“P.S. I Love You”

(Producing Science of Primarily Soft Stuff via Particle Simulations Plus Statistics Plus Supercomputing, from the Pico Scale to the Pedestrian Scale)

Gerald J. Wang

”2020” Howes Scholar Talk

July 19, 2021

M⁵ LAB

Carnegie Mellon University

Civil & Environmental Engineering

There is a simple animating principle behind particle-based simulations… (“it’s classic!”)

$$m\frac{d^2\vec{r}}{dt^2} = \vec{F}$$

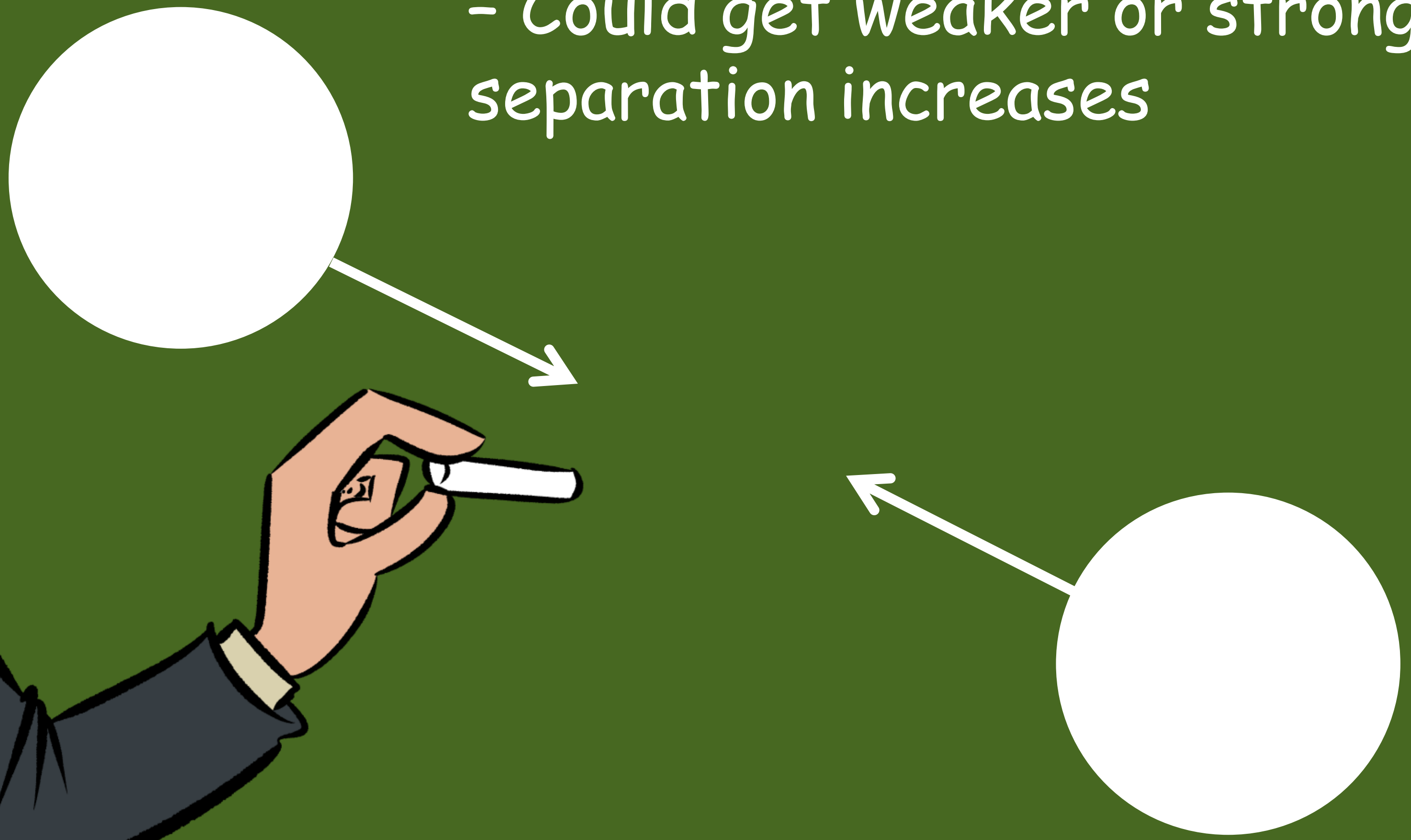
“As long as you tell me the inter-particle forces,
I’ll tell you the particle trajectories.”

(And there are a lot of places
where you might get these forces from!)

A Few Types of Forces between Particles

(1) CENTRAL FORCES:

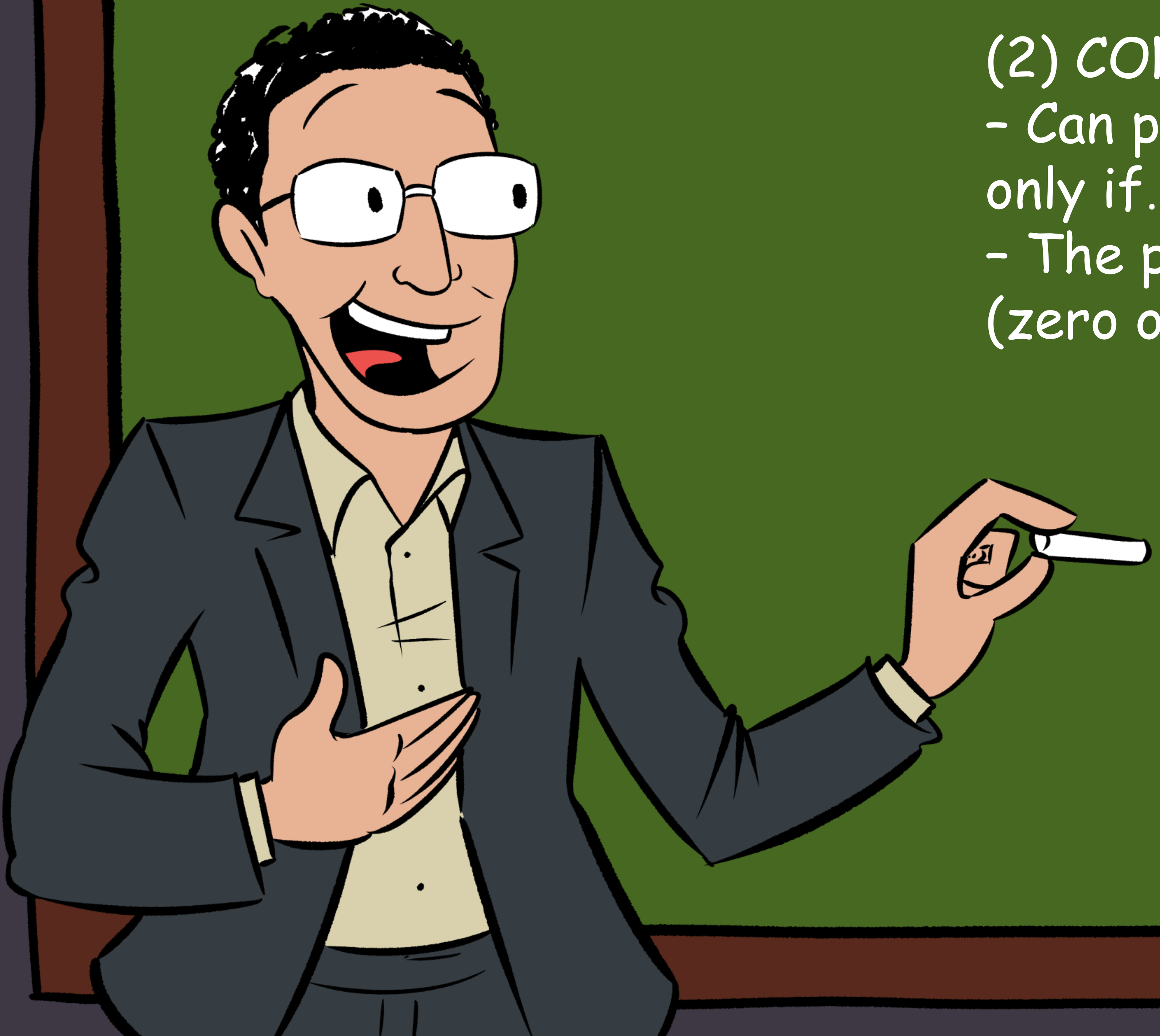
- Act along the particles' line-of-center
- Could get weaker or stronger as separation increases

