Bridging Molecular and Continuum Scales in Wetting

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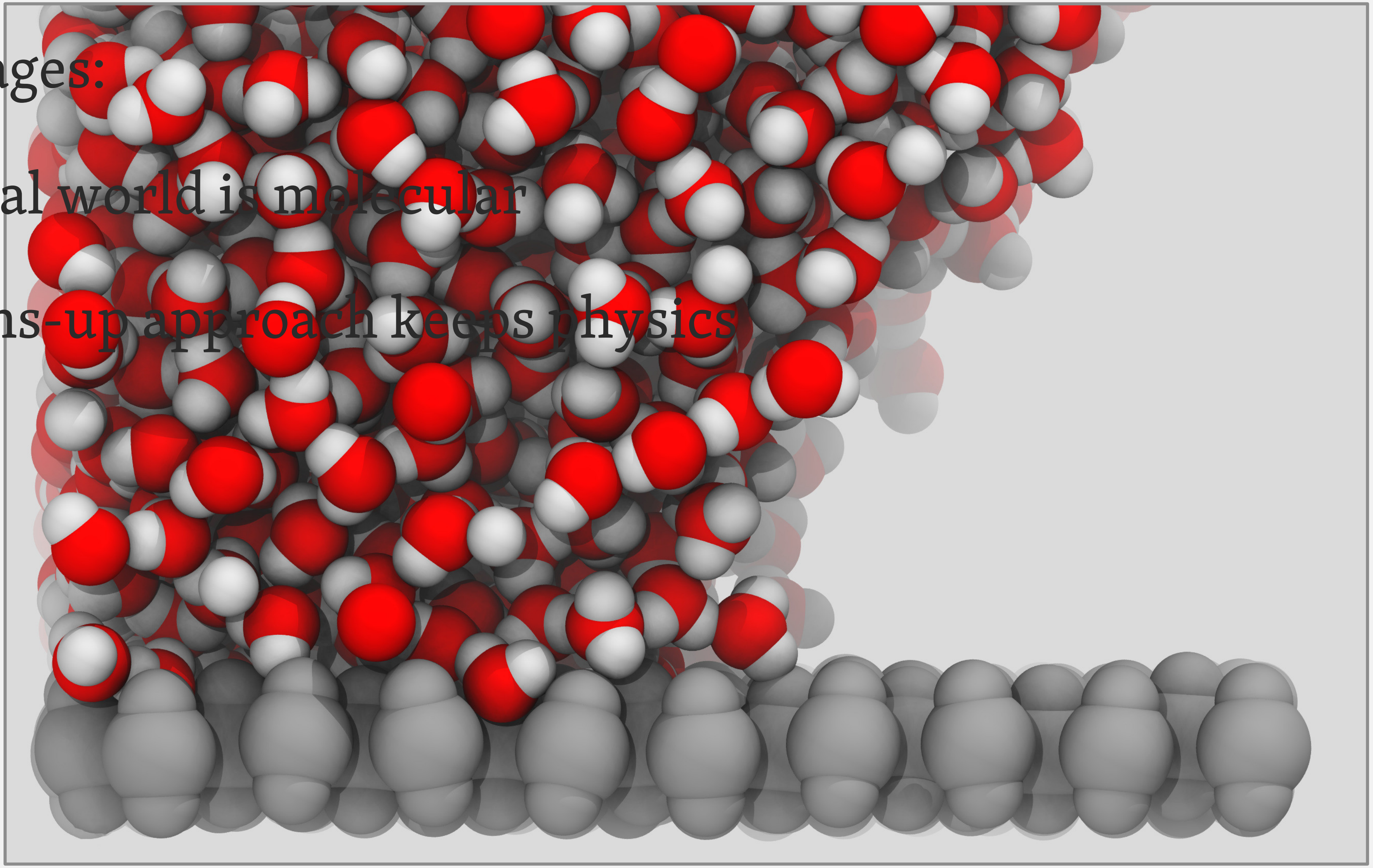
OUTLINE

- Molecular and continuum views of wetting
- Problems of purely molecular systems
- Example of multiscale simulation: Contact line friction in wetting
- (Bonus study: Realistic (?) electrowetting)

