Rigidity theory in statistical mechanics

Miranda Holmes-Cerfon
Courant Institute of Mathematical Sciences

Collaborators

Thanks to:

Michael Brenner (Harvard)

Bob Connelly (Cornell)

Steven Gortler (Harvard)

Yoav Kallus (Sante Fe Institute)

John Ryan (NYU/Cornell)

Louis Theran (St Andrew's University)

and

US Dept of Energy & NSF

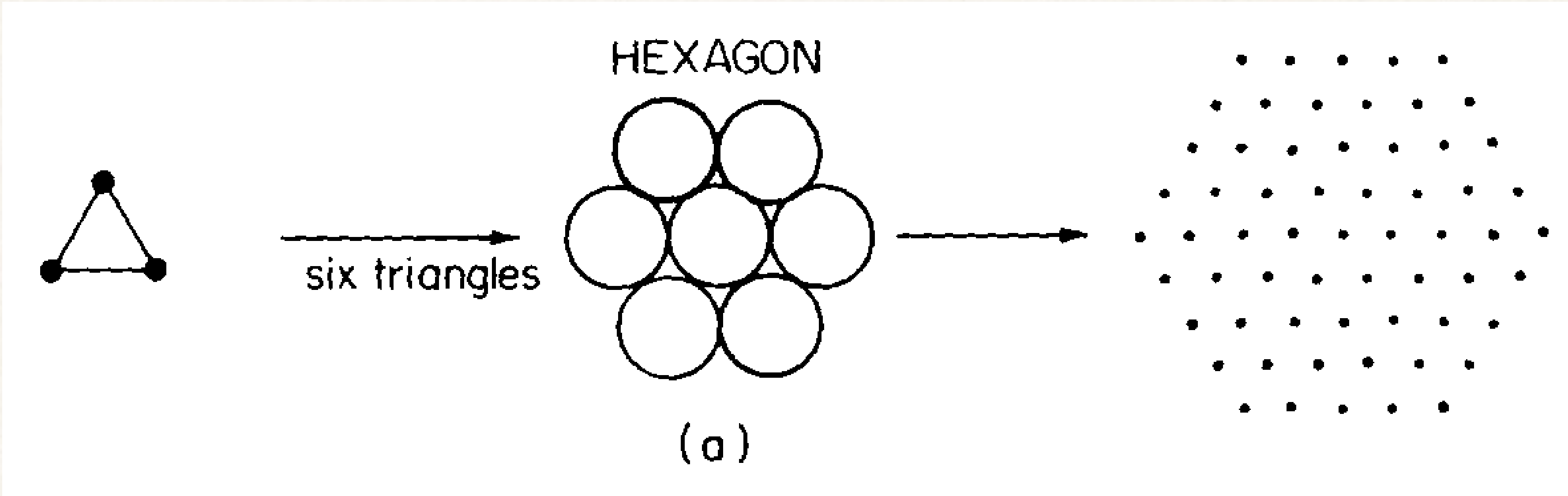
Guiding motivation:

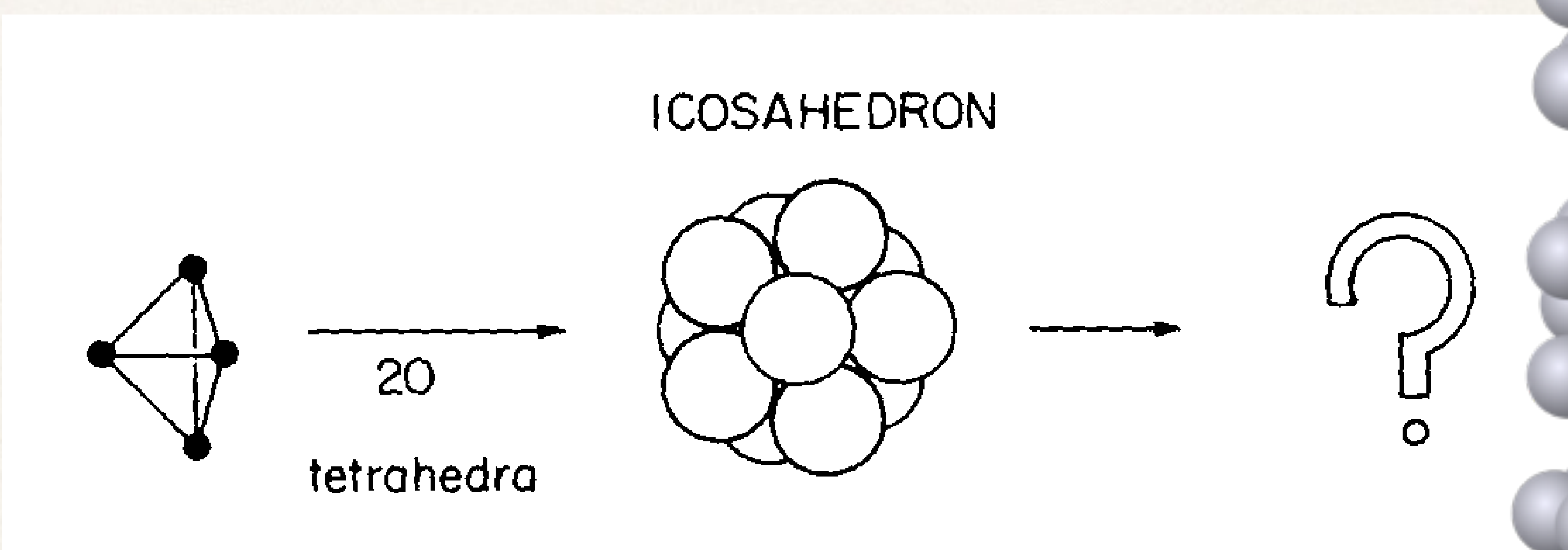
Physics is interesting because we live in 3 dimensions

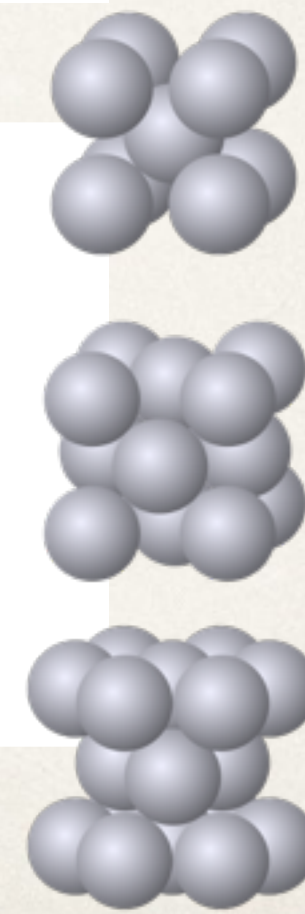
—> Geometrical Frustration

What is Geometrical Frustration?