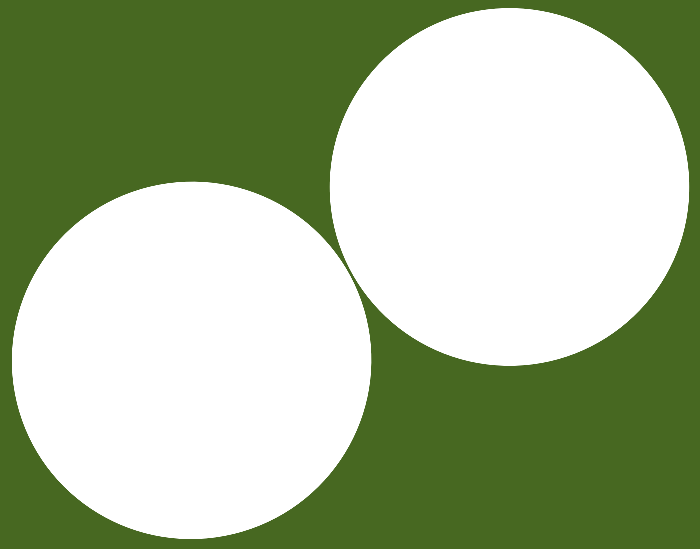


A Few Types of Forces between Particles

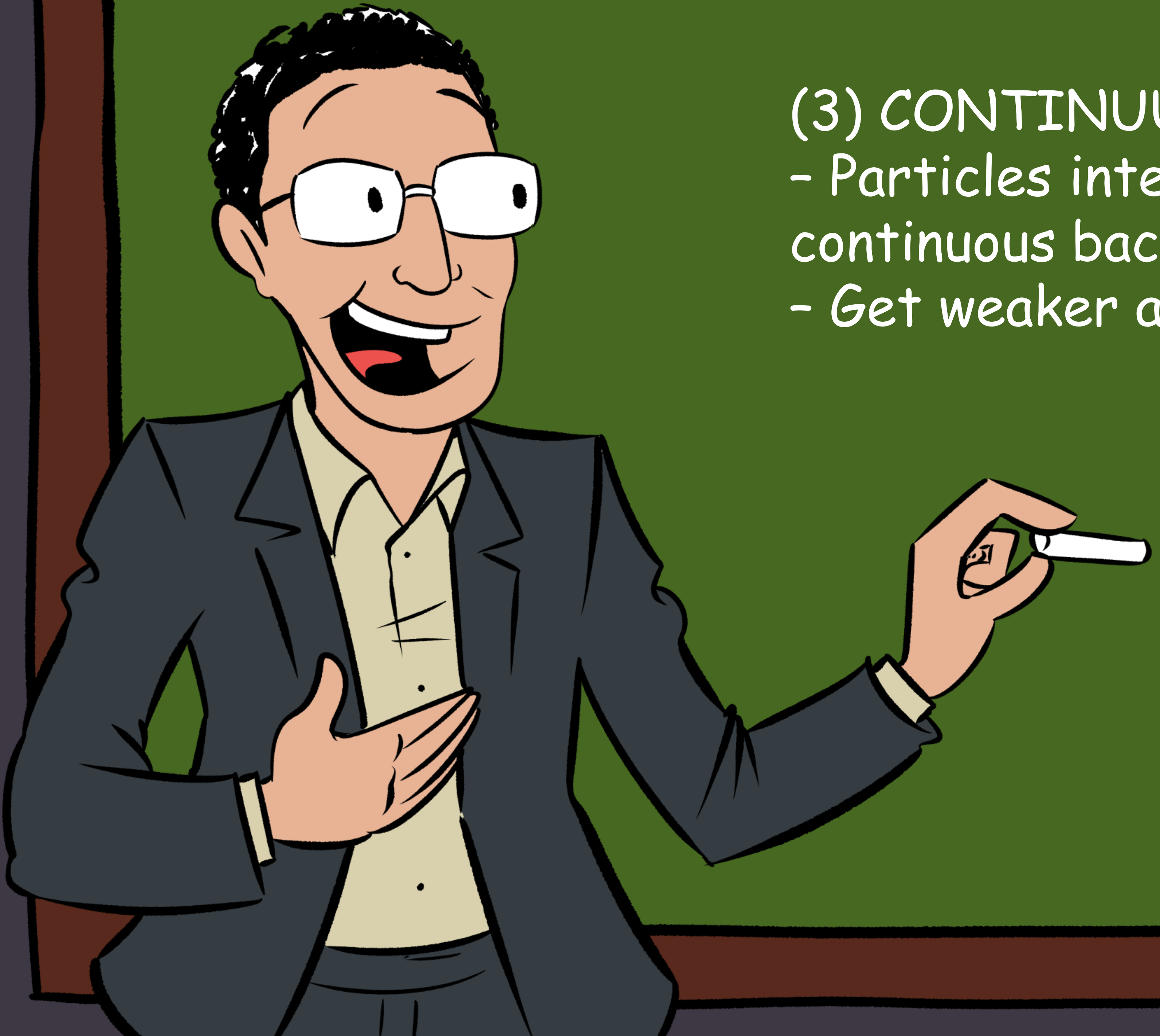
(2) CONTACT FORCES:

- Can push in many possible directions, but only if…
- The particles are touching (zero otherwise)





A Few Types of Forces between Particles



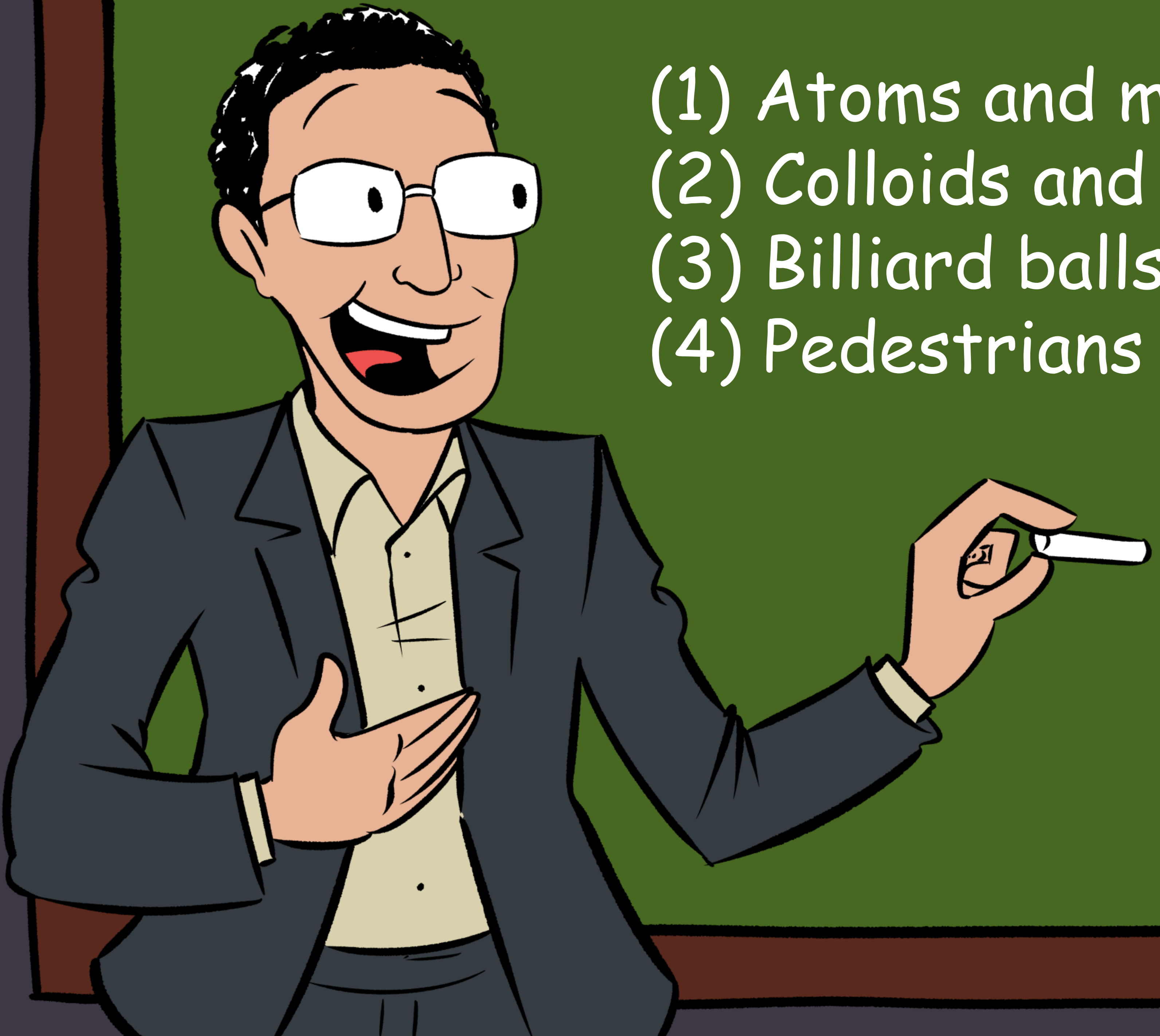
(3) CONTINUUM-MEDIATED FORCES:

- Particles interact indirectly through a continuous background medium
- Get weaker as separation increases

Video demo!


trending
NOW
Kids will be Kids
#GOATSONATRAMPOLINE #CANADA #BRITISHCOLOMBIA
40 85°
4
Pause (k)
CBS Miami
SUBSCRIBE

Particle Simulations at Every Length Scale



(1) Atoms and molecules
(2) Colloids and polymers
(3) Billiard balls
(4) Pedestrians

Particle Simulations at Every Length Scale

(1) Atoms and molecules
(2) Colloids and polymers
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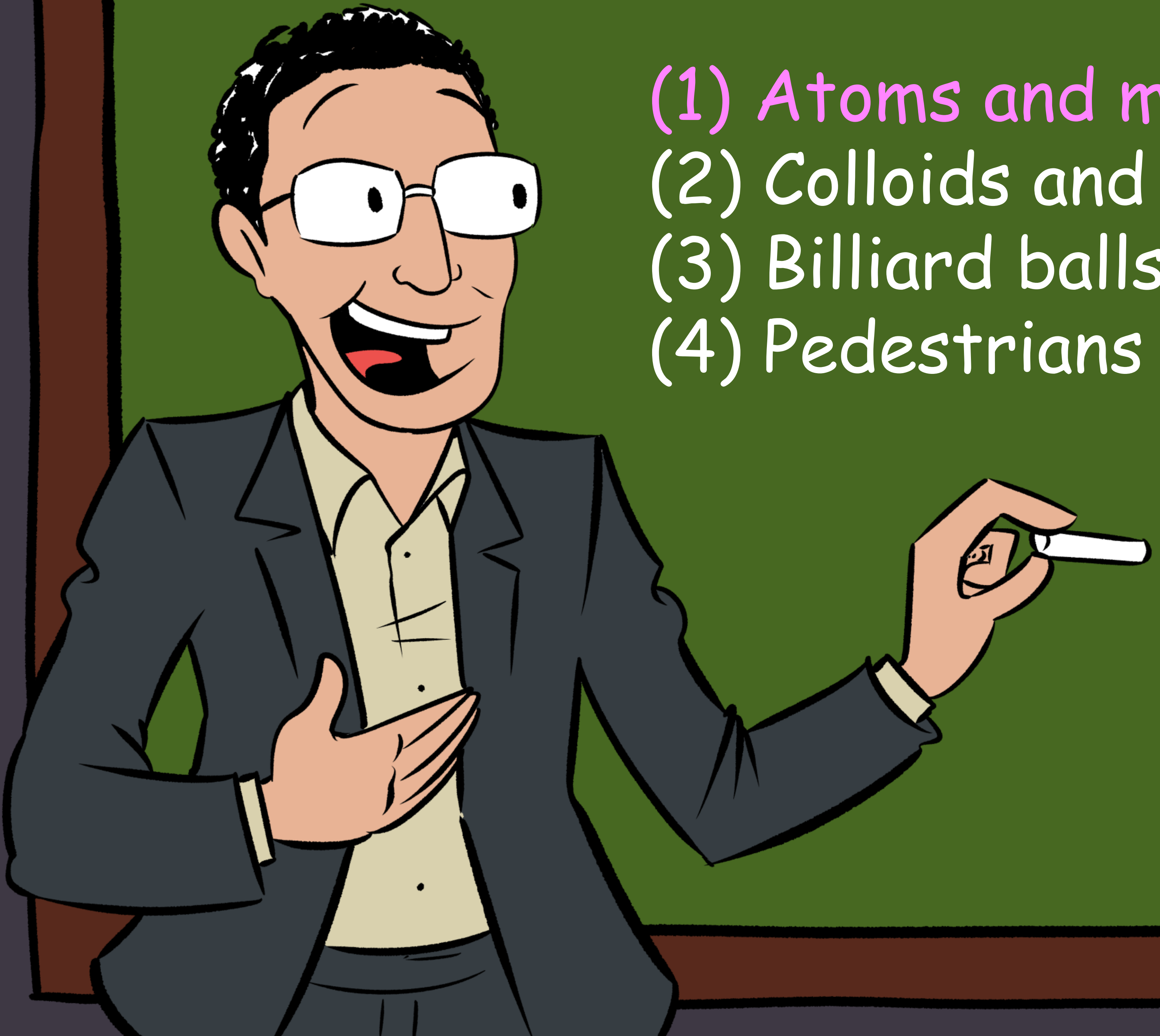
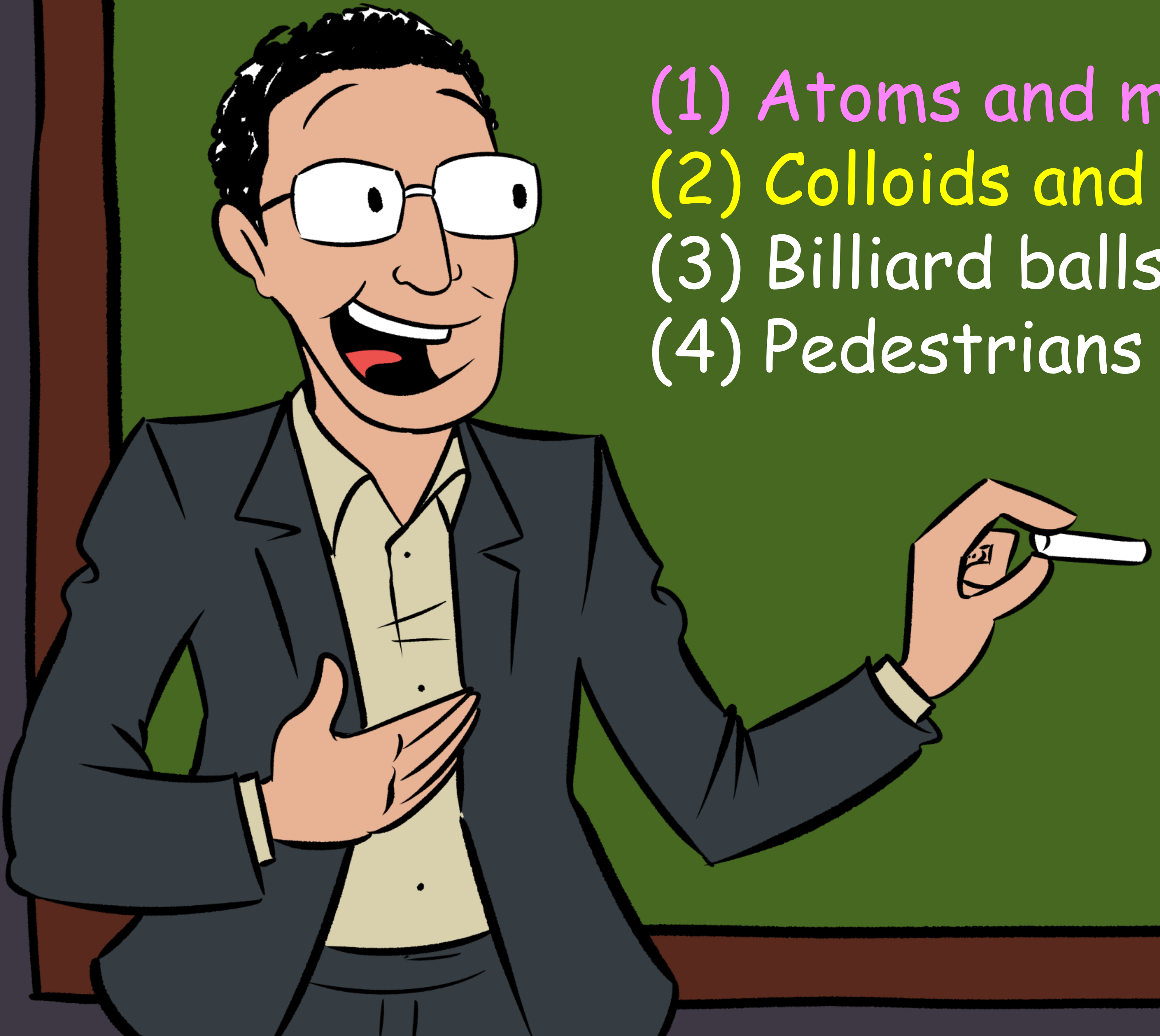


