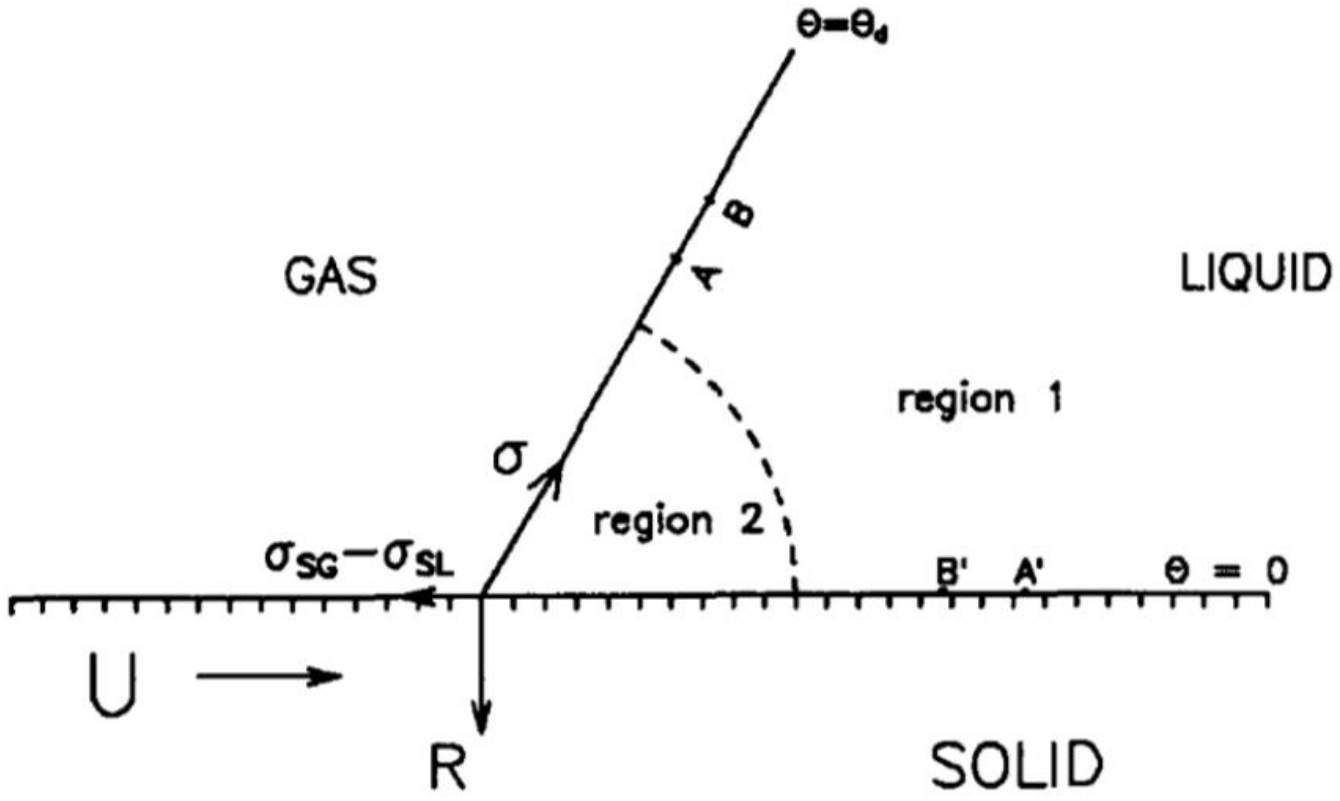
Moving Contact Line

Report, Apr. 2020

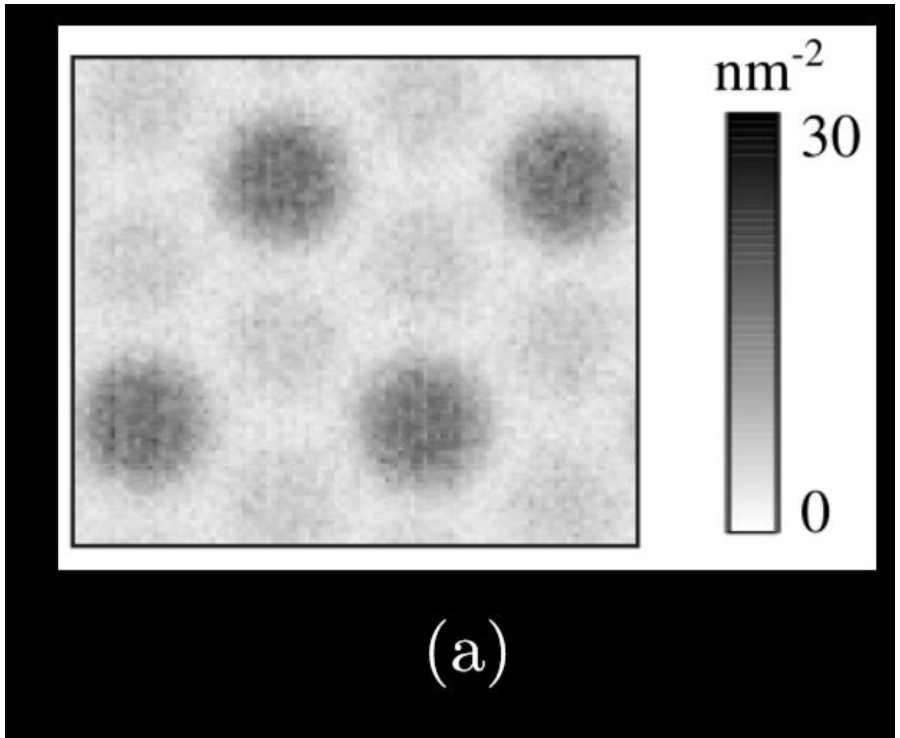
Recap: the singularity