D. Nelson, F. Spaepen, Solid State Phys. 42, 1 (1989)







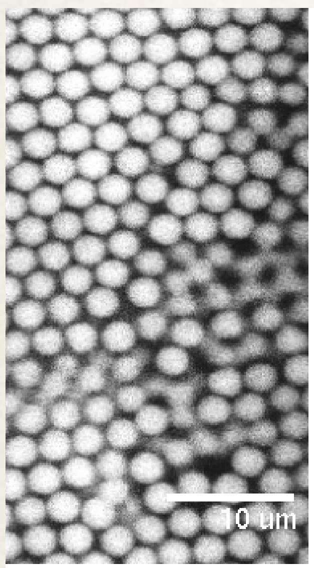
bcc unit cell

fcc unit cell

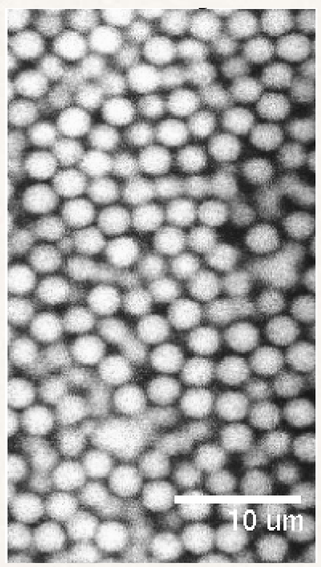
hcp unit cell

Geometric frustration: locally preferred order ≠ globally preferred order

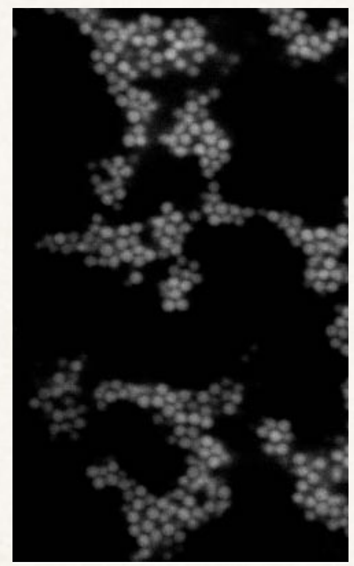
Frustration —> disordered phases



crystal

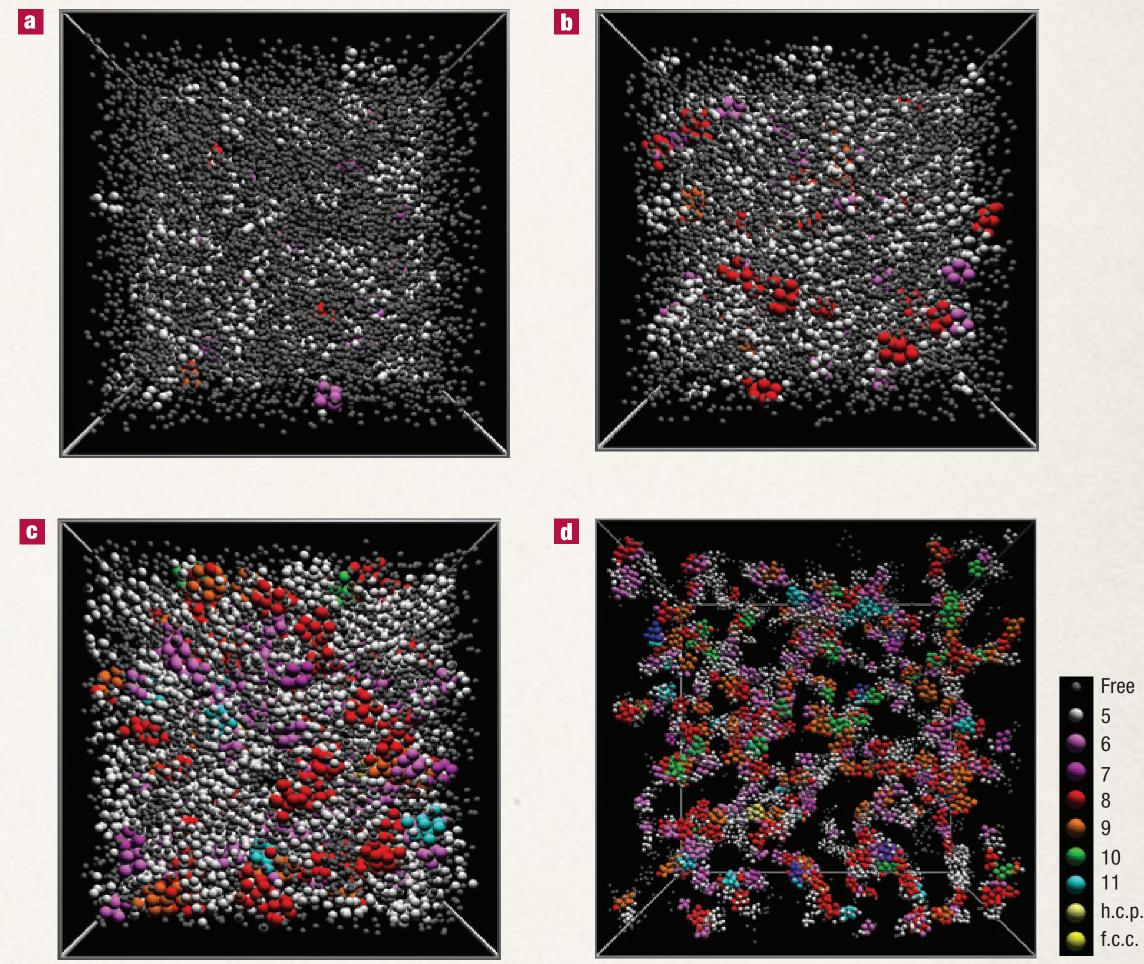


glass



gel

(D. Weitz, webpage)