✓ Forces are... CENTRAL
✓ Origins include...
QUANTUM MECHANICS
and E&M

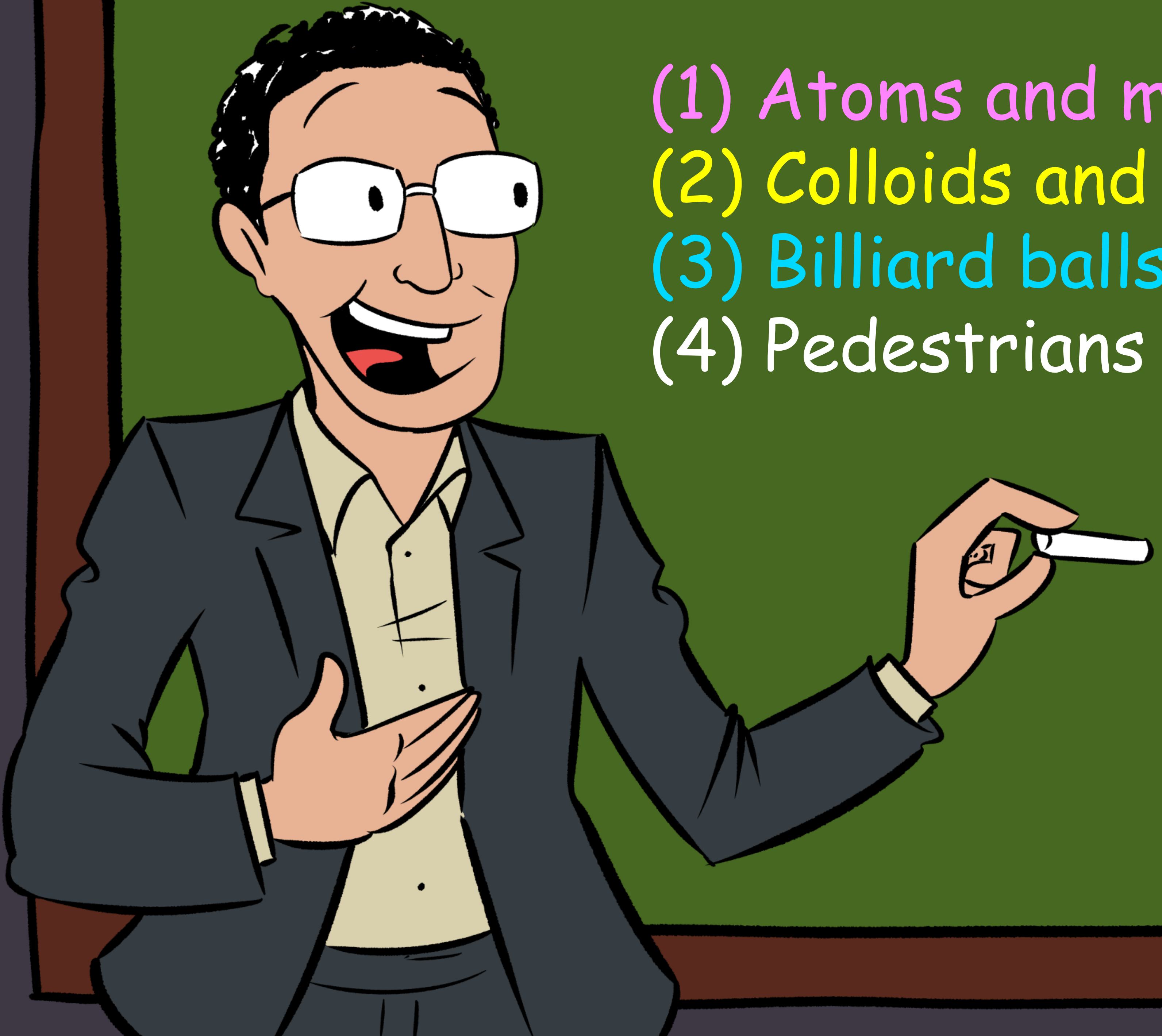
Particle Simulations at Every Length Scale



(1) Atoms and molecules
(2) Colloids and polymers
(3) Billiard balls
(4) Pedestrians

- ✓ Forces are... CENTRAL and CONTINUUM-MEDIATED
- ✓ Origins include... E&M, THERMODYNAMICS, and HYDRODYNAMICS

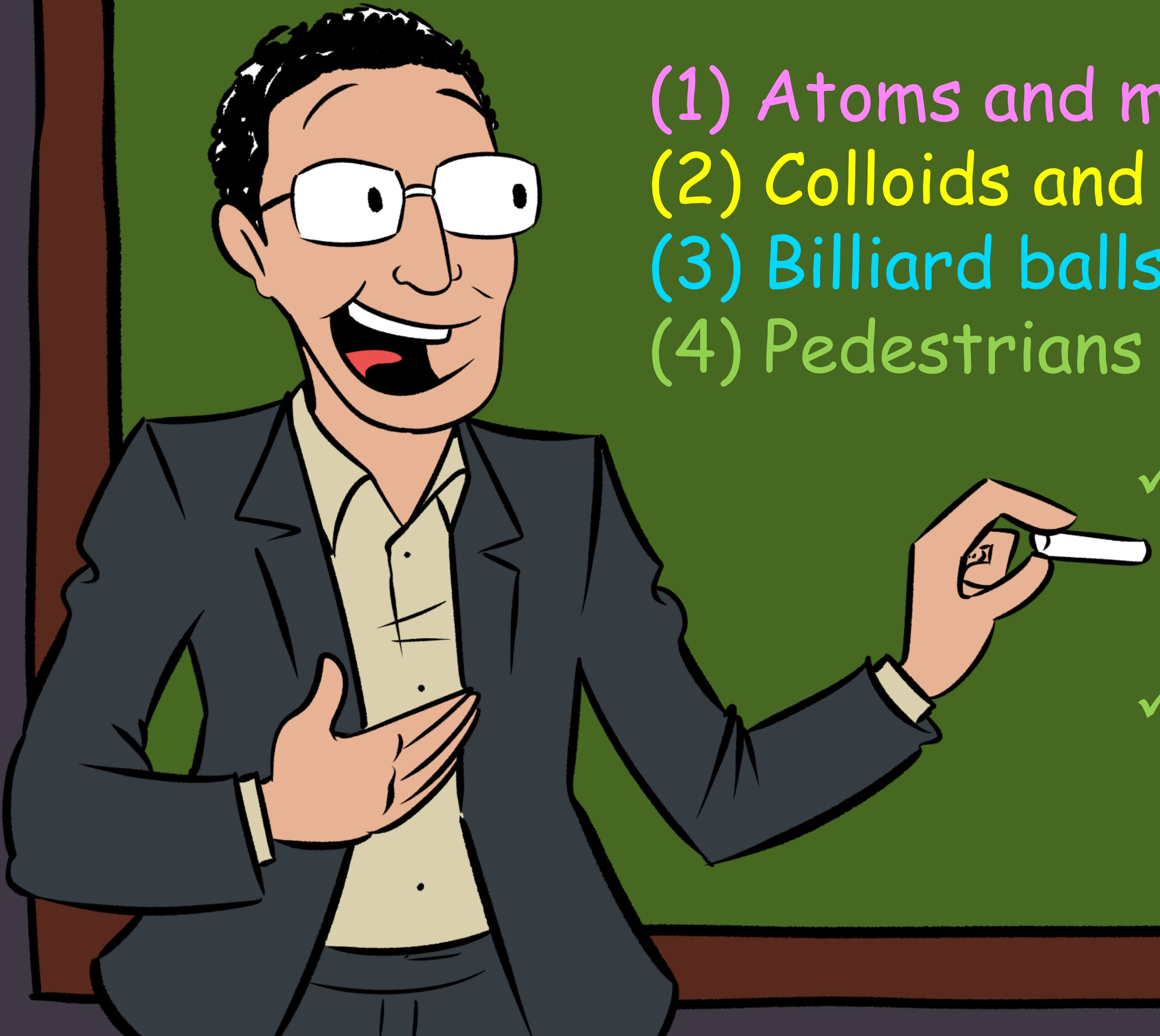
Particle Simulations at Every Length Scale



(1) Atoms and molecules
(2) Colloids and polymers
(3) Billiard balls
(4) Pedestrians

✓ Forces are… CONTACT
✓ Origins include… ELASTICITY and FRICTION

Particle Simulations at Every Length Scale

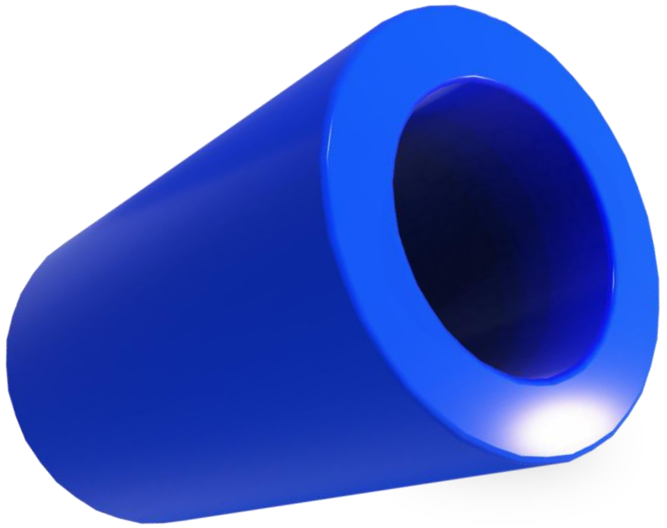


(1) Atoms and molecules
(2) Colloids and polymers
(3) Billiard balls
(4) Pedestrians

- ✓ Forces are... CONTACT and CENTRAL (and INTERNALLY SUPPLIED!)
- ✓ Origins include...
  FRICTION and
  PSYCHOLOGY and CAKE

“P.S. Something old, something new, something borrowed, something blue.”