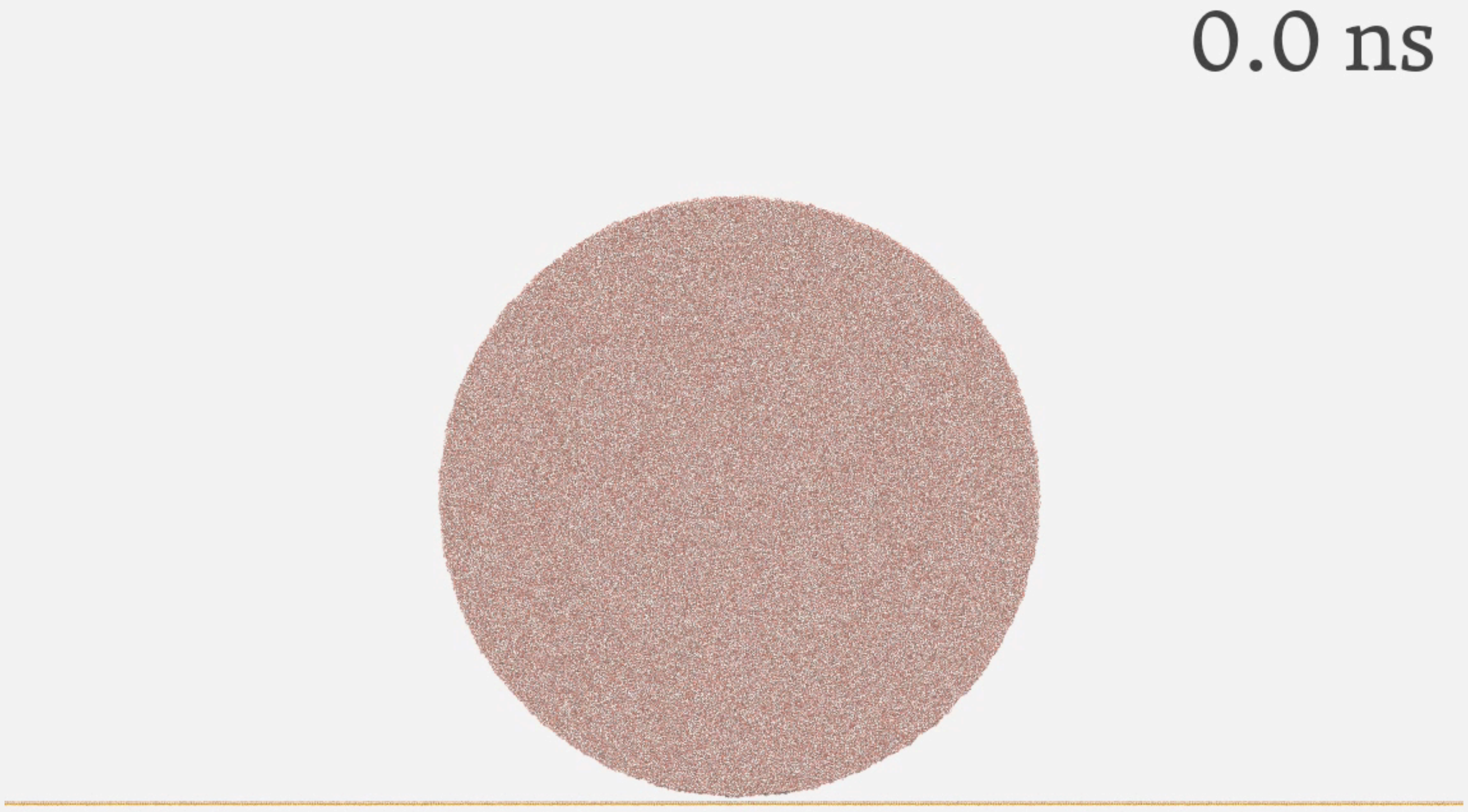
MOLECULAR VIEW

Advantages:

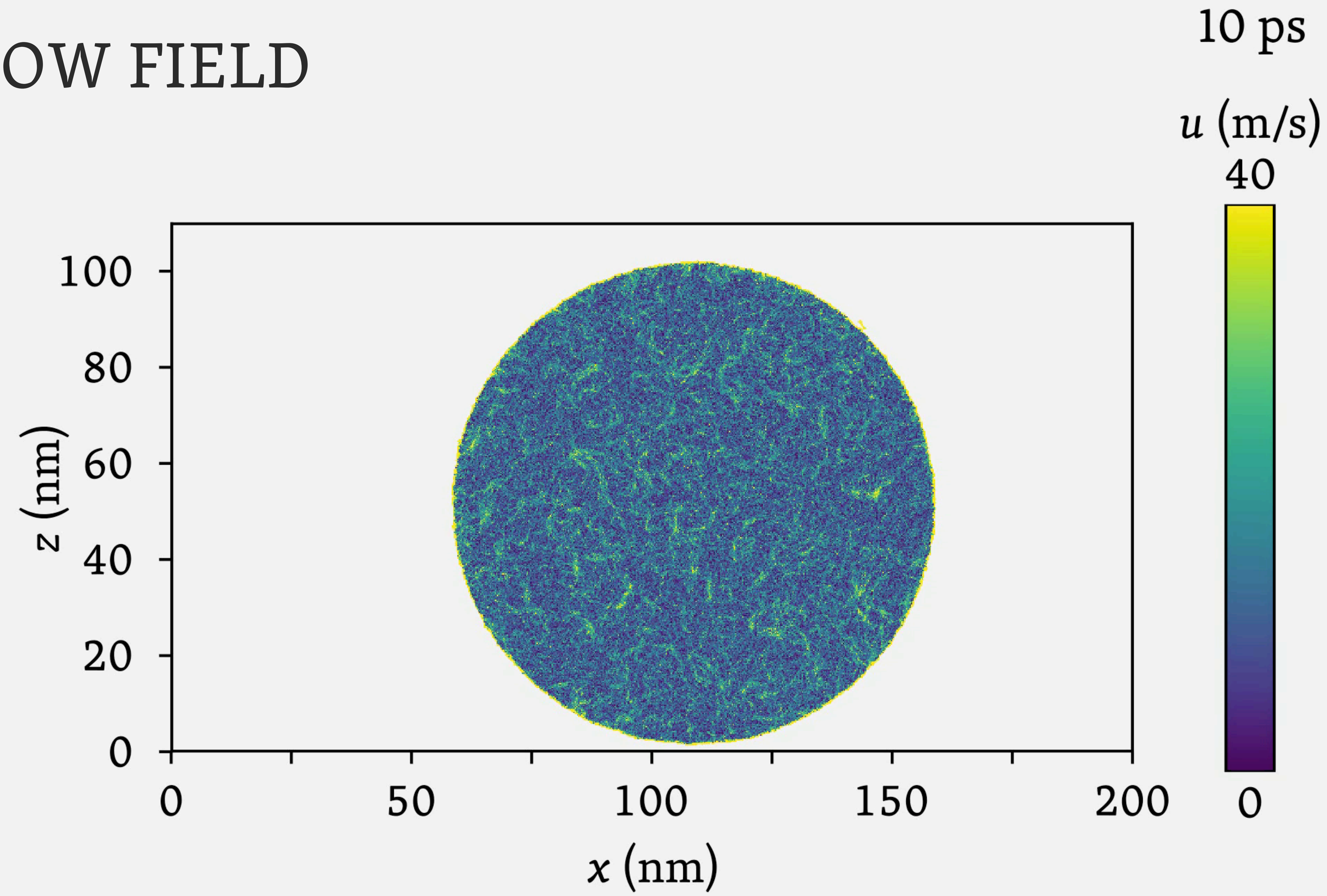
- Physical world is molecular
- Bottoms-up approach keeps physics