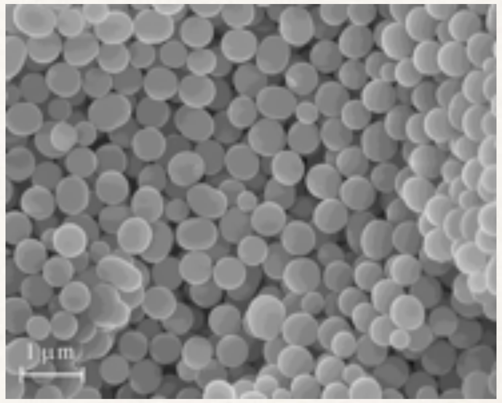
C. Patrick Royall, S. R. Williams, T. Ohtsuka, H. Tanaka, Nat. Mater. 7, 556 (2008)

creation of local "global minima" leads to gel formation

Colloidal particles (colloids)

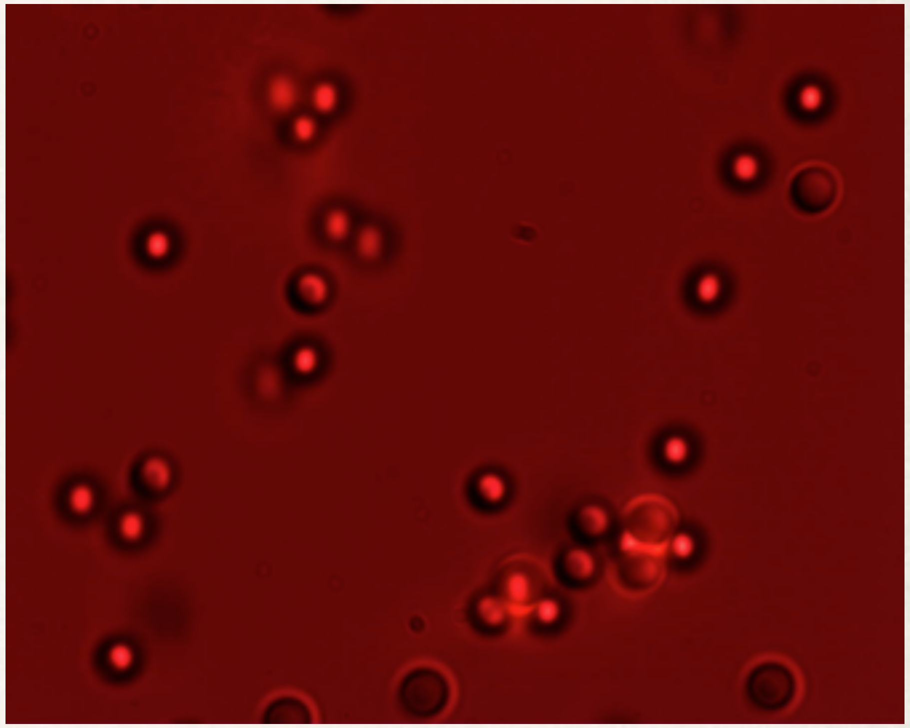
- *Colloidal* particles: diameters ~ 10^{-8}-10^{-6} m. (» atoms, « scales of humans)
- Range of interaction « diameter of particles (unlike atoms)

