Computational geometry of soft matter

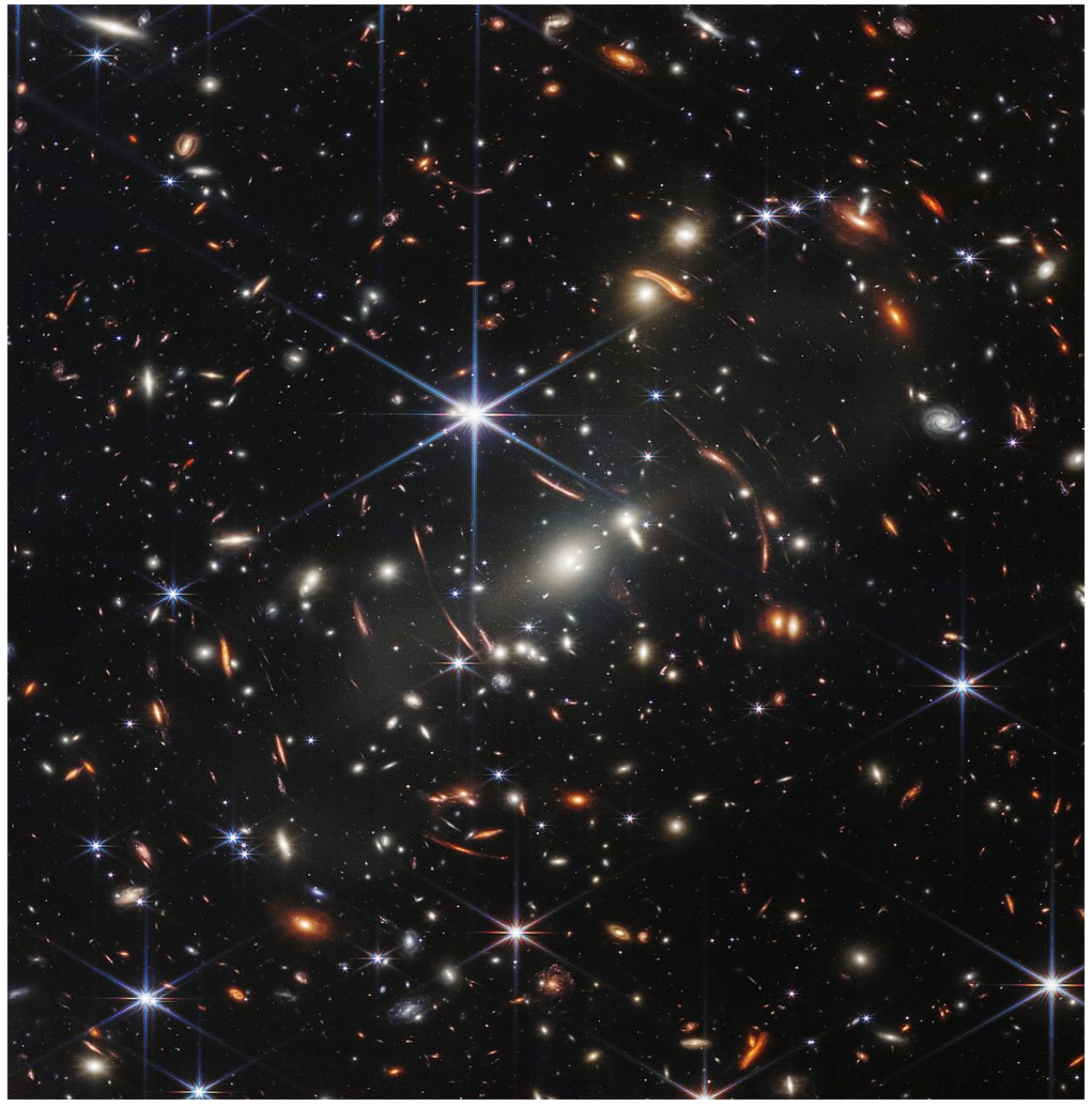
UMass Summer School on Soft Solids and Complex Fluids 2024

Lecture 1 (Monday June 3)

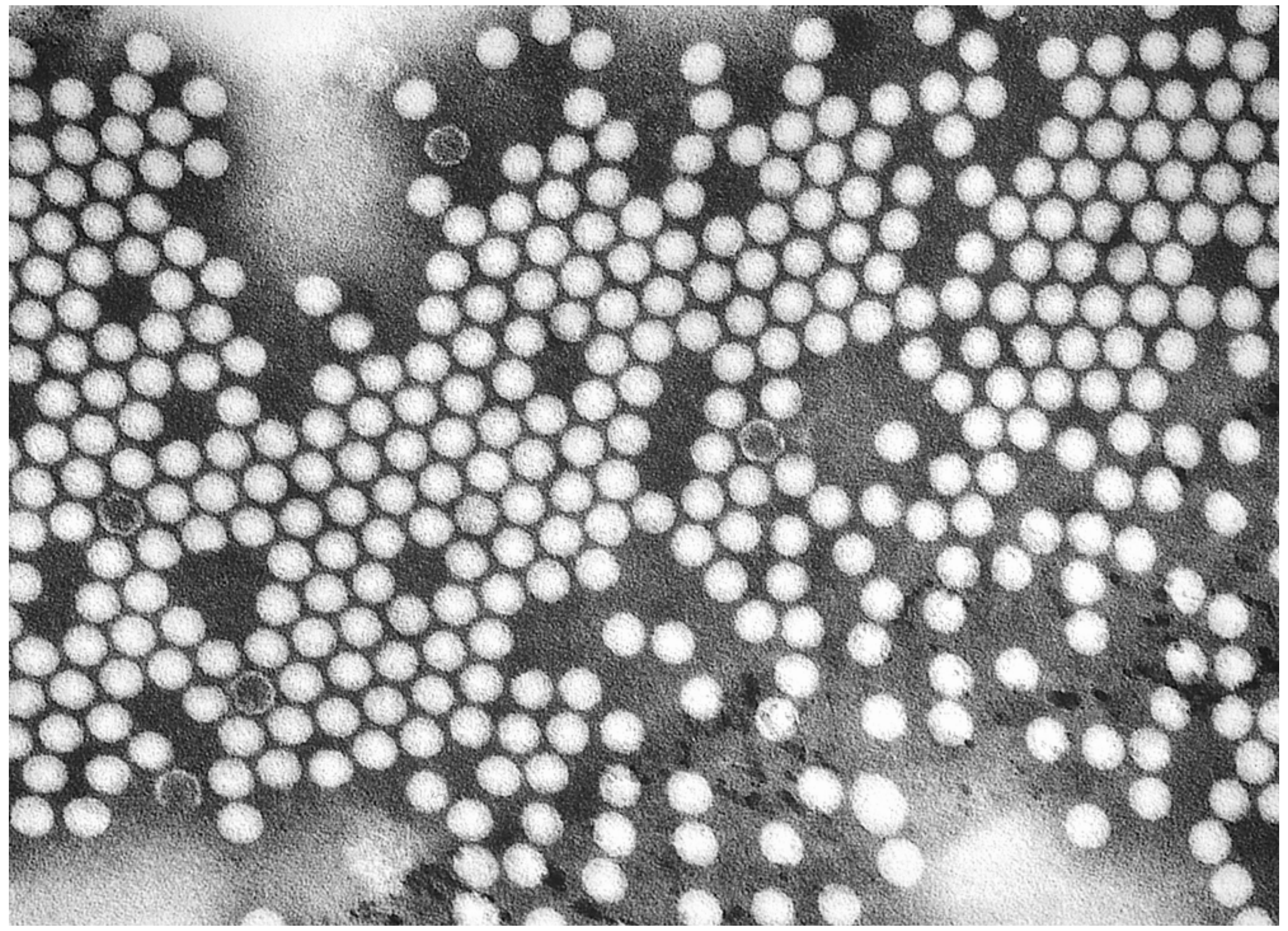
Chris H. Rycroft, University of Wisconsin–Madison
(chr@math.wisc.edu)

Introduction

- Geometry is everywhere! From the scale of atoms to the scale of galaxies, we use geometry to describe the world around us
- Geometry underpins many physical theories that we develop*
- There are many different ways to think about geometry, from the discrete to the continuum
- Nowadays, with increases in data-collection ability, we often need computational approaches to handle geometry



SMACS 0723 galaxy cluster
James Webb Space Telescope

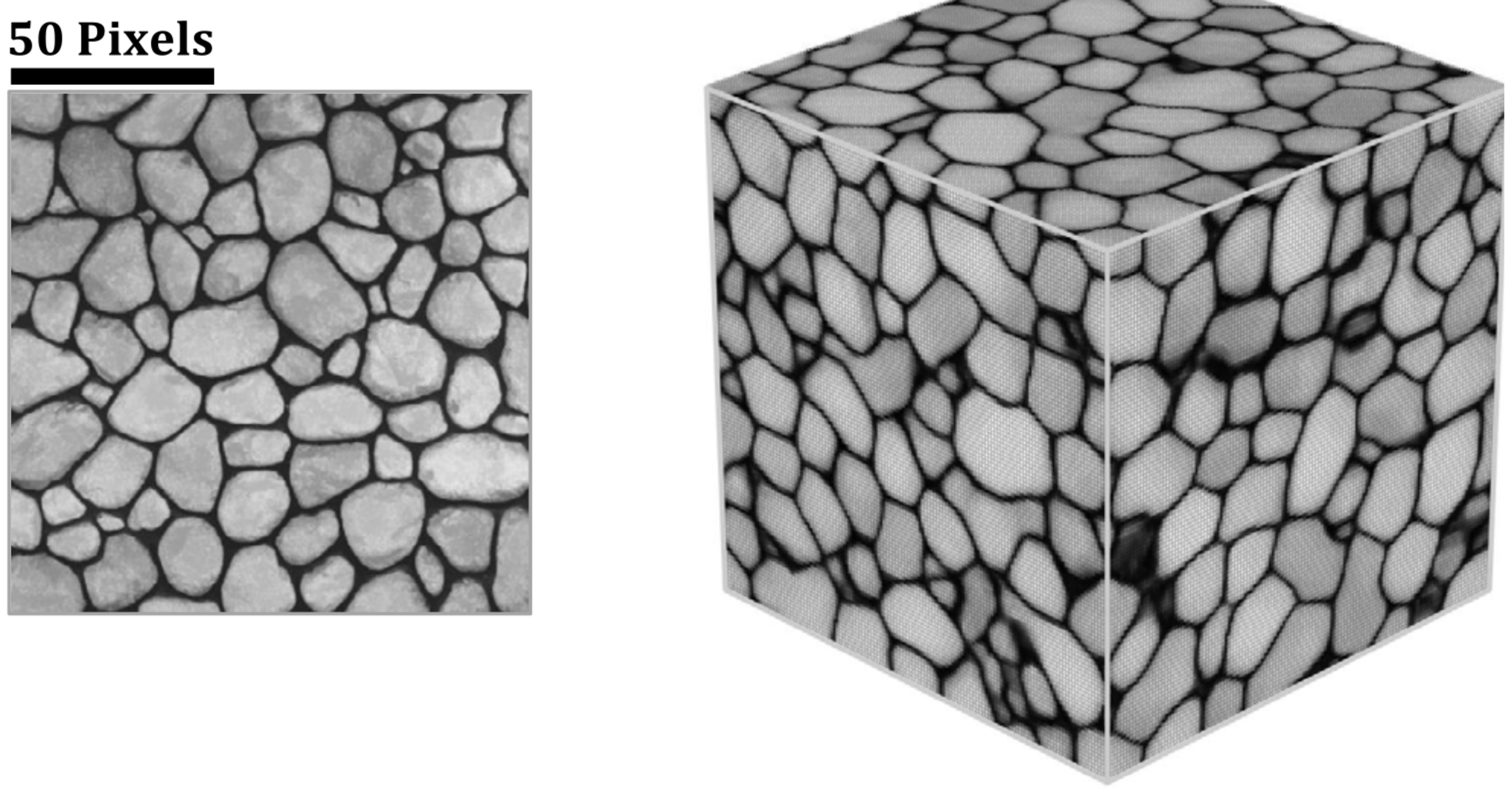


TEM image of polio virus
(CDC public image library)

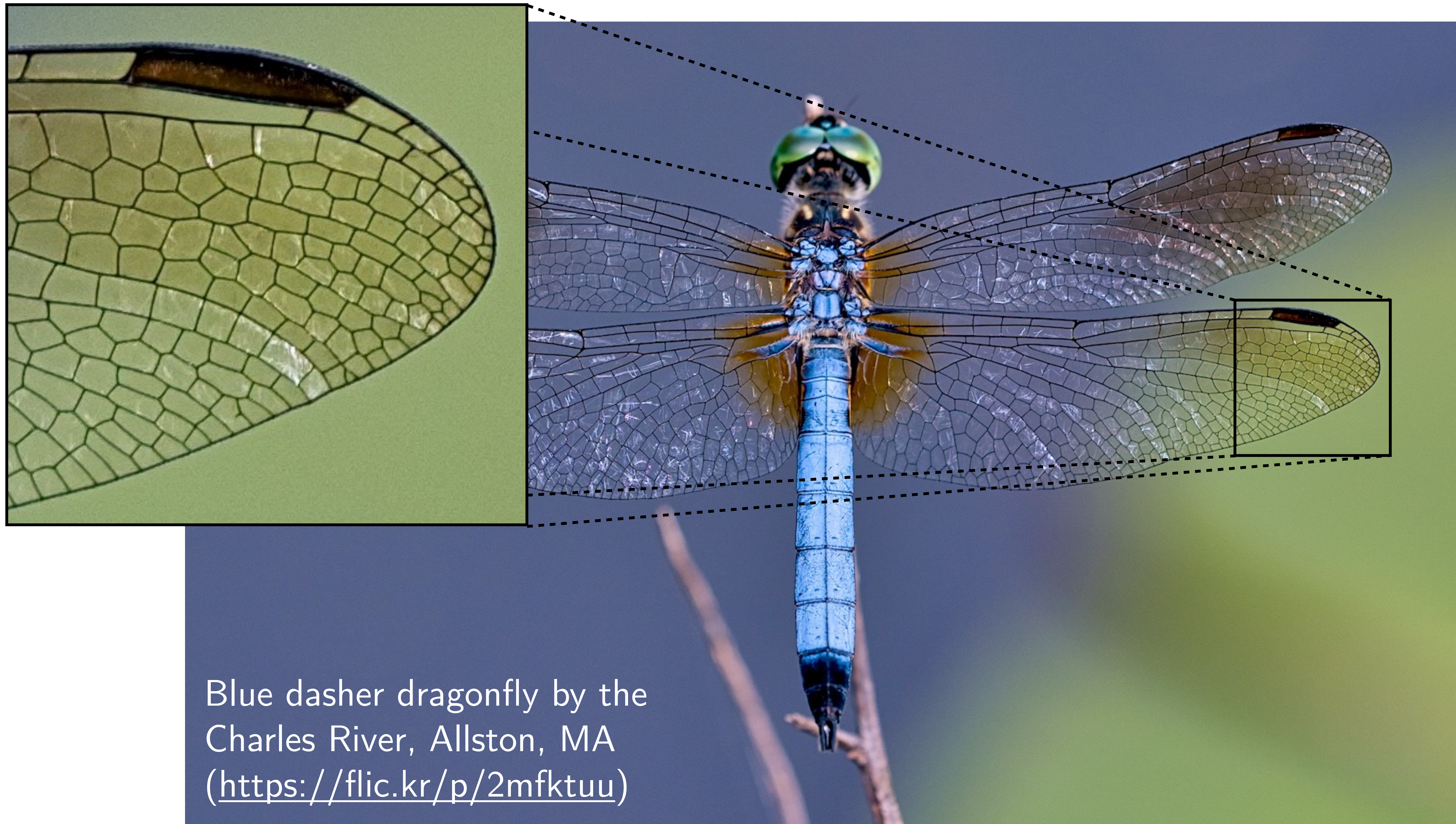
* We have already seen this from the other lectures

Some background

- I studied mathematics as an undergraduate
- I started the MIT Ph.D. program aiming to study string theory ...
- ... but instead became interested in soft matter and its real-world applications
- Since then I have found that within a wide range of research collaborations, much time has spent working on mathematics and software for geometry.
- There are many commonalities between supposedly unrelated systems



Polycrystalline material*


Blue dasher dragonfly by the Charles River, Allston, MA (https://flic.kr/p/2mfktuu)

*I. Javaheri and V. Sundararaghavan, Computer-Aided Design **120**, 102806 (2020).

Program files and photos

- These lectures have an associated GitHub repository:

  https://github.com/chr1shr/uma_ss2024

  It contains example codes in C++ and Perl, along with scripts for creating graphs and movies

- Some associated photos are available on Flickr:

  https://flic.kr/s/aHBqjByDR9

Outline

Monday

- A model of dense granular drainage
- Voronoi analysis of granular flow
- Neighbor relations

Tuesday

- Development of the Voro++ library
- Netwok analysis for CO_2 capture
- Alternative models and methods

Wednesday

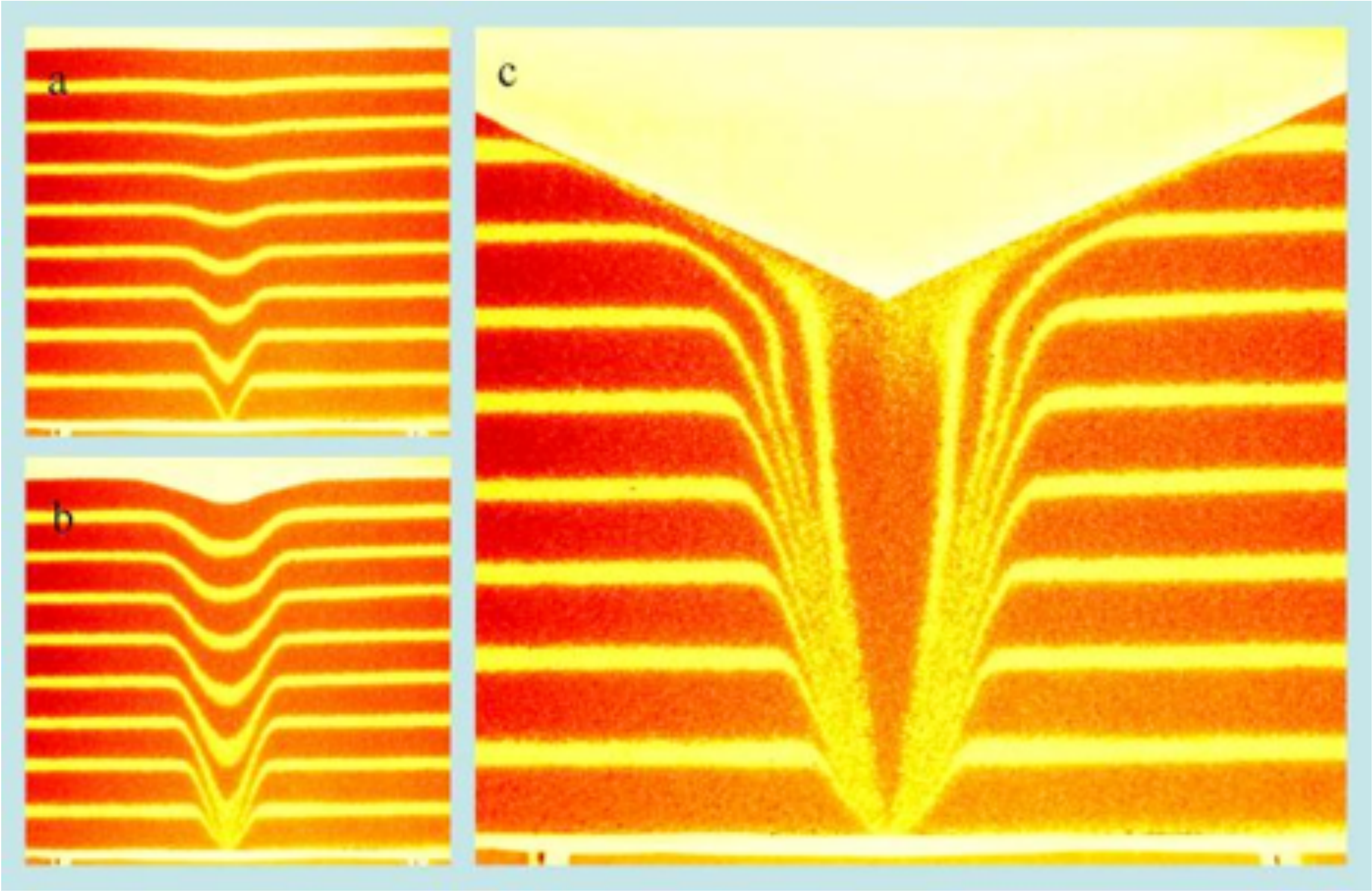
- Topological Voronoi analysis
- Lloyd's algorithm and meshing
- Insect wing structure

Thursday

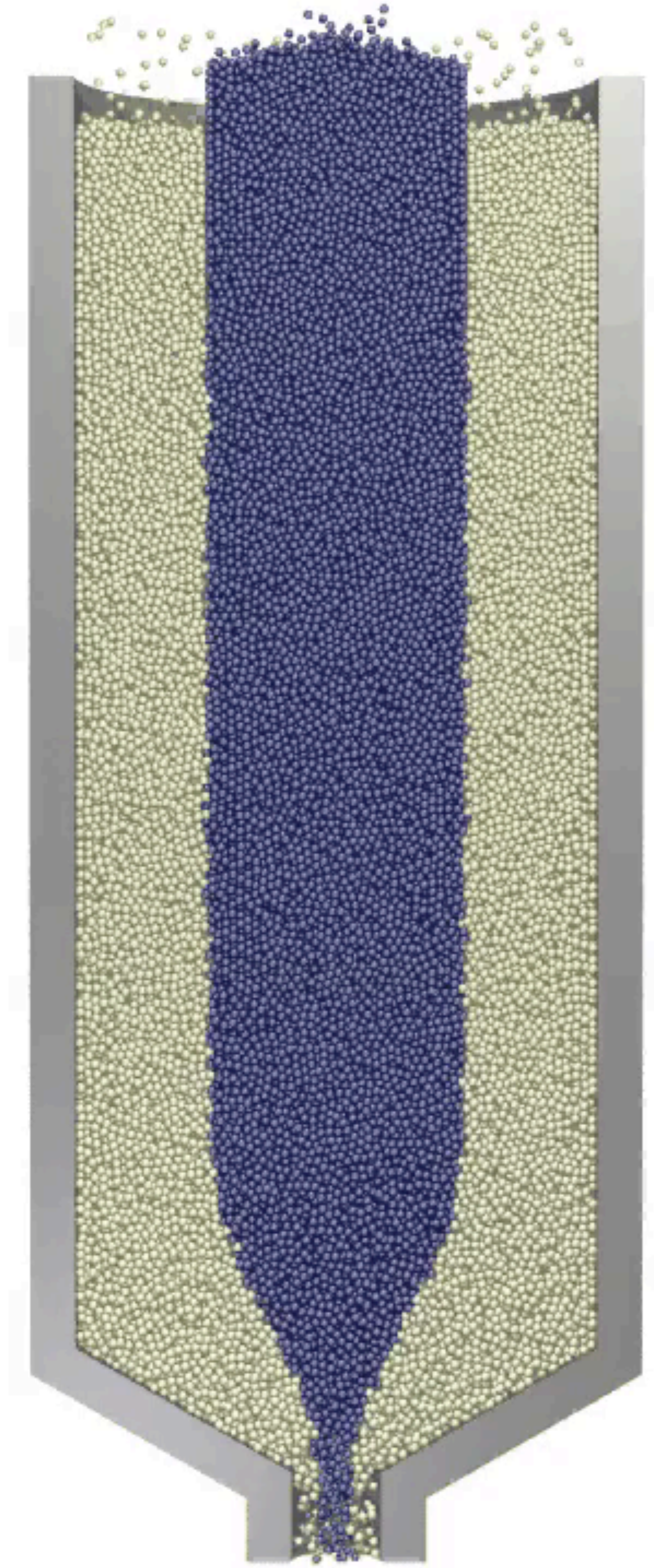
- Continuum representations of deformation
- The reference map technique
- Fluid–structure interaction

Mixing in dense granular drainage

- Many industrial processes involve powders and grains draining through silos
- Fundamentally different engineering challenges to draining fluid tanks
- Some experiments show a parabolic flow region above the orifice
- Particles also mix, but this happens slowly