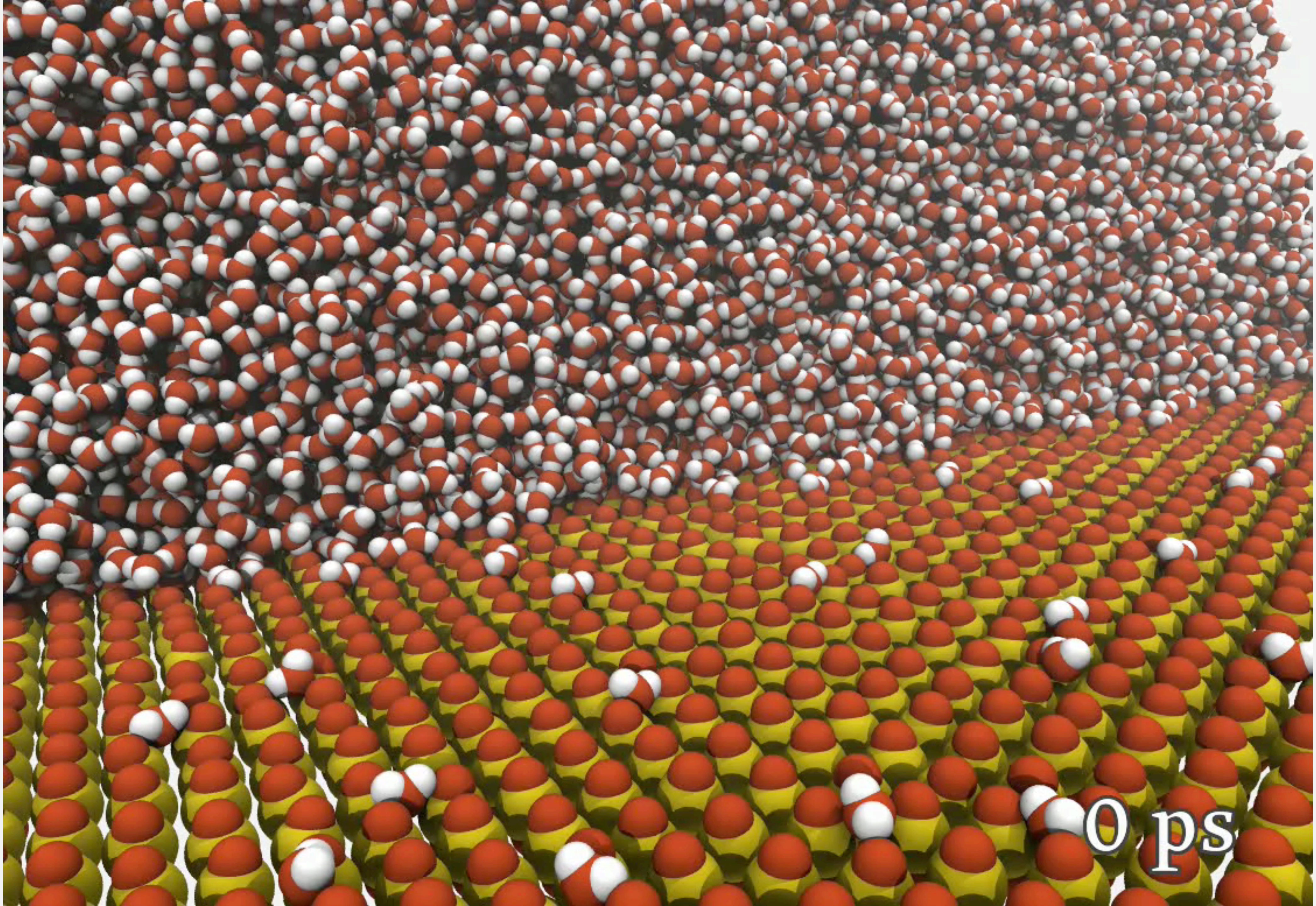
MOLECULAR SIMULATIONS



FLOW FIELD



BUT: WHAT DO WE GET FROM THIS?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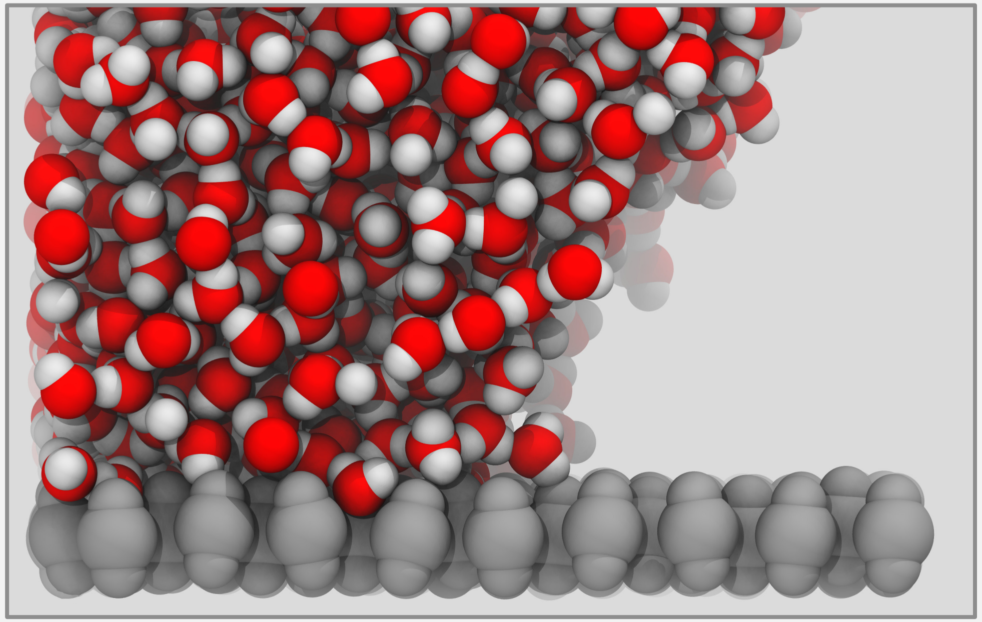
MOLECULAR VIEW

Advantages:

- Physical world is molecular
- Bottoms-up approach keeps physics

Disadvantages:

- How do we interpret the data?
- Molecules are expensive to model



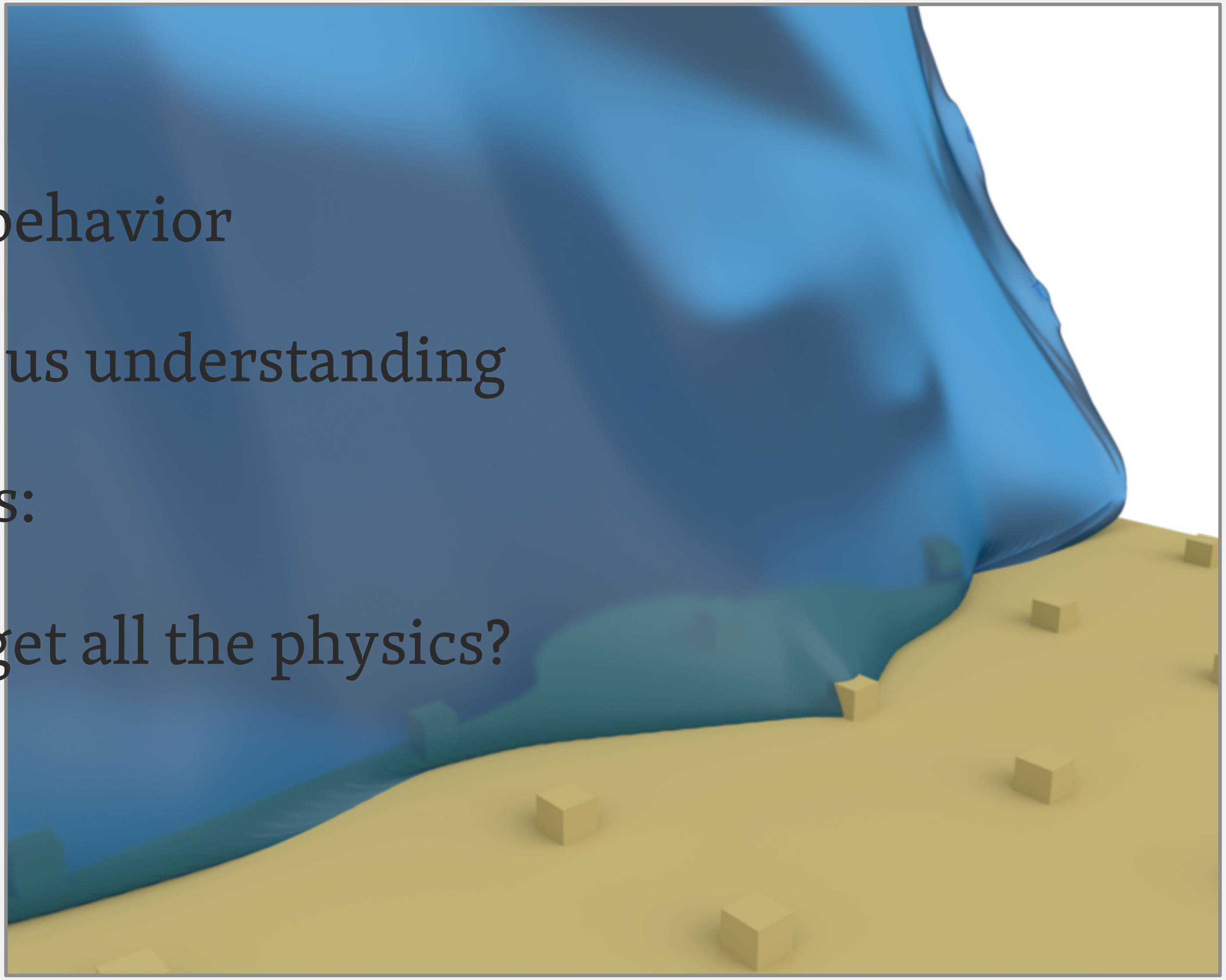
CONTINUUM MODELS

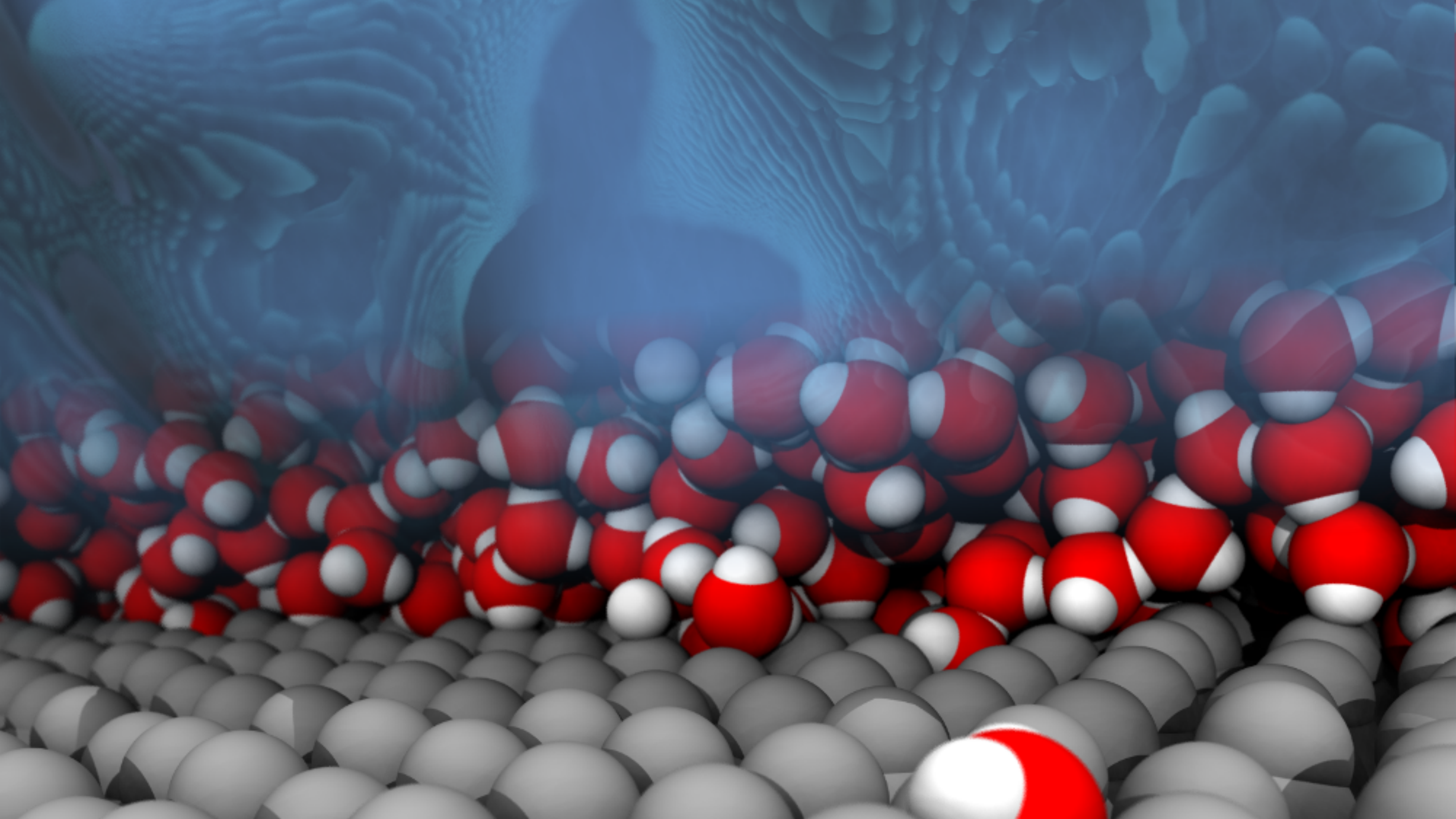
Advantages:

- Large scale behavior
- Models give us understanding

Disadvantages:

- How do we get all the physics?





EXAMPLE: CONTACT LINE FRICTION BOUNDARY CONDITION

CONTACT LINE FRICTION

What is it?

- Energy dissipation from some process at the contact line Important for mesoscopic or sensitive systems
- Theorized to be due to slippage or substrate defects
- But: also appears for perfect no-slip substrates

Our desire: *characterize* this term for molecular systems and derive a *boundary condition*.

