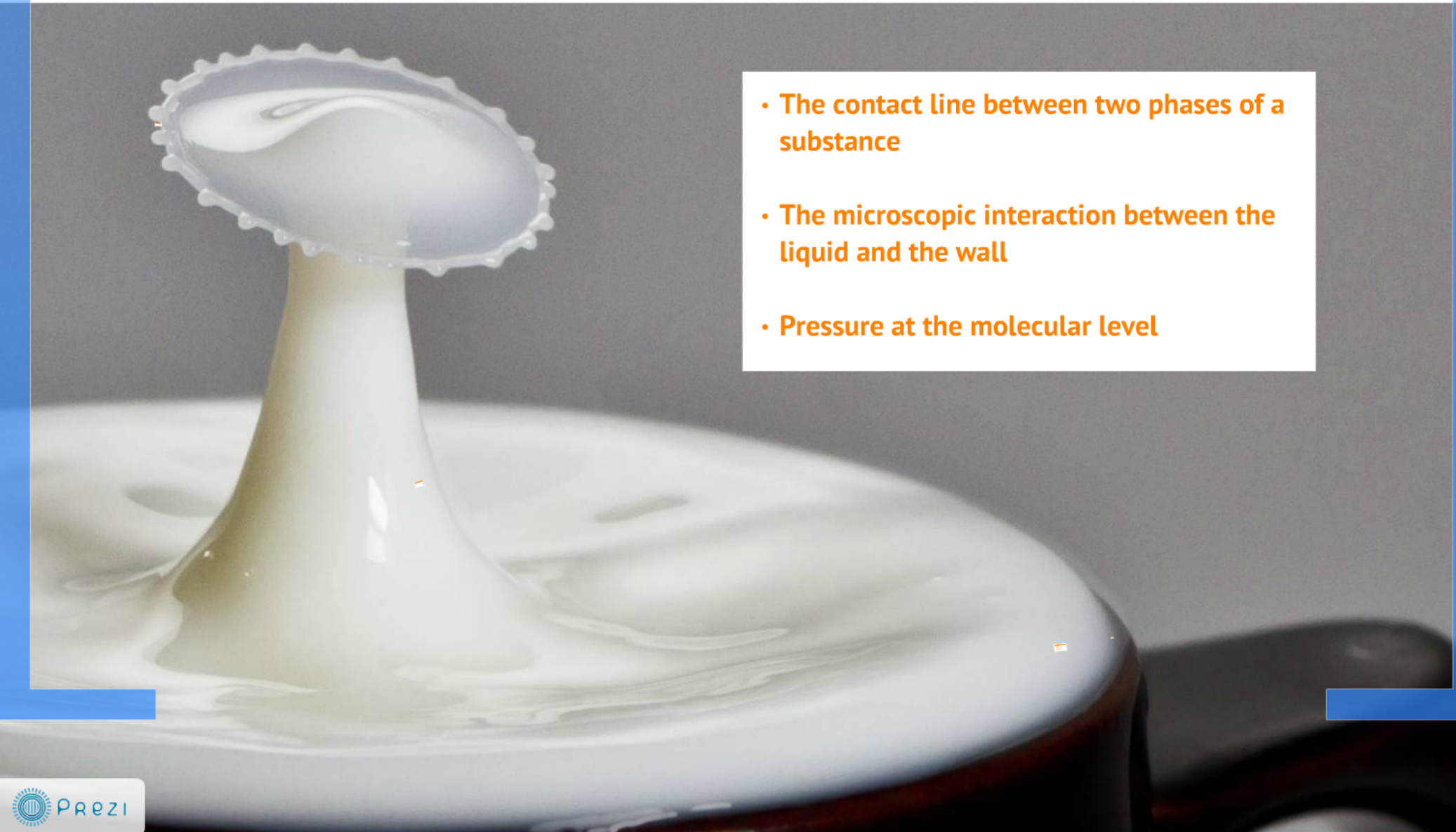## Limitations of the Continuum Description