Drainage of layers of sand between glass plates



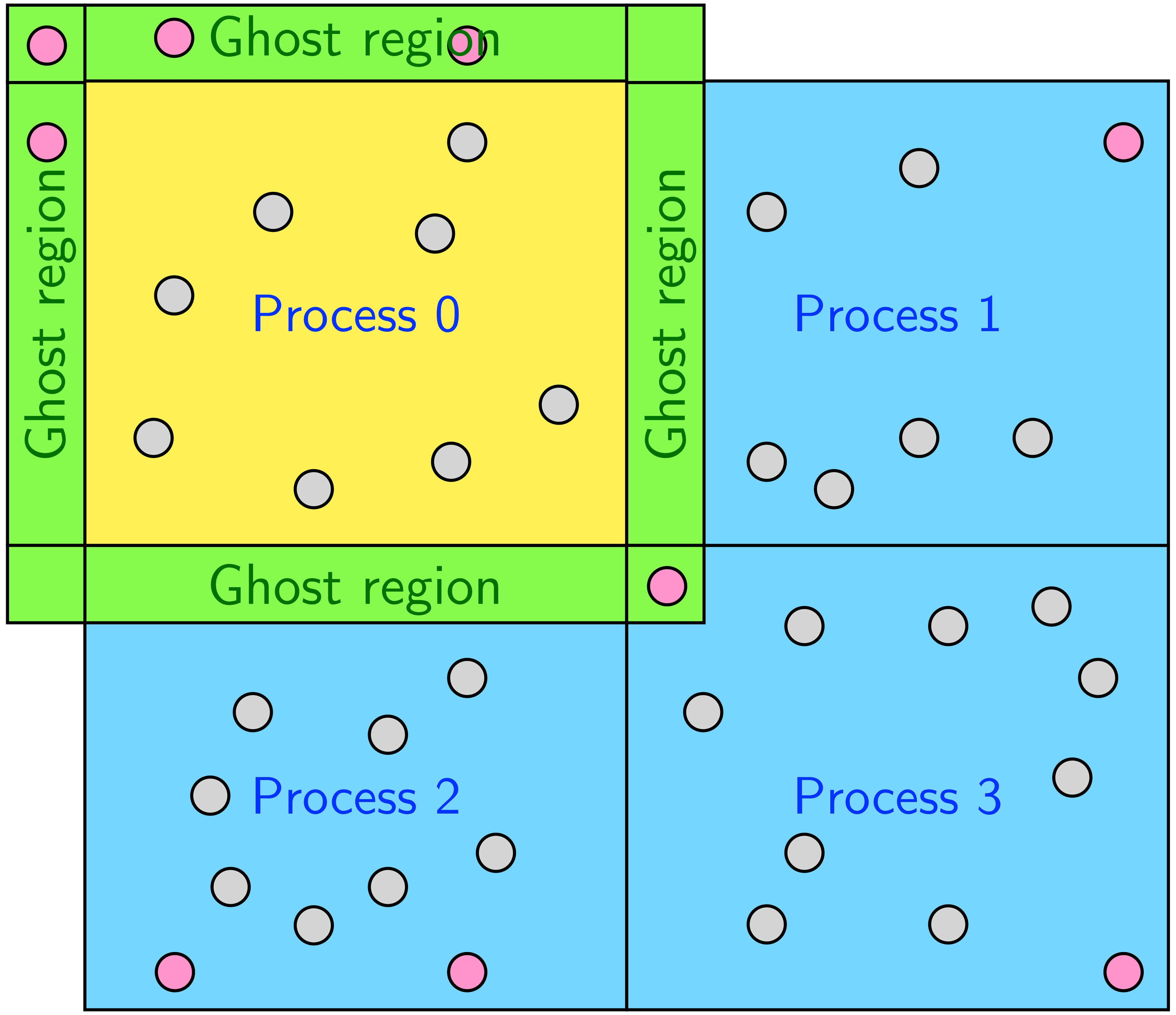
Cutaway of 440,000 particles in a cylindrical hopper

A. Samadani *et al.*, Phys. Rev. E **60**, 7203–7209 (1999).

Discrete-element simulation with LAMMPS

LAMMPS: Large Atomic/Molecular Massively Parallel Simulator (https://lammps.sandia.gov)

- Developed at Sandia National Laboratories since the late 90's
- General platform for simulating atoms and particles using the discrete element method* (DEM)
- Many different options and force models: Lennard-Jones, granular, embedded atom model, ...
- Provides computational infrastructure for efficient parallel simulation



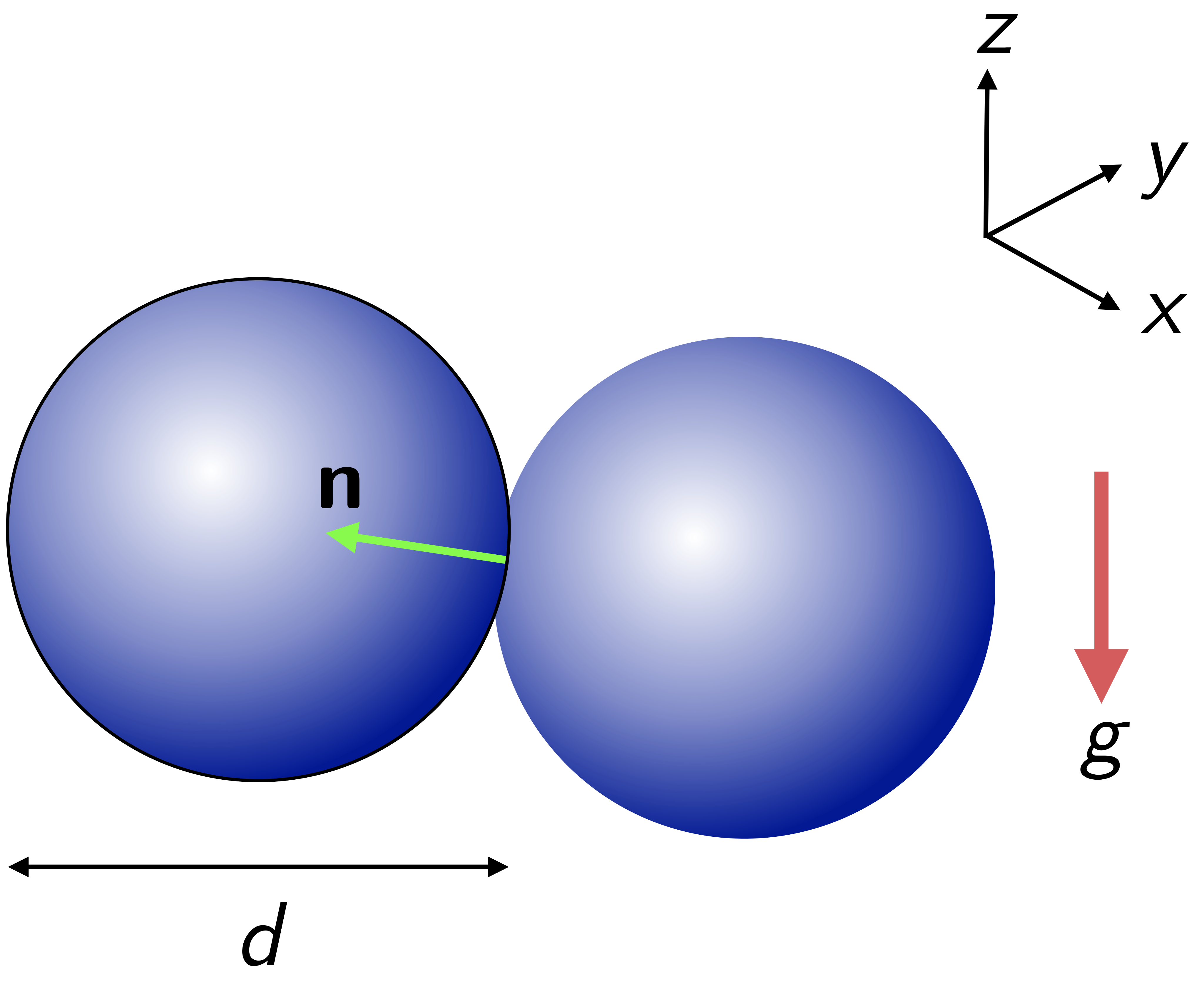
Example LAMMPS simulation with four processors and periodic boundary conditions

* Closely related to molecular dynamics (MD). DEM usually includes particle rotation.

Granular contact model

(simulation scales)

- Lengths measured in terms of a particle diameter d
- Defines a natural time unit according to $\tau = \sqrt{d/g}$
- Mass m is defined so that particles have density m/d^3



P. A. Cundall and O. D. L. Strack, Geotechnique **29**, 47 (1979).

K. L. Johnson, *Contact mechanics*, Cambridge University Press, 1999.

L. E. Silbert *et al.*, *Granular flow down an inclined plane: Bagnold scaling and rheology*, Phys. Rev. E **64**, 051302 (2001).

Granular contact model

(simulation scales)

- Contact force model

$$\mathbf{F}_n = f(\sqrt{\delta/d})\left(k_n\delta\mathbf{n} - \frac{\gamma_n\mathbf{v}_n}{2}\right)$$

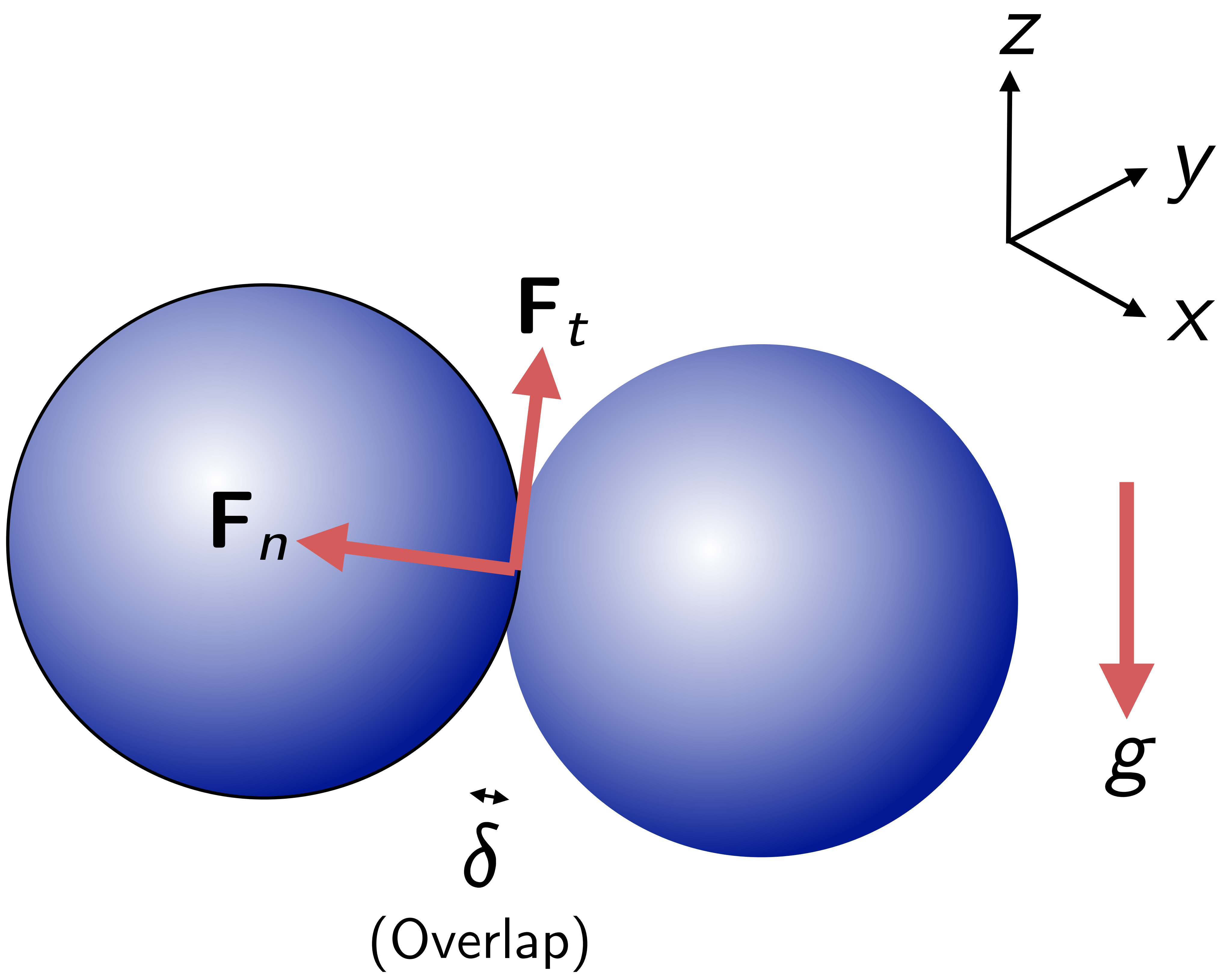
$$\mathbf{F}_t = f(\sqrt{\delta/d})\left(-k_t\mathbf{\Delta s}_t - \frac{\gamma_t\mathbf{v}_t}{2}\right)$$

- Two common options

$$f(\lambda) = \begin{cases} 1 & \text{for Hookean contacts} \\ \sqrt{\lambda} & \text{for Hertzian contacts} \end{cases}$$

- Coulomb friction

$$|\mathbf{F}_t| \leq \mu|\mathbf{F}_n|$$



Typical parameter choices

Symbol	*Description*	*Value*
k_n	Normal elastic constant	$2 \times 10^6 mg/d$
k_t	Tangential elastic constant	$2k_n/7$
γ_n	Normal viscoelastic constant	$50\sqrt{10}\tau^{-1}$
γ_t	Tangential viscoelastic constant	$25\sqrt{10}\tau^{-1}$
μ	Coulomb friction coefficient	0.5

Friction

- Friction is a subtle aspect of the simulation
- When two particles come into contact, the tangential displacement $\mathbf{\Delta s}_t$ is tracked over the lifetime of the contact
- If $|\mathbf{F}_t|$ exceeds $\mu|\mathbf{F}_n|$, then it is rescaled to have magnitude $\mu|\mathbf{F}_n|$ and $\mathbf{\Delta s}_t$ is adjusted so that (†) holds

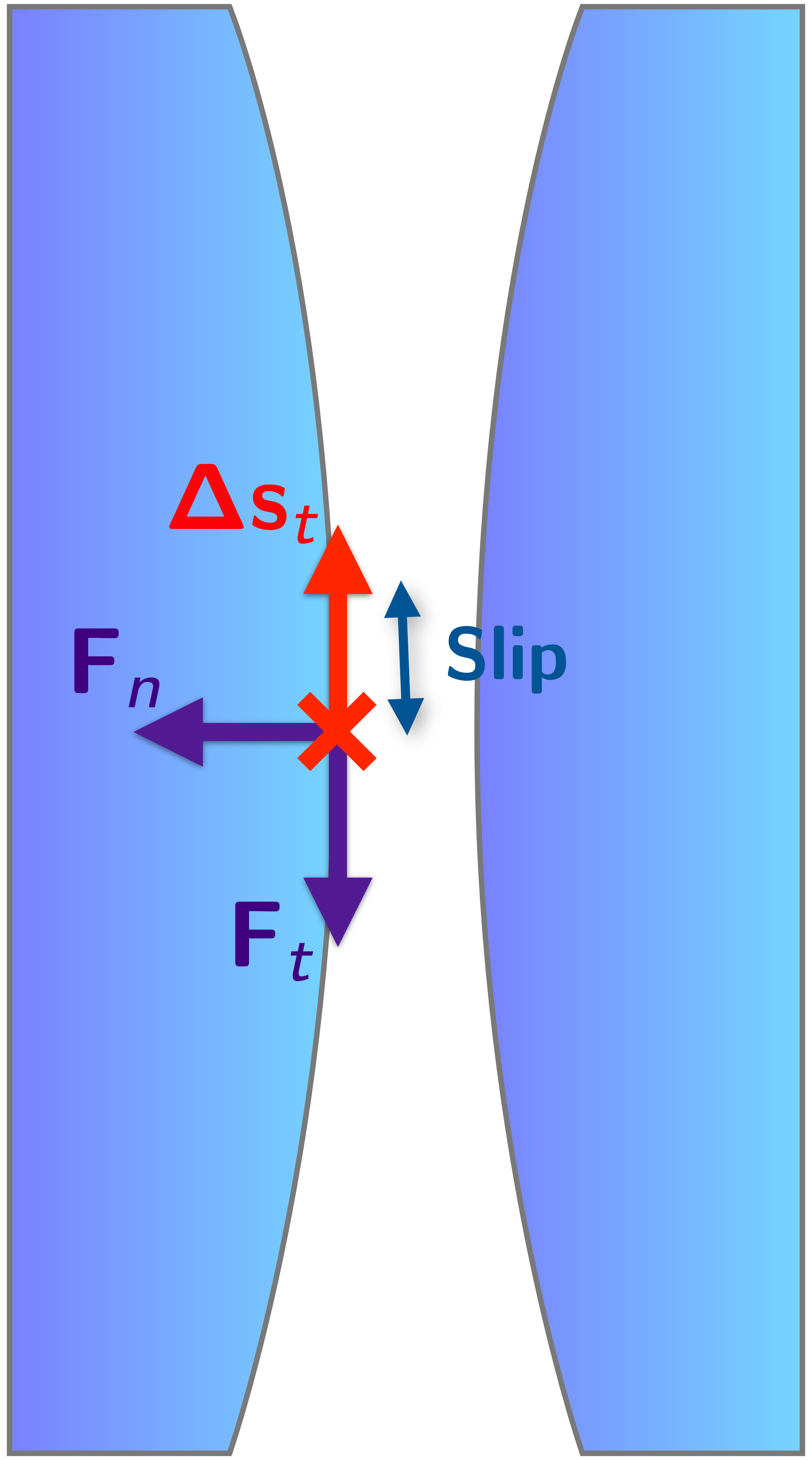
Normal and tangential forces

$$\mathbf{F}_n = f(\sqrt{\delta/d})\left(k_n\delta\mathbf{n} - \frac{\gamma_n\mathbf{v}_n}{2}\right)$$

$$\mathbf{F}_t = f(\sqrt{\delta/d})\left(-k_t\mathbf{\Delta s}_t - \frac{\gamma_t\mathbf{v}_t}{2}\right) \quad (\dagger)$$

Coulomb friction

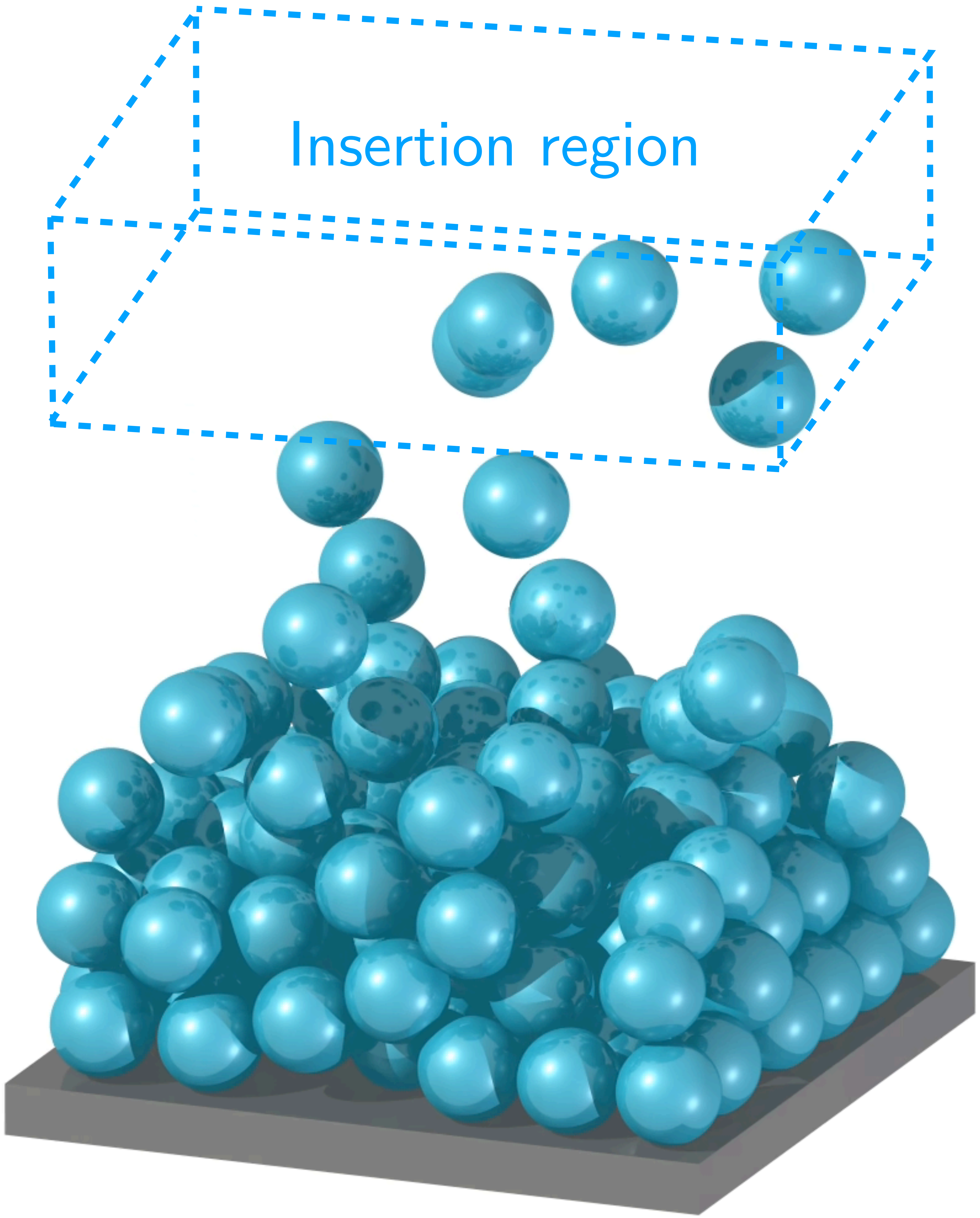
$$|\mathbf{F}_t| \le \mu|\mathbf{F}_n|$$



Creating a particle packing

(using pouring)

- The example simulation creates a packing of 350 particles
- Particles are randomly inserted in groups into a region
- Once a group falls out of the region, a new group is added
- End of simulation is a roughly $7d$ by $7d$ by $7d$ packing



LAMMPS input file

- LAMMPS is run using a text configuration file, which specifies:
  - Particle interaction model
  - Numerical timestep
  - Output types
  - Simulation domain
- Run with command

```
mpirun -np 4 ./lmp_openmpi <input1.lmp
```

Creates four processes using the MPI (Message Passing Interface) library

```
# Pouring LAMMPS input file
atom_style granular
boundary  fm fm fm
newton  off
communicate  single vel yes

# Region setup
region reg block -3.5 3.5 -3.5 3.5 0 10 units box
create_box   1 reg

# Neighbor computation setup
neighbor     0.2 bin
neigh_modify delay 0

# Pair interaction
pair_style   gran/hooke/history 2000000 \
             NULL 158.113883 NULL 0.5 0
pair_coeff   * *
timestep     0.000025

...
```

input1.lmp

LAMMPS output

- Typically LAMMPS will save two types of output:
  - The dump file containing frequent snapshots of the particle positions with a numerical IDs, in text format
  - Restart files at infrequent intervals, which contain a complete information about the simulation (*e.g.* including history-dependent contact information)
- Dump files can be used for a wide-range of post-processing

```
ITEM: TIMESTEP
1000
ITEM: NUMBER OF ATOMS
13
ITEM: BOX BOUNDS
-3.5 3.5
-3.5 3.5
0 10
ITEM: ATOMS id type xs ys zs
1 1 0.823044 0.764876 0.923205
2 1 0.25138 0.516107 0.938156
3 1 0.381063 0.390279 0.92573
4 1 0.389969 0.920736 0.948707
5 1 0.89836 0.588533 0.920575
6 1 0.577129 0.805506 0.904006
7 1 0.731278 0.441968 0.779584
8 1 0.764215 0.301355 0.87453
9 1 0.682624 0.42572 0.909503
10 1 0.552108 0.279713 0.949857
11 1 0.53695 0.0874061 0.948688
12 1 0.0893446 0.329288 0.93171
13 1 0.391378 0.603187 0.944647
...
```