MEASURING THE DISSIPATION

- Symptomized as a decrease in contact line velocity ν
- In a damped regime:

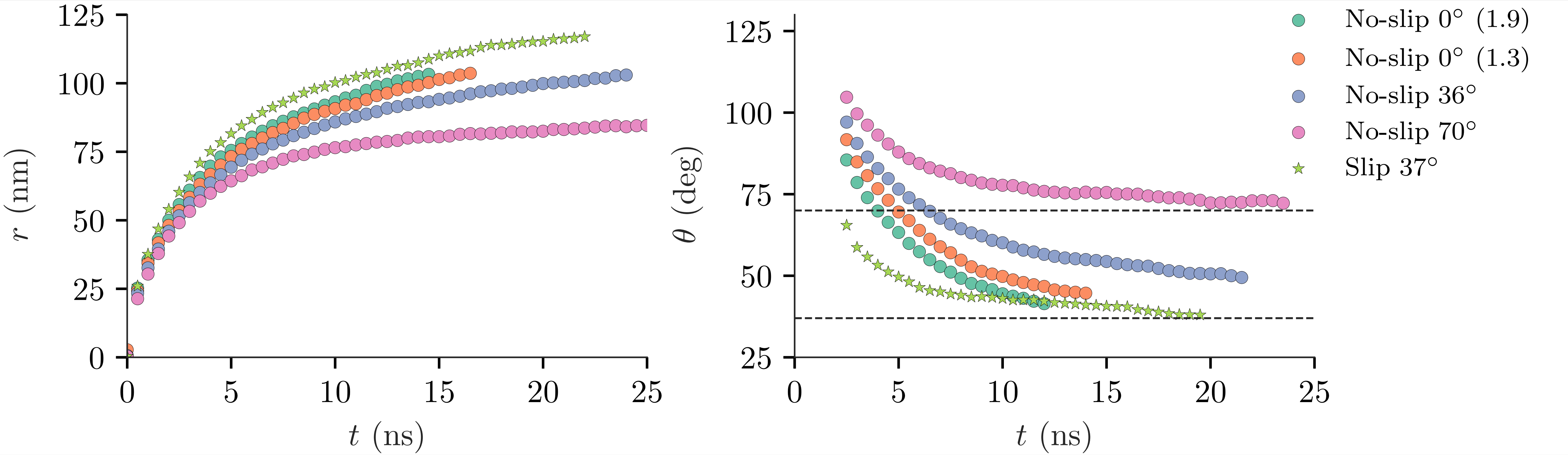
  $v = \frac{F}{\mu_f}$, where

  $F = \gamma\,(\cos\theta_0 - \cos\theta)$ is the Young driving force, and

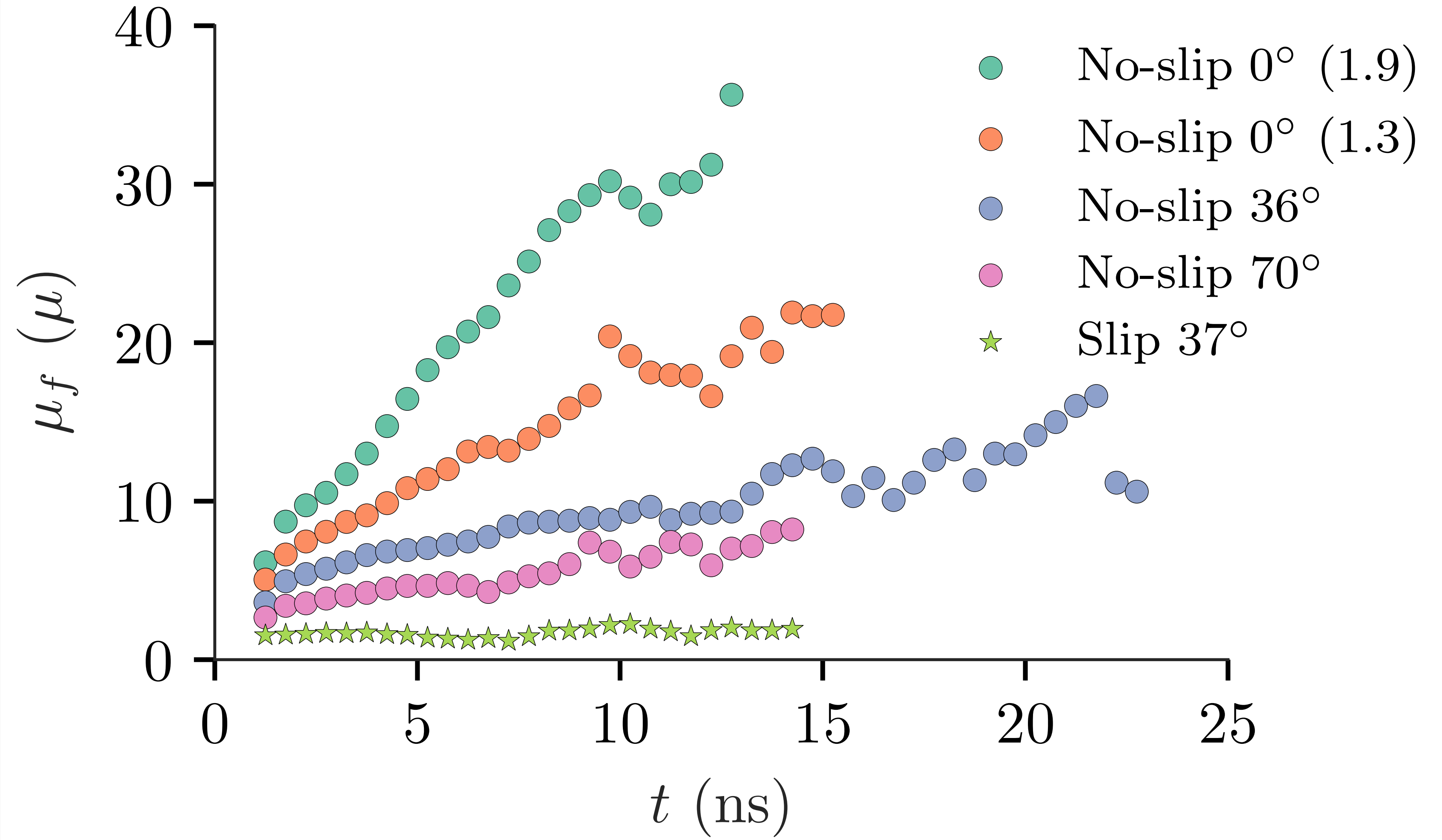
  μ_f is the contact line friction (dissipation)
- Thus:

  $\mu_f = \mu_f(v, \theta)$ for given γ and θ_0 (system energetics).