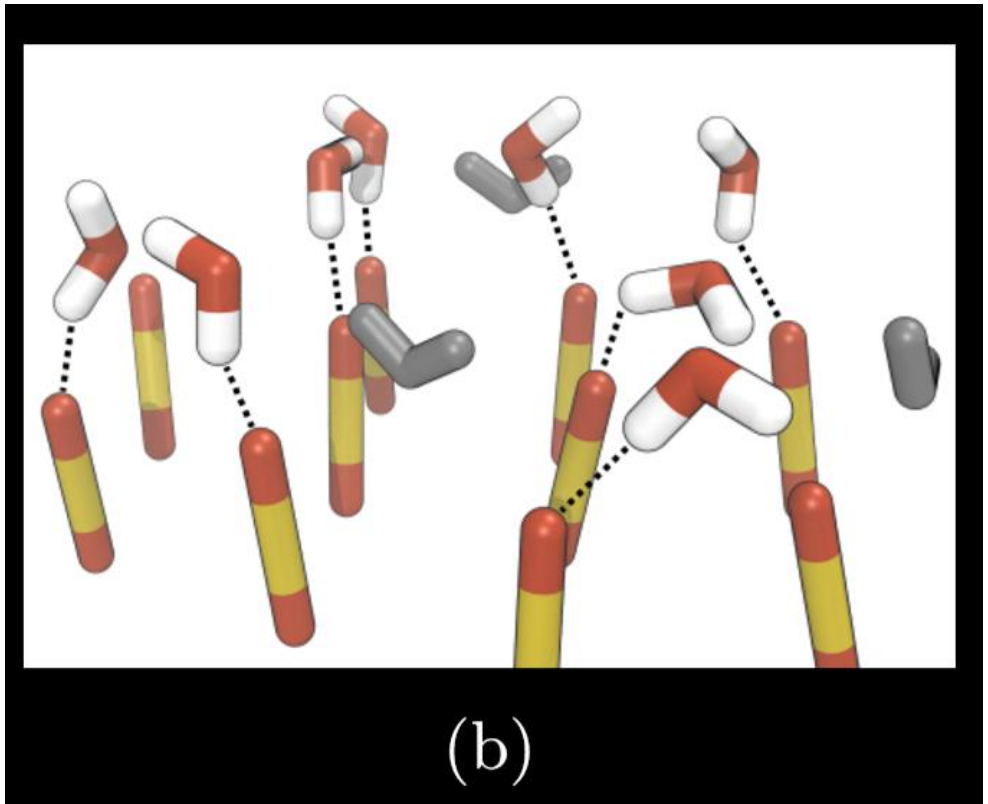
- No-slip



The nature of no-slip

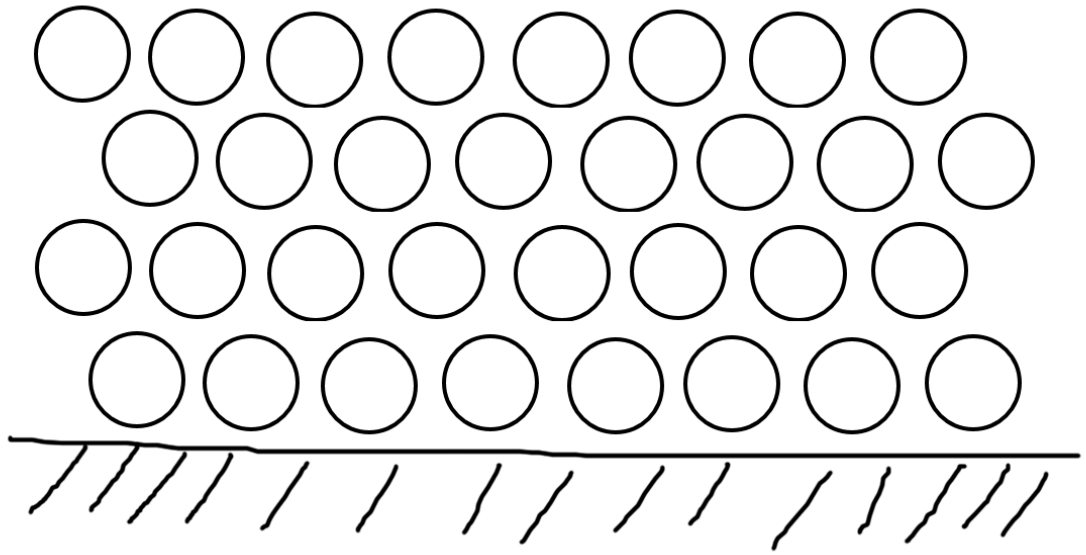
- Hydrophilic surface + water = no-slip
- A 2015 study has shown that the no-slip condition in dynamic wetting is a consequence of liquid molecules forming hydrogen bonds with substrate molecules