mayonnaise

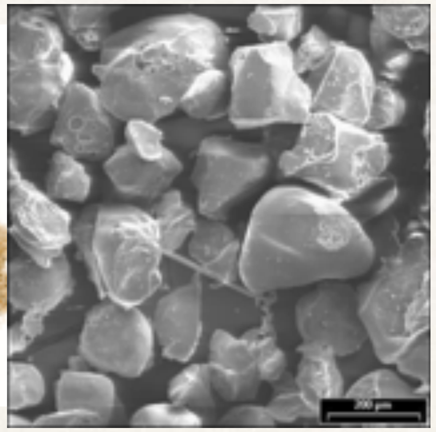


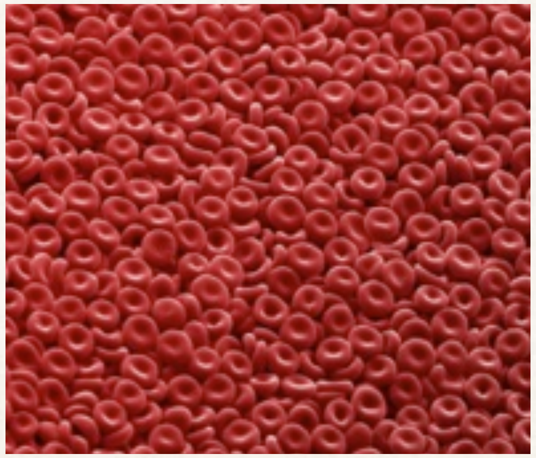
opal

red blood cells

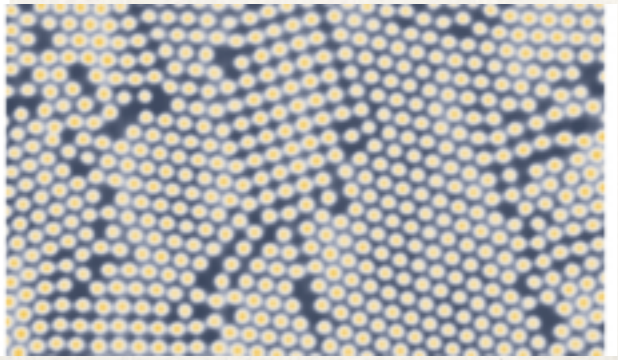


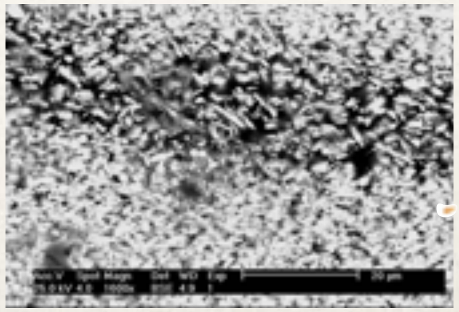
sand





cornstarch

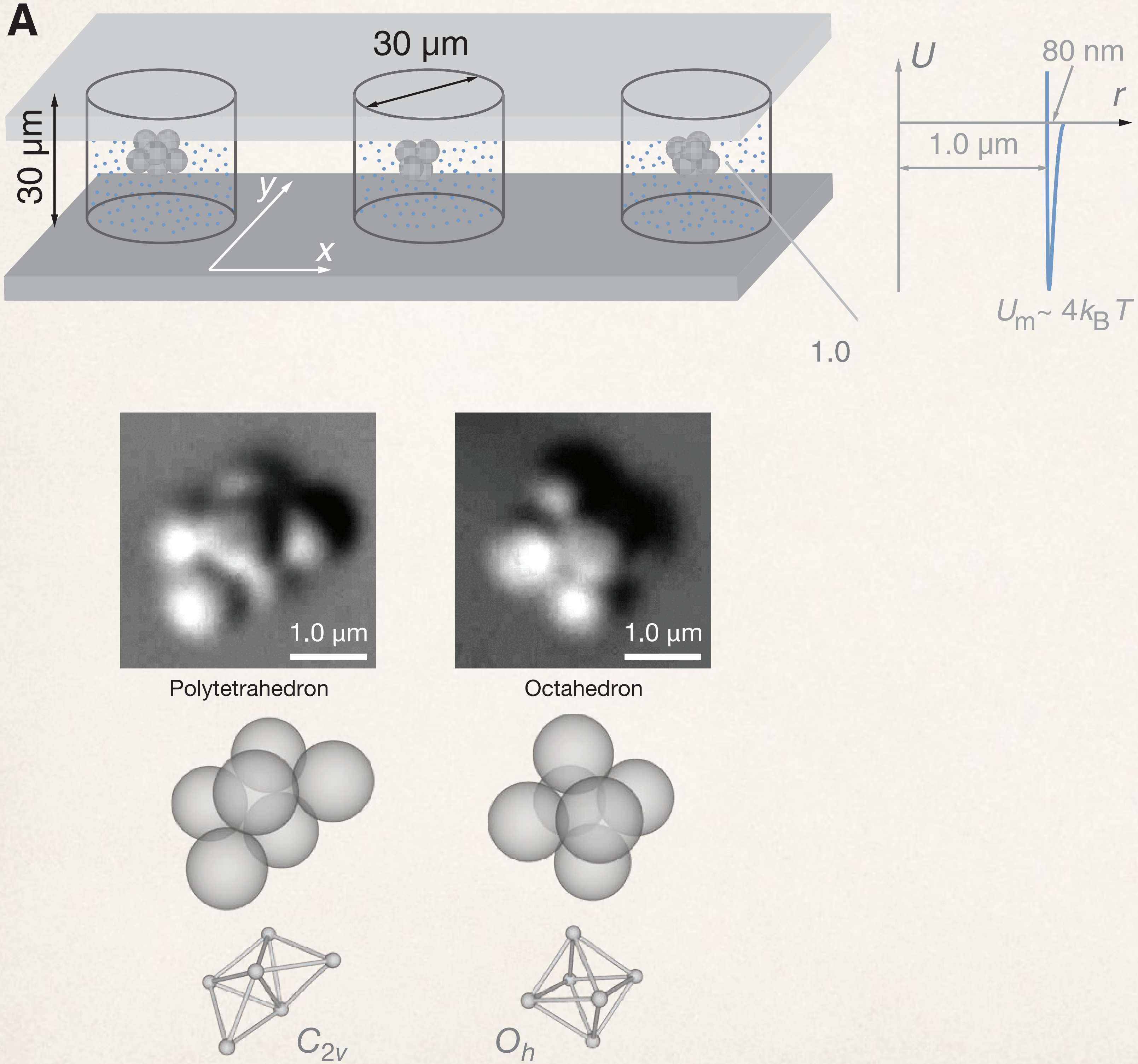


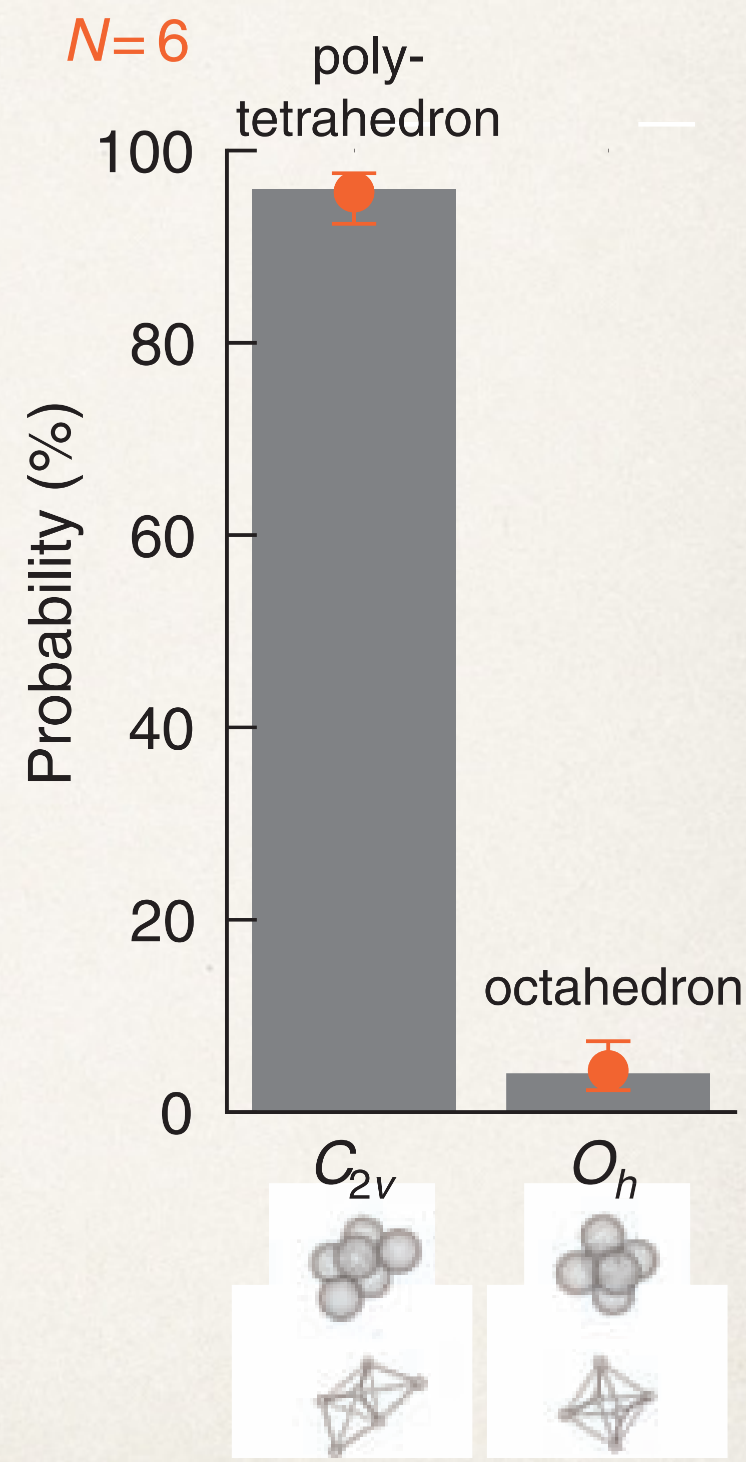


paint

ketchup

Small clusters of colloids like to be asymmetric





G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

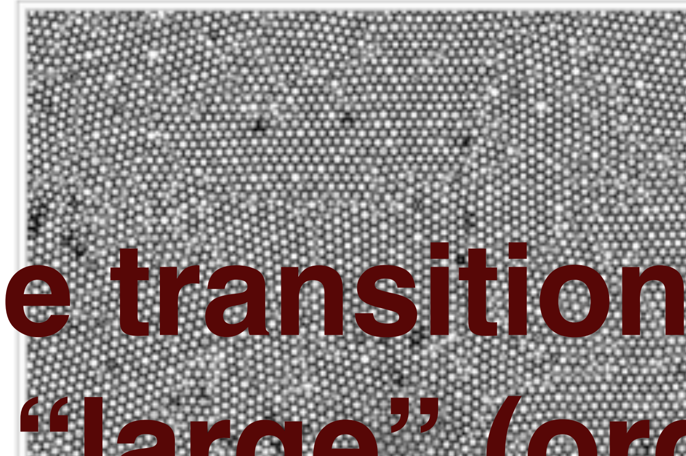
Large collections of colloids like to form crystals

Colloidal crystal

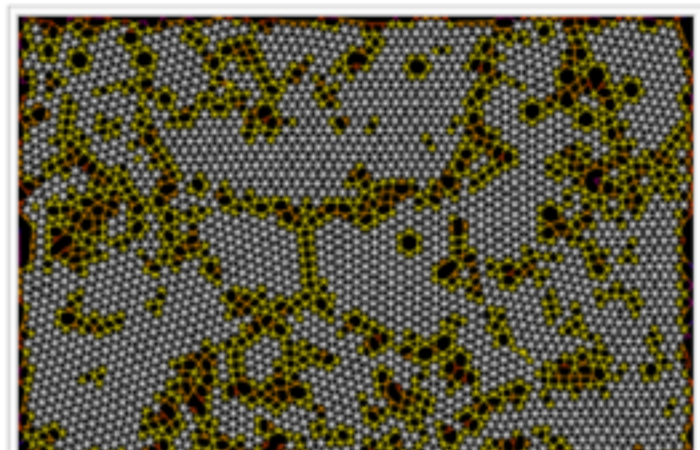
From Wikipedia, the free encyclopedia

A **colloidal crystal** is an ordered array of colloid particles, analogous to a standard crystal whose repeating subunits are atoms or molecules.