- The contact line between two phases of a substance
- The microscopic interaction between the liquid and the wall
- Pressure at the molecular level

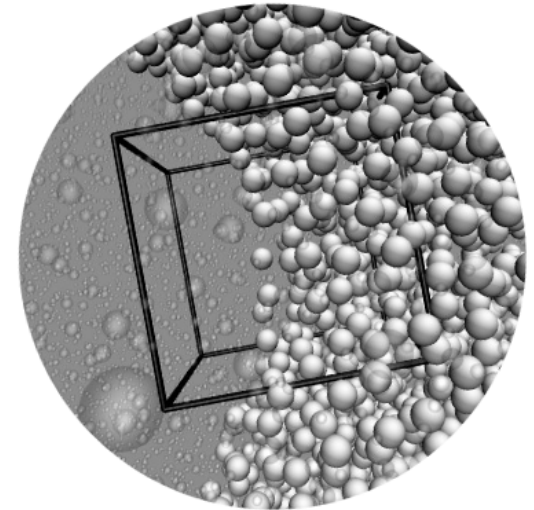# Limitations of the Continuum Description

- The contact line between two phases of a substance

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Contact Lines

- **Continuum mechanics cannot adequately model the contact line between two phases**

- **Interface tracking required and extra modelling assumptions must be invoked**

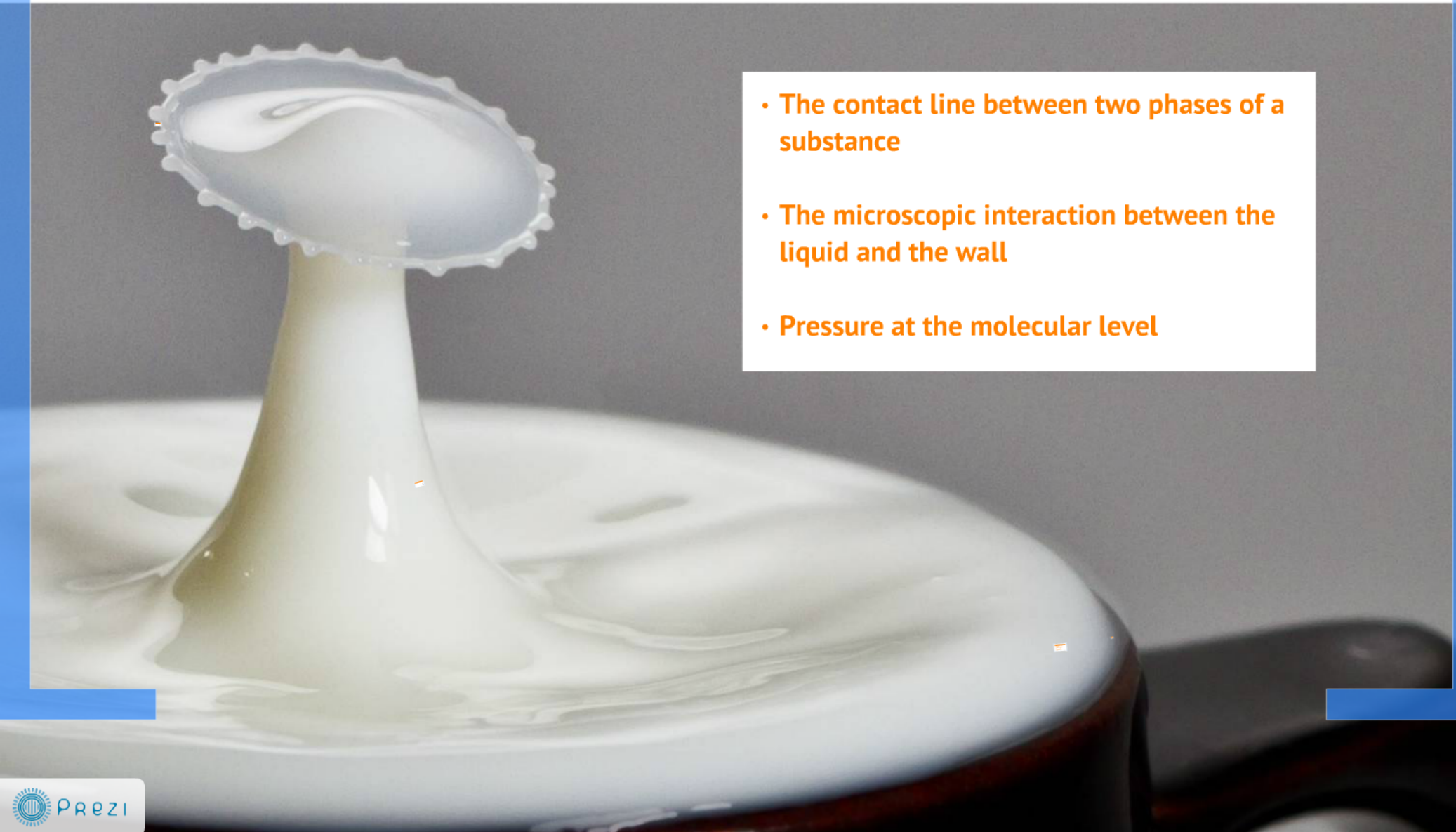- **Discrete molecular dynamics captures phase change and interaction naturally***

