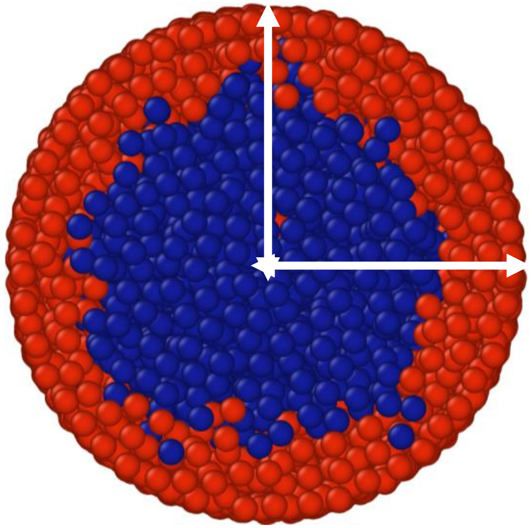


Metastable state broken and complete phase separation obtained

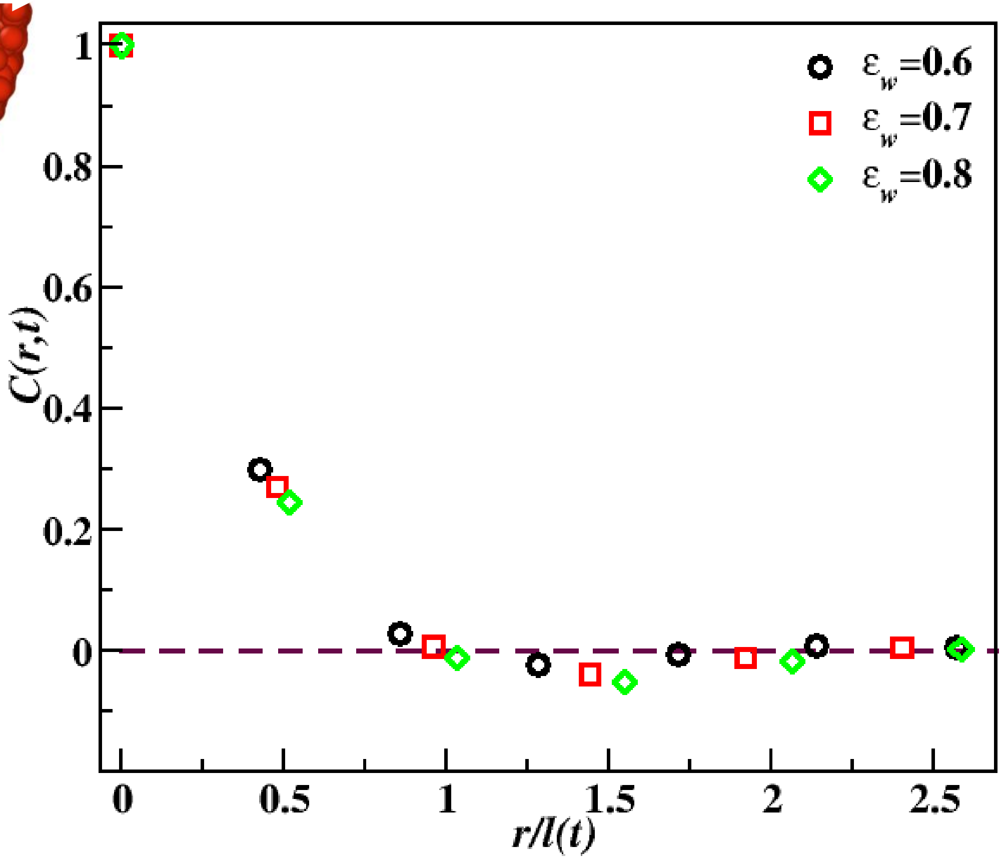
COMPLETE WETTING (CW)