LAMMPS dump file excerpt

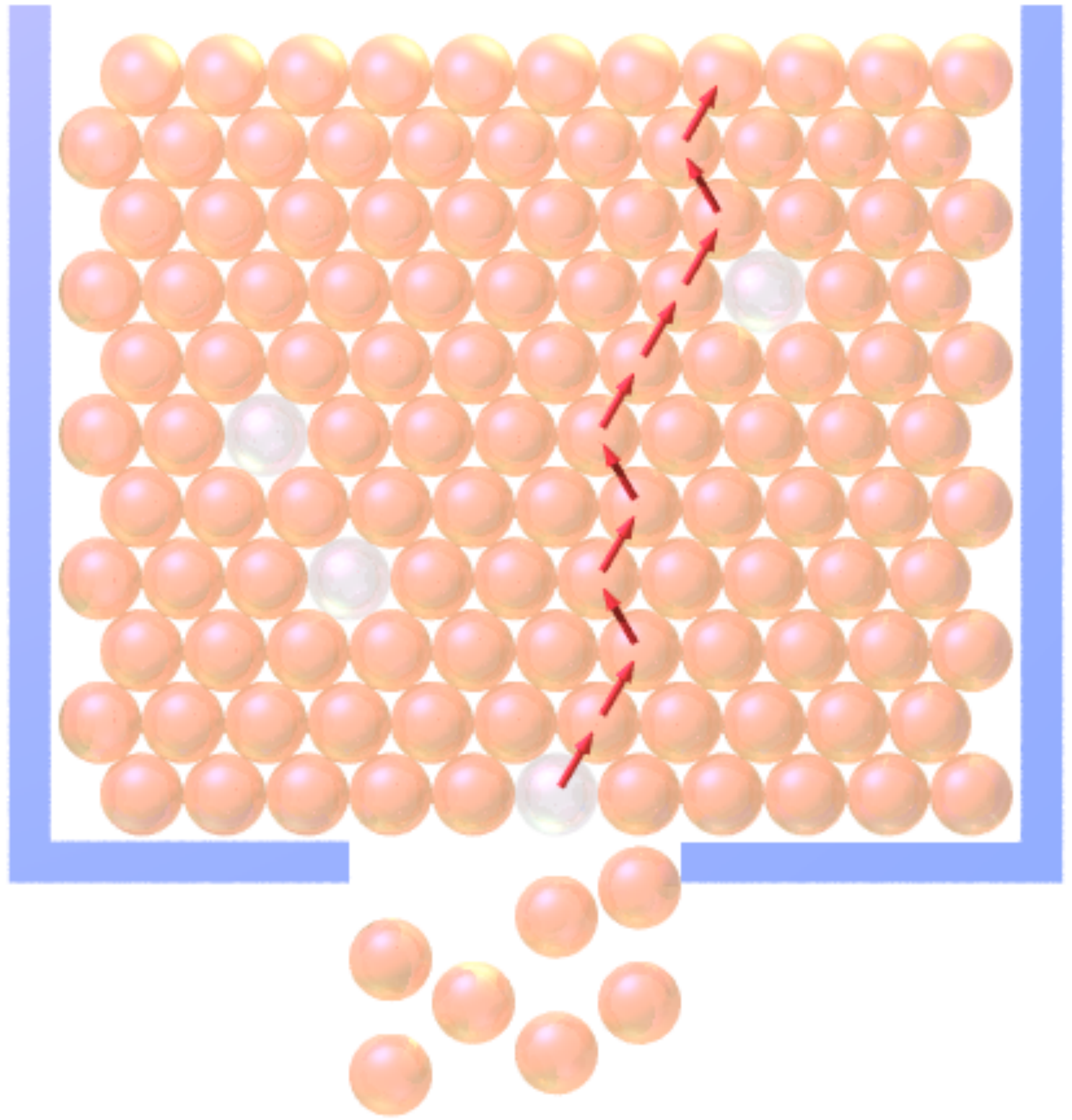
The void model

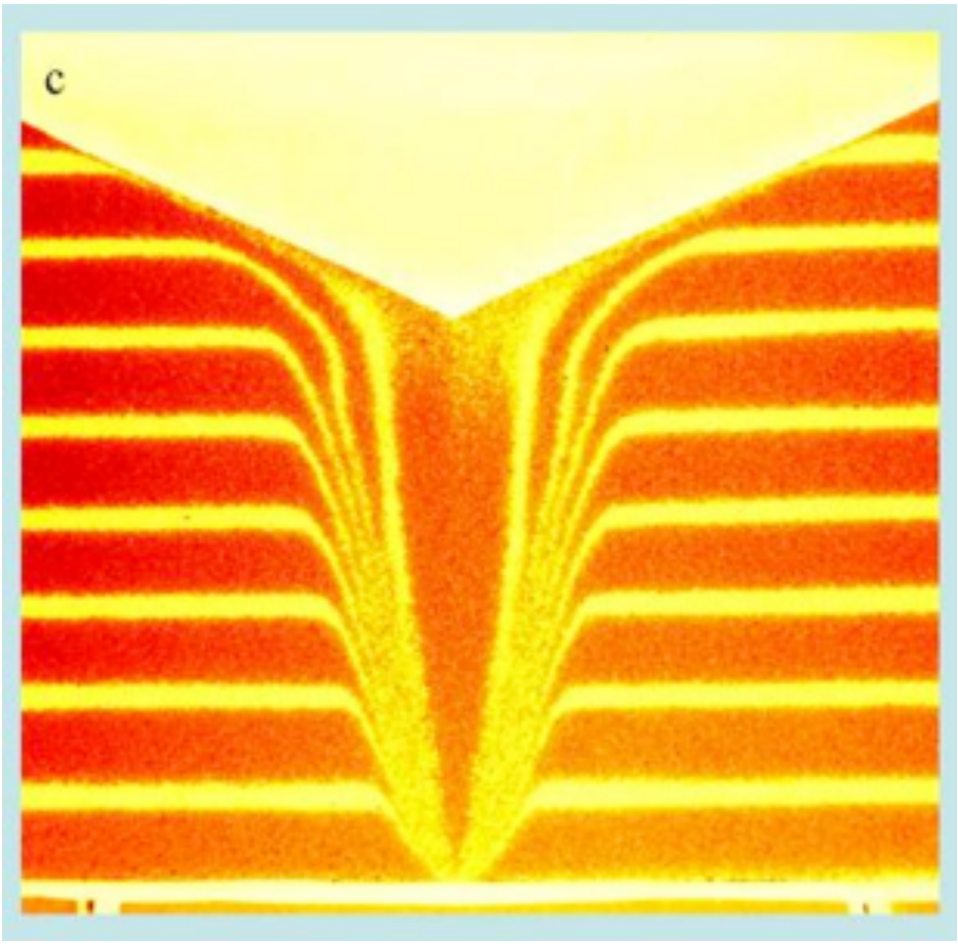
- Treat particles as on a 2D hexagonal lattice
- Voids introduces at orifice and do random walks upward
- Continuum limit for vertical velocity v_z

$$\frac{\partial v_z}{\partial z} = b\frac{\partial^2 v_z}{\partial x^2}$$

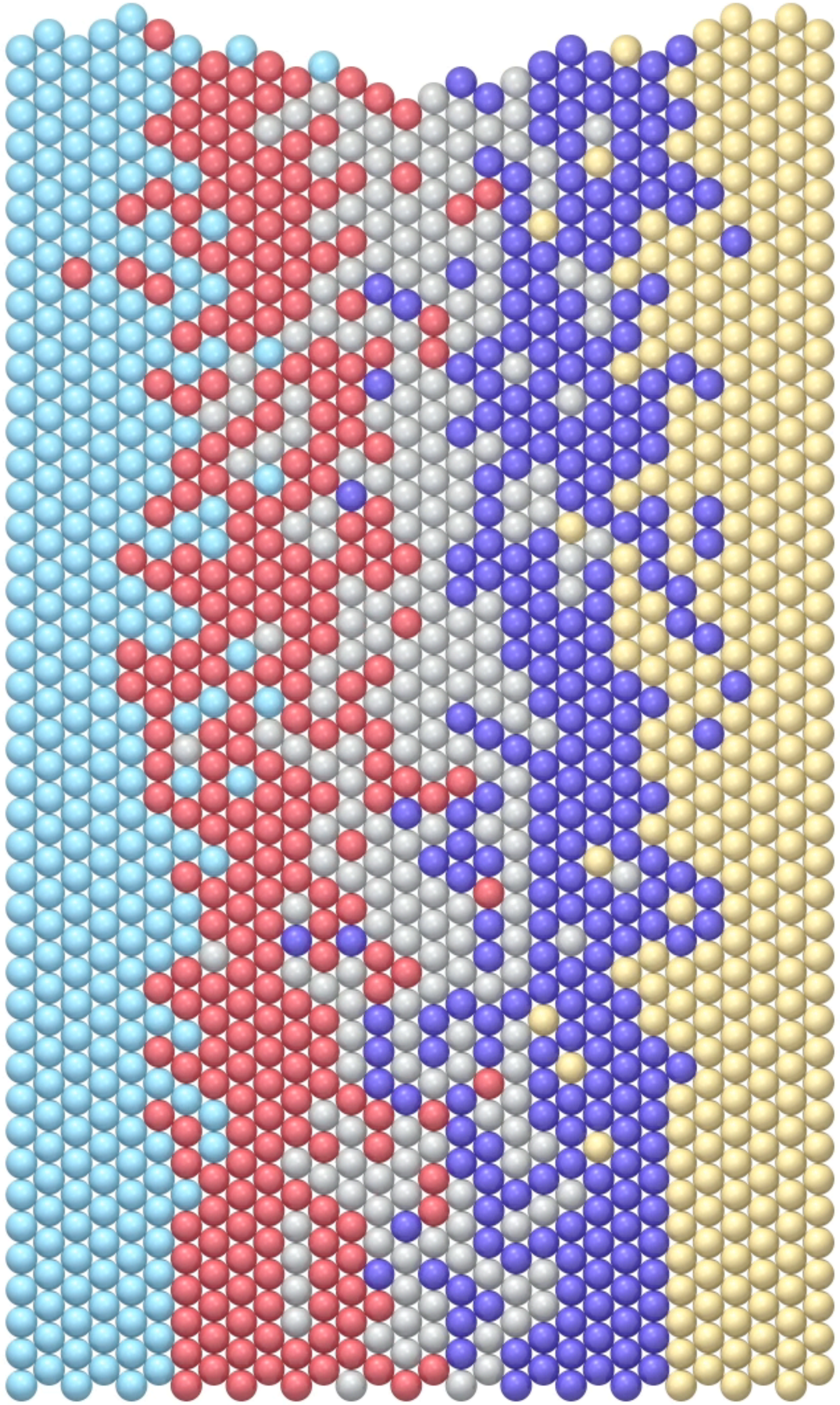
- Limit of particle PDF

$$-\frac{\partial v_z}{\partial z} = b\frac{\partial^2 v_z}{\partial x^2} - 2b\frac{\partial}{\partial x}\left(\rho\frac{\partial}{\partial x}\log v_z\right)$$





Samadani *et al.* (1999)



W. W. Mullins, *Stochastic theory of particle flow under gravity,* J. Appl. Phys. **43**, 665–678 (1972).
H. Caram and D. C. Hong, *Random-walk approach to granular flows,* Phys. Rev. Lett. **67**, 828–833 (1991).

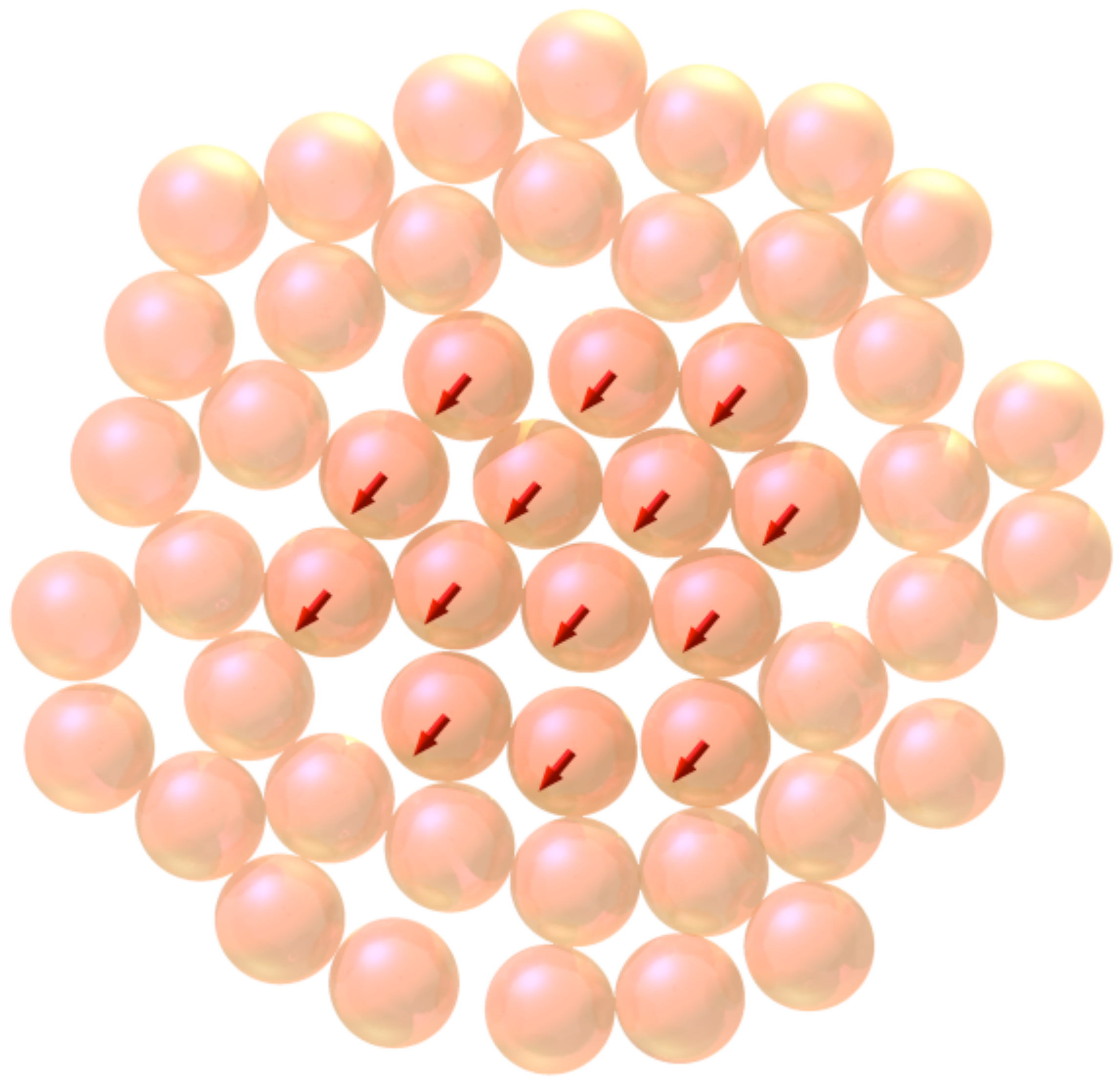
Velocity correlations

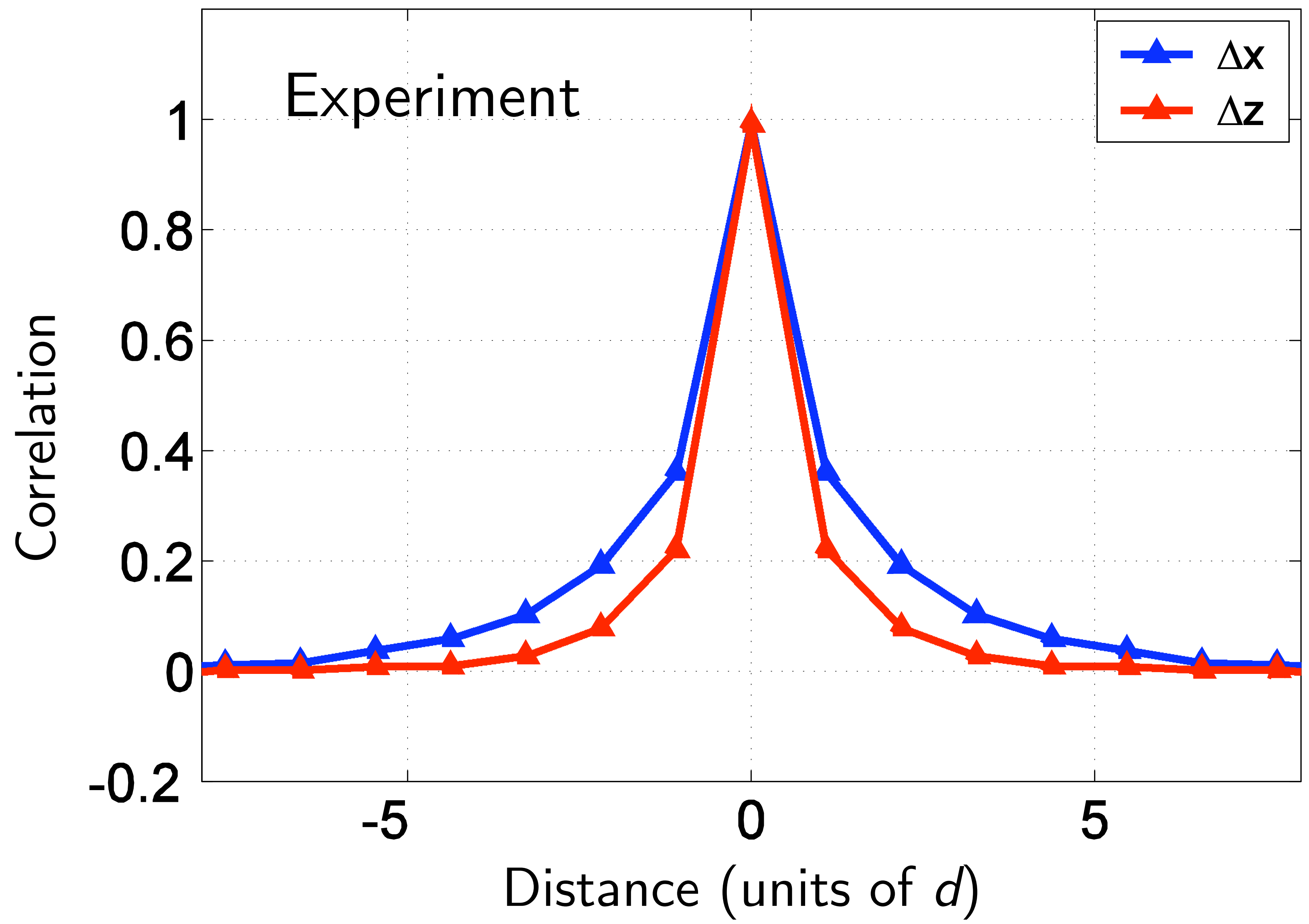
(in experiments and simulations of granular drainage)

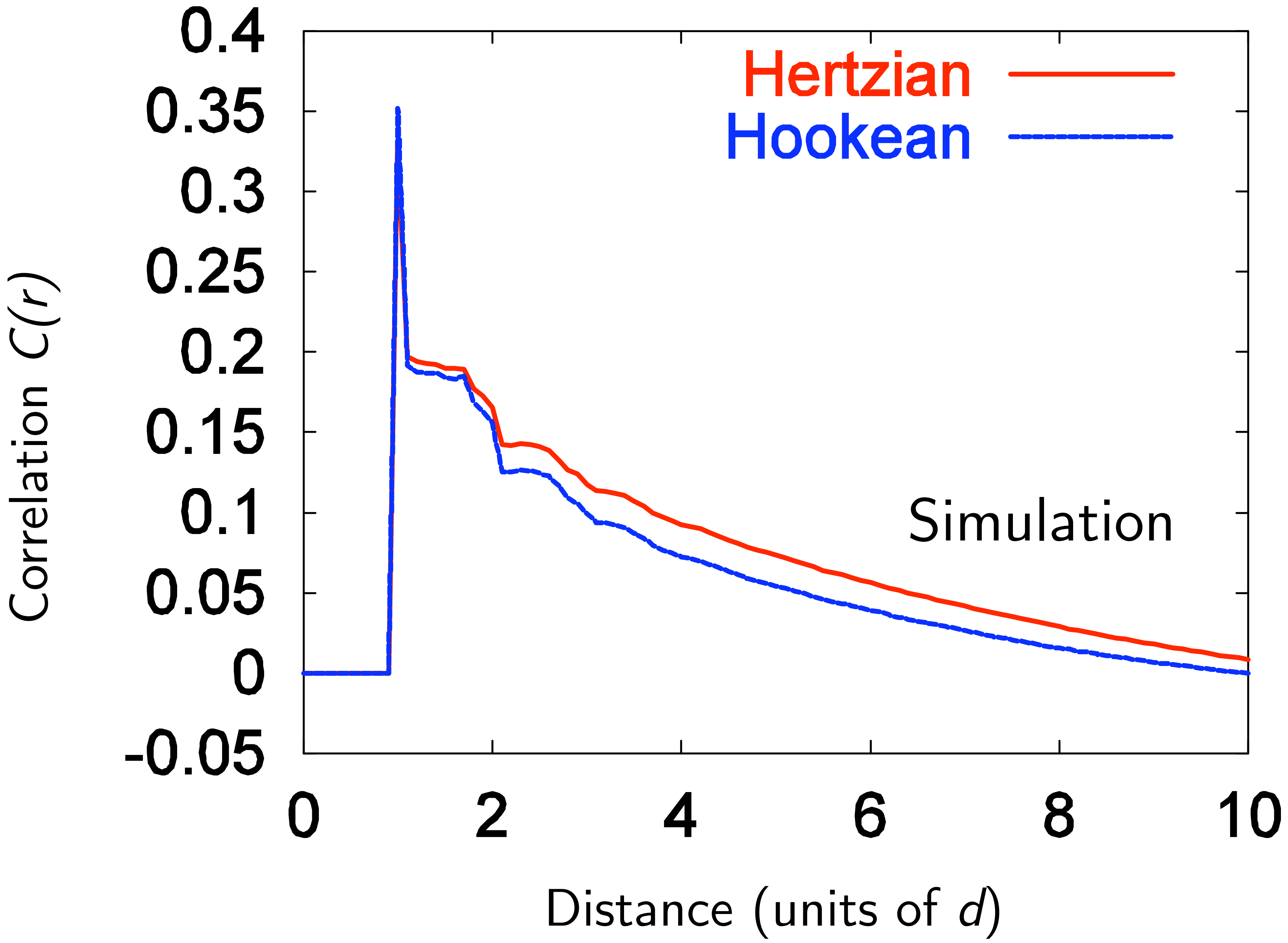
Compute local velocity correlations using

$$C(r) = \frac{\langle \mathbf{v}(0)\mathbf{v}(r) \rangle}{\sqrt{\langle \mathbf{v}(0)^2 \rangle \langle \mathbf{v}(r)^2 \rangle}}$$

Suggests correlated motion

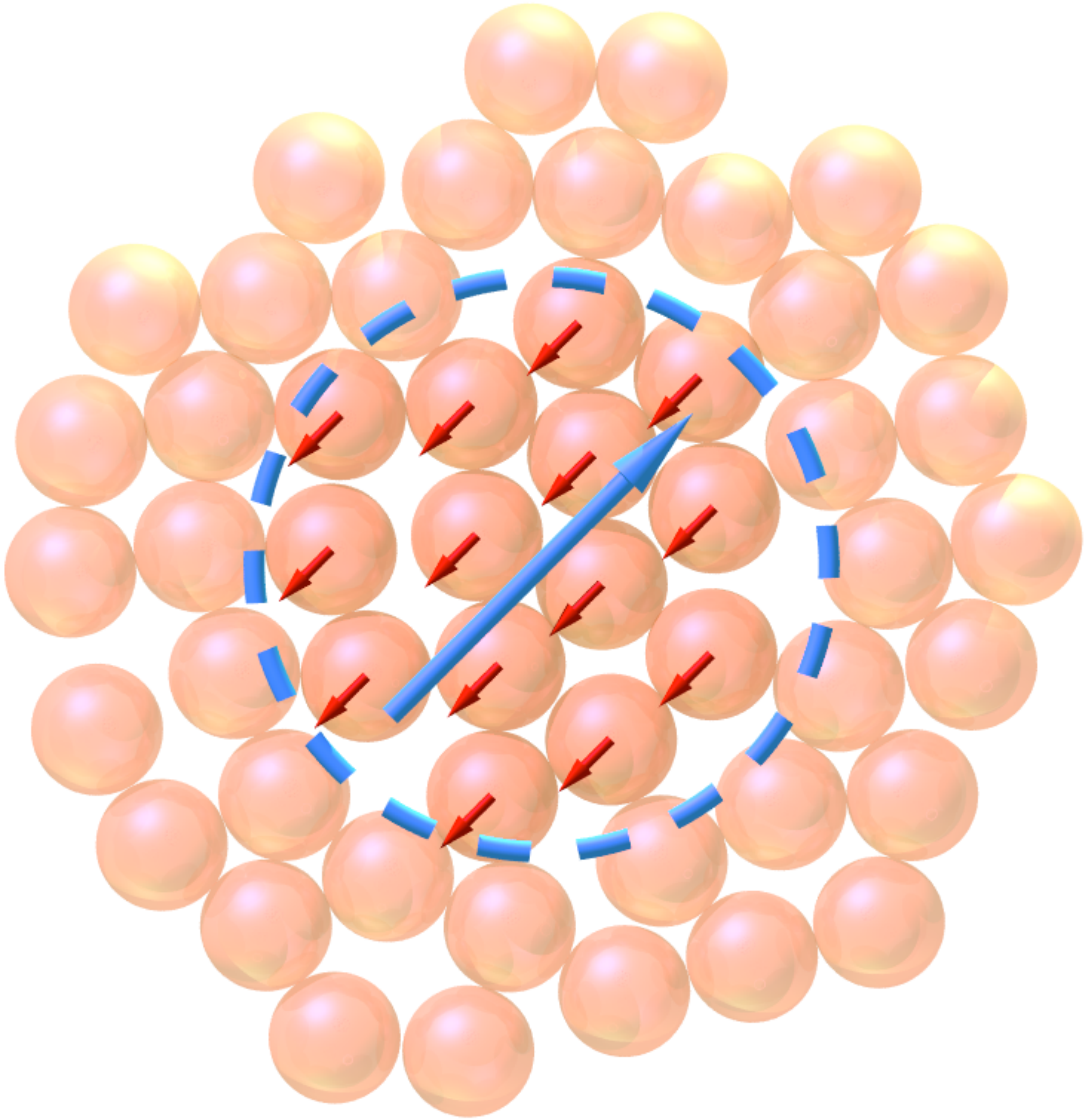






J. Choi, *Transport-limited aggregation and dense granular flow*, Ph.D. thesis, MIT, 2005.
C. H. Rycroft *et al.*, *Dynamics of random packings in granular flow*, Phys. Rev. E **73**, 051306 (2006).