At the nanoscale, fluid slip is a big deal…

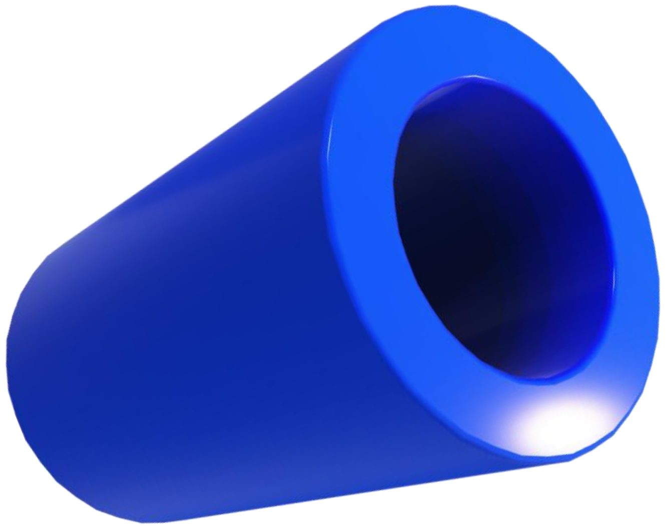


Pipe Flow

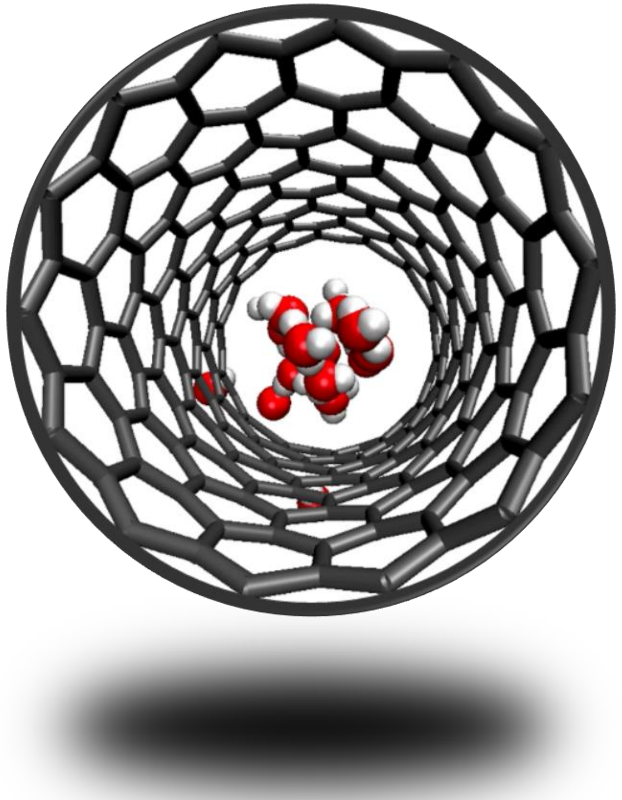
$Q \sim R^4$ (Hagen-Poiseuille, no slip)

$Q_{\text{slip}} \sim l_{\text{slip}} R^3$ (additional flow due to slip)

At the nanoscale, fluid slip is a big deal...



Pipe Flow



$$Q \sim R^4$$ (Hagen-Poiseuille, no slip)

$$Q_{\text{slip}} \sim l_{\text{slip}} R^3$$ (additional flow due to slip)

$$\frac{l_{\text{slip}}}{R} \sim 1$$ (exciting and **non-negligible** slip phenomena appear)

NANOSCALE HYDRODYNAMICS

Enhanced flow in carbon nanotubes

Mainak Majumder*, Nitin Chopra*,
Rodney Andrews†, Bruce J. Hinds*
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LETTER

doi:10.1038/nature19315

Massive radius-dependent flow slippage in carbon nanotubes

Eleonora Secchi[1], Sophie Marbach[1], Antoine Niguès[1], Derek Stein[1,2], Alessandro Siria[1] & Lydéric Bocquet[1]

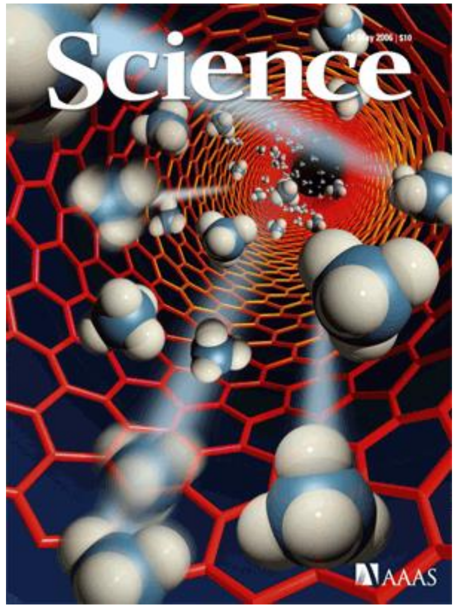
Fast Mass Transport Through Sub-2-Nanometer Carbon Nanotubes

Jason K. Holt[1,*], Hyung Gyu Park[1,2,*], Yinmin Wang[1], Michael Stadermann[1], Alexander B. Artyukhin[1], Costas P. Grigoropoulos[2], Aleksandr Noy[1], Olgica Bakajin[1,†]

[1] Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA.
[2] Department of Mechanical Engineering, University of California, Berkeley, CA 94720, USA.
† To whom correspondence should be addressed. E-mail: bakajin1@llnl.gov

* These authors contributed equally to this work.
– Hide authors and affiliations

Science 19 May 2006:
Vol. 312, Issue 5776, pp. 1034-1037
DOI: 10.1126/science.1126298