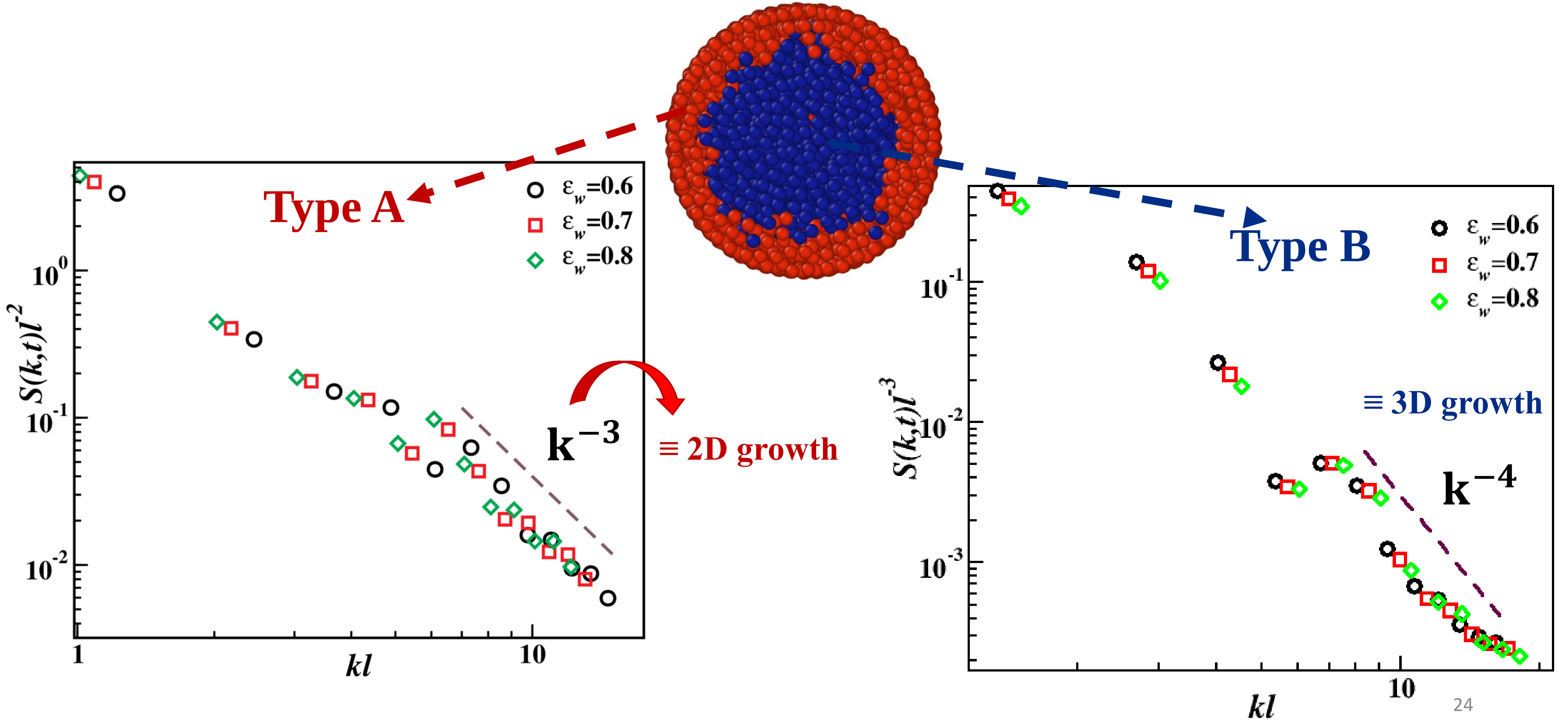
Time evolution of the system