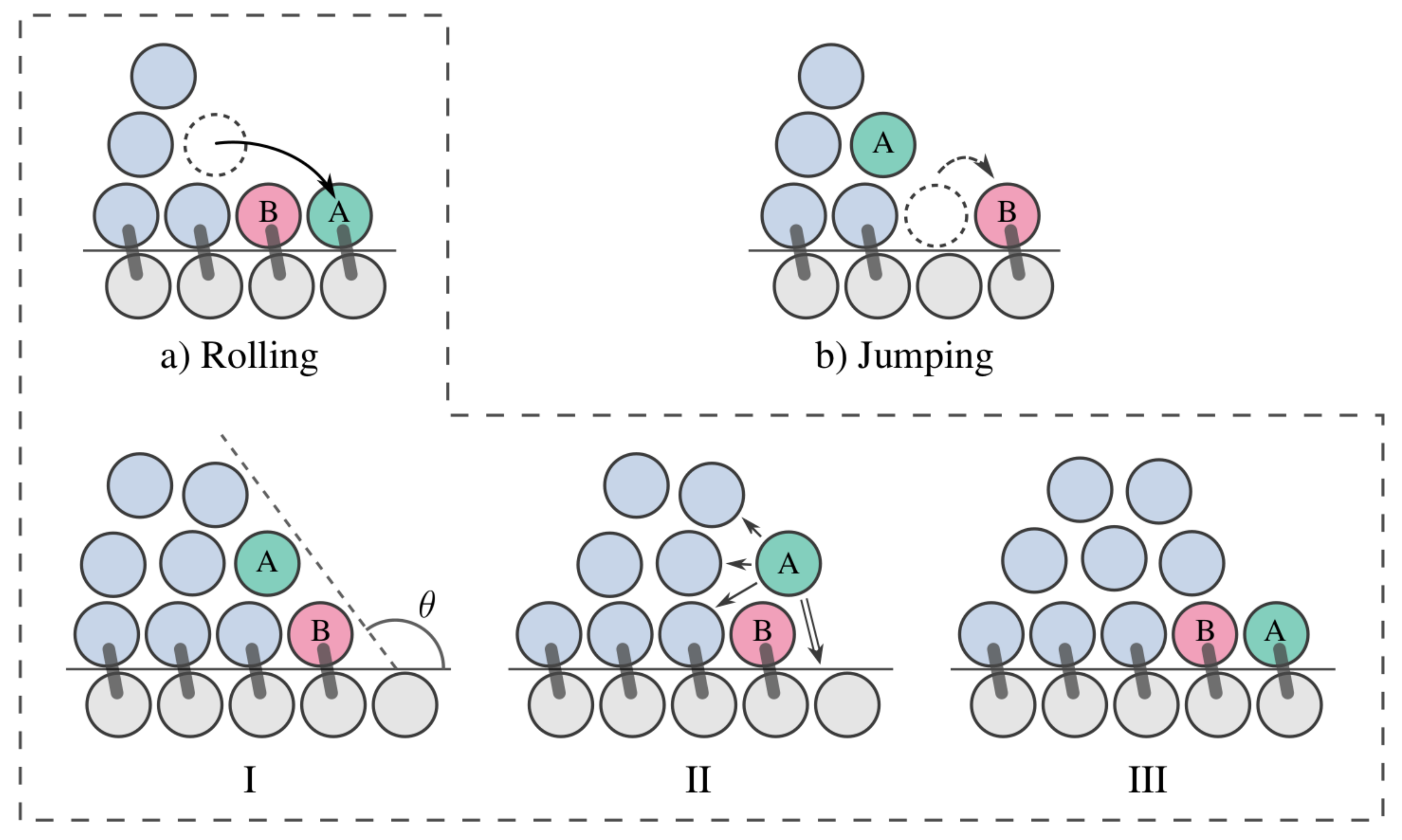
MEASUREMENTS



CONTACT LINE FRICTION INCREASE



MODEL OF ADVANCEMENT GIVES BARRIER

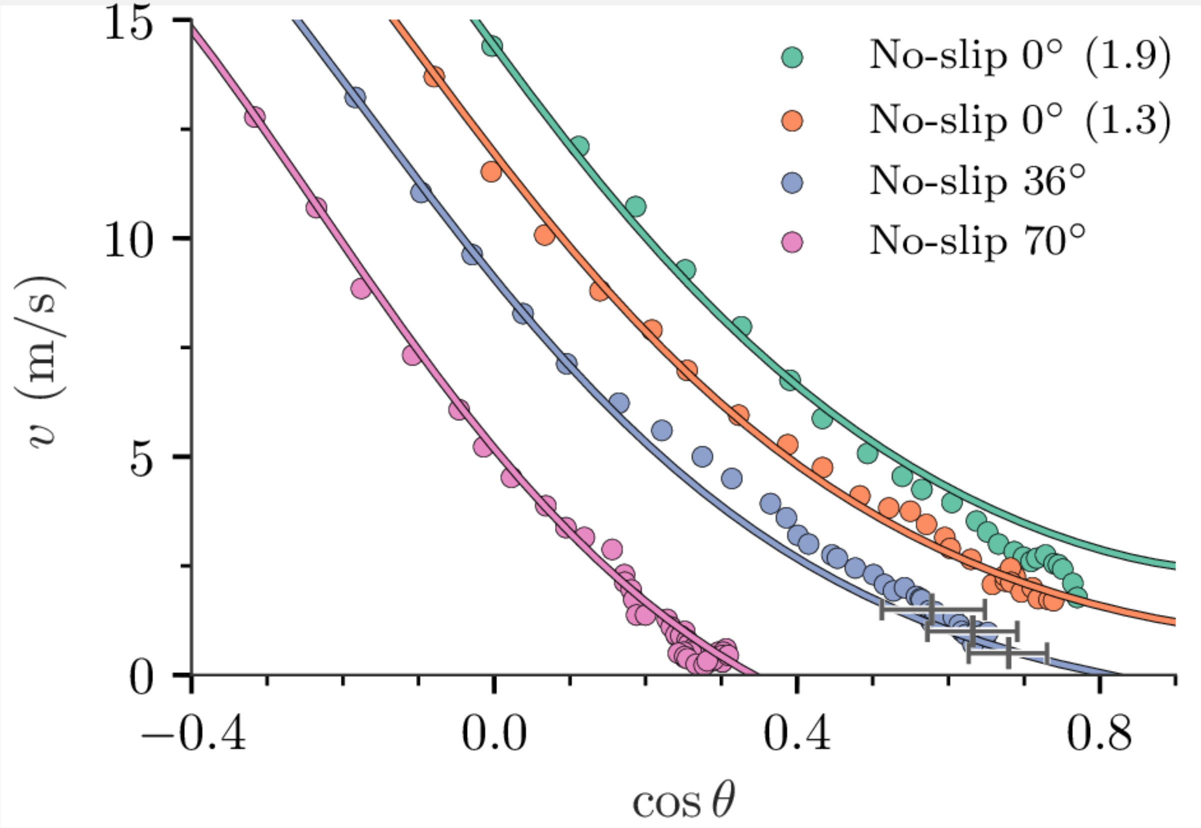


BARRIER SETS DISSIPATION

- Barrier $\Delta E(\theta)$ is the required thermal fluctuation
- Advancement rate (velocity) decreases by an exponential:

$$v = \frac{F}{\hat{\mu}_f} \exp(-a\Delta E)$$

- Good match to data! Boundary condition constructed.