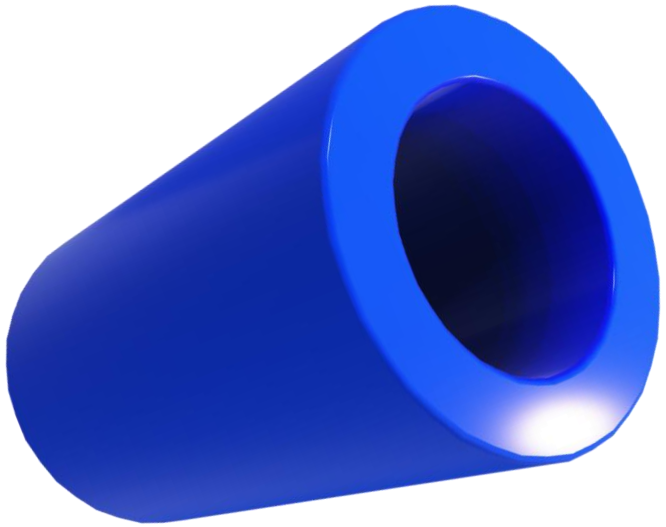


Fluid flow in carbon nanotubes and nanopipes

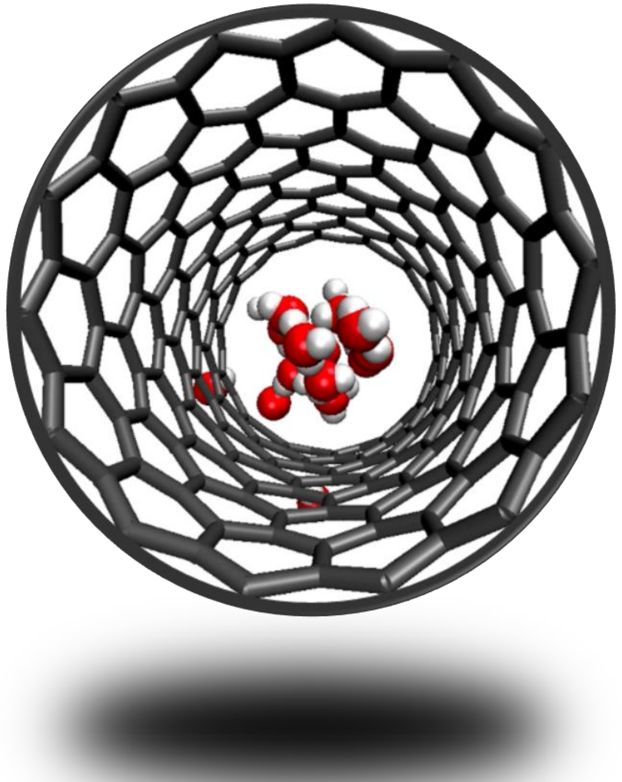
M. Whitby & N. Quirke

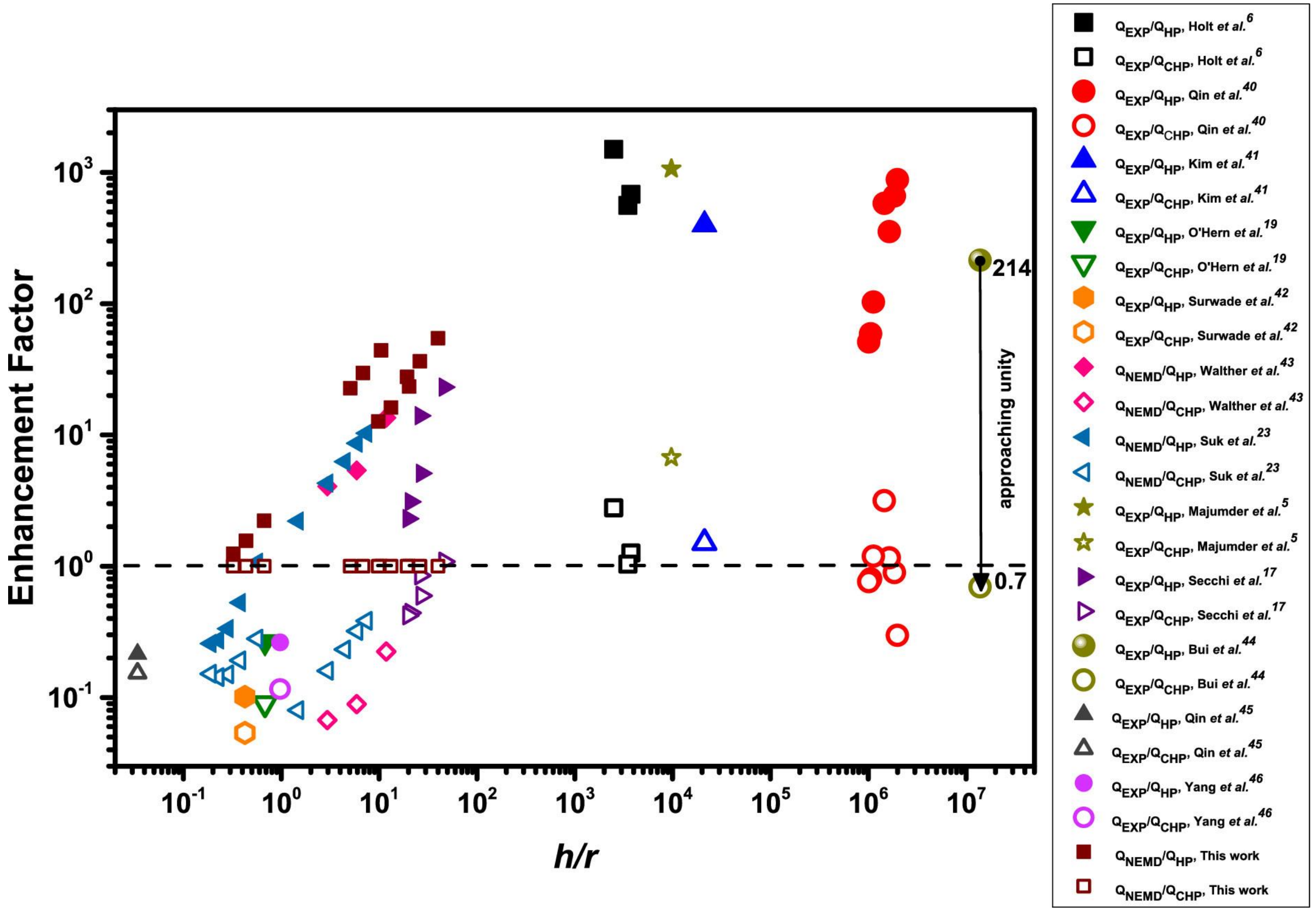
Nature Nanotechnology 2, 87–94(2007) | Cite this article

At the nanoscale, fluid slip is a big deal…



Pipe Flow





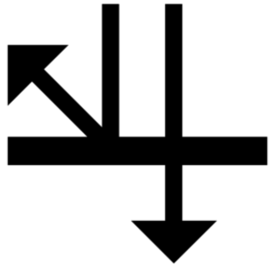
[Heiranian and Aluru,
ACS Nano 2020, 14, 1, 272–281]

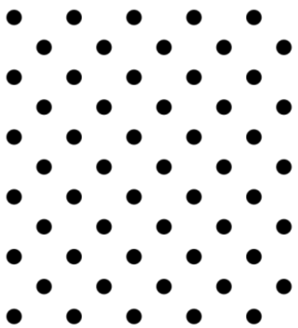
$Q \sim R^4$ (Hagen-Poiseuille, no slip)

$Q_{\text{slip}} \sim l_{\text{slip}} R^3$ (additional flow due to slip)

$\frac{l_{\text{slip}}}{R} \sim 1$ (exciting and **non-negligible** slip phenomena appear)

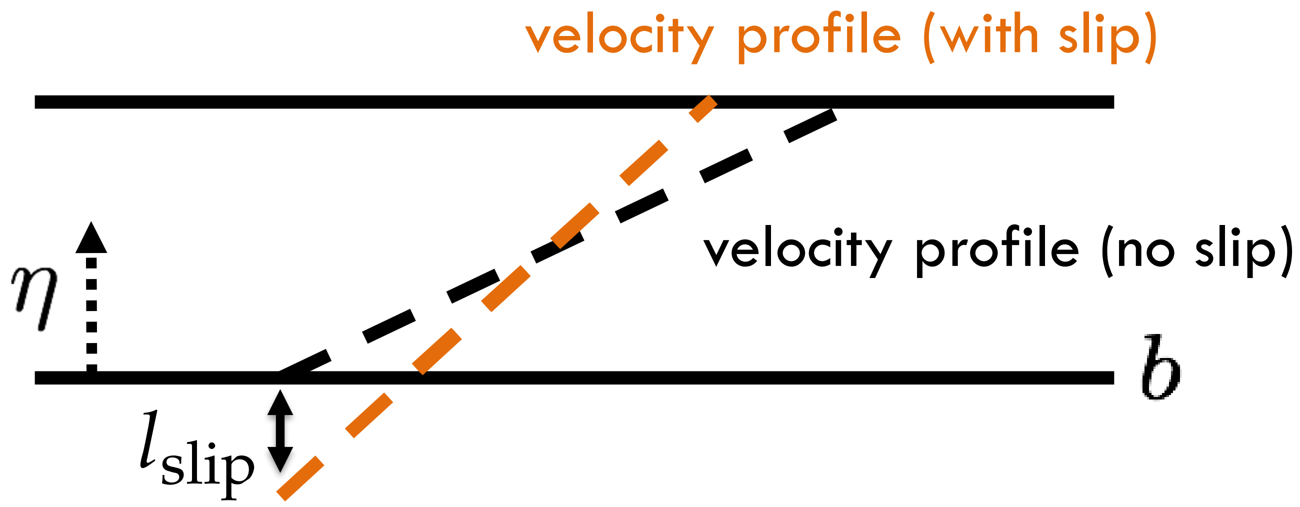
Applications galore ("something blue")…





”Business as usual” is the Navier slip condition…

- Assumption: Slip velocity is **linear** in the velocity gradient at the boundary.
- Slip length is the distance within the boundary at which the (extrapolated) velocity profile matches the boundary velocity.
- The Navier slip condition has been shown (rigorously) to hold **for dilute fluids**.
- **Key question: What is the appropriate slip condition for dense fluids?**



$$u_{\text{slip}} = l_{\text{slip}} \frac{\partial u}{\partial \eta}\bigg|_b$$

To model slip, Molecular-Kinetic Theory (MKT) is a jump in the right direction.

$$u_{\text{slip}} = \frac{2l_{\text{j}}}{\tau_{\text{j}}} \exp\left(-\frac{\alpha\varepsilon}{k_{\text{B}}T}\right) \sinh\left(\frac{l_{\text{j}}\mu}{2\sigma_{\text{FL}}k_{\text{B}}T}\dot{\gamma}\right)$$

Viscosity

Shear rate

Length scale for jumps

Time scale for jump attempts

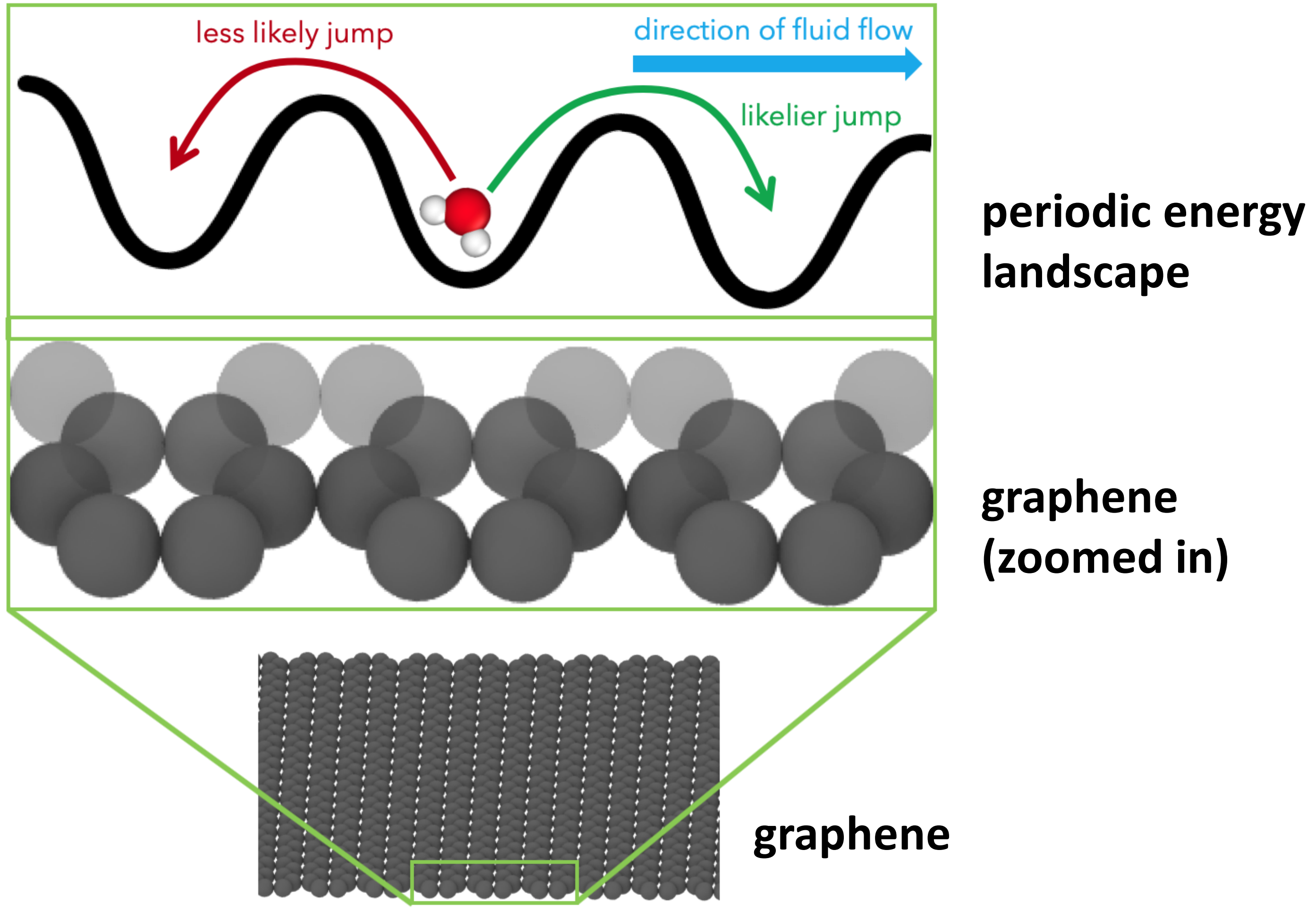
Fluid-solid interaction energy

Surface density of interfacial fluid layer

[Wang and Hadjiconstantinou, *Phys. Rev. Fluids* 2019, 4(6), 064201]

[Wang and Hadjiconstantinou, *Phys. Rev. Fluids* 2017, 2(9), 094201]

[Blake and Haynes, *J. Colloid Interface Sci.* 30 (1969)]



In the appropriate limit, MKT recovers the Navier slip condition:

$$u_{\text{slip}} = l_{\text{slip}}\dot{\gamma}$$

$$l_{\text{slip}} = \frac{l_{\text{j}}^2 e^{-\alpha\varepsilon/(k_{\text{B}}T)}\mu}{\tau_{\text{j}}\sigma_{\text{FL}}k_{\text{B}}T}$$

Slip length directly linked to microscopic parameters!