[1] A natural example of this phenomenon can be found in the gem opal, where spheres of silica assume a close-packed locally periodic structure under moderate compression.[2][3] Bulk properties of a colloidal crystal depend on composition, particle size, packing arrangement, and degree of regularity. Applications include photonics, materials processing, and the study of self-assembly and phase transitions.

Contents [hide]



A collection of small 2D colloidal crystals with grain boundaries between them. Spherical glass particles (10 μm diameter) in water.

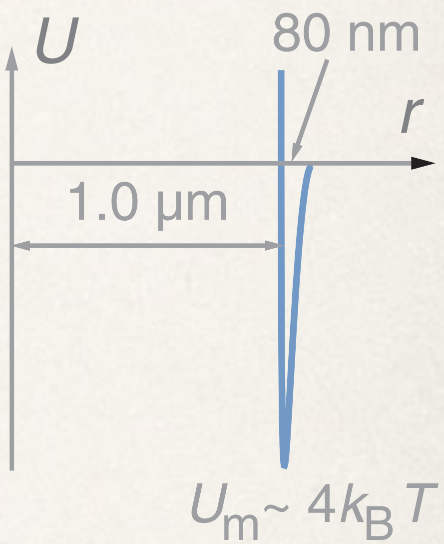


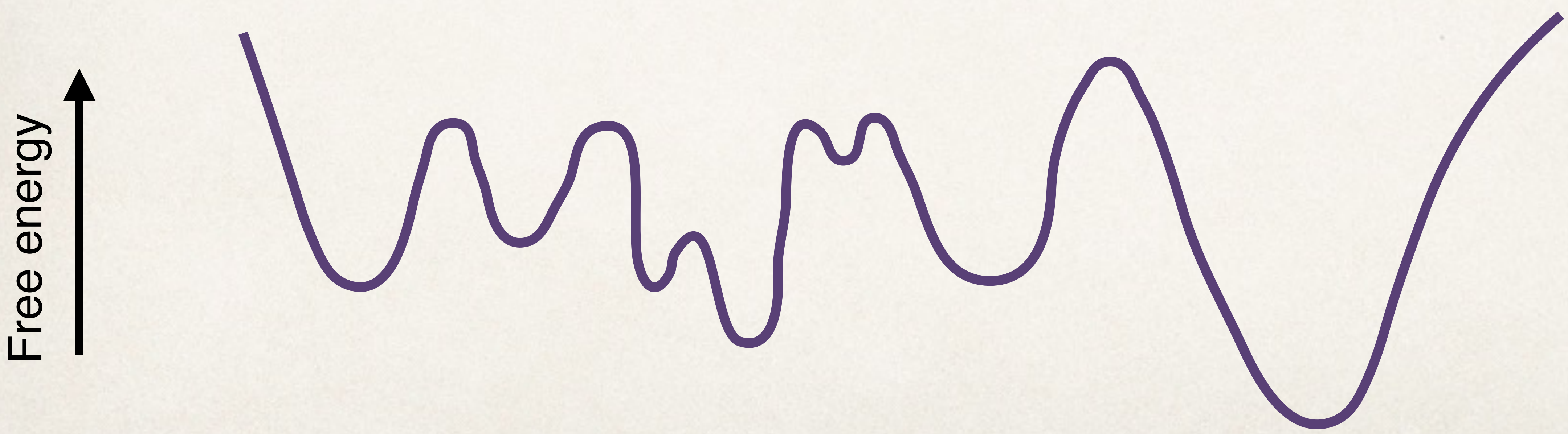
The connectivity of the crystals in the colloidal crystals above. Connections in white indicate that

When and how does the transition from "small" (disordered) to "large" (ordered) happen?