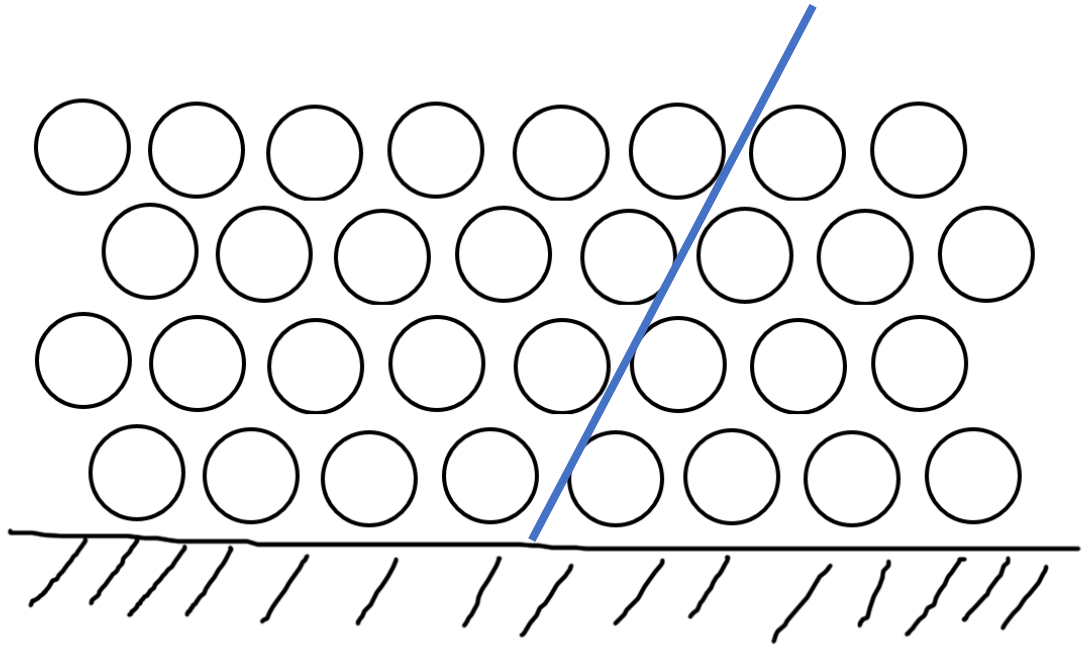
Strong vs weak friction

- No-slip is a good assumption because…

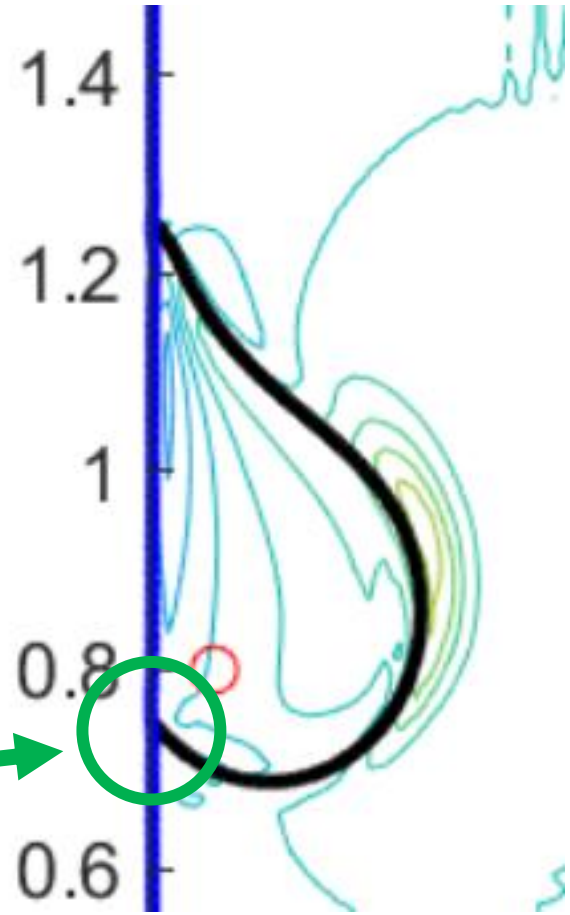


Strong vs weak friction

- However, when there is moving contact line…



- Hydrogen bonds CAN break. And it takes energy.