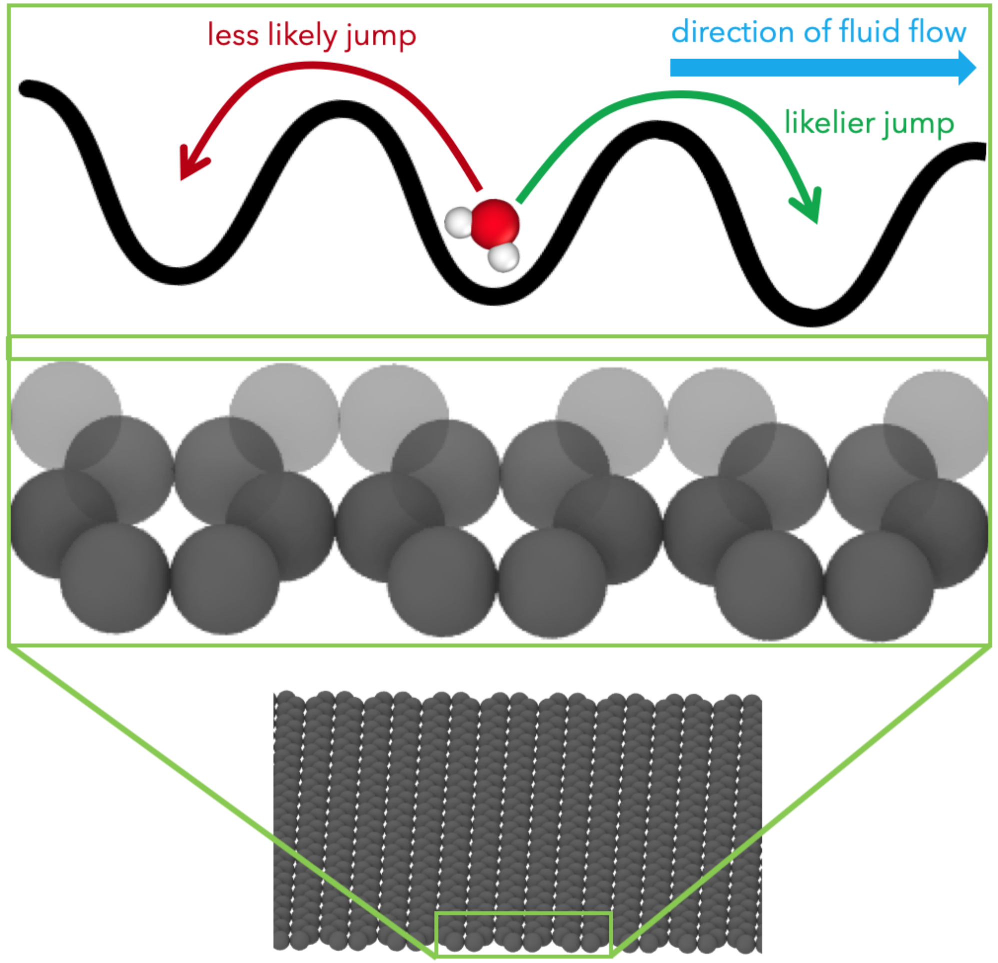
To model slip, Molecular-Kinetic Theory (MKT) is a jump in the right direction.

[Wang, under review]

[Wang and Hadjiconstantinou, *Phys. Rev. Fluids* 2019, 4(6), 064201]

[Wang and Hadjiconstantinou, *Phys. Rev. Fluids* 2017, 2(9), 094201]

$$u_{\text{slip}} = \frac{2l_{\text{j}}}{\tau_{\text{j}}} \exp\left(-\frac{\alpha\varepsilon}{k_{\text{B}}T}\right) \sinh\left(\frac{l_{\text{j}}\mu}{2\sigma_{\text{FL}}k_{\text{B}}T}\dot{\gamma}\right) \qquad l_{\text{slip}} = \frac{l_{\text{j}}^2 e^{-\alpha\varepsilon/(k_{\text{B}}T)}\mu}{\tau_{\text{j}}\sigma_{\text{FL}}k_{\text{B}}T}$$

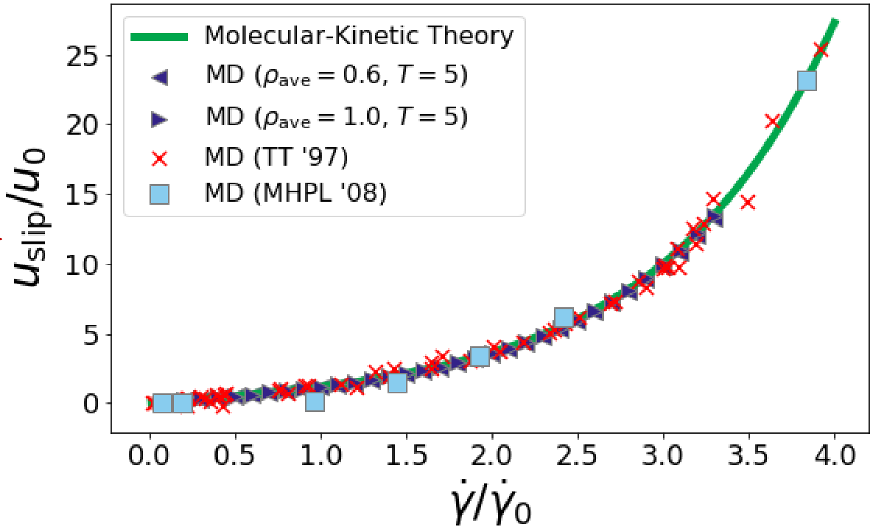


MKT has been validated against:

MD simulations (in house and from literature)

[Thompson and Troian, *Nature* 1997, 389]

[Martini, Hsu, Patankar, and Lichter, *Phys. Rev. Lett.* 2008, 100]



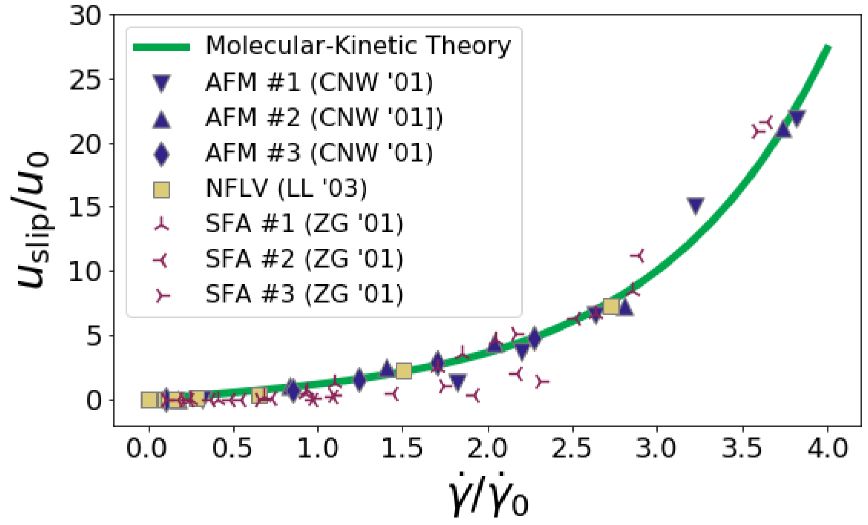
and

experiments

[Craig, Neto, and Williams, *Phys. Rev. Lett.* 2001, 87]

[Zhu and Granick, *Phys. Rev. Lett.* 2001, 87]

[Léger, *J. Phys.: Cond. Matt.* 2003, 15]



Governing equations for pedestrian dynamics

$$\vec{F} = m\frac{\vec{v}_{\text{desired}} - \vec{v}_{\text{instantaneous}}}{\tau} - \vec{\nabla}U + \vec{R}$$

The "selfish" term: Each pedestrian has a desired velocity and tries to stick to that velocity (proportional control).

The "social interaction" term: Pedestrians experience forces that depend on spatial configuration relative to other pedestrians.

The "random" term: Each pedestrian is given a *tiny* random (Gaussian) kick to reduce stalling events.

$$U = U_{\text{far}} + U_{\text{near}}$$

The "collision avoidance" term: Pedestrians try to avoid each other in general, with a characteristic "personal space" set by d_0. **This is the focus of our work.**

$$U_{\text{far}}(d) = Ke^{-d/d_0}$$

The "brushing shoulders" term: In the event two pedestrians are near contact, they experience a frictional force.

For more on social force models, see, e.g. →

[Helbing and Molnar, *Phys. Rev. E* 1995, 51(5), 4282–4286]
[Helbing, Farkas, and Vicsek, *Nature* 2000, 407, 487–490]
[Koyama *et al.*, *Artif. Life Robot.* 2020, 25, 529–536]

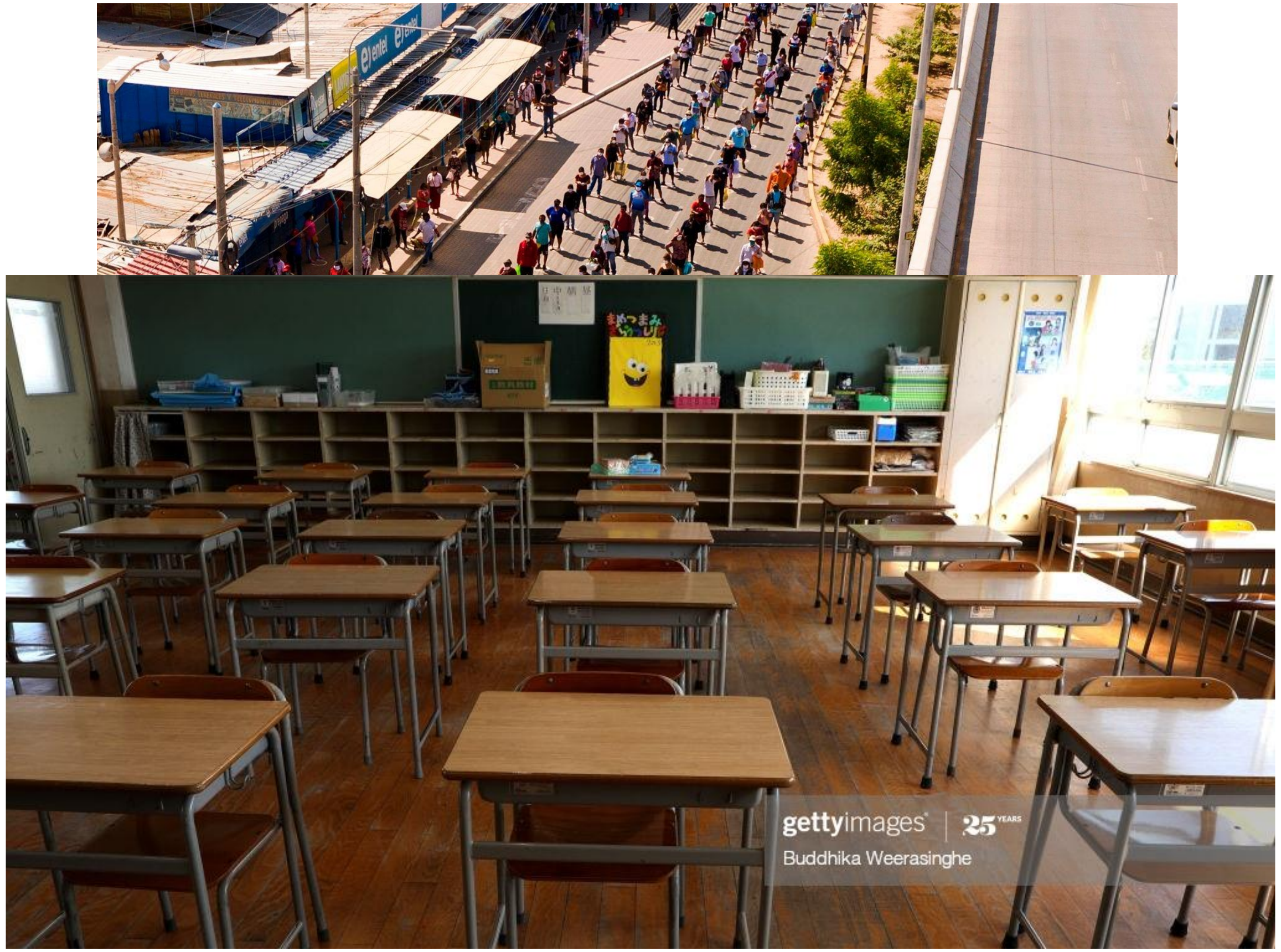
How does the need for increased social distancing affect pedestrian flows in confined environments?