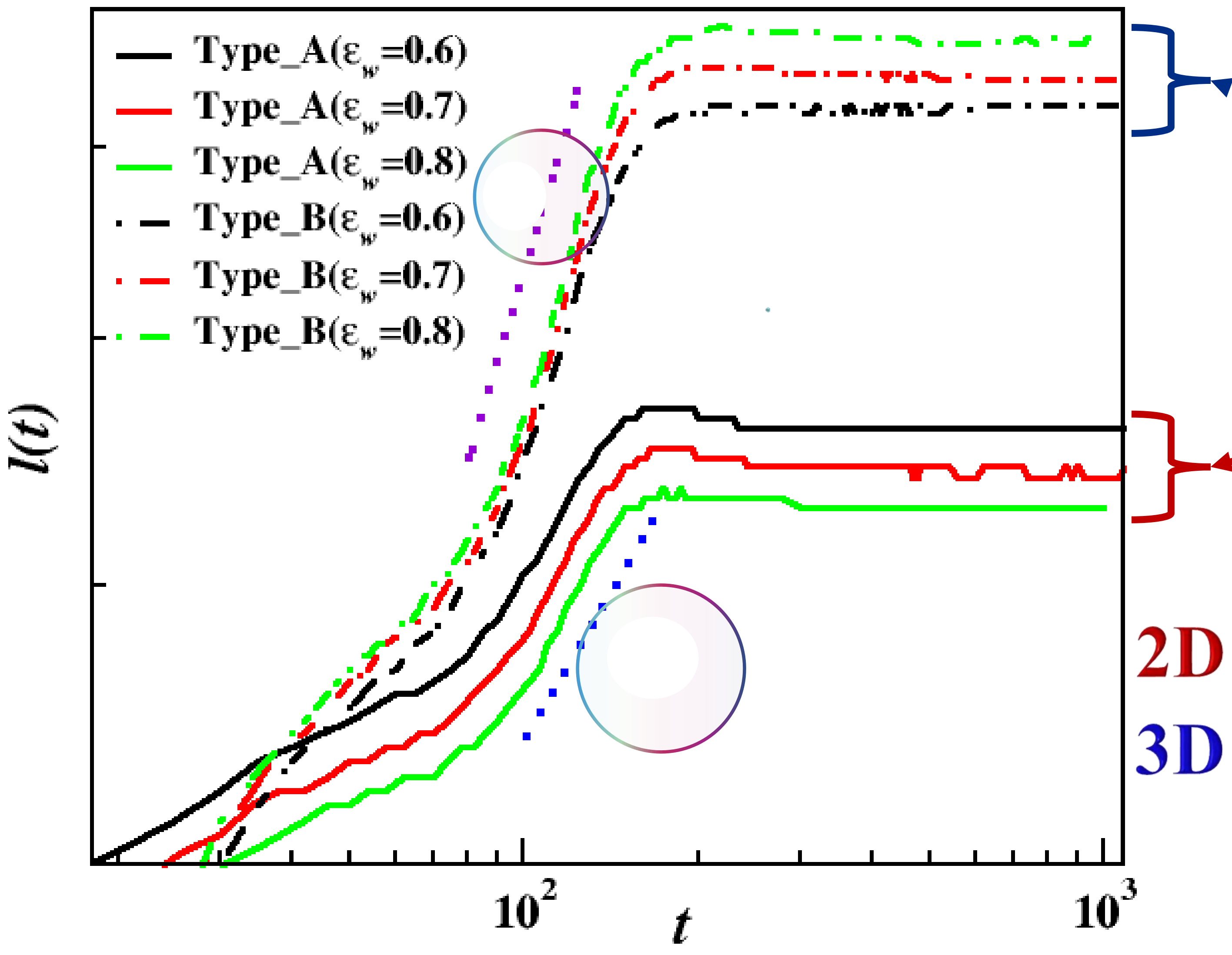
Correlation calculated radially from the center of the cylinder.