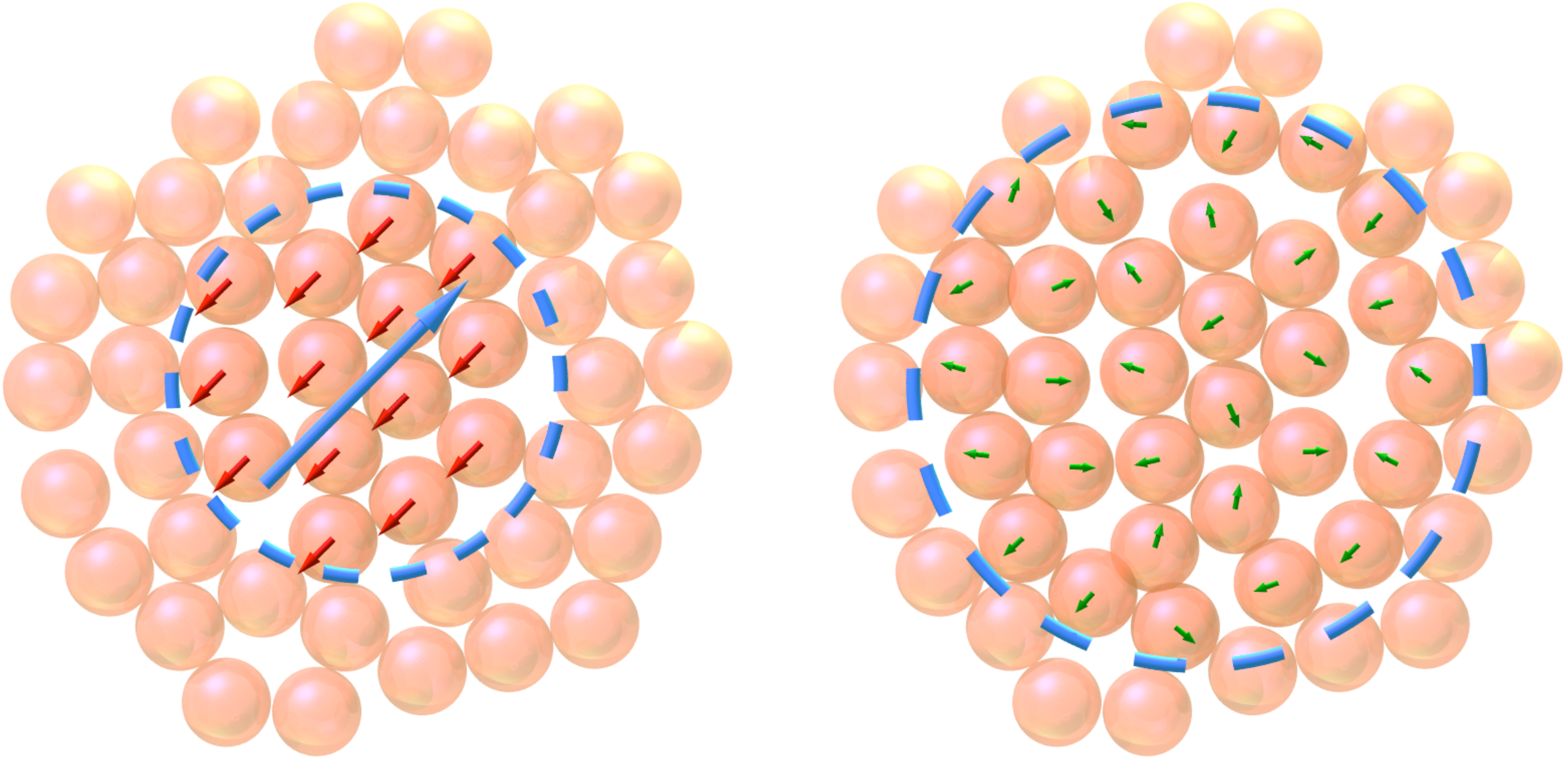
The spot model for random packing dynamics



- A spot is an extended region of slightly enhanced interstitial volume
- Spots cause correlated displacements of passive, off-lattice particles within range

M. Z. Bazant, *The Spot Model for random-packing dynamics*, Mech. Mat. **38**, 717 (2005).

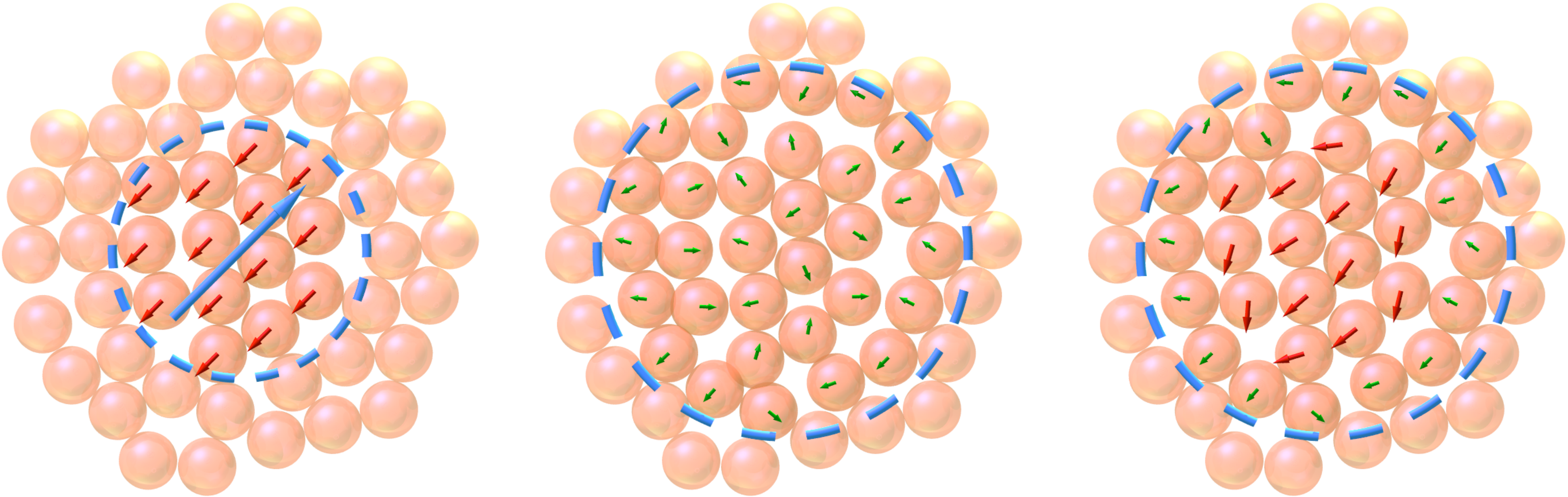
The spot model for random packing dynamics



- Apply elastic relaxation to all particles within range
- All overlapping particles experience a correcting normal displacement

M. Z. Bazant, *The Spot Model for random-packing dynamics*, Mech. Mat. **38**, 717 (2005).

The spot model for random packing dynamics



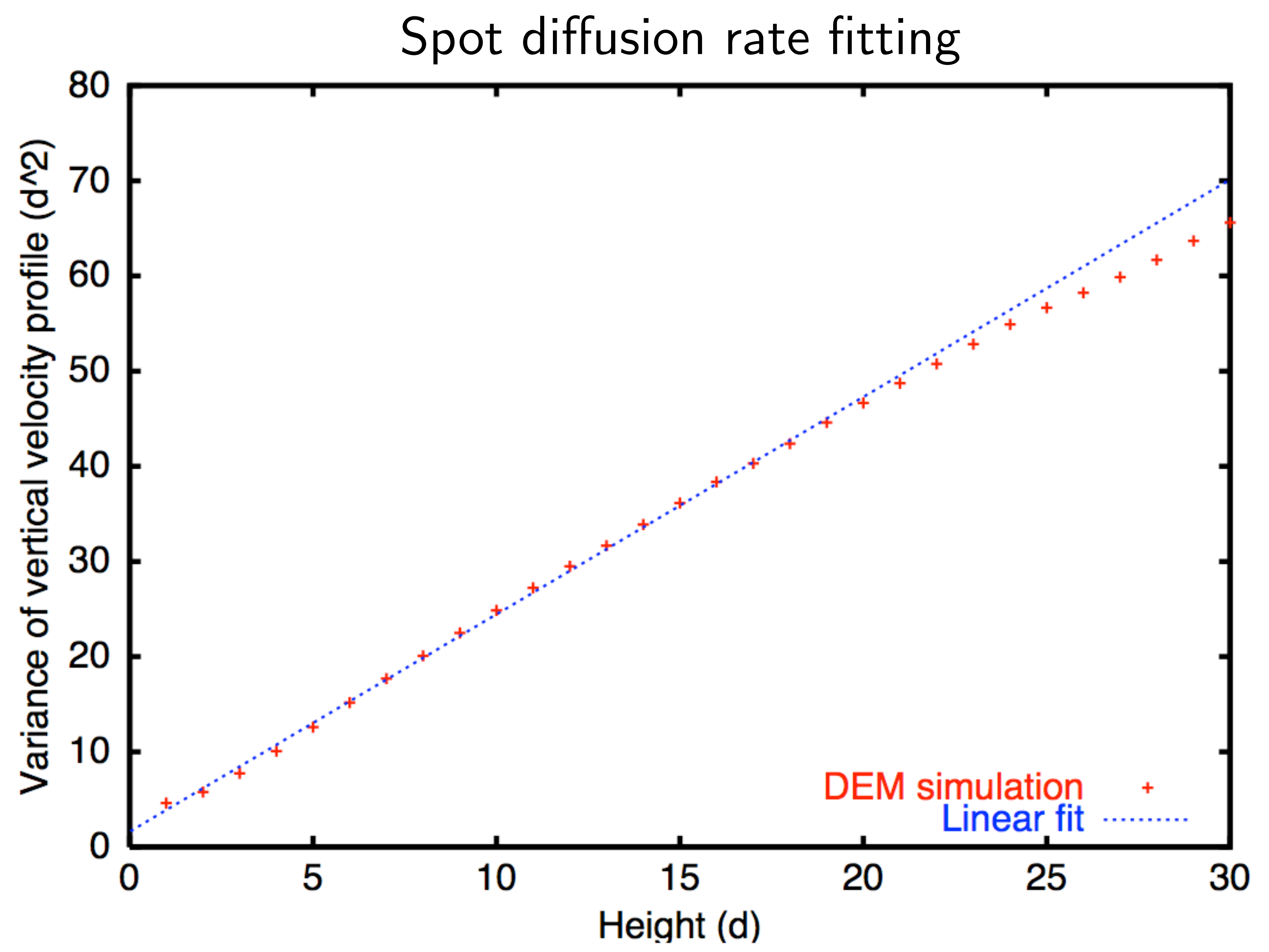
- The combination is a bulk spot motion, while preserving packing geometry
- Not clear *a priori* if this will produce realistic flowing random packings

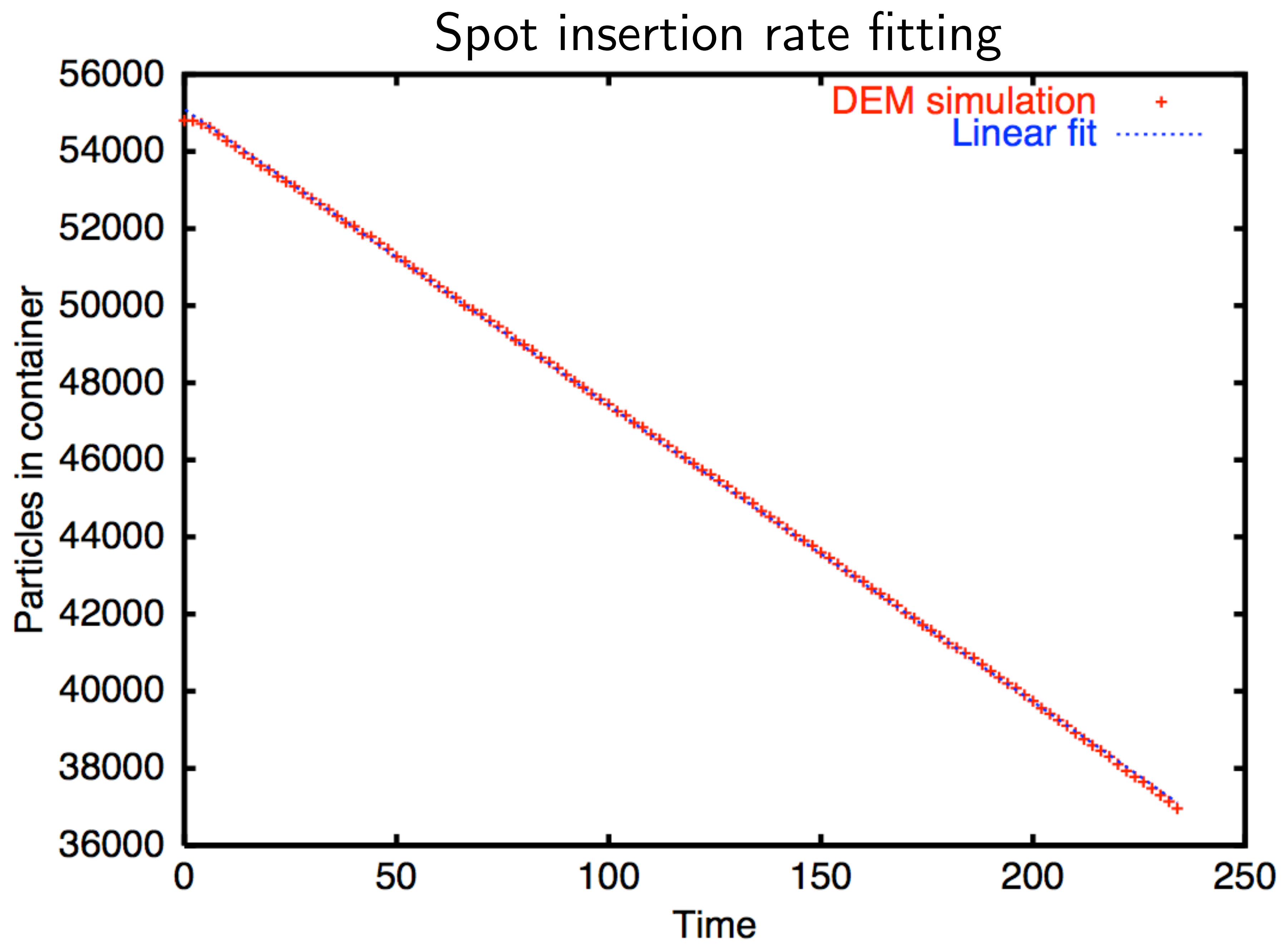
M. Z. Bazant, *The spot model for random-packing dynamics*, Mech. Mat. **38**, 717 (2005).

Choice of spot simulation parameters

- Systematically fit three parameters from DEM:
  - Spot radius R_s
    (from velocity correlations)
  - Spot volume V_s
    (from particle diffusion)
  - Spot diffusion rate b
    (from velocity profile width)

- Two more parameters to capture time dependence:
  - Spot insertion rate
    (from flow rate)
  - Spot velocity
    (from density drop)

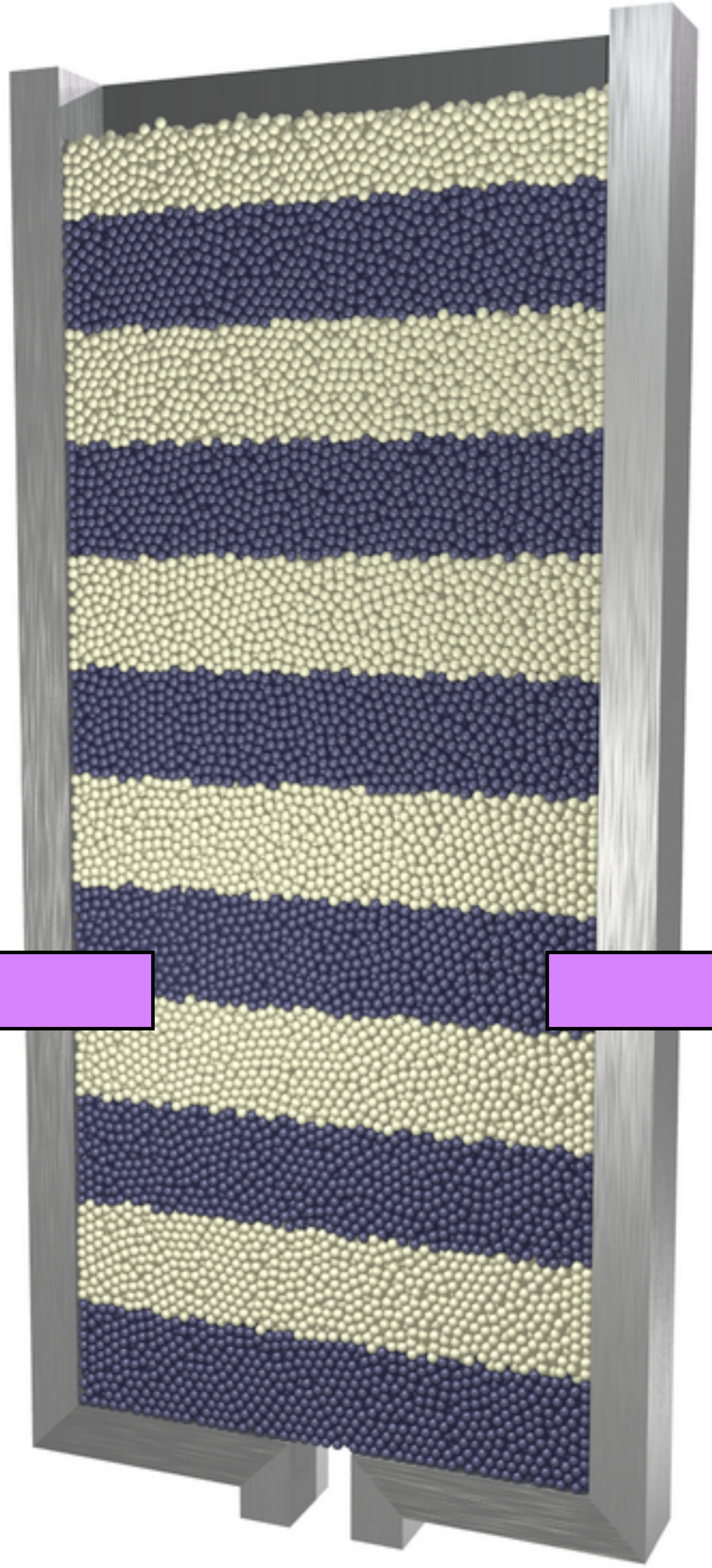




Two very different simulations

DEM

- Particles drained from circular orifice $8d$ across
- Snapshot recorded at fixed intervals
- Run on 24 processors



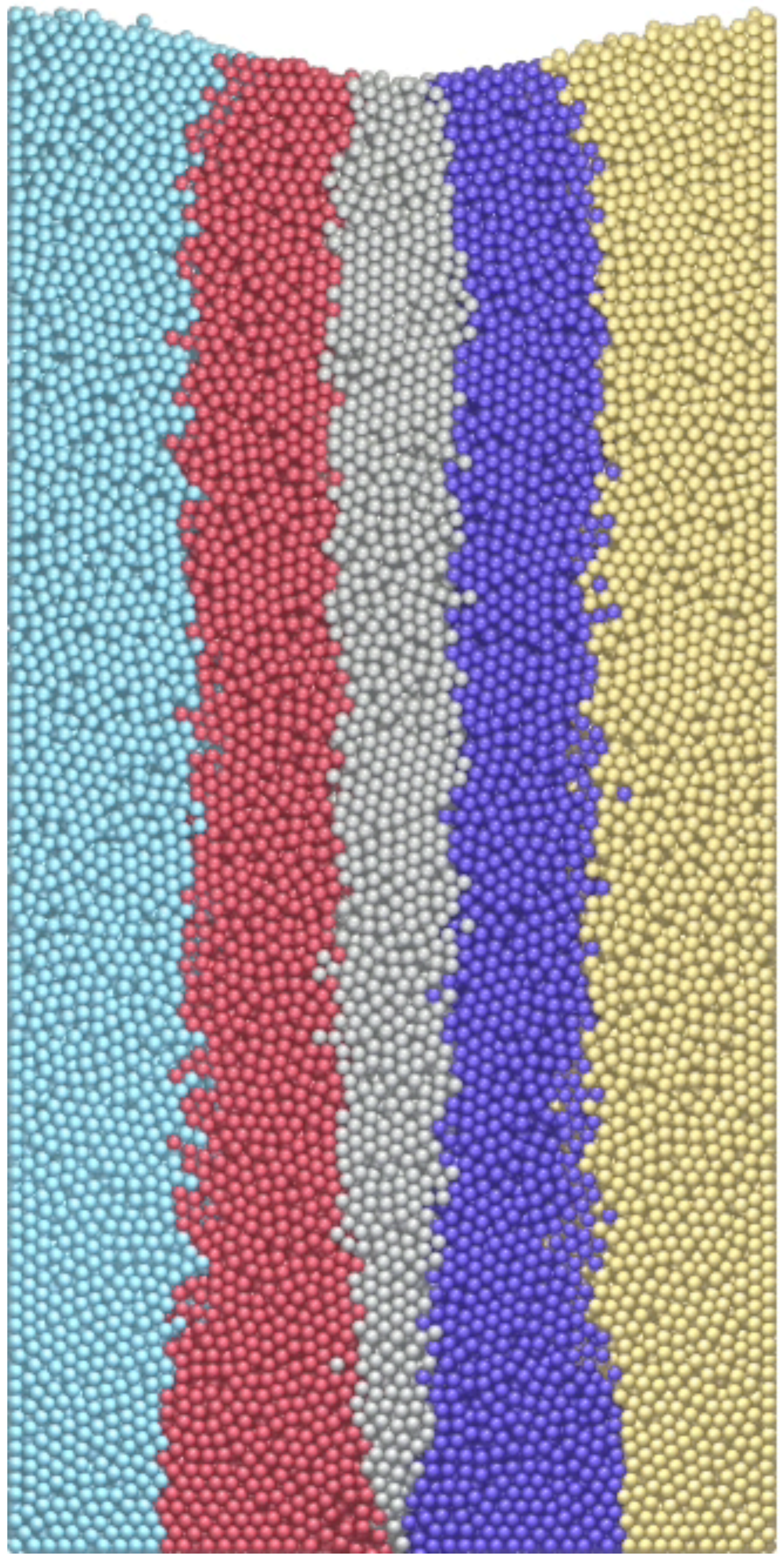
Initial packing of 55000 poured particles from DEM $50d$ by $8d$ by $110d$