*Hadjiconstantinou (1998)
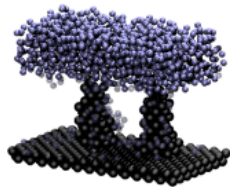
Limitations of the Continuum Description

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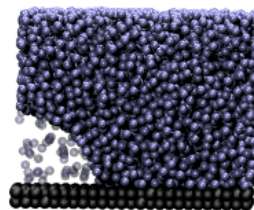- **Pressure at the molecular level**

Fluid-wall interactions

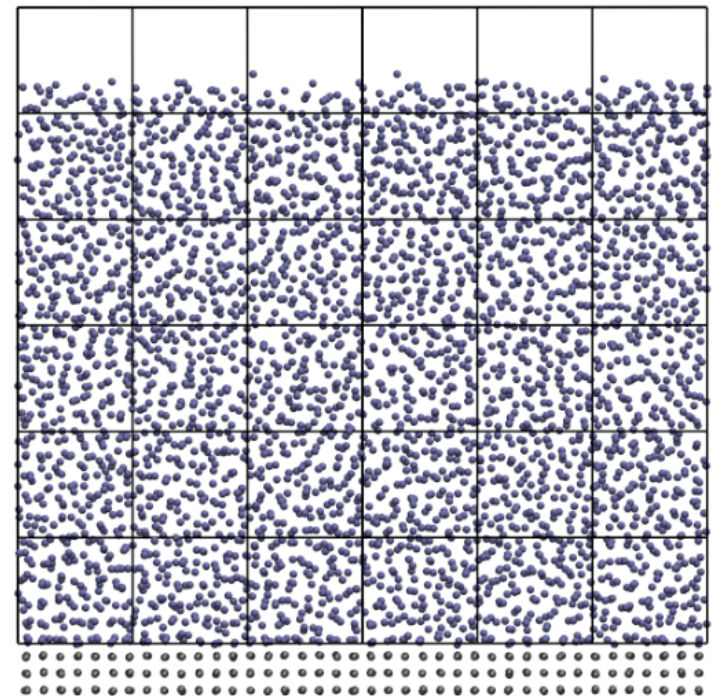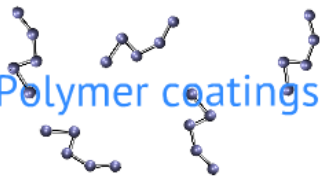- **Molecular Dynamics allows nanoscopic analysis of wall treatments and interactions**