$$\frac{d_0}{d_{\mathrm{walkway}}} \lesssim 1$$

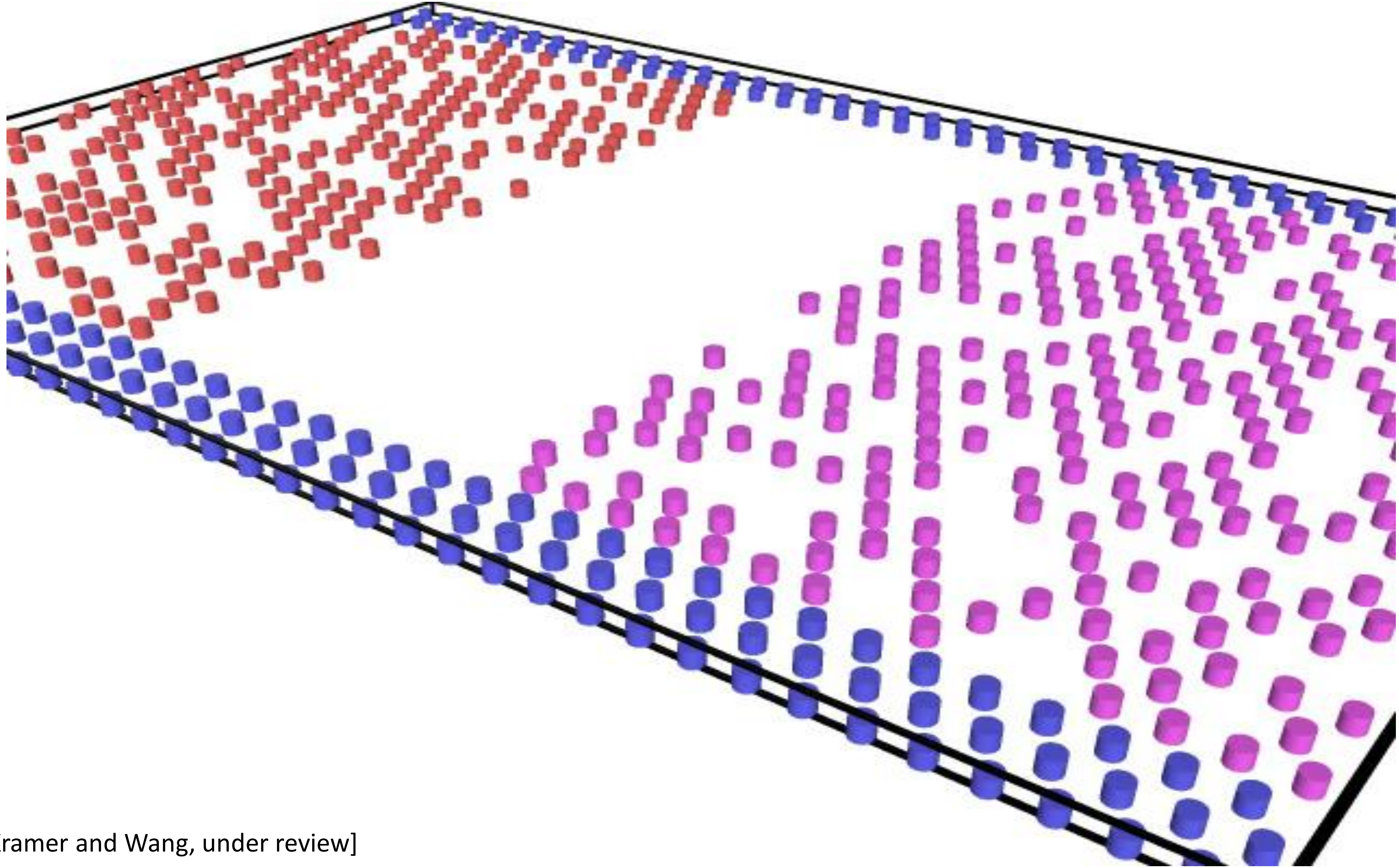
$$\downarrow$$

$$\frac{d_0}{d_{\mathrm{walkway}}} \sim 1$$

Pedestrians in Piura, Peru

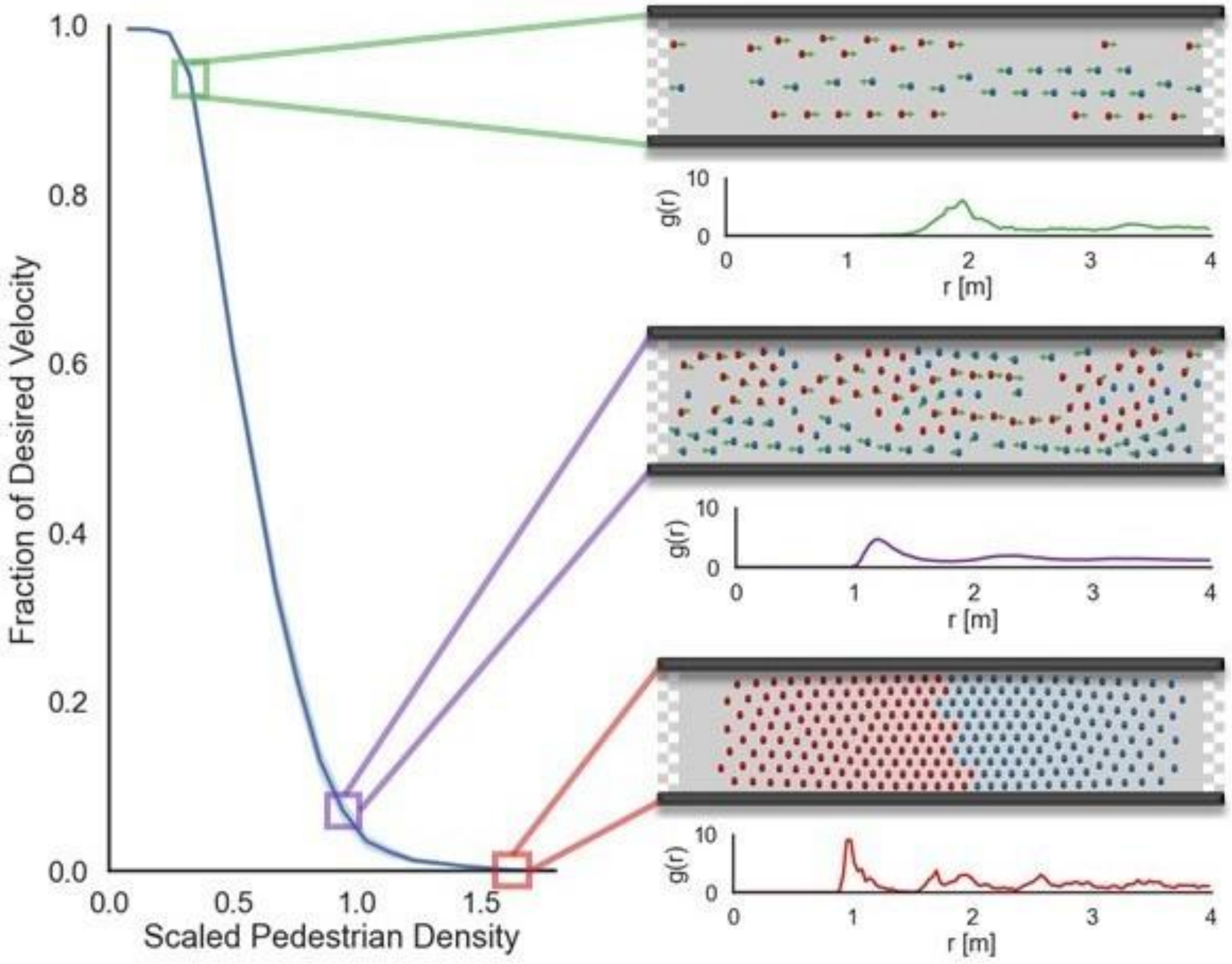


Himeji, Japan – April 06, 2020



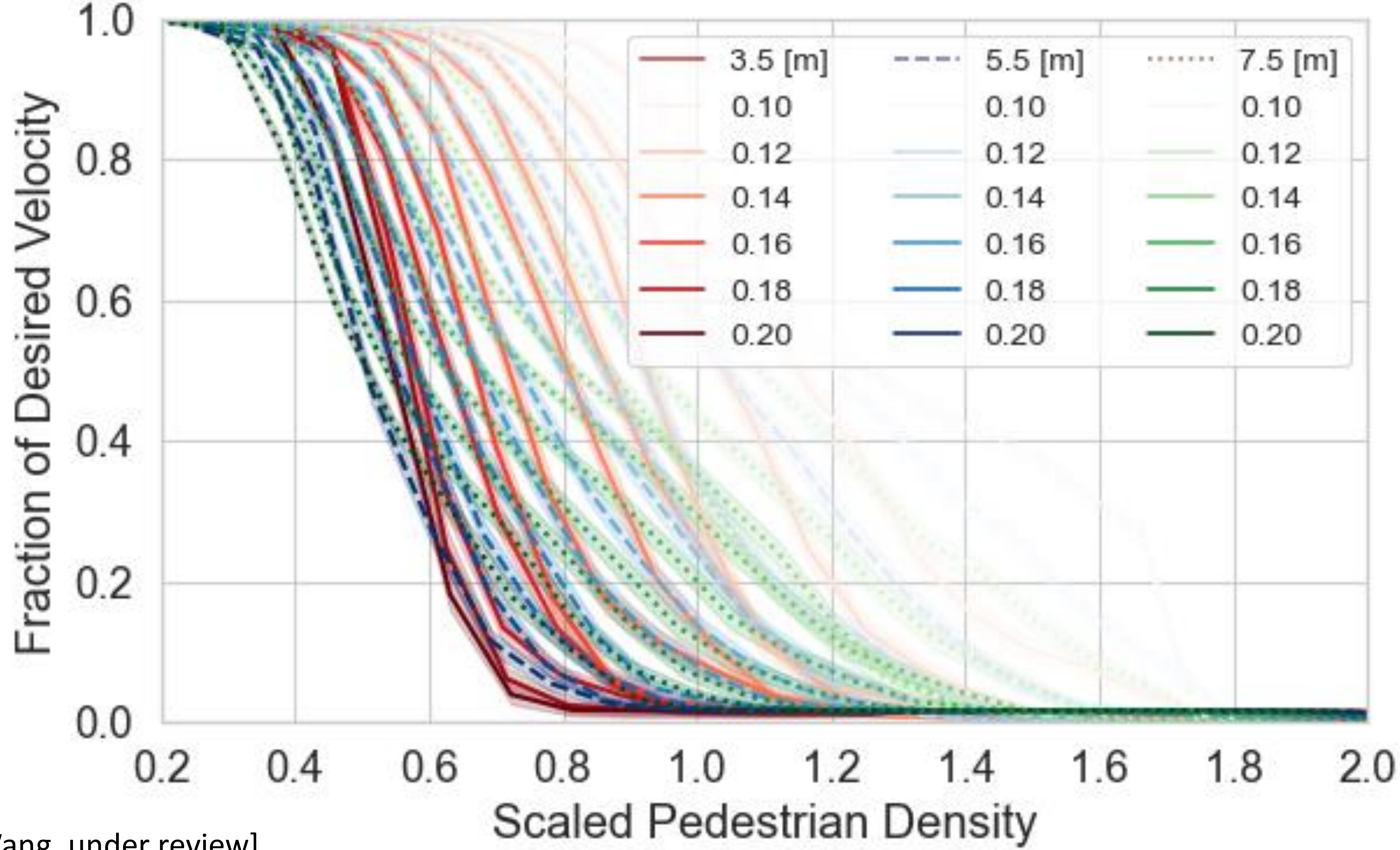
[Kramer and Wang, under review]