Colloids —> Sticky particles

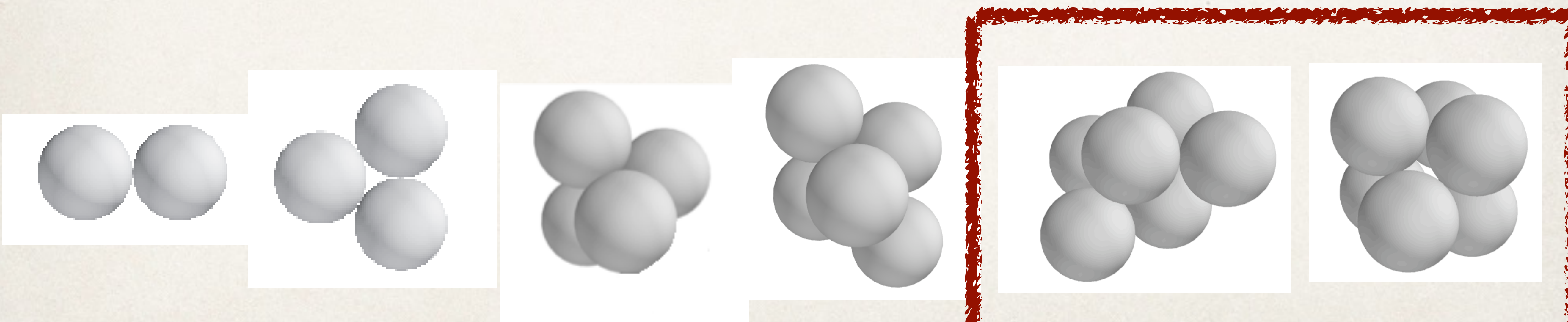
- Model colloids as *sticky*: interacting with infinitesimally short-ranged pair potential
  - ⋆ Allows geometry to be used in statistical mechanics
- Consider finite # N of particles ("cluster")
- Characterize free energy landscape of clusters of sticky particles —> via local minima





What do local minima look like?

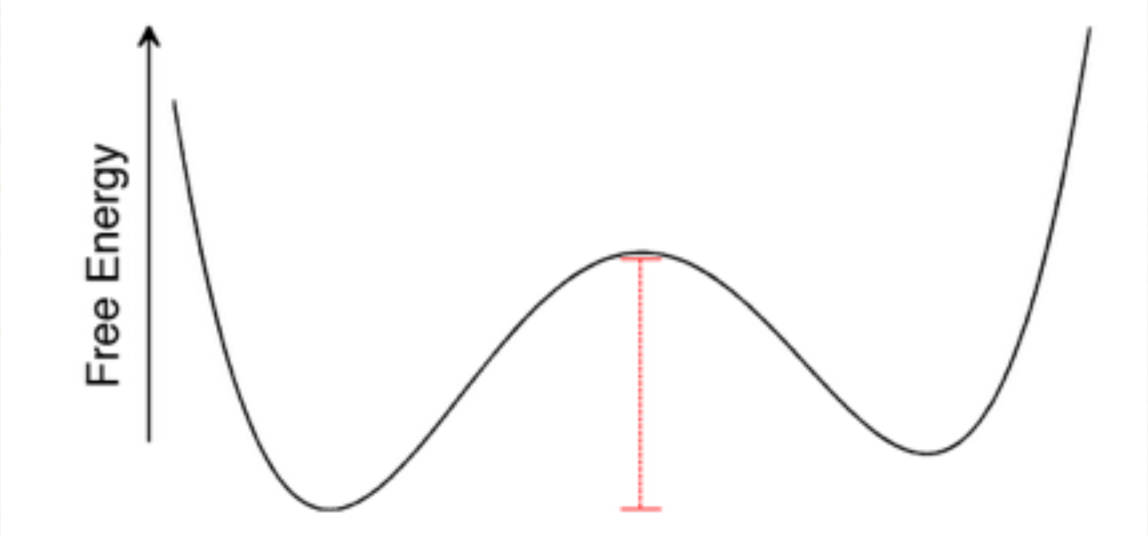
- Spheres are either touching, or not
- Energy of cluster of N spheres ∝ -(# of contacts)
- Lowest-energy clusters = those with maximal number of contacts
- These are (typically) **rigid**: they cannot be continuously deformed without breaking a contact (=crossing an energy barrier.)
- More generally: energetic local minima have a locally maximal number of contacts, so are (typically) rigid.