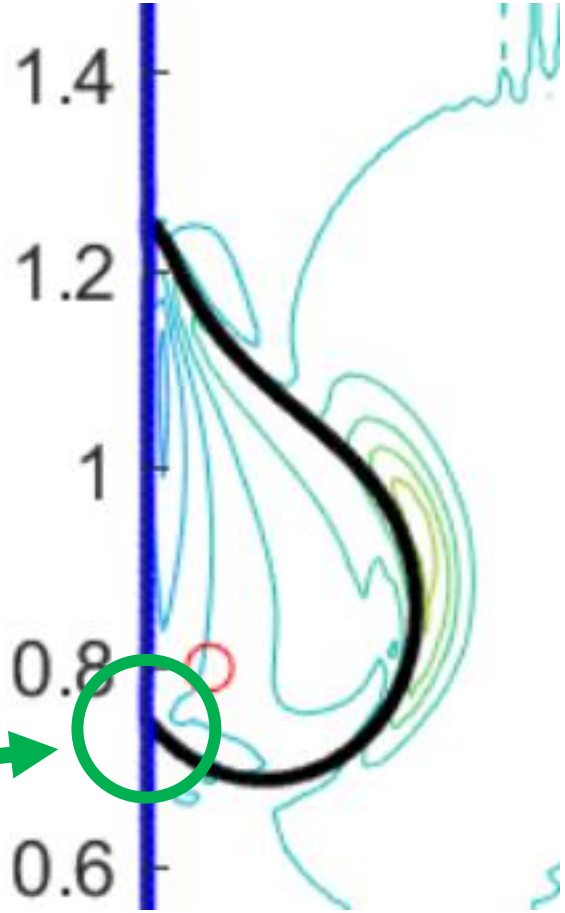
Local area that allows slip

Guanhua suggestion

No-slip

Slip. Apply friction

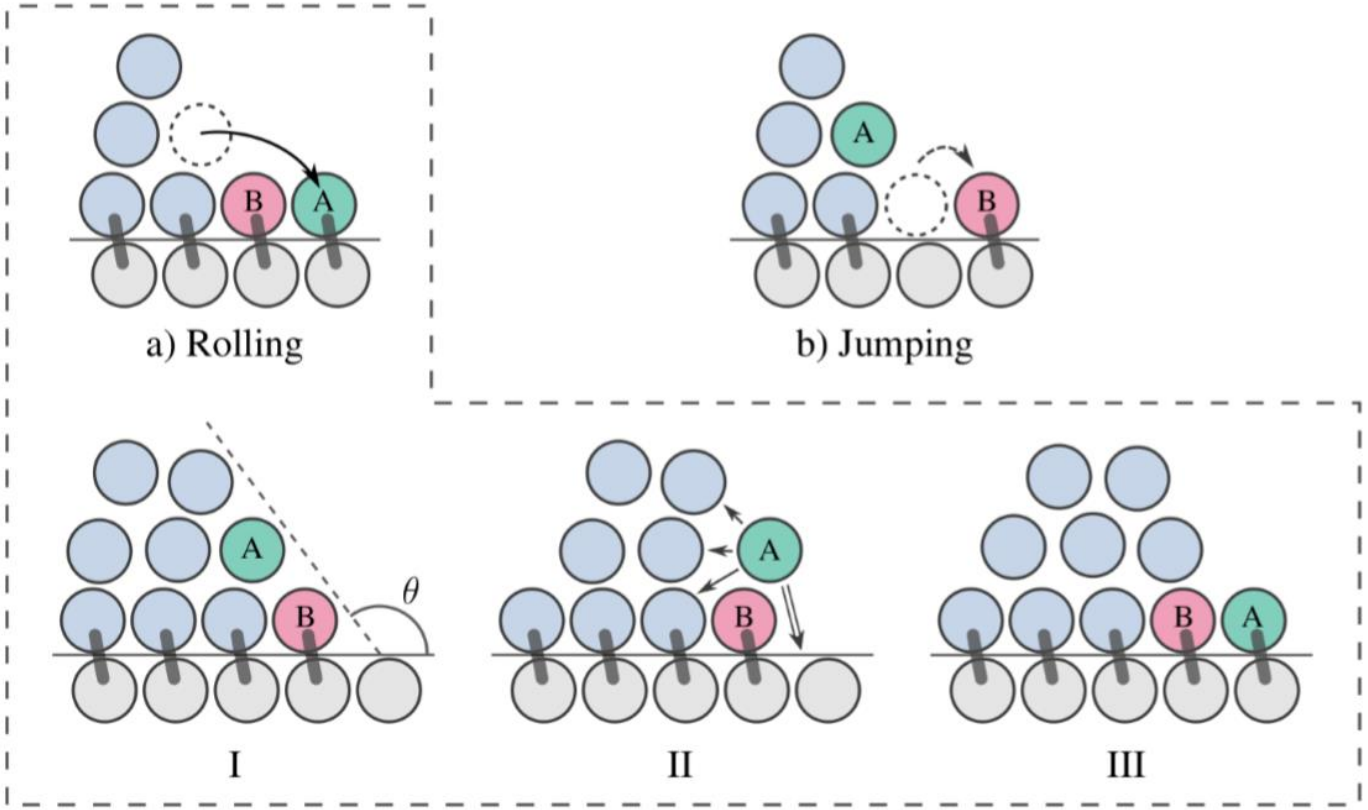
- Hydrogen bonds CAN break. And it takes energy.
- Now we just need a model for friction.



Local area that allows slip

Petter Johansson and Berk Hess's 2018 Study

- Molecular simulation involving 1.2 million water molecules.
  Time step = 1ps



Their conclusion

- Friction depends on contact angle

t (ns)	r (nm)	v (m/s)	θ	μ_f (μ)	f_{MKT}
2.5	50	14	95°	4.4 ± 0.5	0.19 ± 0.01
8.0	80	3.0	64°	9 ± 1	0.49 ± 0.01
12.5	90	1.7	55°	12 ± 2	0.49 ± 0.01