NEED FOR MULTISCALE SYSTEMS

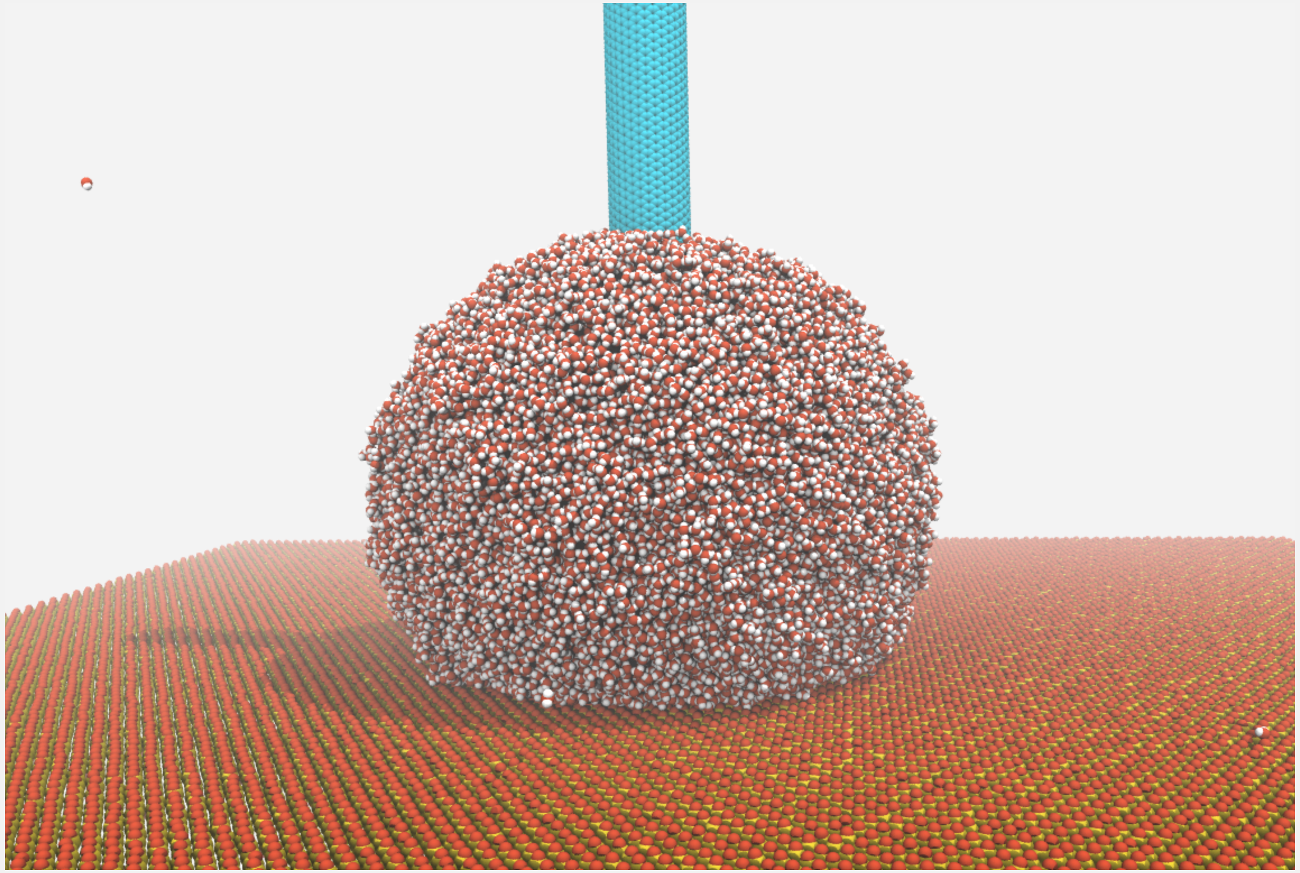
Large systems give:

- Access to slower regimes
- Lots of statistics
- Most importantly: inclusion of molecular processes in otherwise continuum systems

CONTACT LINE FRICTION IN ELECTROWETTING

ELECTROWETTING SYSTEM

- Apply electric potential to spread out droplet
- Our systems: charge distributions, electrode, realistic ionic solutions



APPLY POTENTIAL

Measured contact line friction less than 10% of spontaneous wetting

STATE OF MULTISCALE WETTING

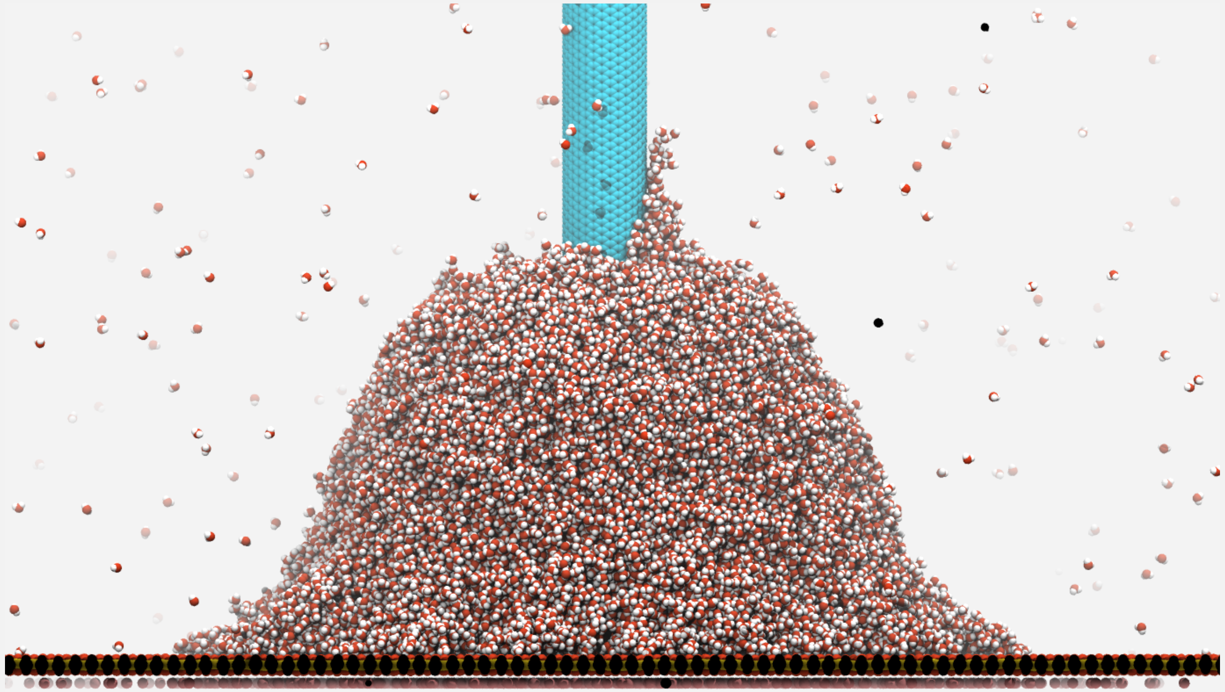
- Need for accurate simulations of multiscale systems
- Pure MD works, but is limited by scaling
- A few different multiscale methods are proving successful
- Can work with limited MD systems to analyze effects to use for larger simulations