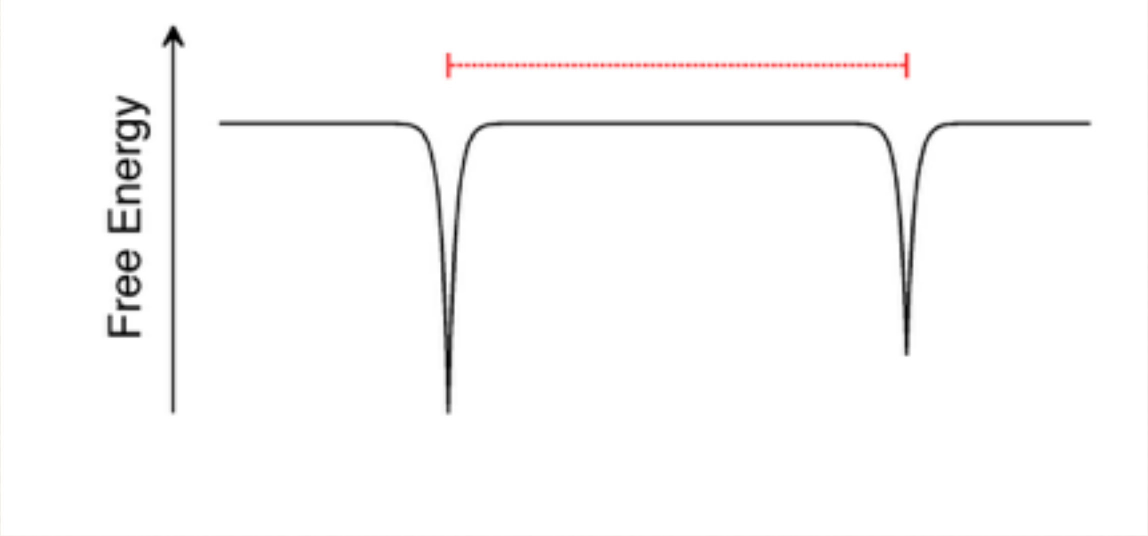
2 rigid clusters for N=6

Energy landscape with very short-range interactions

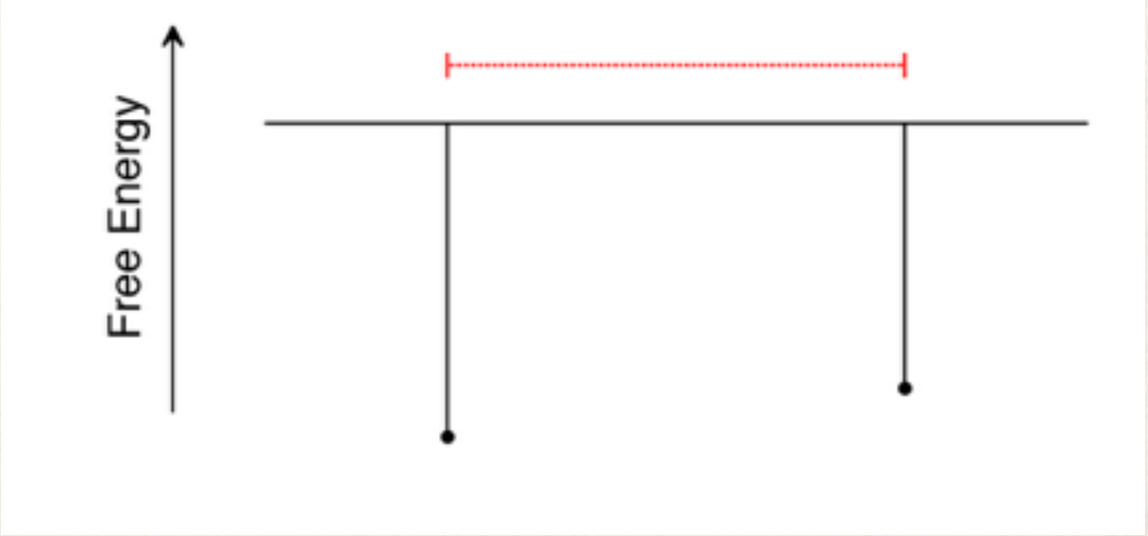
Traditional energy landscape



Colloidal energy landscape



Sticky energy landscape



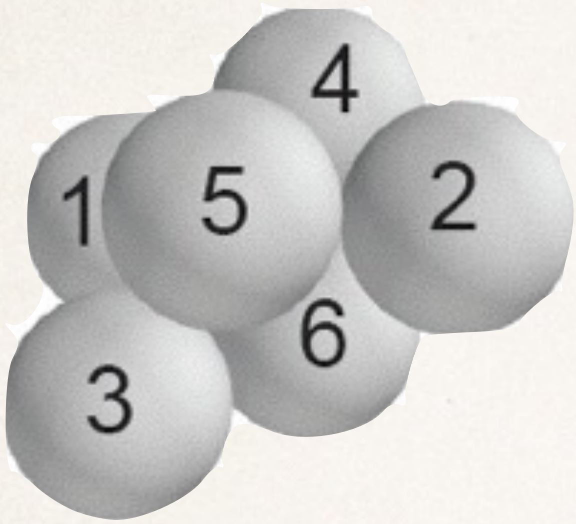
Outline

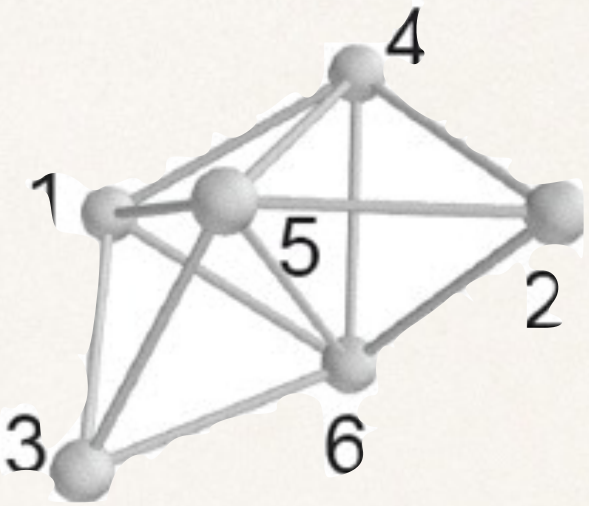
- Rigidity — review: What is rigid? And how can we test it?
- Sphere packings: What are all the ways to arrange N identical spheres into a rigid cluster?
- Statistical mechanics: What are the free energies / probabilities to find each cluster, in equilibrium?

Rigidity — Review

What is a rigid cluster (rigid graph), and how can we test it?

What is rigid?





adjacency matrix A

$$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

- Each adjacency matrix corresponds to a system of quadratic equations and inequalities ($x_i \in \mathbb{R}^3$):

$$|x_i - x_j|^2 = d^2 \qquad \text{if } A_{ij} = 1$$
$$|x_i - x_j|^2 \geq d^2 \qquad \text{if } A_{ij} = 0$$

- A cluster (x,A) with $x = (x_1, x_2, \dots, x_N)$ is *rigid* if it is an isolated solution to this system of equations (modulo translations, rotations) (e.g. Asimow&Roth 1978)
$\Longleftrightarrow$ There is no finite, continuous deformation of the cluster that preserves all edge lengths.