Spot

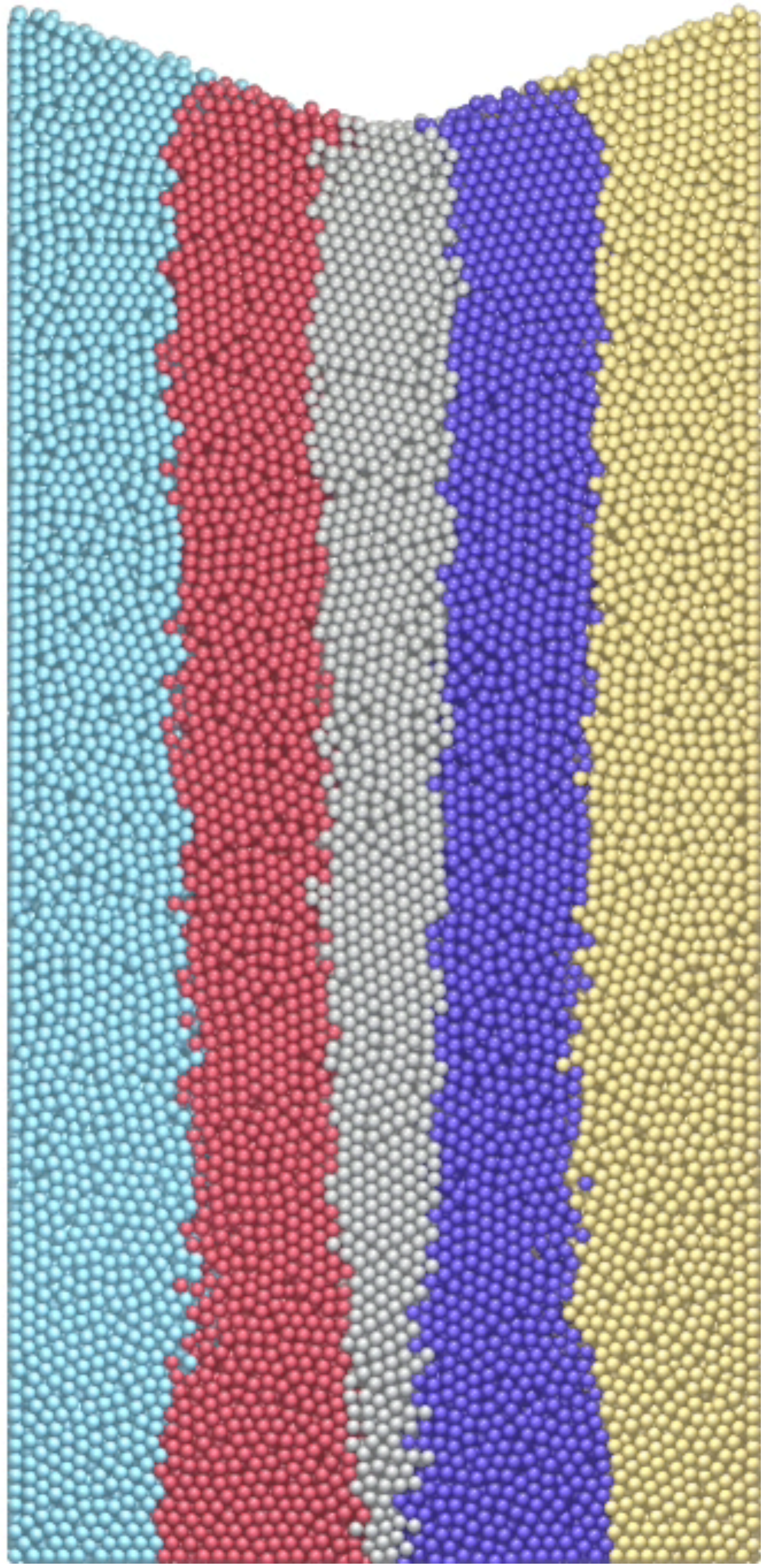
- Spots introduced at orifice
- Event driven
- Spots move upwards and do random walk horizontally
- Calibrate parameters from DEM

Comparison between DEM and spot simulation

- Using the same initial packing in a 50d by 8d by 110d container
- Fitted parameters:
  - $R_s = 2.6d$
  - $V_s = 0.2V_p$
  - $b = 1.14d$
- Reproduces flowing random particle packing with a factor of 100 speedup



DEM simulation
(3 days, 24 processors)



Spot simulation
(8 hours, single processor)

C. H. Rycroft *et al.*, *Dynamics of random packings in granular flow*, Phys. Rev. E **73**, 051306 (2006).
C. H. Rycroft *et al.*, *Fast spot-based multiscale simulations of granular flow*, Powder Technol. **200**, 1–11 (2010).

Question 1: tracking density changes

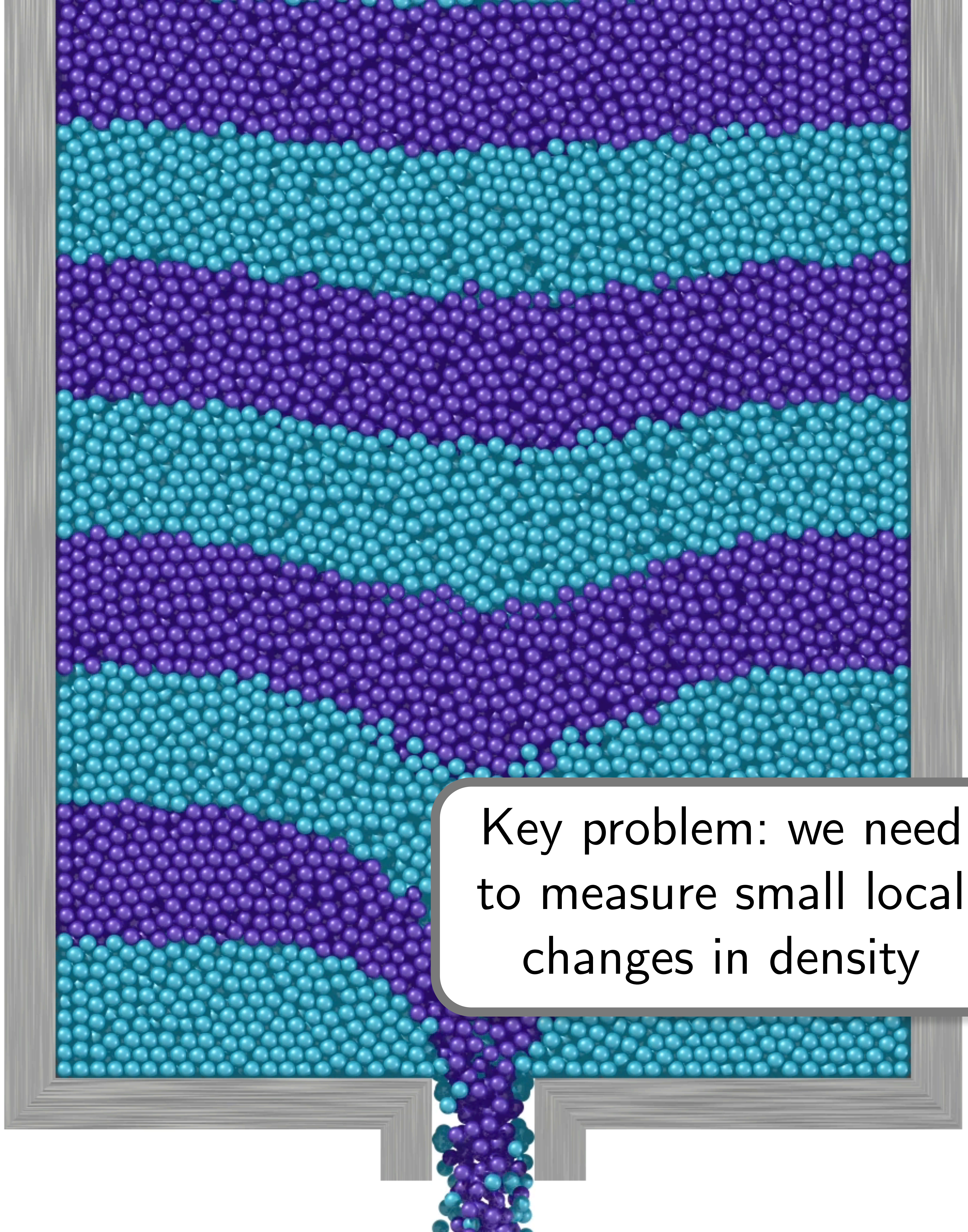
Question

If we believe the spot model, where would expect the packing density to be reduced during flow?

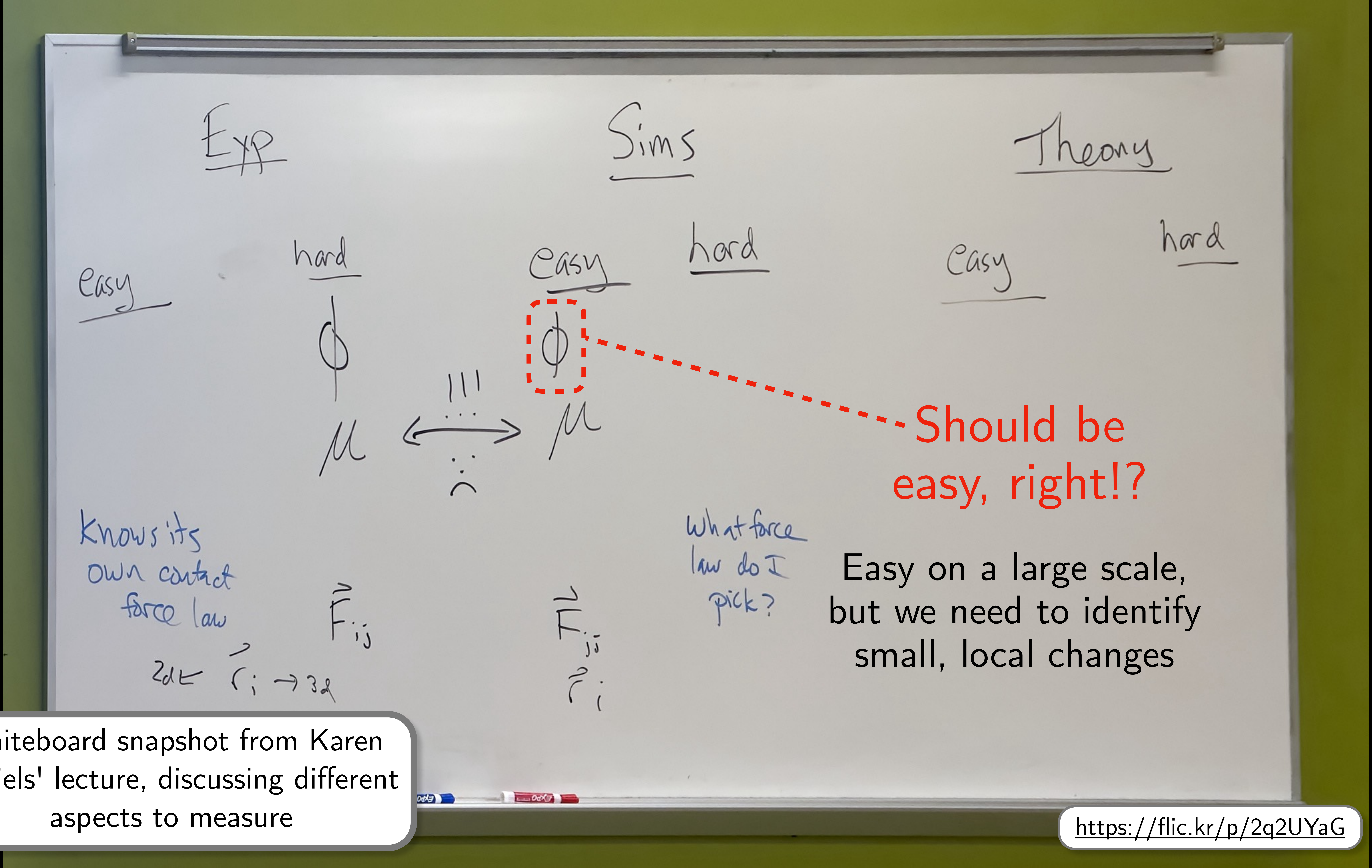
Answer

Spots carry negative volume, and cause downward velocity

We'd expect the largest density drop above the orifice.



Key problem: we need to measure small local changes in density



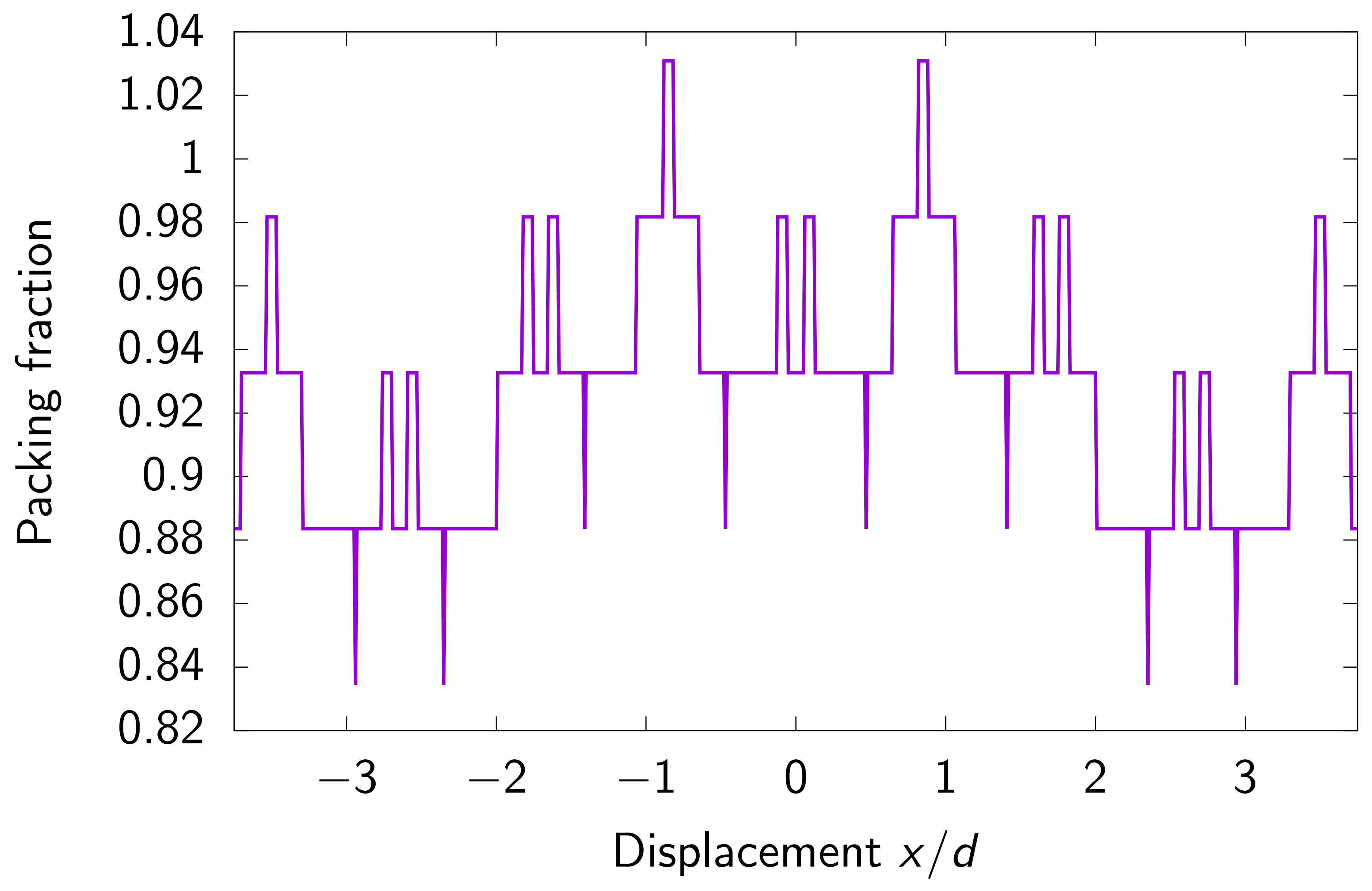
Should be easy, right!?

Easy on a large scale, but we need to identify small, local changes

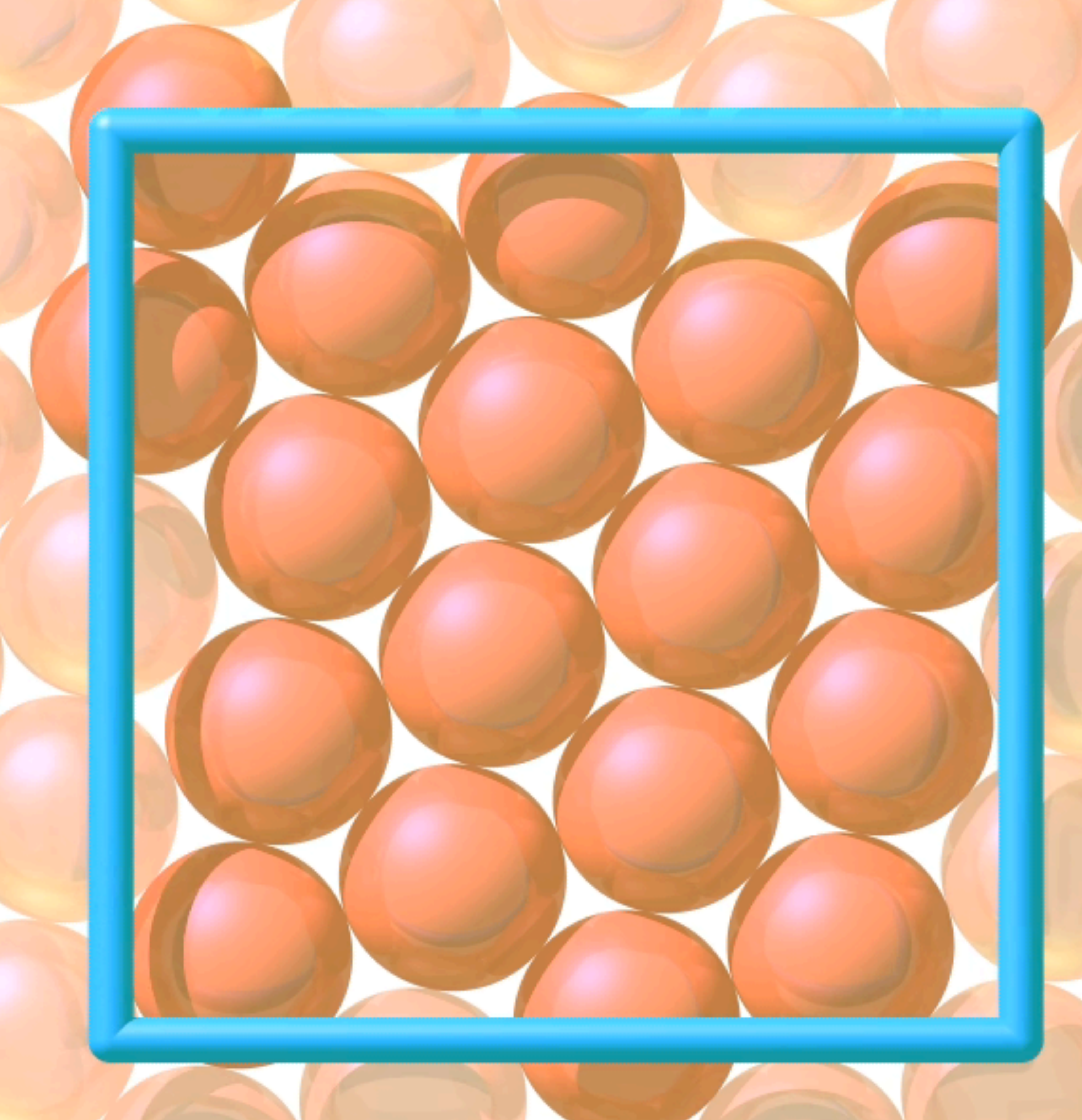
Whiteboard snapshot from Karen Daniels' lecture, discussing different aspects to measure

https://flic.kr/p/2q2UYaG

Measuring 2D density (version 1)