ACKNOWLEDGMENTS

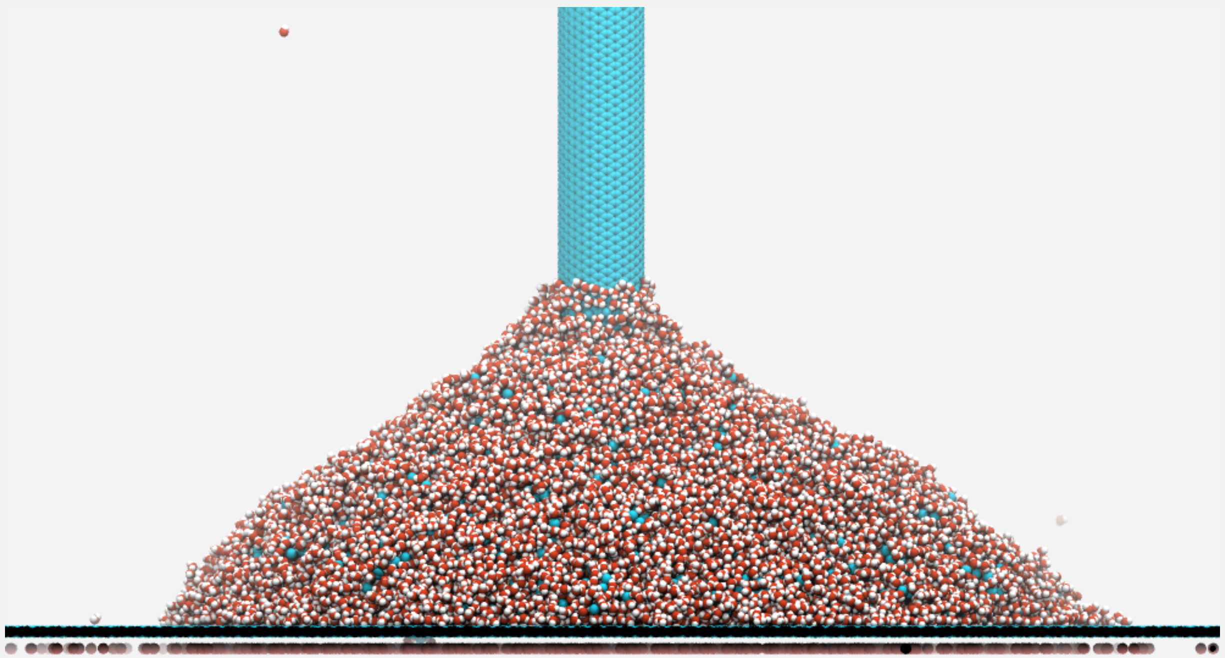
SERC
Swedish e-Science Research Centre

erc
European Research Council
Established by the European Commission

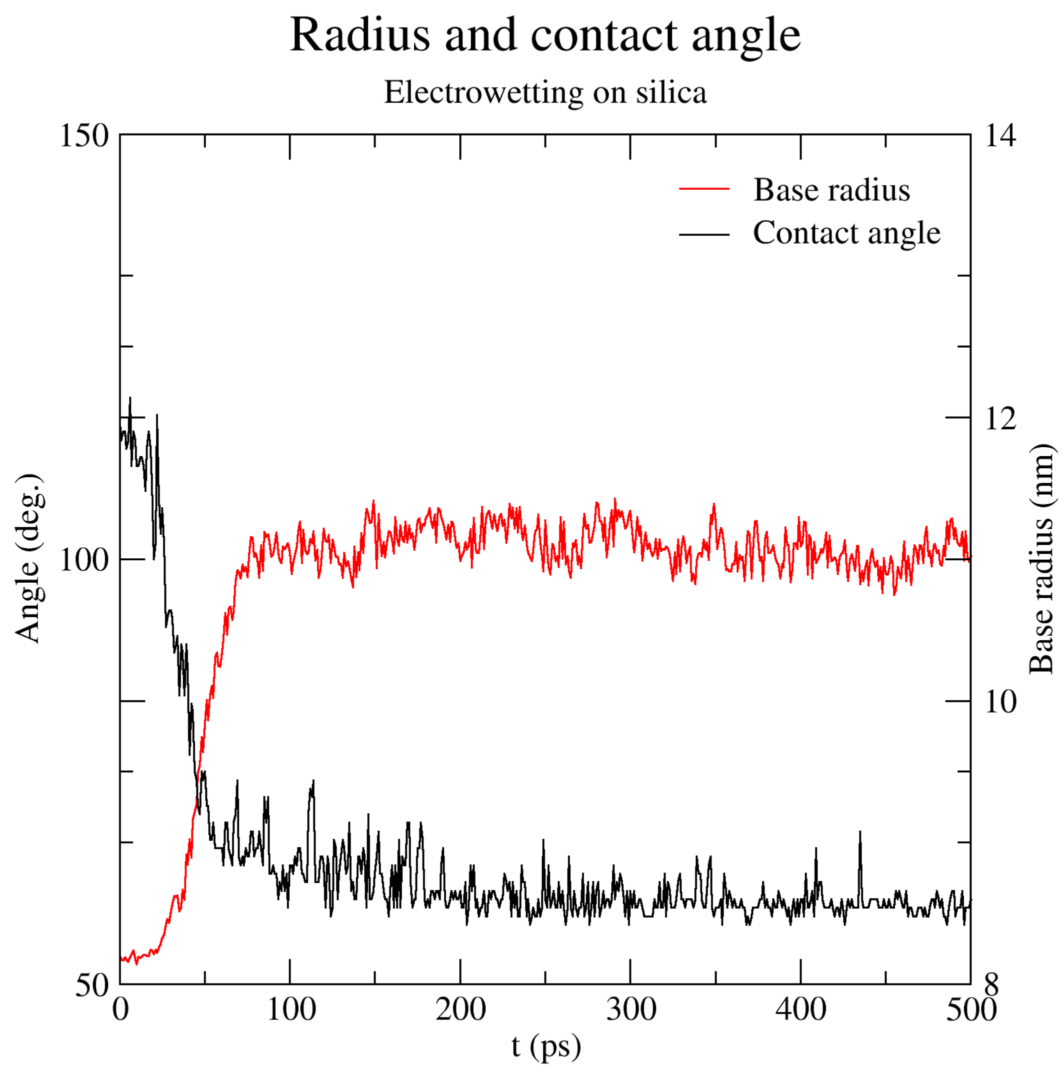
THANK YOU FOR LISTENING!



Pure water



KCl solution



Radius and contact angle
Electrowetting on silica
Base radius
Contact angle
150
100
50
14
12
10
8
0
100
200
300
400
500
Angle (deg.)
Base radius (nm)
t (ps)