  - Nano-scale surface roughness

  - Polymer coatings

  - Nucleation
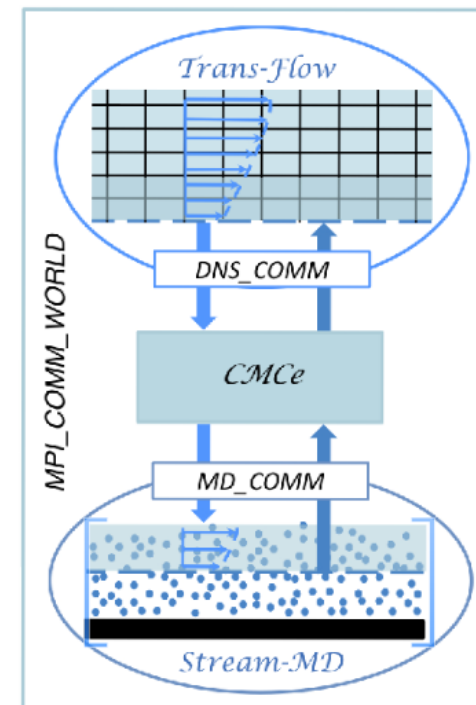
Continuum to Molecular coupling

- Simulate molecular dynamics where discrete effects are important

- The bulk of the domain is simulated by the continuum solver

- A discrete form of Reynolds' transport theorem is required to provide a consistent framework
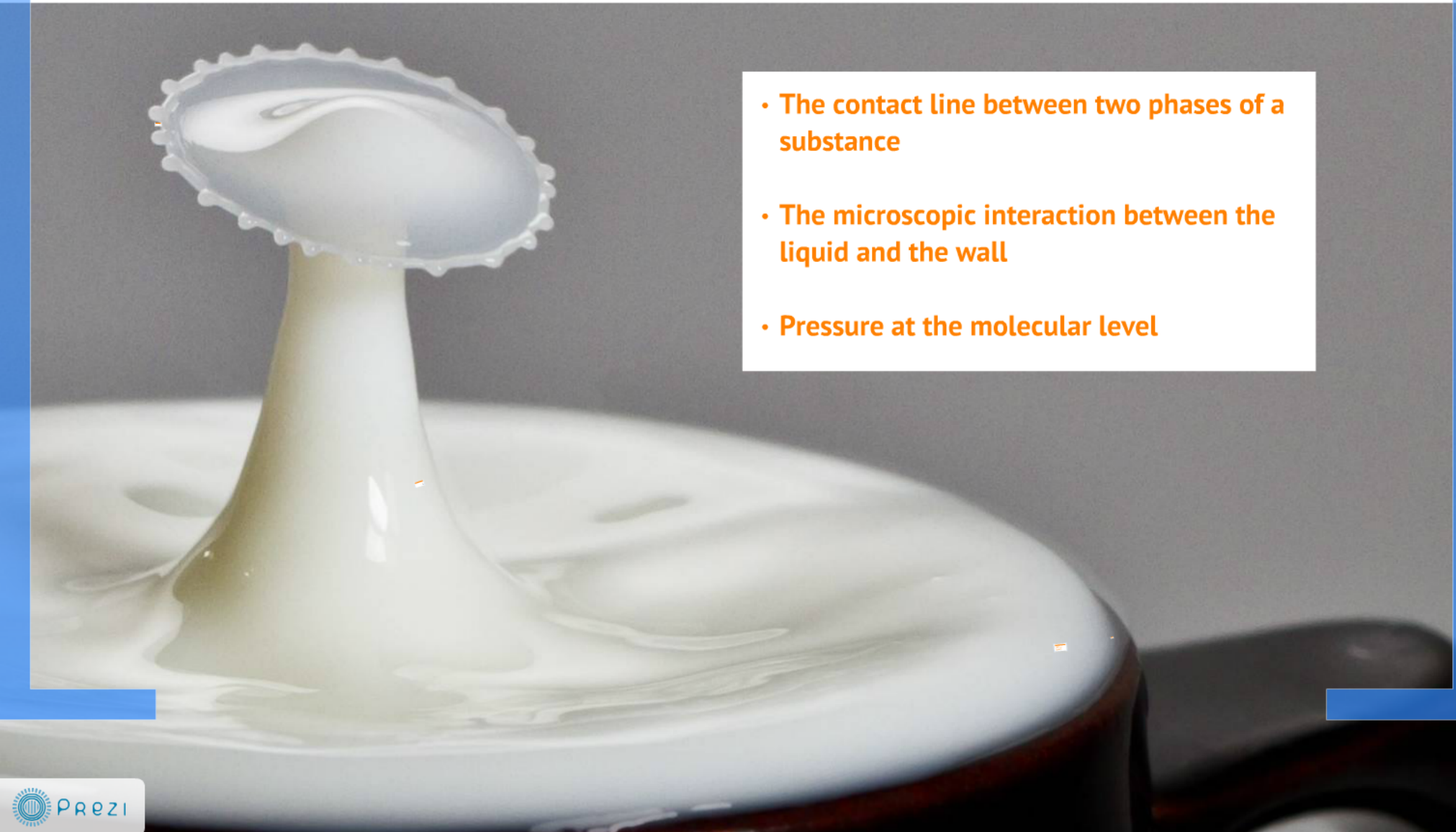