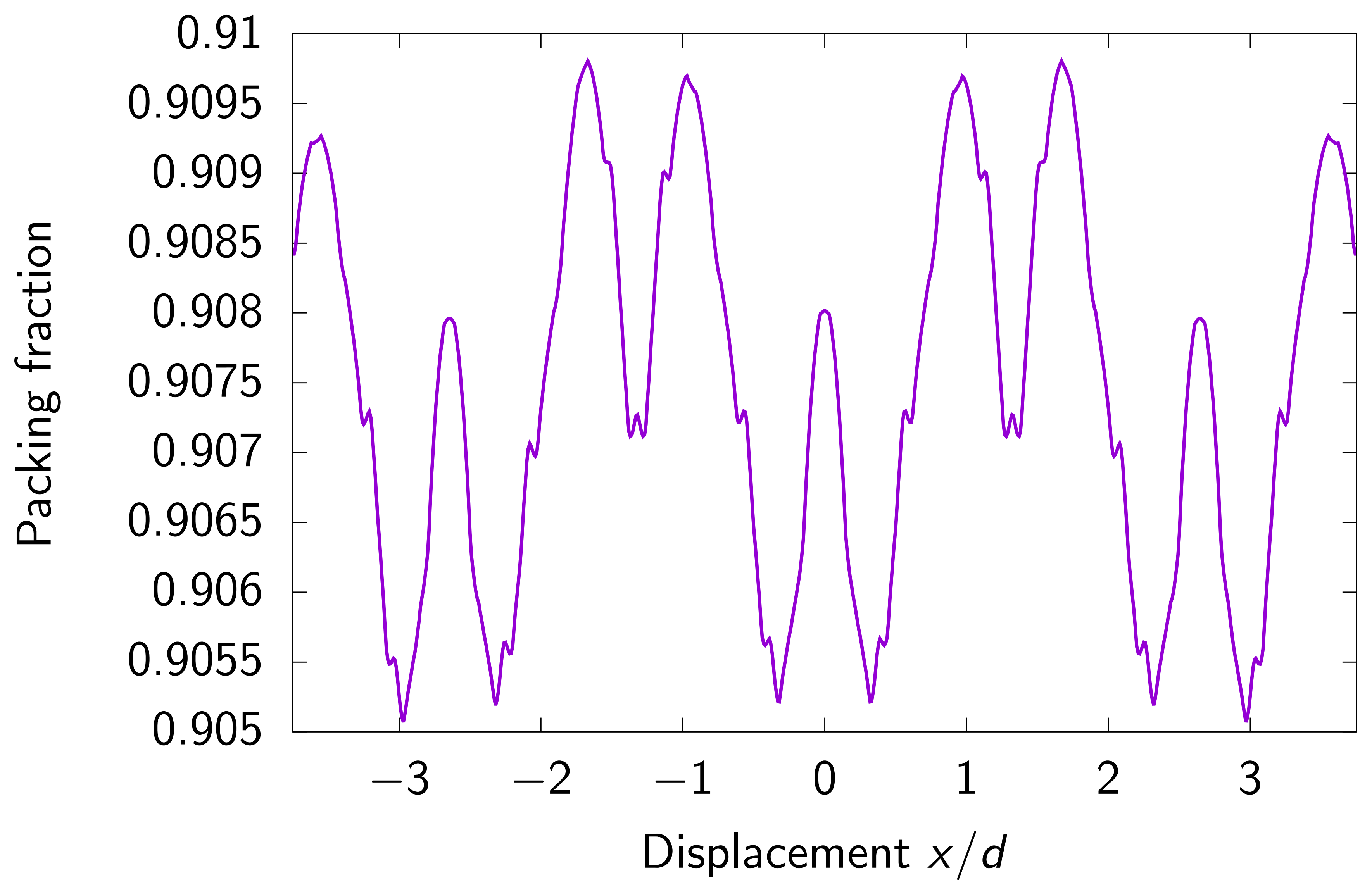


Packing fraction varies by 20%, and sometimes exceeds 100%

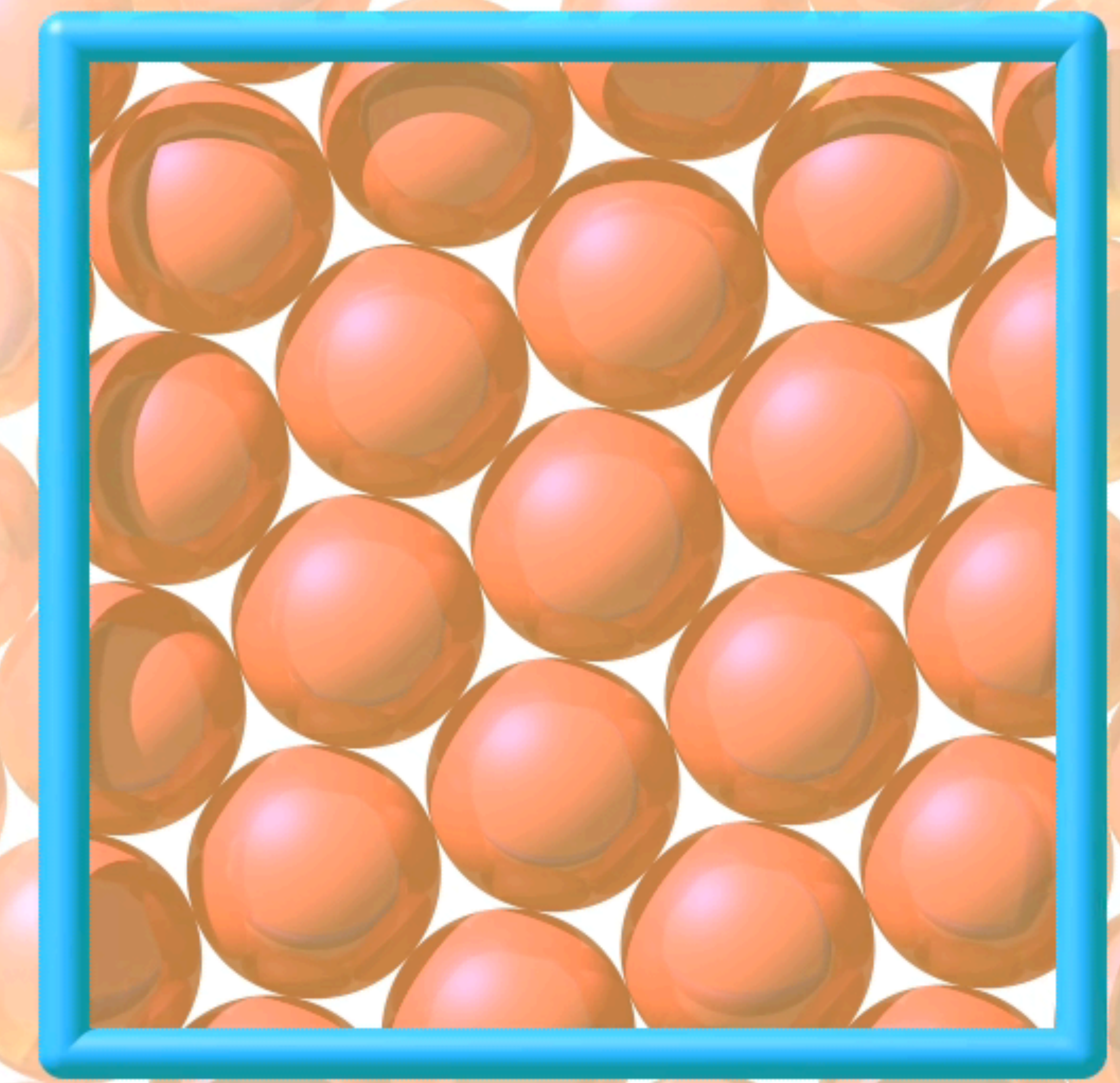


We use **packing fraction**, the proportion of space occupied by particles, as a proxy for density

Measuring 2D density (version 2)



More accurate, but still has variations of 0.5%

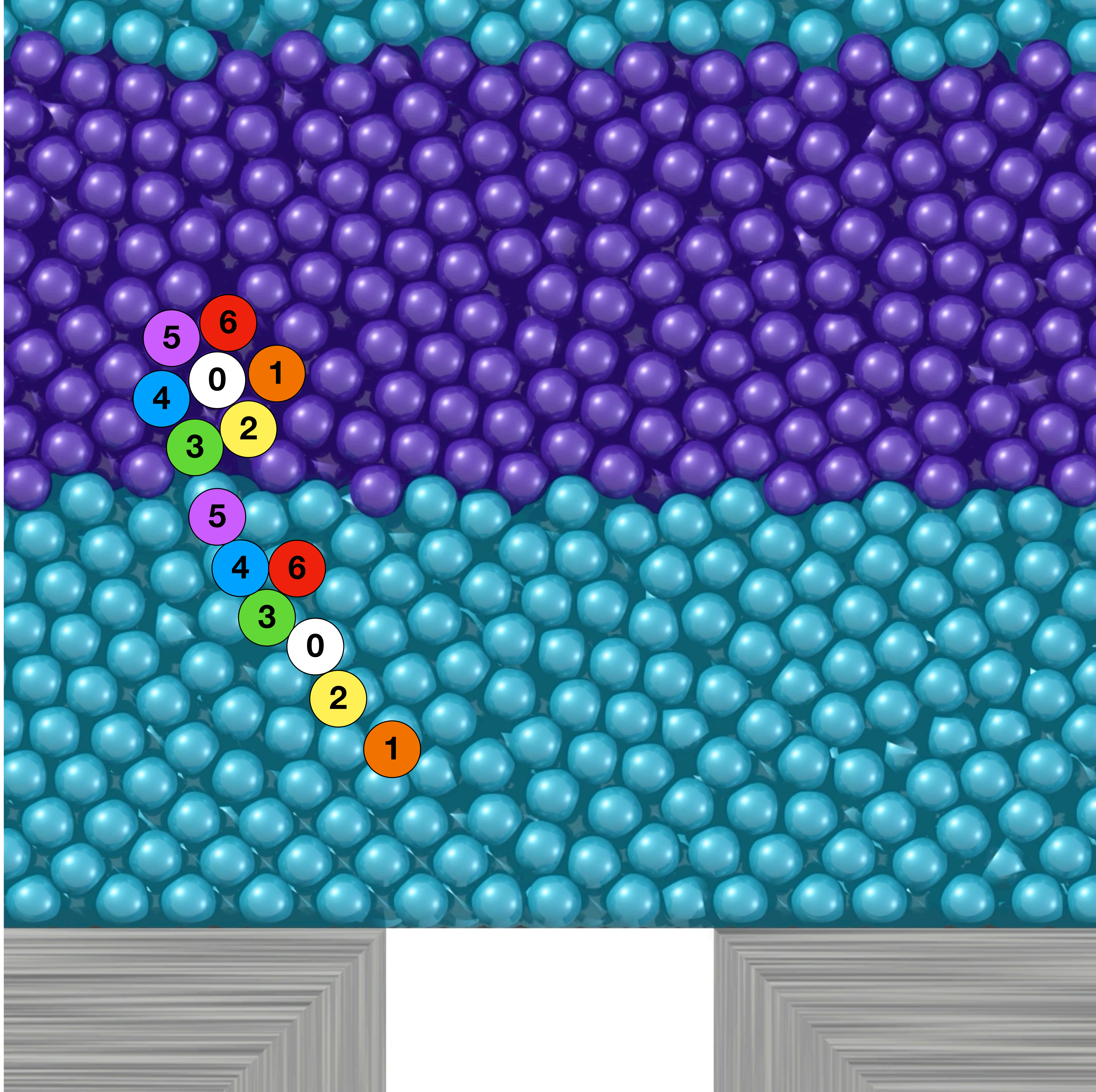


Question 2: packing structure

Question

The DEM simulation realistically models how particles move past each other*

Does the spot model do the same? Are the statistics of neighbor relations similar?



* C. H. Rycroft *et al.*, *Physical test of a particle simulation model in a sheared granular system*, Phys. Rev. E **80**, 031305 (2009).

Question 2: packing structure

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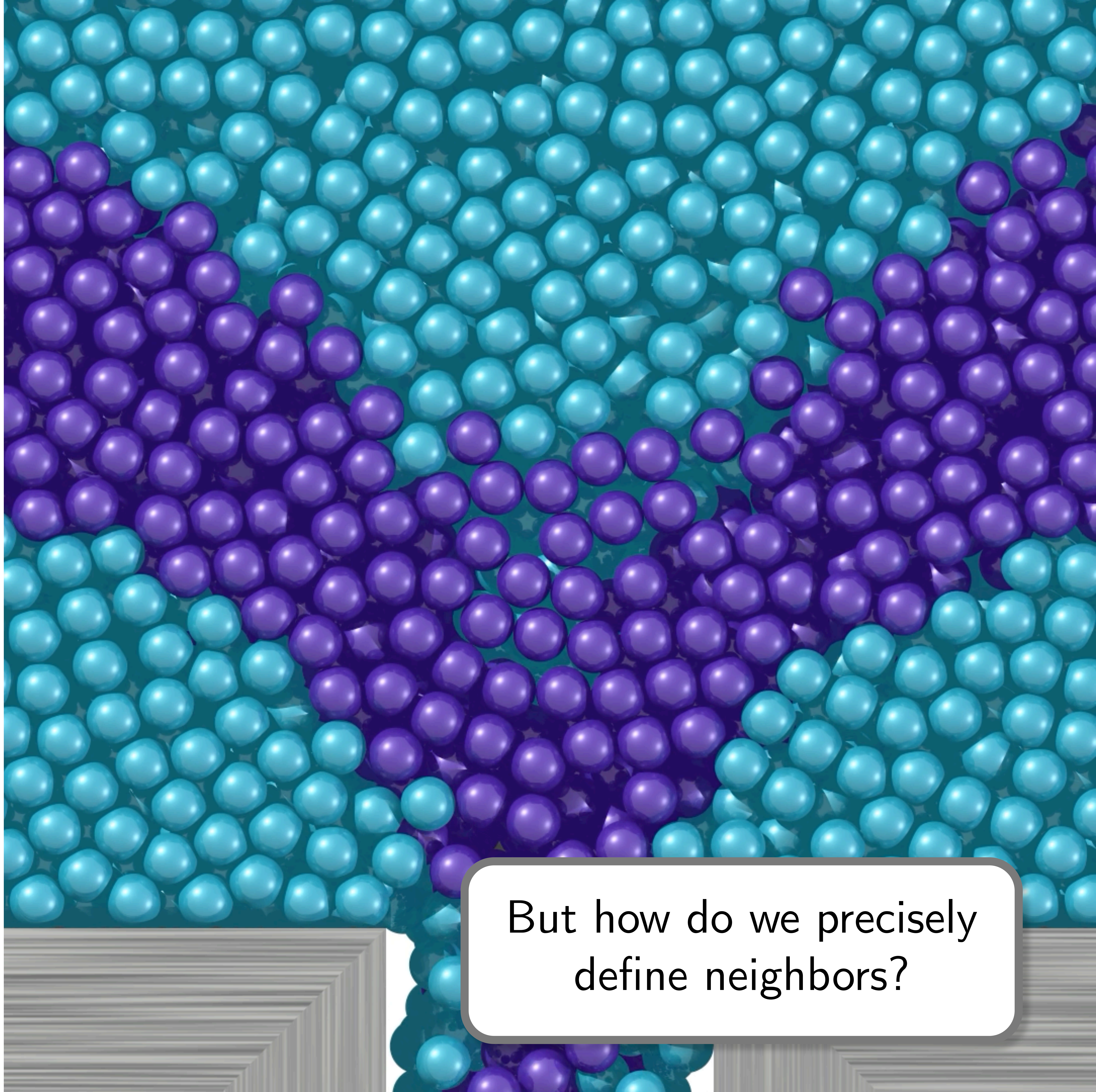
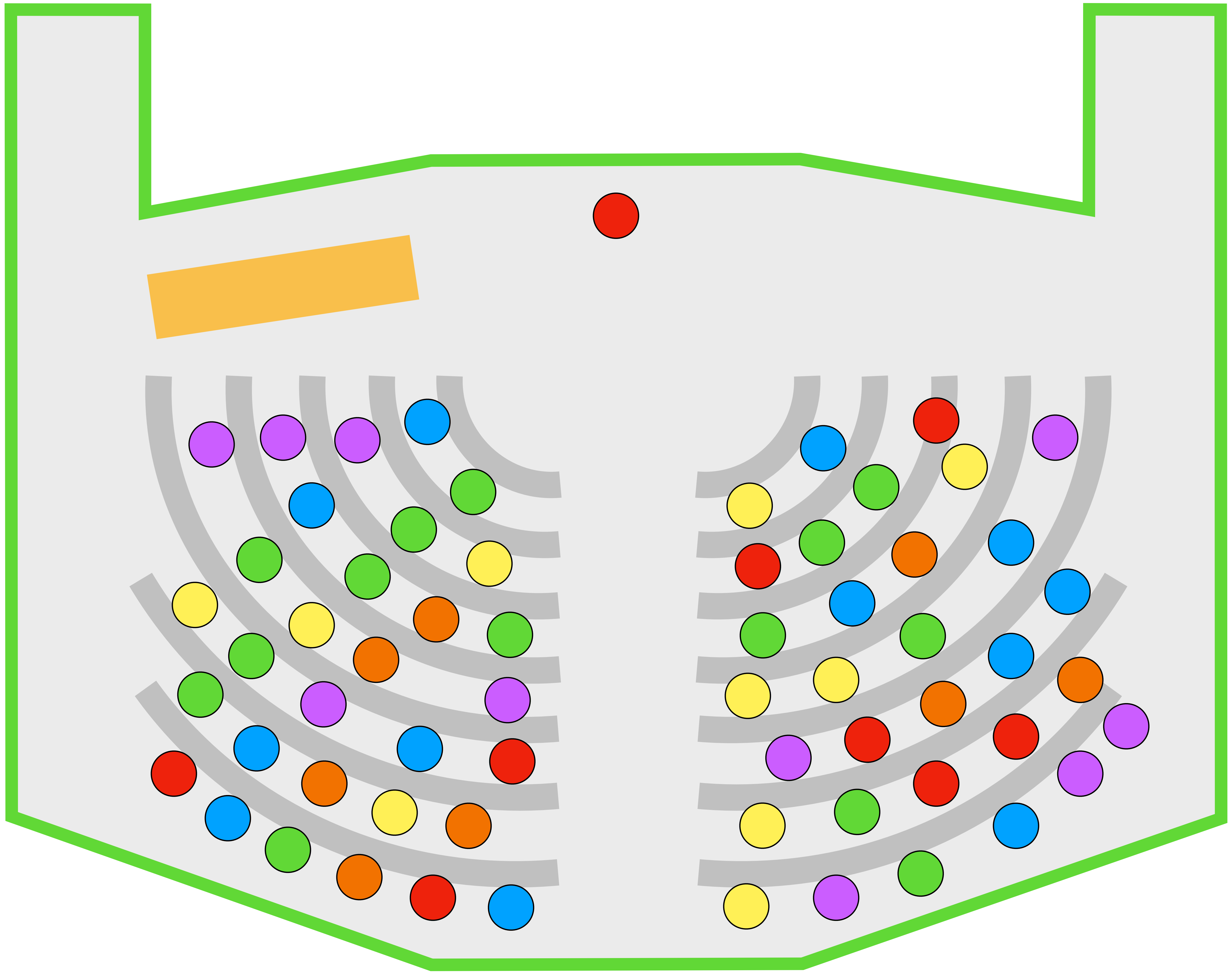


* C. H. Rycroft *et al.*, *Physical test of a particle simulation model in a sheared granular system*, Phys. Rev. E **80**, 031305 (2009).

Neighbor relations test

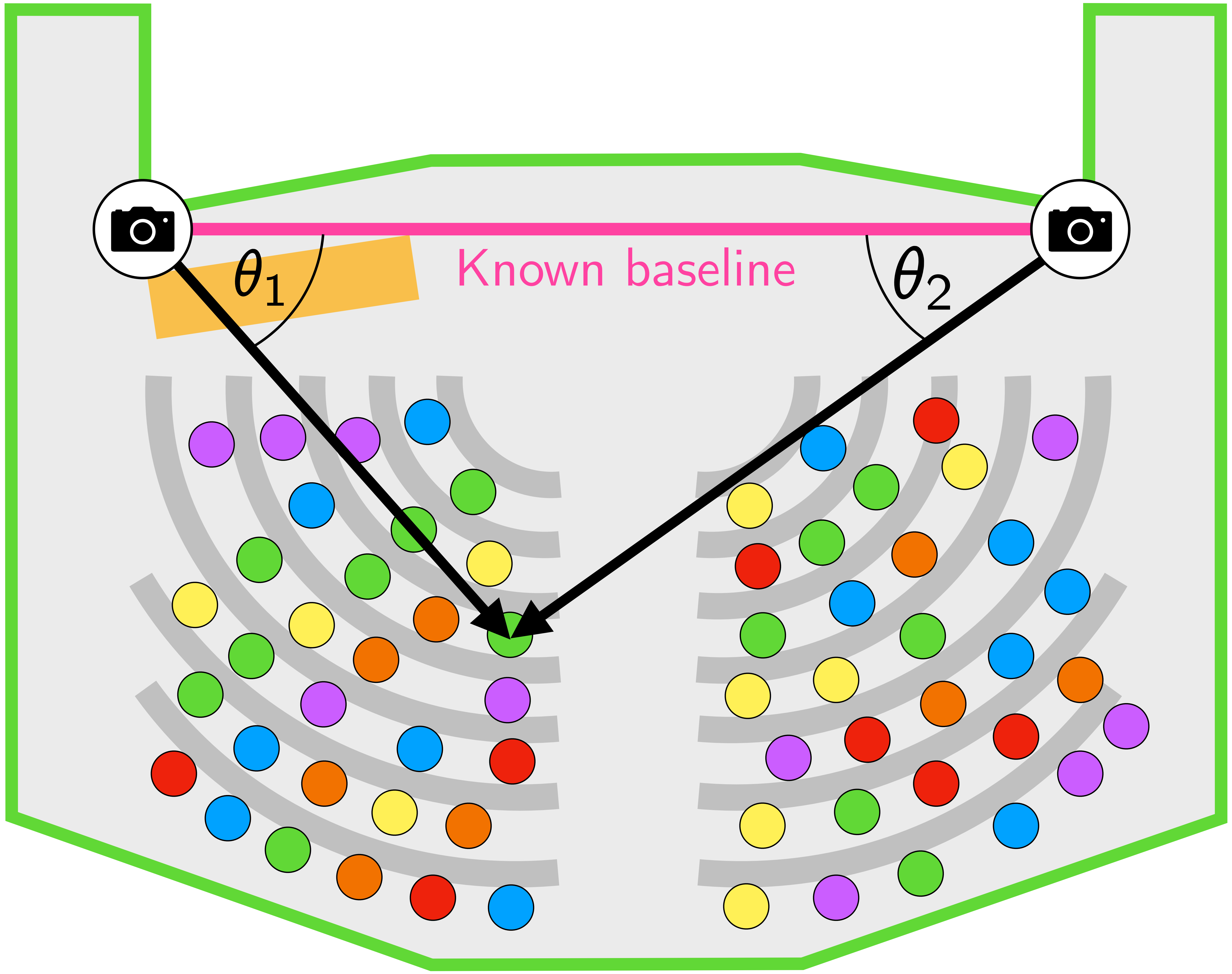
- Suppose everyone in the room is a particle
- Who would you define as your particle neighbors?
- I will give everyone a rainbow-colored ID number
- Please hold it up, and write down in **A** the IDs of all of your neighbors



The lecture room

Triangulation

- I am going to build a map of particle positions using triangulation
- From photos at two ends of a known baseline, I can determine everyone's position
- I will build a map visualizing the neighbor relations



The lecture room

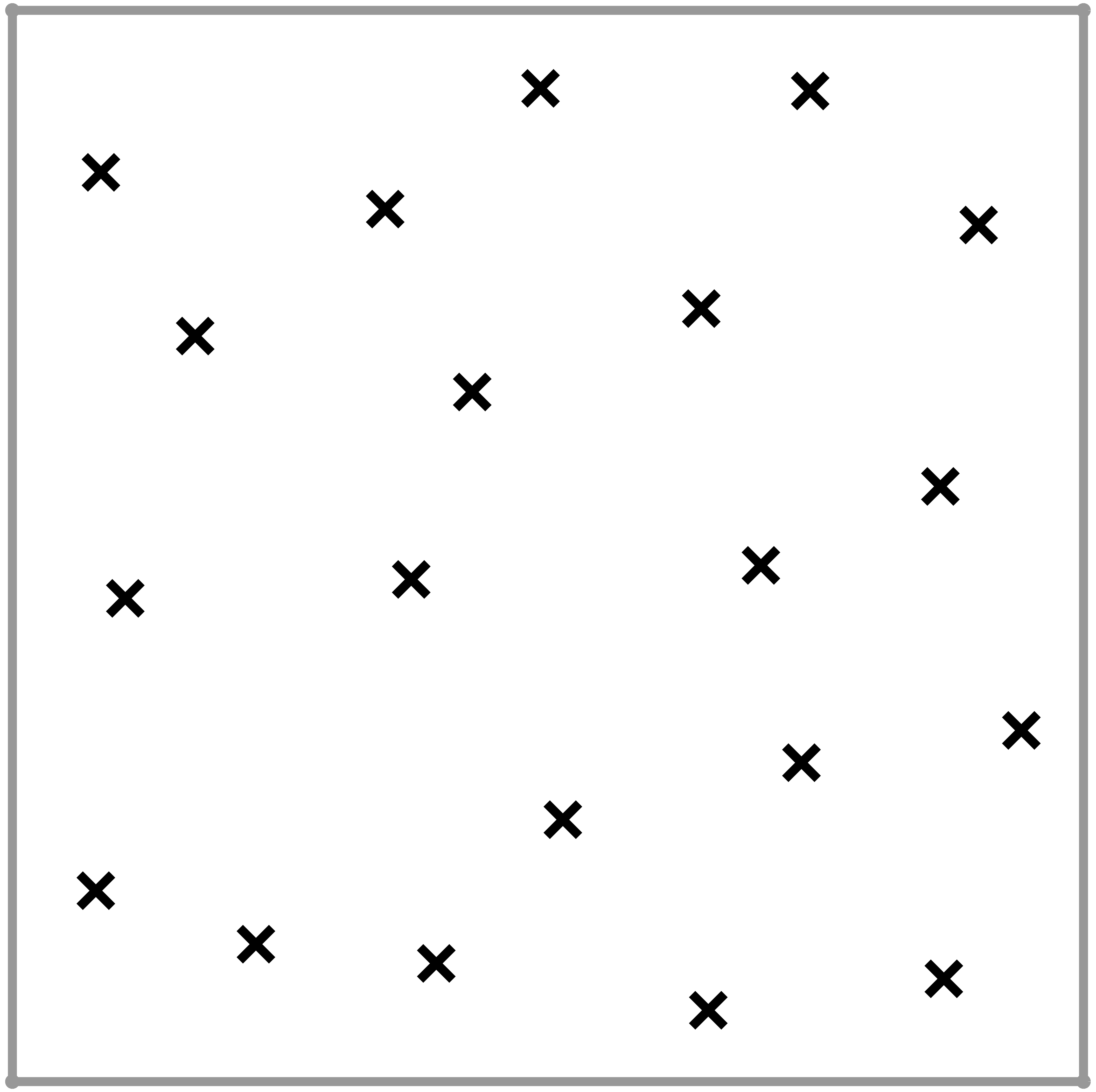
A technique from computational geometry

- Consider a domain Ω with distance metric d, and introduce a set of points x_i
- The Voronoi cell for point* x_i is the space x that satisfies

$$d(x, x_i) < d(x, x_j)$$

  for any $j \neq i$

- Together the Voronoi cells form the Voronoi tessellation of Ω



* We can think of *point* and *particle* as synonymous in this definition

A. Okabe *et al.*, *Spatial tessellations: Concepts and Applications of Voronoi Diagrams*, Wiley, 2000.
E. A. Lazar *et al.*, *Voronoi cell analysis: the shapes of particle systems*, Am. J. Phys. **90**, 469 (2022).