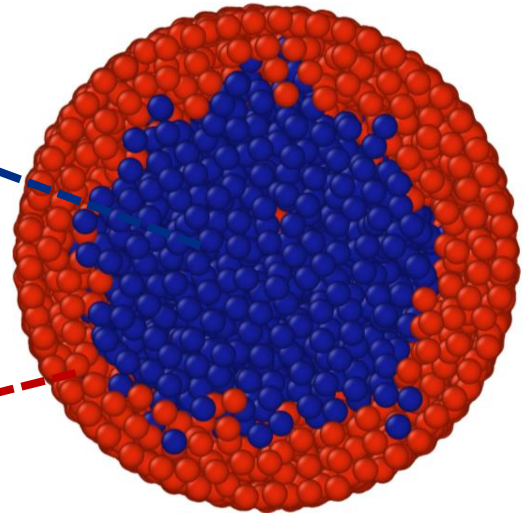


CW: Structure Factor



CW: Domain Growth



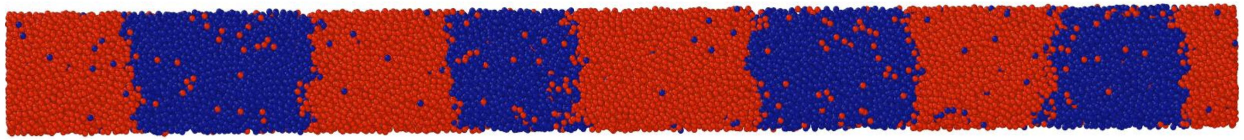


2D Viscous hydrodynamics,α=1/2

3D Viscous hydrodynamics, α=1

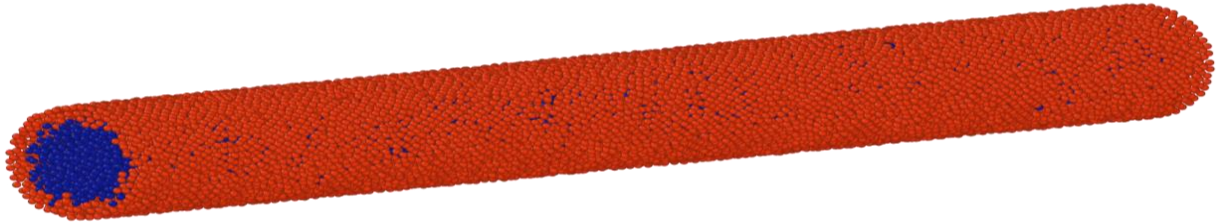
SUMMARY

- Surface-directed spinodal decomposition of binary liquid inside a cylindrical pore is studied
- Type A particles → wetting interaction and Type B particles → inert to wall.
- **Partial Wetting** : -



  - ✓ Domains → Metastable with increasing domain size w.r.t increasing $\in_w$
  - ✓ Growth laws → Diffusive LS law ~ $t^{1/3}$, Inertial hydrodynamic law ~ $t^{2/3}$

- **Complete Wetting**:-



  - ✓ Domains → Cylindrical or Tube like fully separated domains
  - ✓ Growth laws → Viscous hydrodynamic growths:
    - Type A ~ $t^{1/2}$ (≡ 2D Growth)
    - Type B ~ t (≡ 3D Growth)

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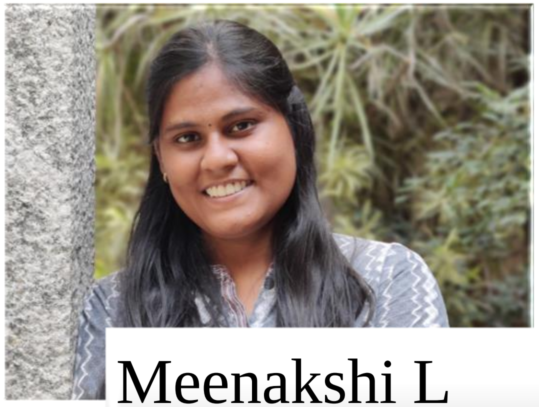

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