Three models

More Assumptions

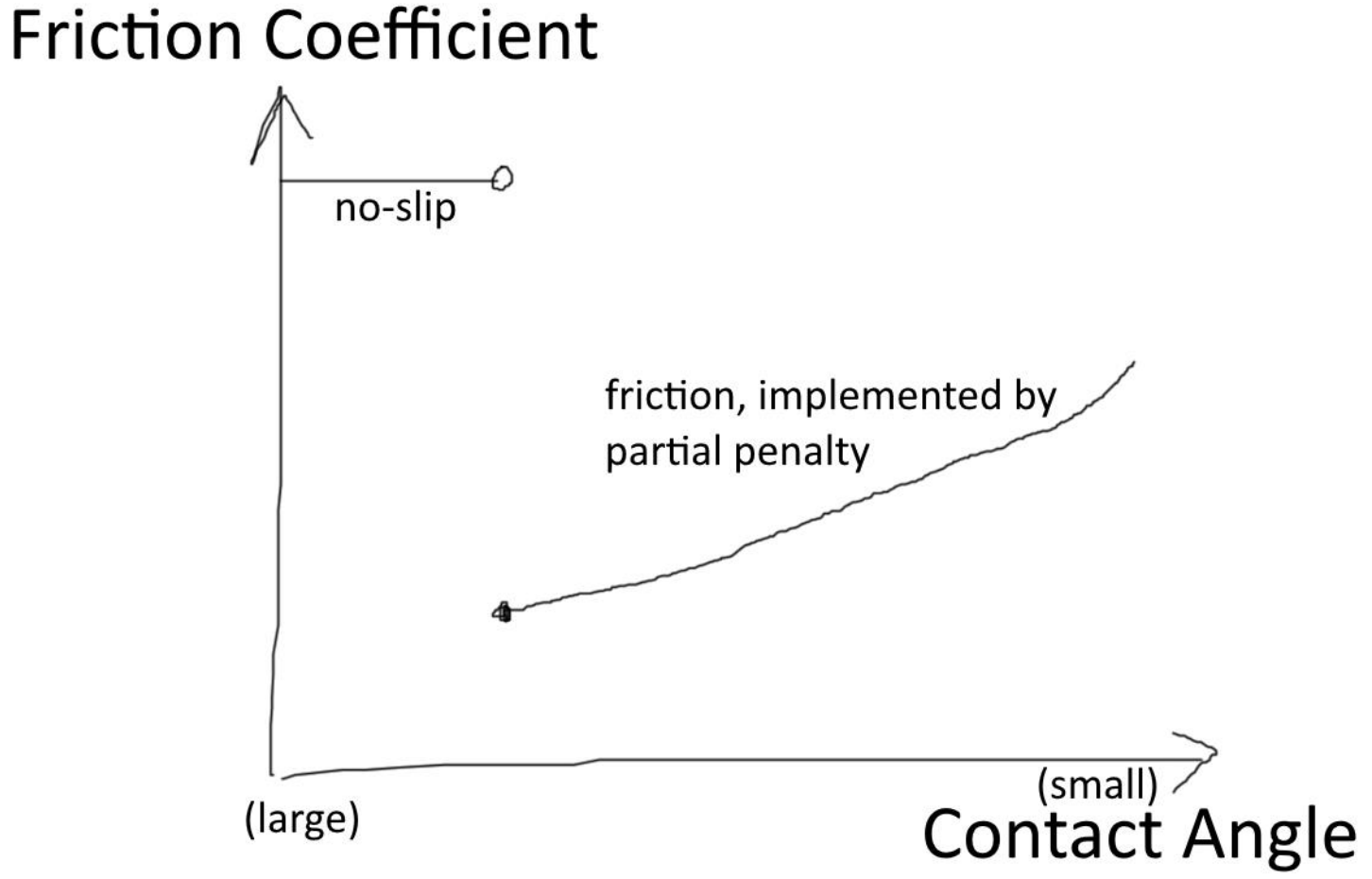
More Assumptions

Microscopic	**Macroscopic**	**Numerical**
Johansson's molecular model	Naiver-stokes with added friction	Penalty IBM with dynamic boundary properties

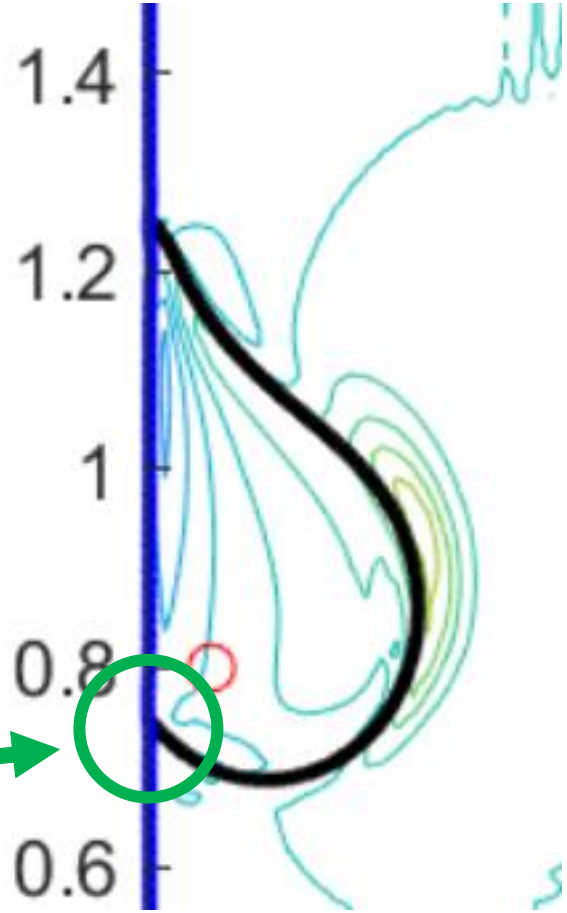
Naiver-stokes with added friction

The Navier boundary condition:

$$\beta u_s = \hat{\mathbf{t}} \cdot \tau \cdot \hat{\mathbf{n}}$$

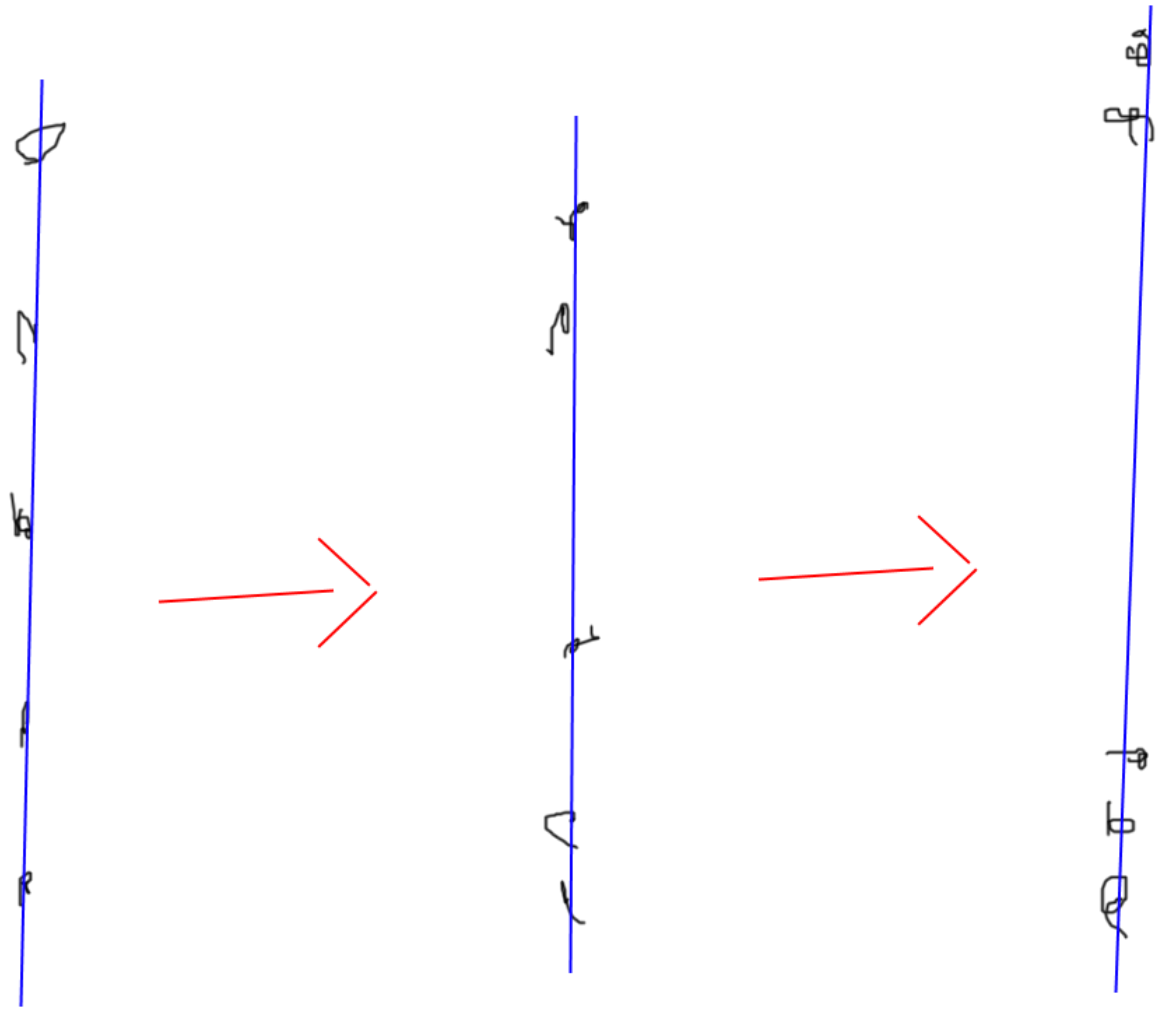


Penalty IBM with dynamic boundary properties

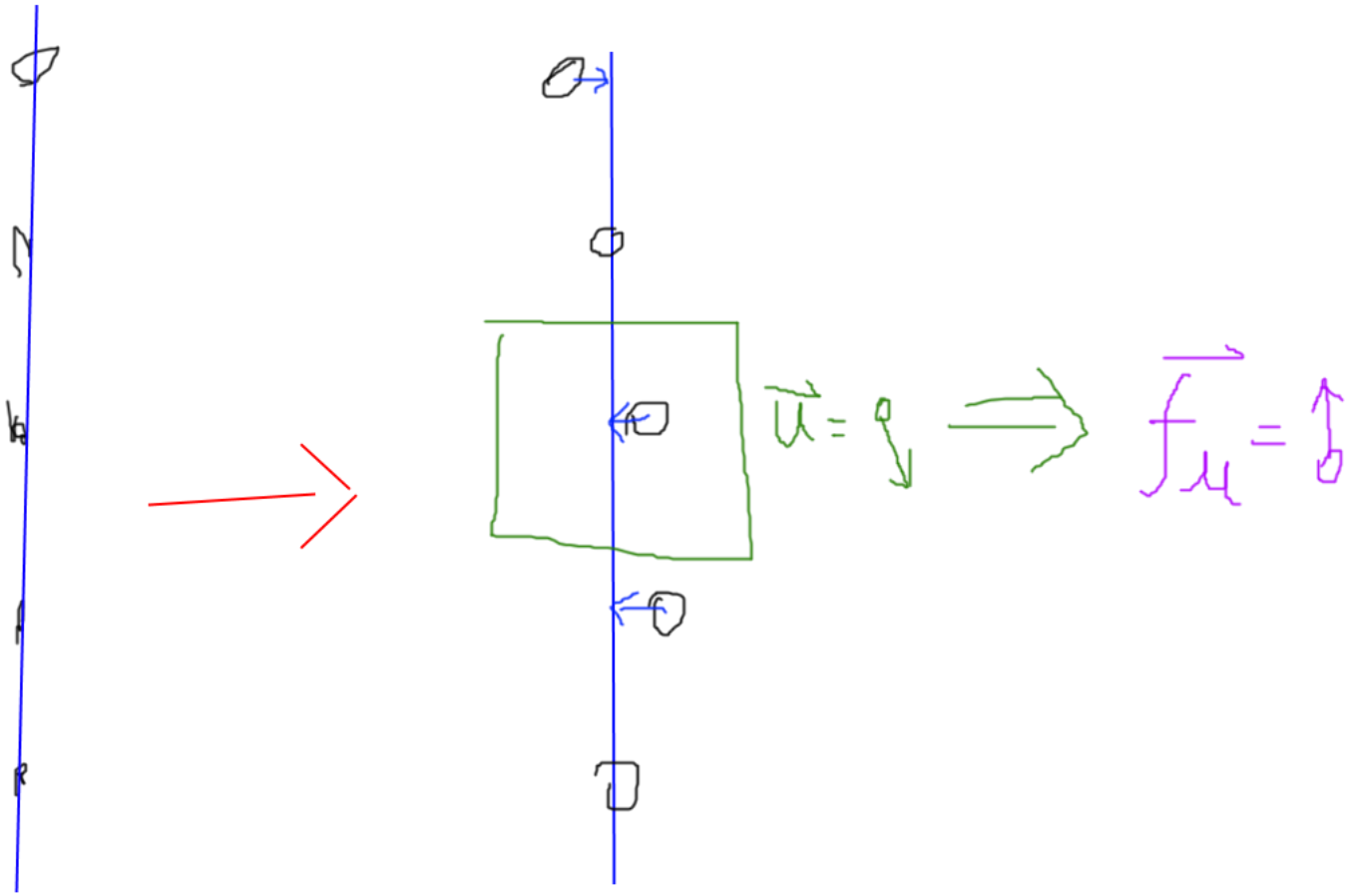


Local area that allows slip

Problem with naïve penalty



Solution



References

- Petter Johansson and Berk Hess, “Molecular Origin of Contact Line Friction in Dynamic Wetting”
- P.Johansson, A.Carlson, andB.Hess,“Water–substrate physico-chemistry in wetting dynamics,” J. Fluid Mech. 781, 695–711 (2015).
- Y. D. SHIKHMURZAEV , THE MOVING CONTACT LINE ON A SMOOTH SOLID SURFACE.

Penalty can handle solid – fluid

- The Guanhua paper simulates a piece of stone in fluid flow

Use penalty to simulate water – air?