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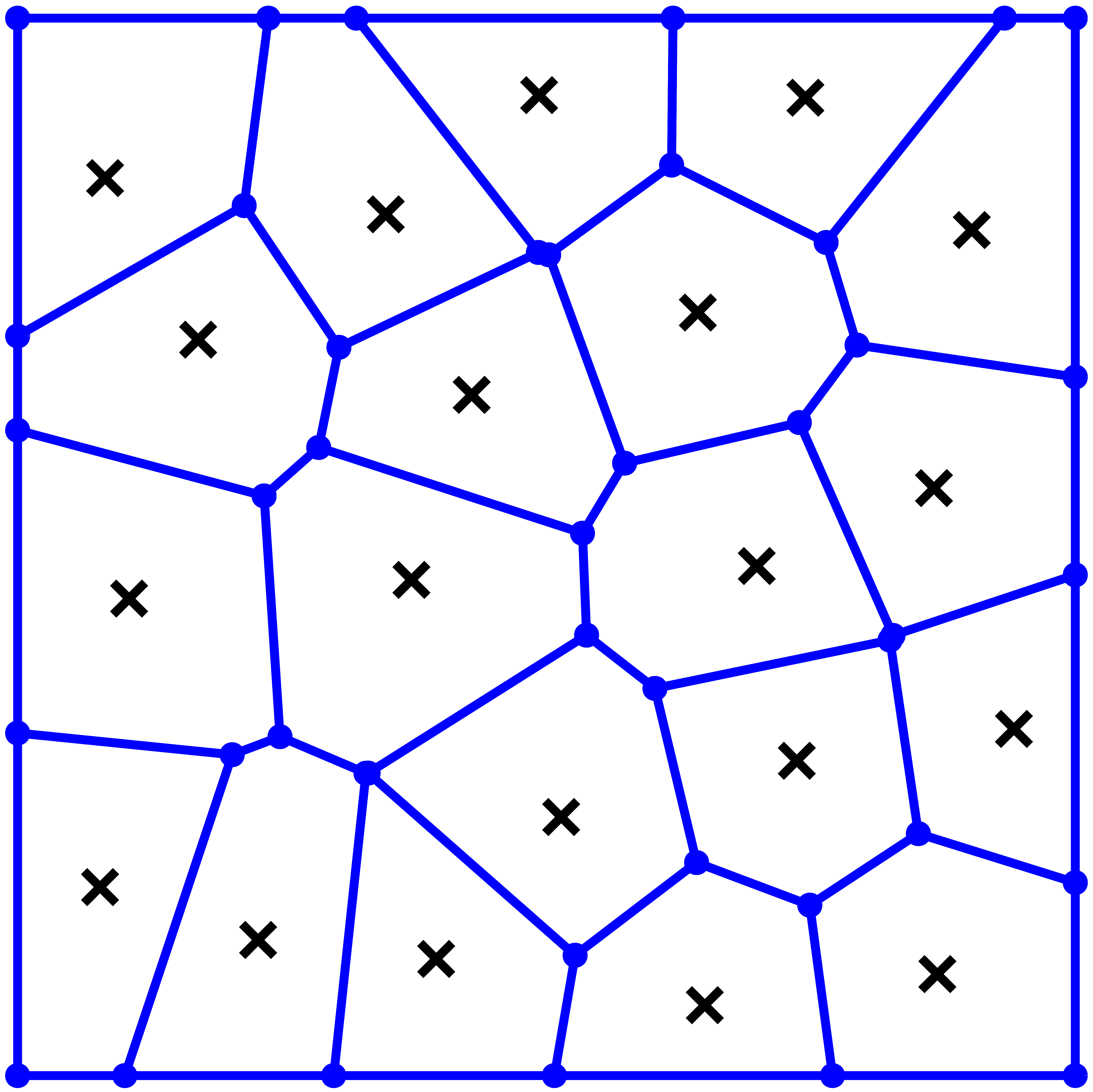

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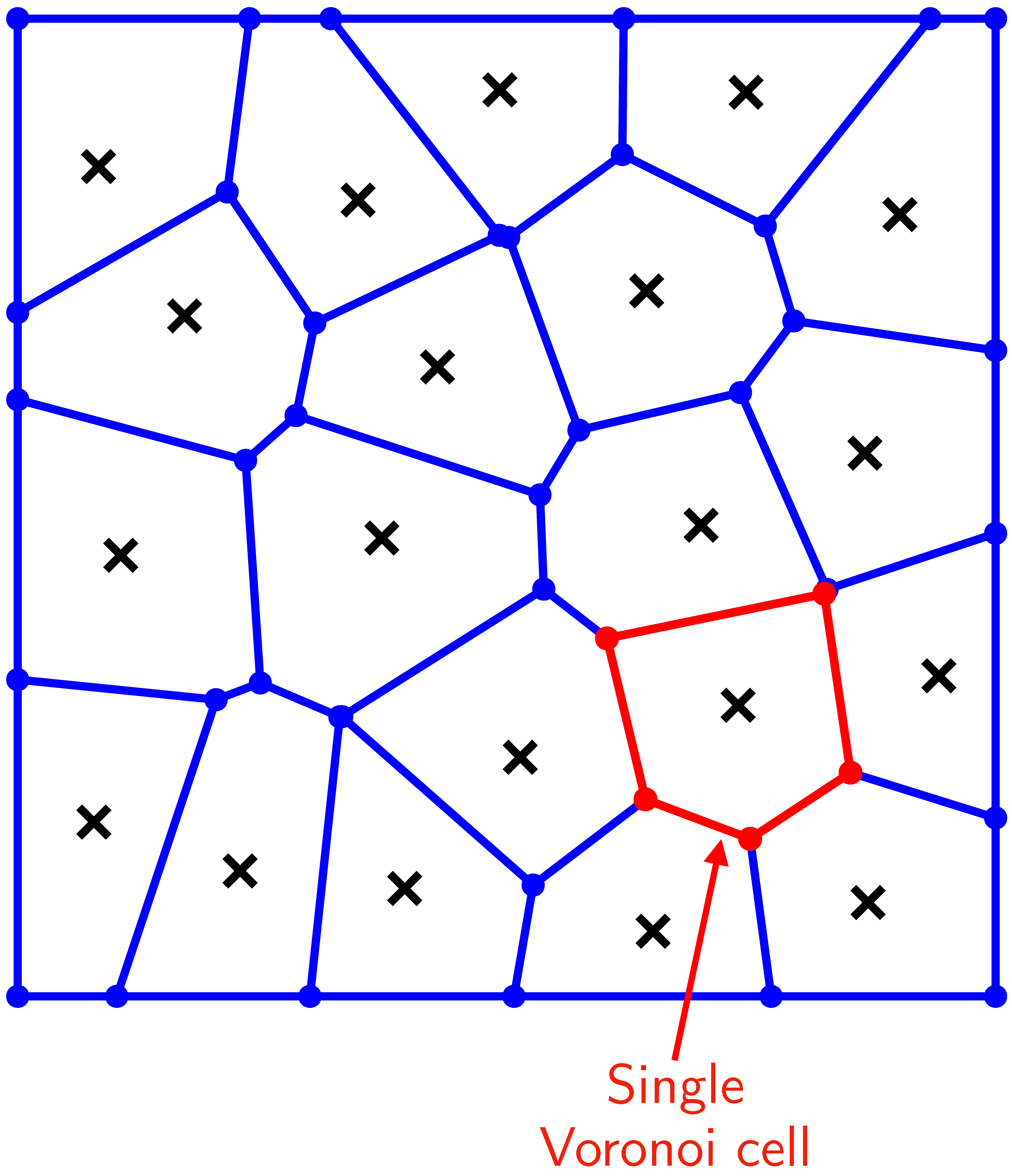
for any $j \neq i$

- Together the Voronoi cells form the Voronoi tessellation of Ω



* We can think of *point* and *particle* as synonymous in this definition

A. Okabe *et al.*, *Spatial tessellations: Concepts and Applications of Voronoi Diagrams*, Wiley, 2000.

E. A. Lazar *et al.*, *Voronoi cell analysis: the shapes of particle systems*, Am. J. Phys. **90**, 469 (2022).

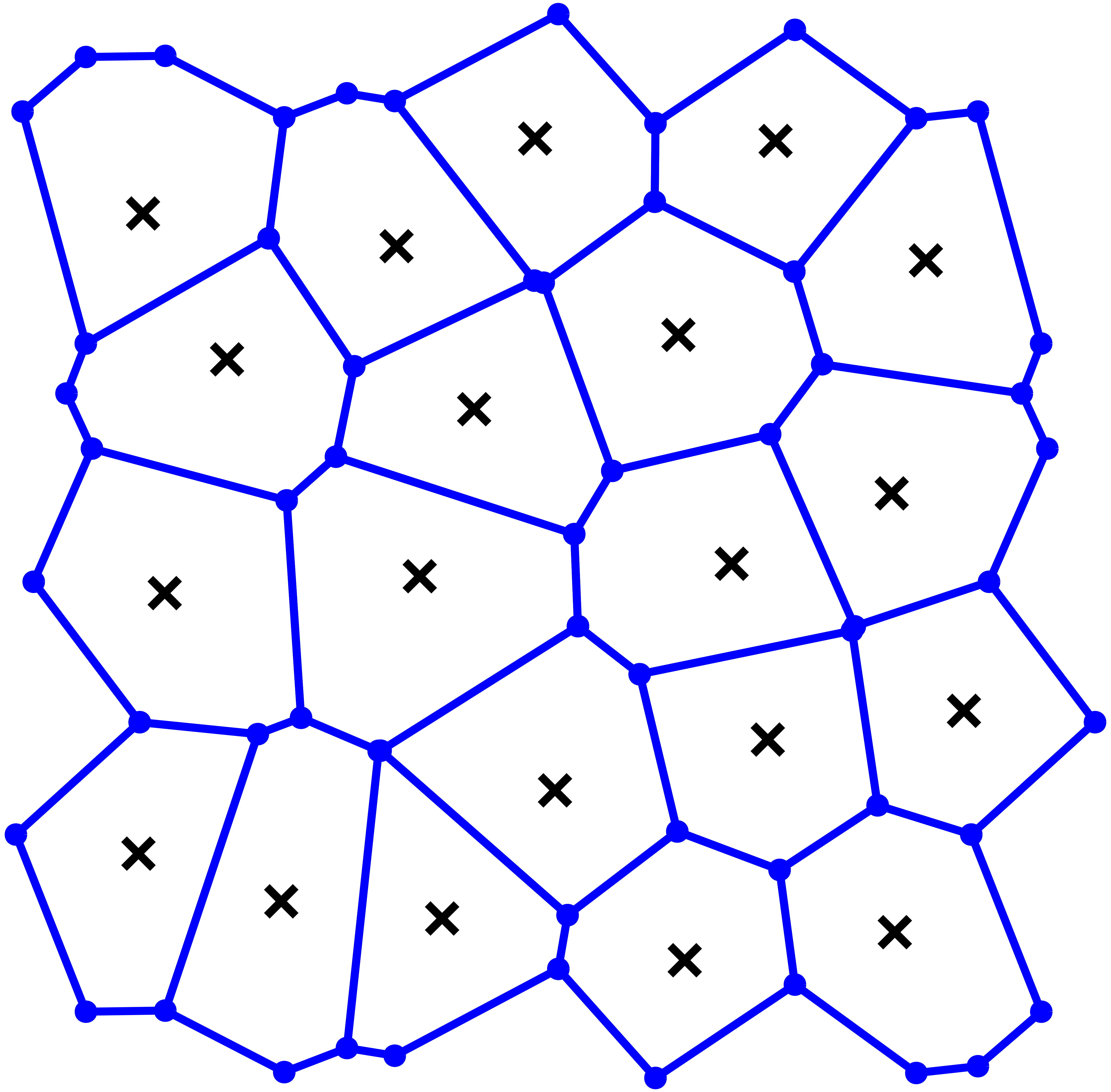
A technique from computational geometry

- Consider a domain Ω with distance metric d, and introduce a set of points x_i
- The Voronoi cell for point* x_i is the space x that satisfies

$$d(x, x_i) < d(x, x_j)$$

for any $j \neq i$

- Together the Voronoi cells form the Voronoi tessellation of Ω



(Can also use periodic boundary conditions)

* We can think of *point* and *particle* as synonymous in this definition

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Some history

- Developed by Georgy Voronyi (1868–1908) in Imperial Russia (present day Ukraine)
- Introduced in two pure mathematics papers in 1908
- Commemorated in 2008 in Ukraine with two-hryvnia coin

G. Voronoï, *Nouvelles applications des paramètres continus à la théorie des formes quadratiques. Premier mémoire ...*, J. reine angew. Math. **133**, 97–179 (1908).
G. Voronoï, *Nouvelles applications des paramètres continus à la théorie des formes quadratiques. Deuxième mémoire ...*, J. reine angew. Math. **134**, 198–287 (1908).

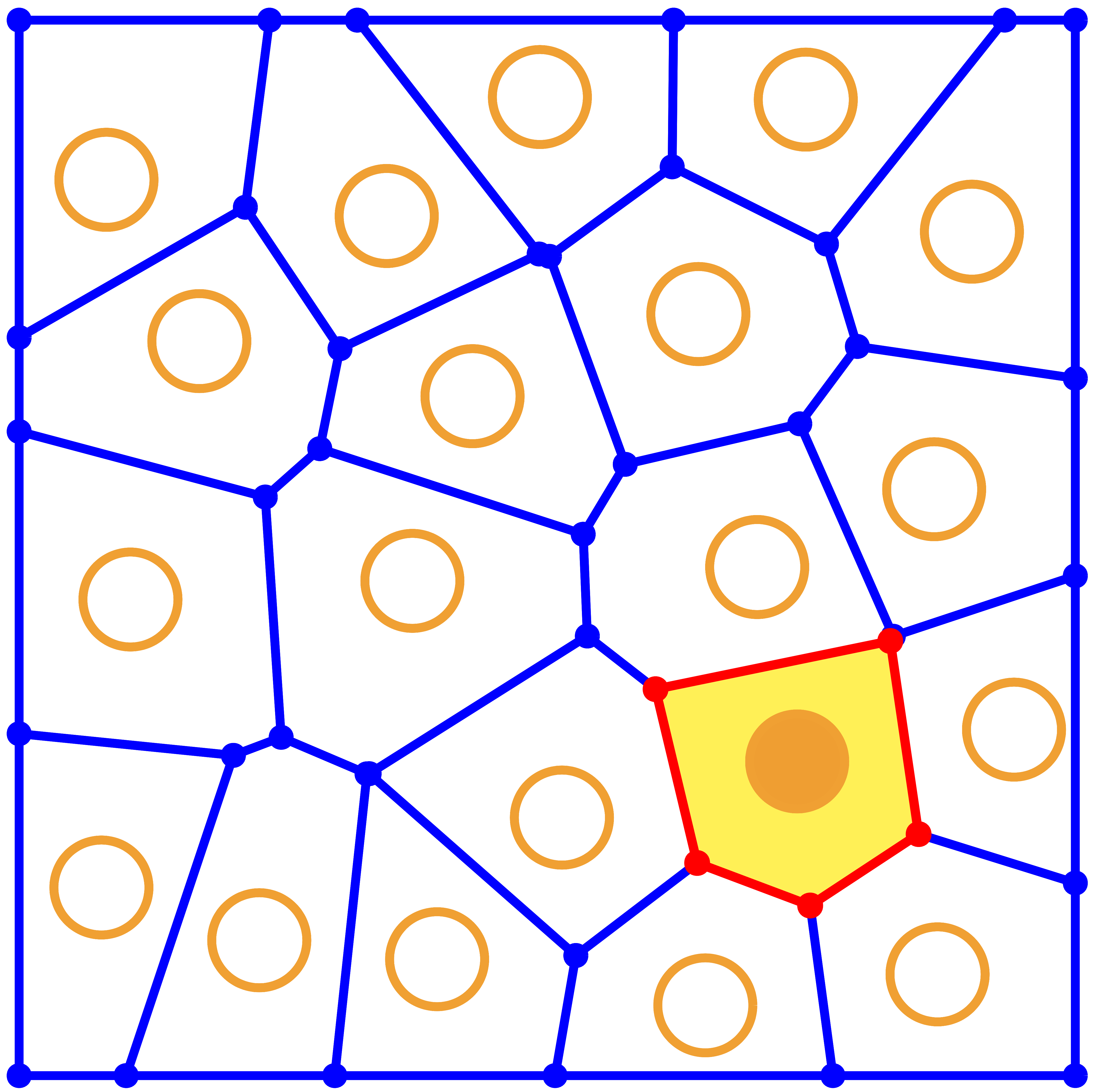
Accurate density measurements

- The Voronoi tessellation provides method to compute the packing fraction ϕ accurately

- For a single particle, measure packing fraction as

$$\phi = \frac{\text{Particle volume}}{\text{Voronoi cell volume}}$$

- Could also be average over several particles and Voronoi cells



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Revisiting 2D hexagonal packing