More people, more problems…



[Kramer and Wang, under review]

... and more preference for social distance, more "problems" too…

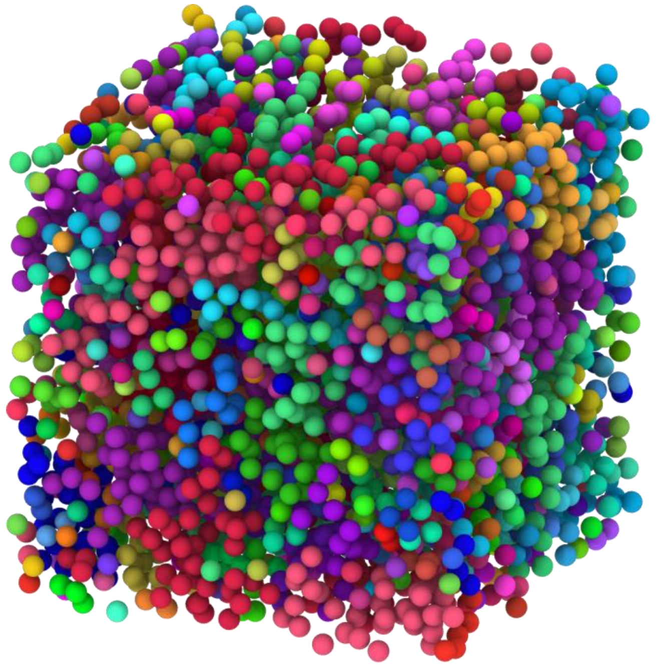


[Kramer and Wang, under review]

“P.S. A picture is worth a thousand words.”

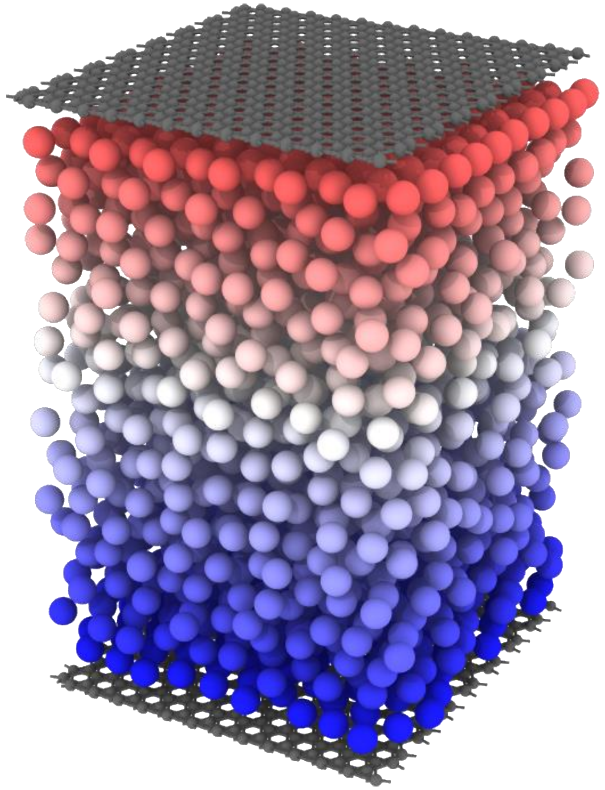
Laboratory for Mechanics of Materials via Molecular and Multiscale Methods (M^5 Lab at CMU)

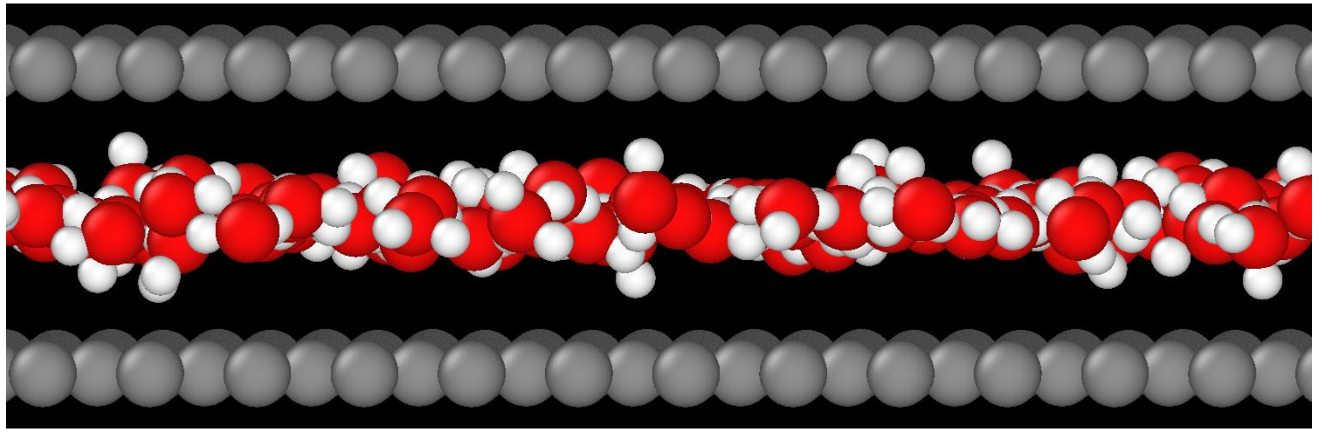
- Statistical physics and molecular-scale mechanics of fluids, polymers, soft matter, and active matter.
- Micro- and nanoscale transport phenomena.
- High-performance computational science and engineering (both theory- and data-driven).
- Molecular-scale design principles for sustainability.
- Physics of livable and equitable urban systems.



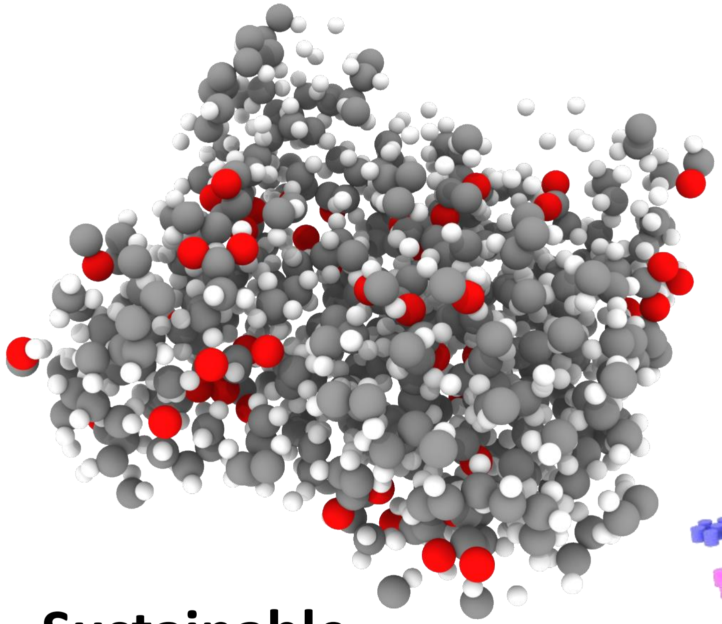
Hydrodynamics of suspensions

Nanoscale heat transfer



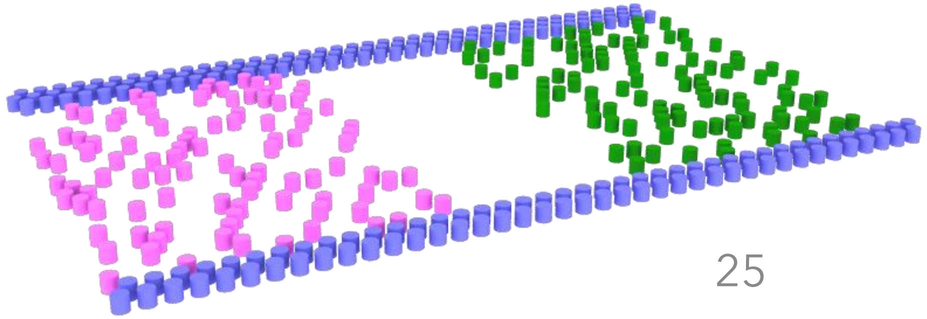


Nanoscale hydrodynamics



Sustainable polymers

Pedestrian flows



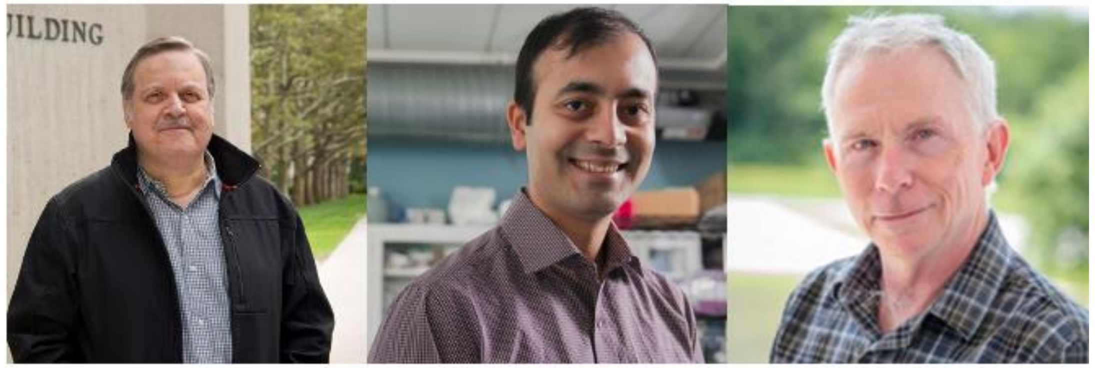
“P.S. One good turn deserves another.”

P.S. Something old, something new, something borrowed, something blue.

P.S. A picture is worth a thousand words. (or at least 10 extra minutes of talk time :P)

P.S. One good turn deserves another.

Nicolas Hadjiconstantinou MIT Mechanical Engineering — **Petros Koumoutsakos** ETHZ Computational Science — **Ju Li** MIT Nuclear Engineering



Daniel Blankschtein MIT Chemical Engineering — **Rohit Karnik** MIT Mechanical Engineering — **Stephen Gray** ANL Center for Nanoscale Materials

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- **Mehul Bapat (G)**
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- **Kelby Kramer ('22)**
- **Leo Li (G)**
- **Divya Rana (BS '23)**
- **Ryan Rusali (BS '21)**
- **Saptarshi Saha (G)**
- **Shuyuan Wang (MS '21)**
- **Diana Warren (BS '23)**
- **Chris Wu (G)**

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