O'Connell, Thompson (1995), Flekkoy et al (2000), Delgado Buscalioni(2003), Nie et al (2004)

Limitations of the Continuum Description

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Discrete Pressure Tensor

- **Molecular stress tensor is non-unique**[*]

- **The correct form is a source of big debate in the literature**[^]

- **The discrete Reynolds' transport theorem provides insight**

$$F_{surface} = \oint_S \mathbf{\Pi} \cdot d\mathbf{S} = \int_V \mathbf{\nabla} \cdot \mathbf{\Pi} dV$$

$$\mathbf{\Pi} = P\mathbf{I} + \boldsymbol{\sigma}$$

[*]Schofield, Henderson (1982)

[^]Irving,Kirkwood(1950), Parker (1954), Lutsko (1988), Todd et al (1995), Zhou (2004), Murdoch (2010), Heyes (2011)

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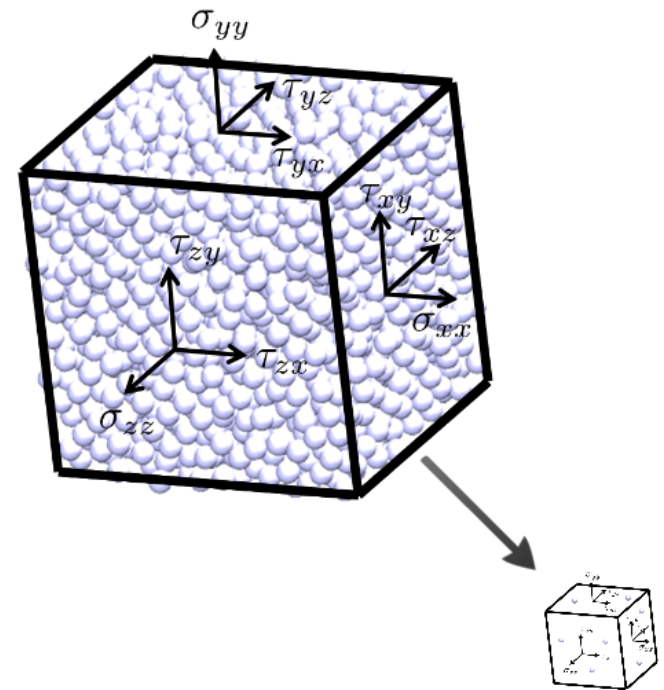
- **Pressure at the molecular level**