Each particle has area

$$V_p = \frac{\pi d^2}{4}$$

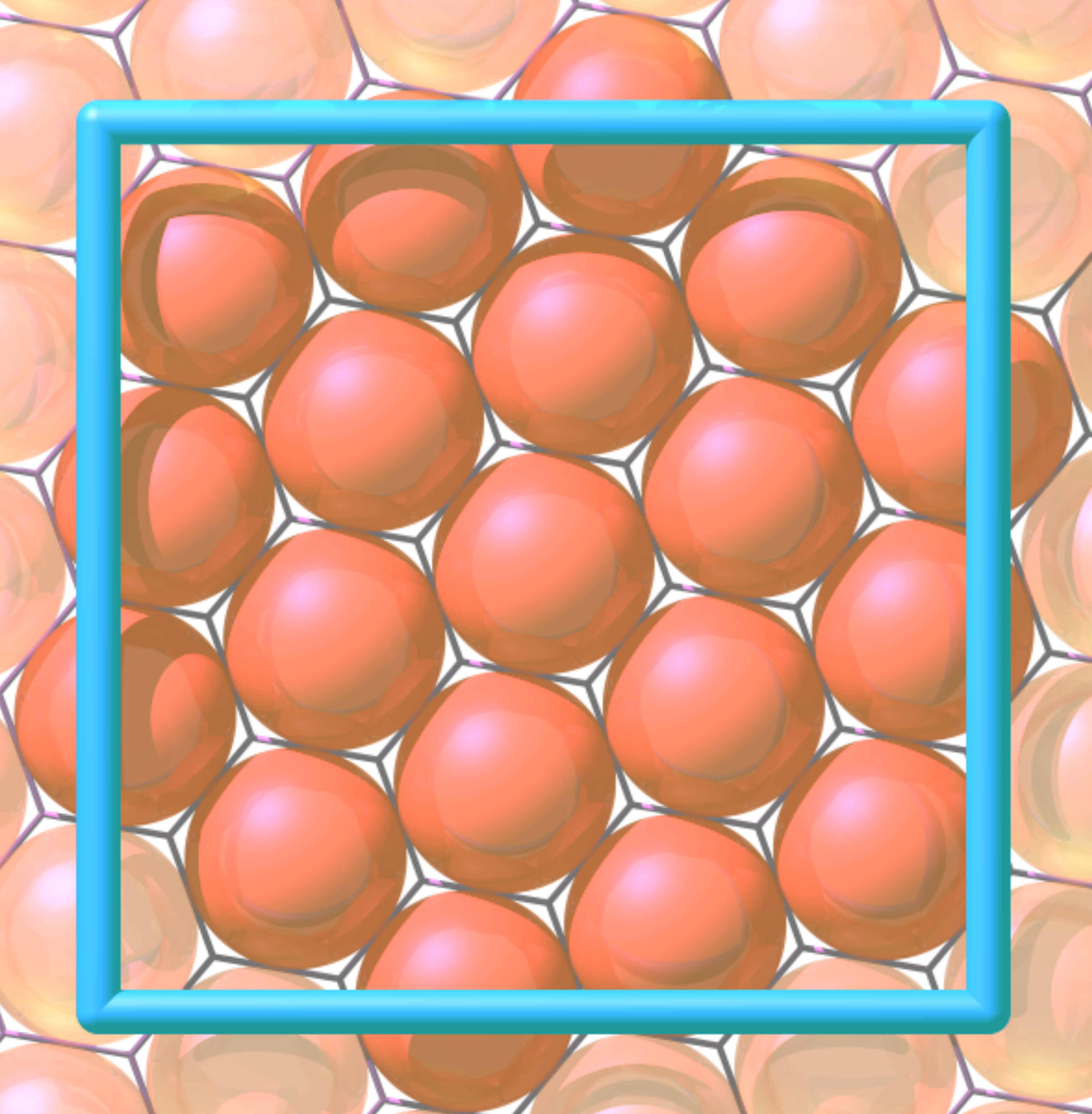
Computing the Voronoi cells

The Voronoi cells will all be regular hexagons

Each has area

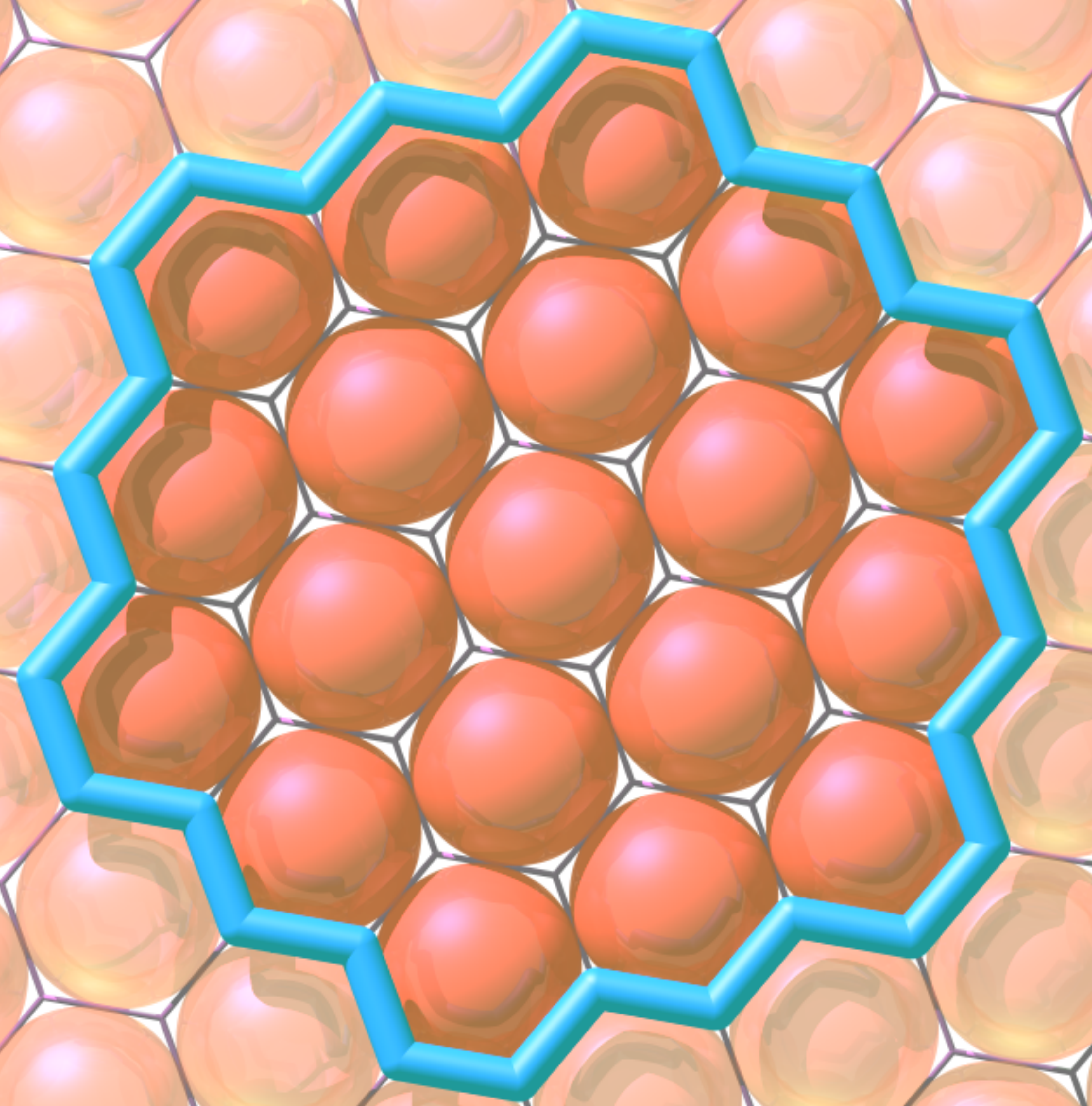
$$V_c = \frac{d^2\sqrt{3}}{2}$$

Examining particles within test box



Consider all of the 19 particles and Voronoi cells within a box

Examining particles within test box



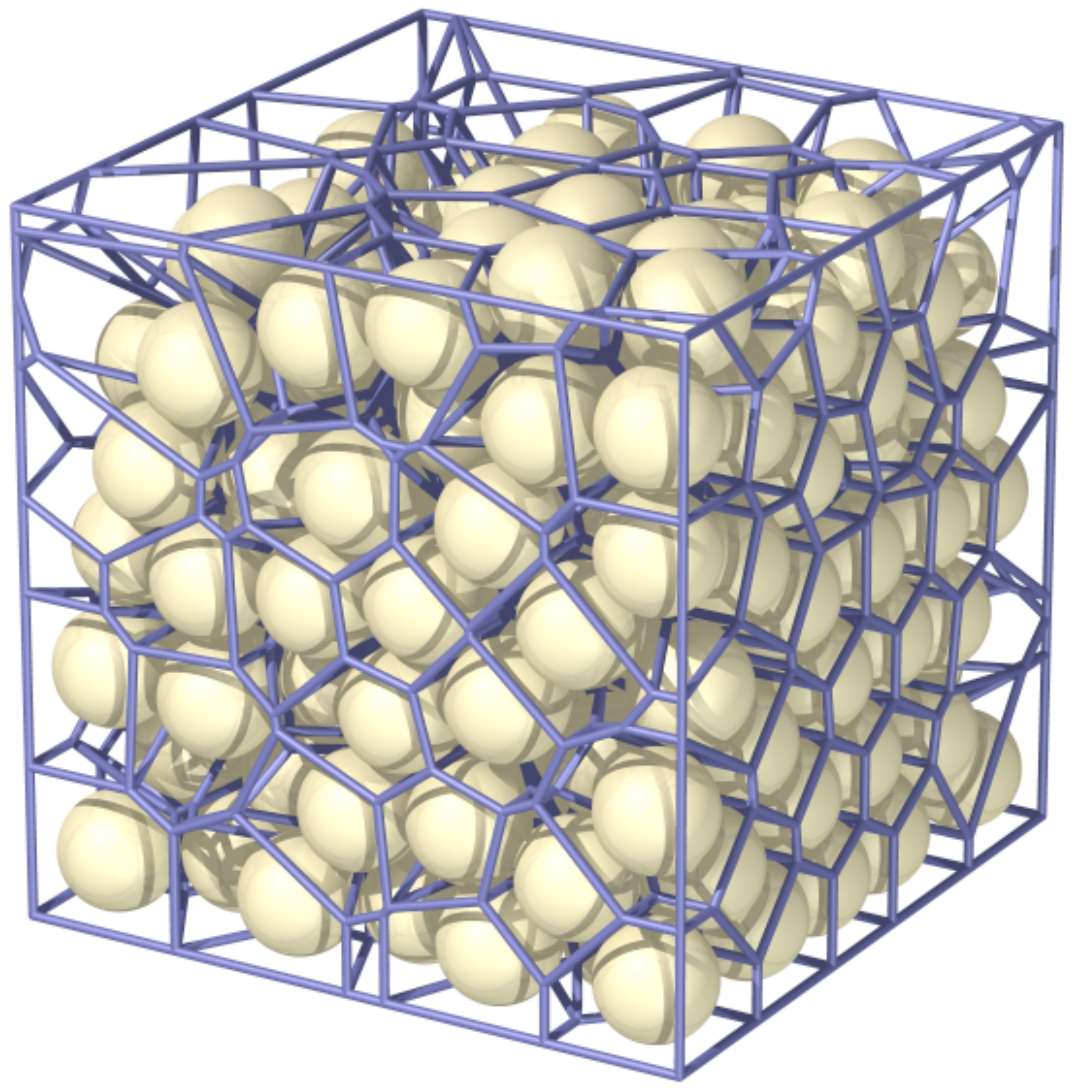
Calculate packing fraction based on

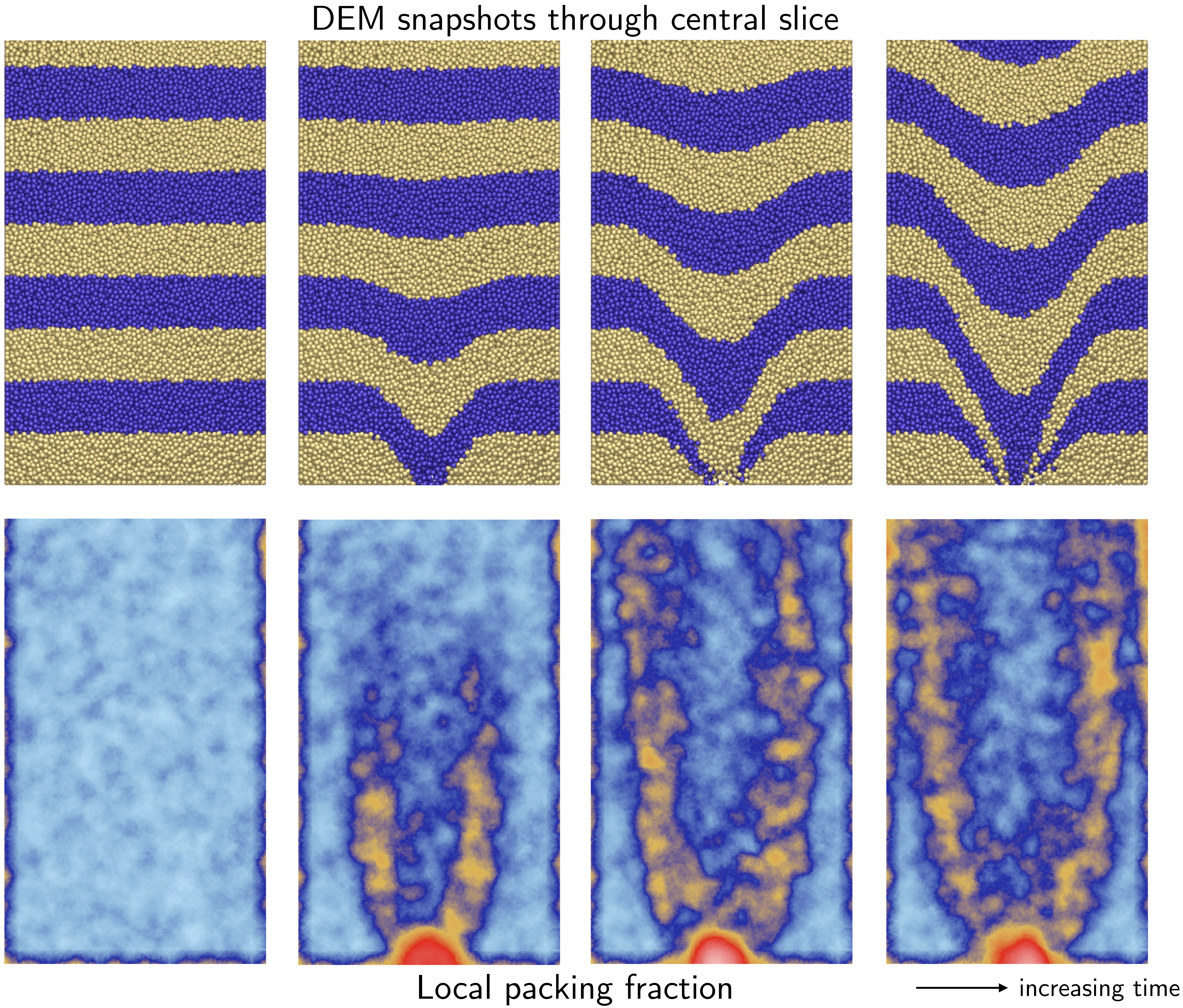
$$\phi = \frac{19V_p}{19V_c} = \frac{\pi}{2\sqrt{3}}$$
$$= 90.69\%$$

Even based on a single particle, this precisely matches the asymptotic value for large regions

Density variations

based on 3D Voronoi cell volumes in local patches





Density variations

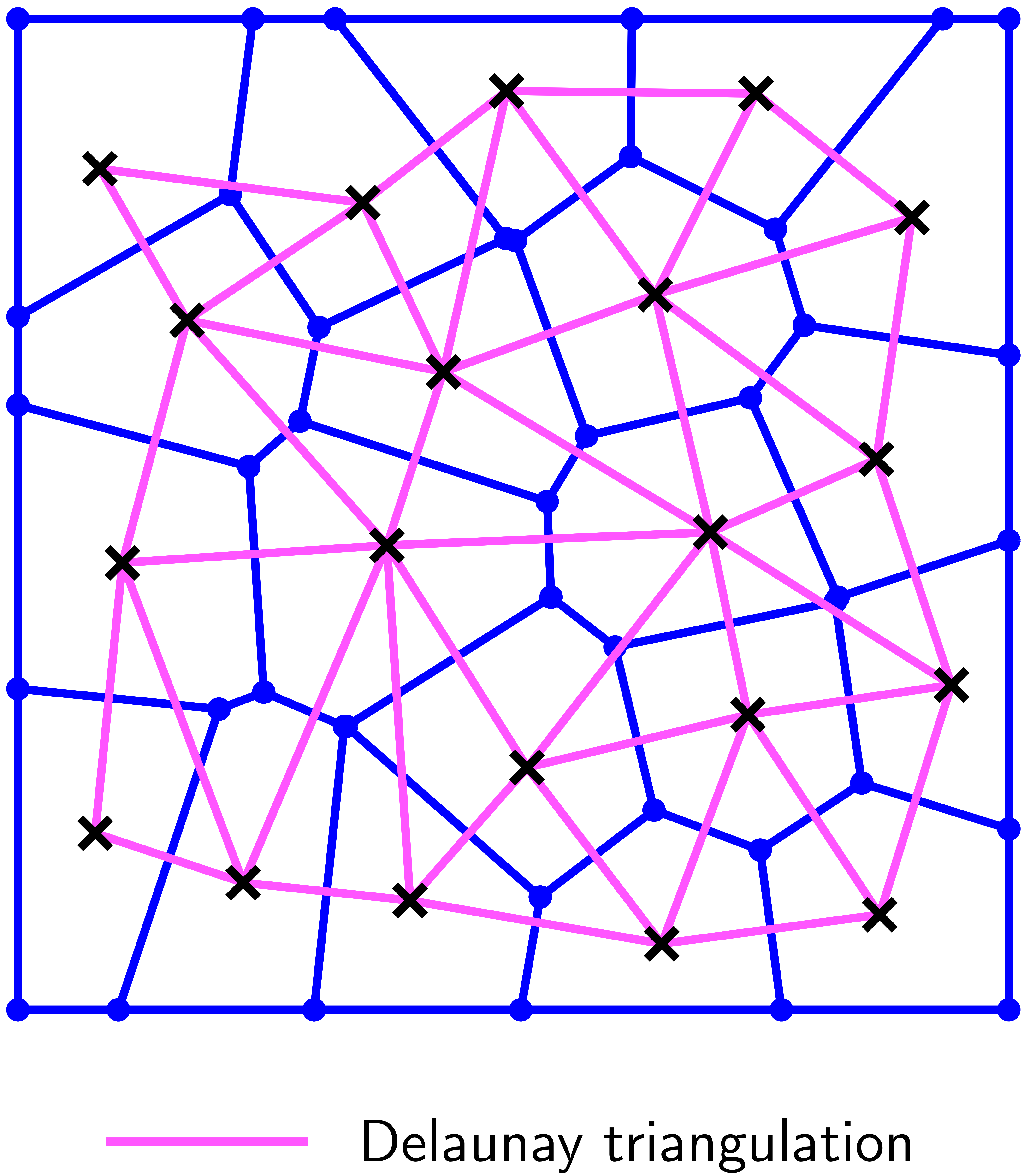
based on 3D Voronoi cell volumes in local patches

Packing fraction is reduced in regions of **highest shear**, not highest velocity

Makes physical sense, since particles need room to flow past each other

A topological definition of neighbors

- We can define two particles as neighbors if their Voronoi cells share a face
- Connecting all these neighbors gives the Delaunay triangulation
- Each Delaunay edge corresponds to a Voronoi face; this is called Voronoi–Delaunay duality



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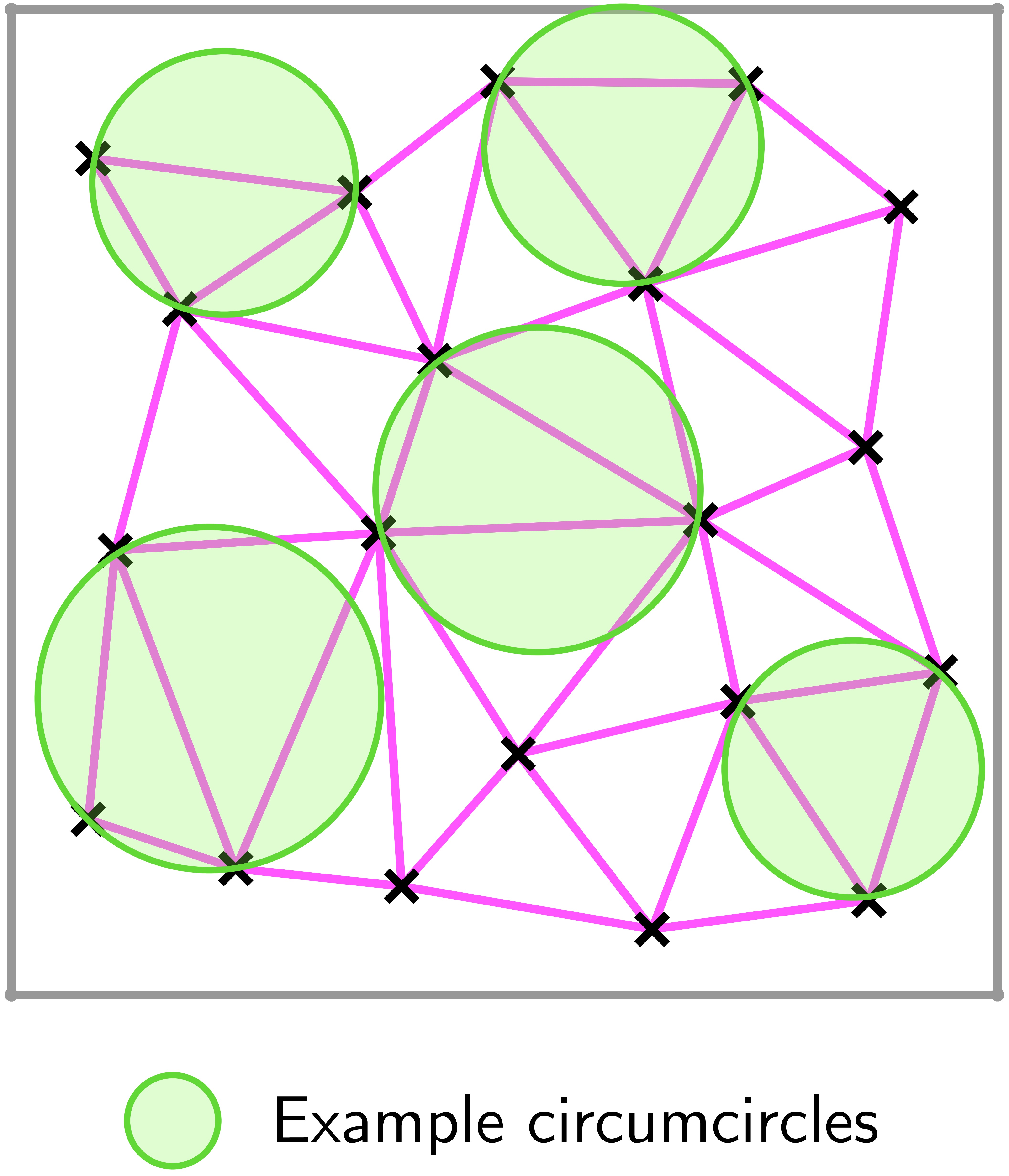
The Delaunay triangulation

- The Delaunay triangulation is interesting in its own right, and can be defined independently of the Voronoi tessellation
- It is the unique triangulation where the circumcircle of each triangle contains no other particle
- Useful basis for triangulation—we will return to this later



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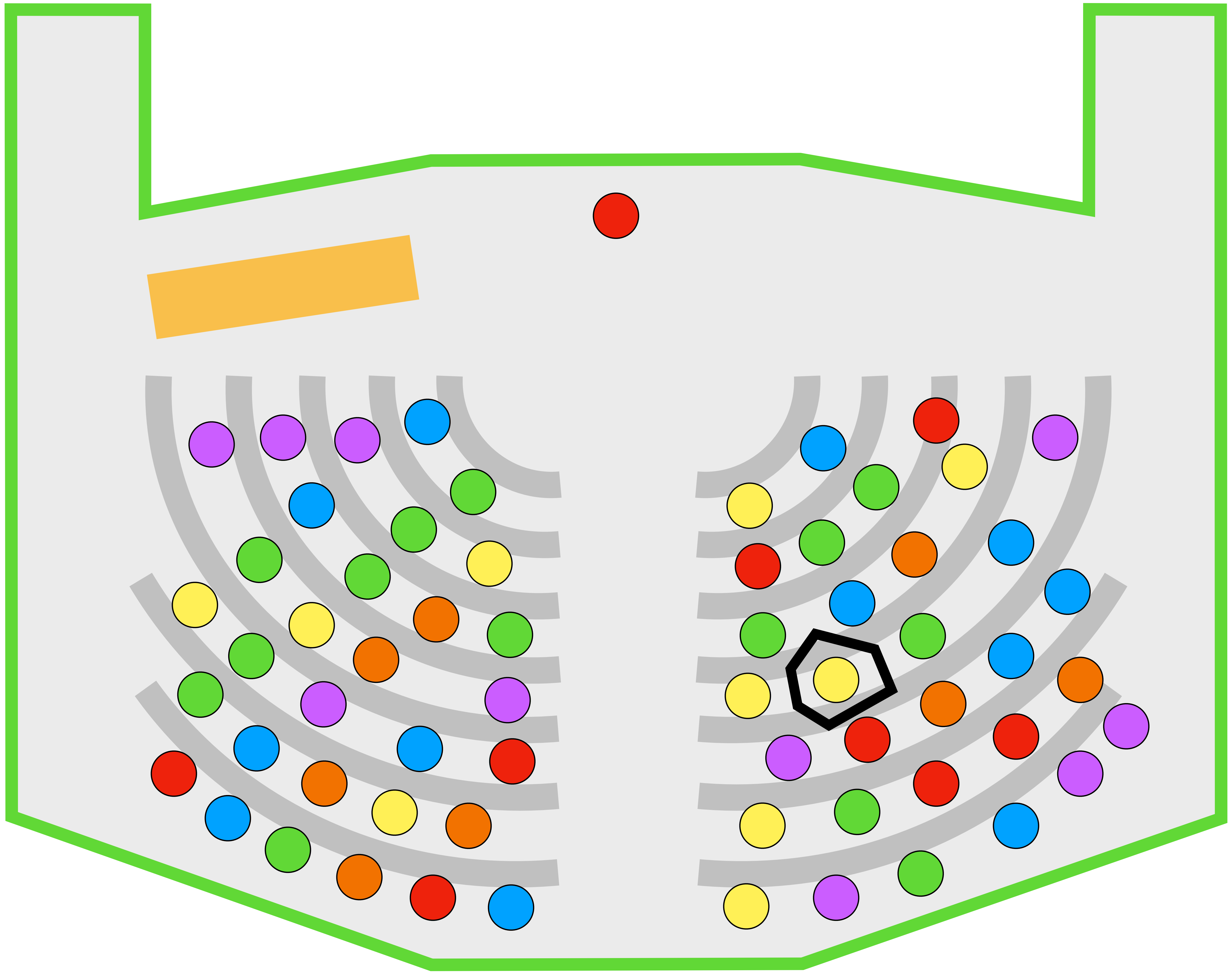
Neighbor relations test (with Voronoi cells)

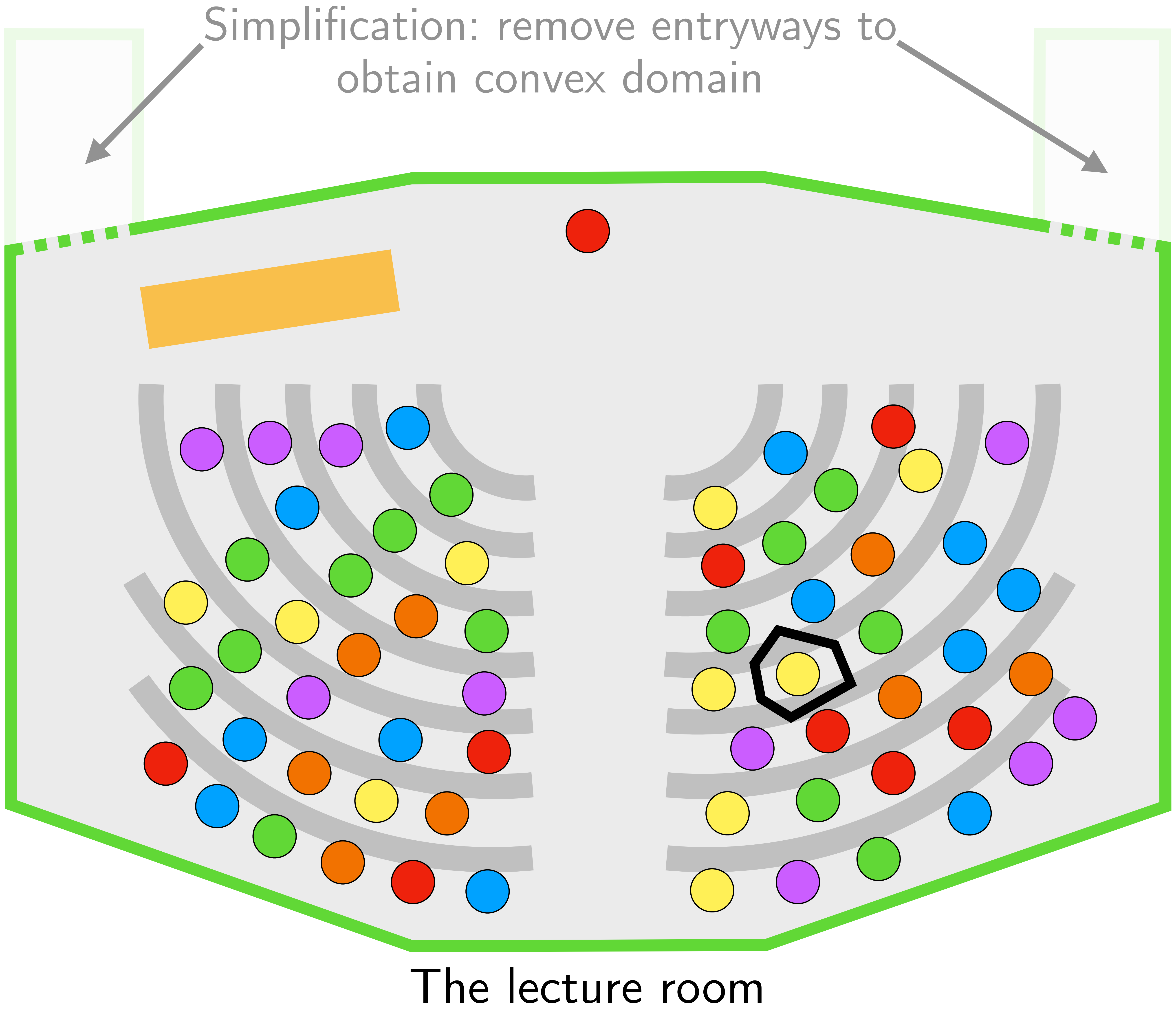
- We'll repeat the neighbor relations test
- But now I want you to visualize the Voronoi cell around you, and write down in **B** your neighbors that share Voronoi face



The lecture room

Neighbor relations test (with Voronoi cells)

- We'll repeat the neighbor relations test
- But now I want you to visualize the Voronoi cell around you, and write down in **B** your neighbors that share Voronoi face
- Extra credit in **C**: estimate the area of your Voronoi cell (include the unit, *e.g.* m^2 or ft^2)



Exercise

- Consider a circular particle of radius 1 centered at (c, d)
- Write a function the proportion of its volume in the region $x<0$, $y<0$