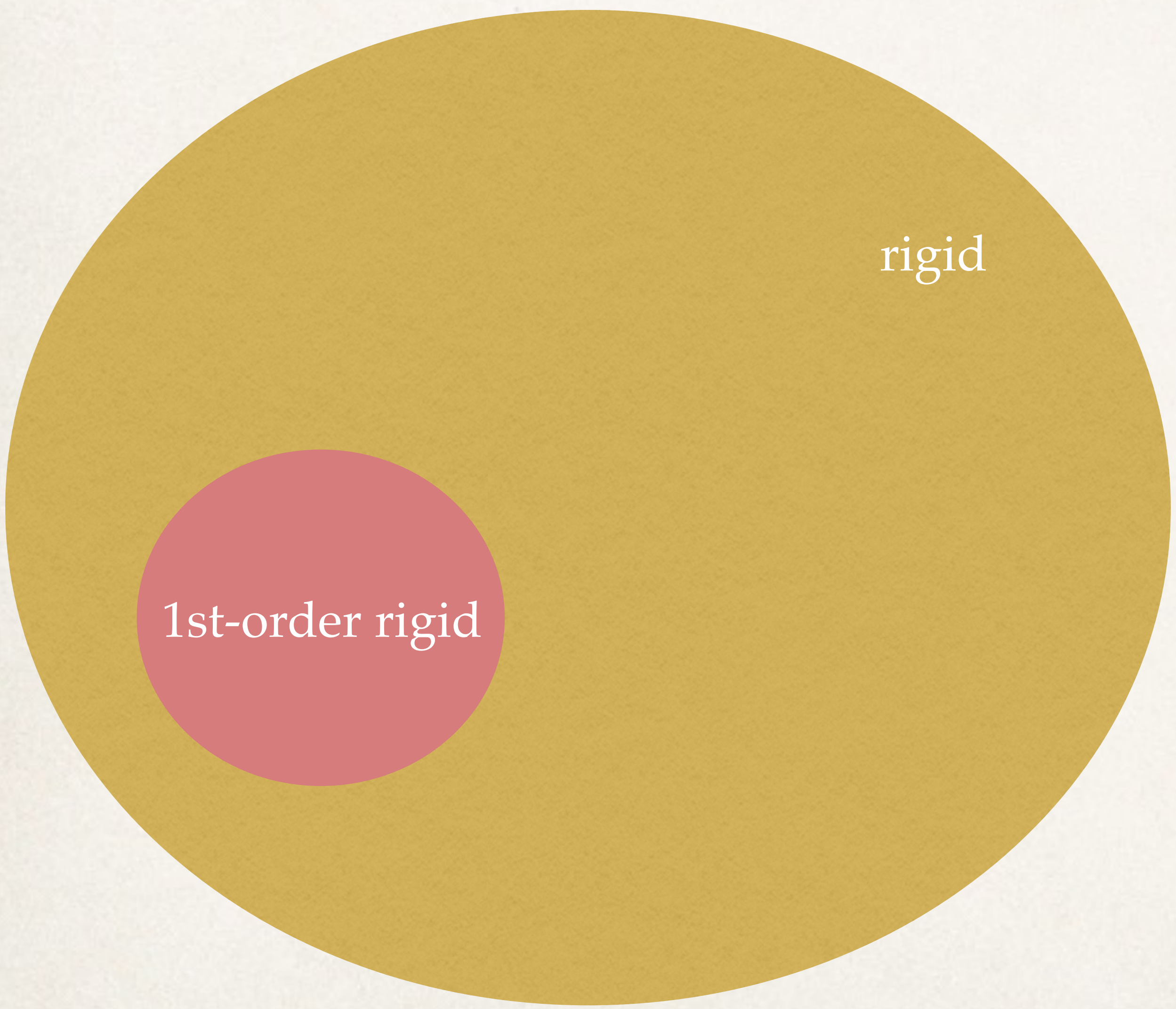
How to test for rigidity?

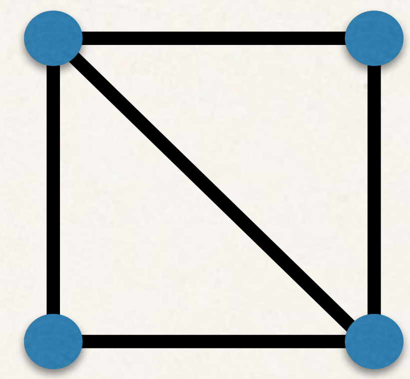
- Testing the full definition is co-NP hard (Abbott, *Master's Thesis*, 2008)
- We will introduce stronger notions of rigidity:
  (based on Connelly & Whiteley, 1996)
  - First-order rigid (too strong/too easy)
  - Second-order rigid (too weak / too hard)
  - Prestress stability (just right)

First-order rigid

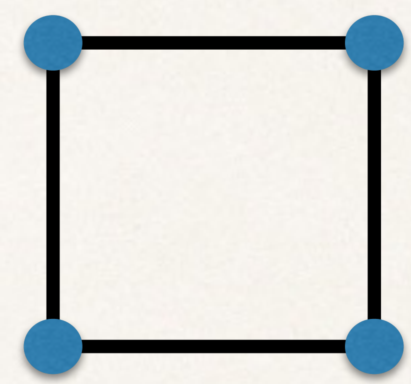
- Let p(t) be a continuous, analytic deformation of cluster with p(0) = x
- Take $d/dt|_{t=0}$ of
$$|x_i - x_j|^2 = d_{ij}^2$$
- Result is
$$(x_i - x_j) \cdot (p_i' - p_j') = 0$$
- Write system as
$$R(x)p' = 0 \qquad (*1)$$
- R(x) is the *rigidity matrix*.
- p′ = p′(0) is the set of velocities we give to the nodes, to deform cluster infinitesimally.
- A cluster is *first-order rigid* if there are no solutions p′ to (*1) except *trivial* solutions (infinitesimal translations, rotations)
- A non-trivial solution p′ to (*1) is a *flex*

- Theorem: (x,A) is first order rigid ⇒ (x,A) is rigid (consequence of Implicit Function Theorem, if isostatic)
- Easy to test first order rigid
- But too restrictive!

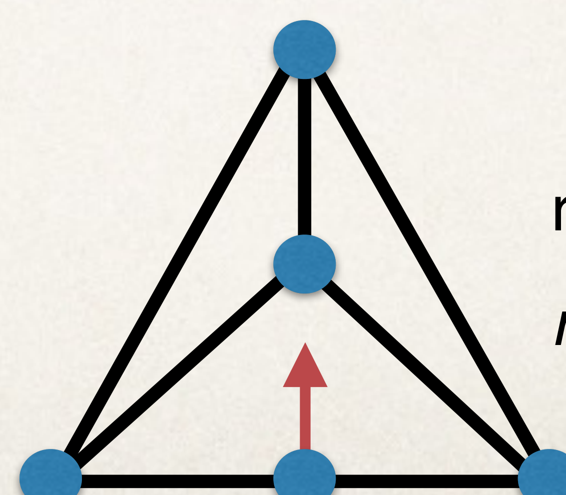




first-order rigid (in R^2)
floppy (in R^3)



floppy (in R^2,R^3)



rigid (R^2)

not first-order rigid (R^2)

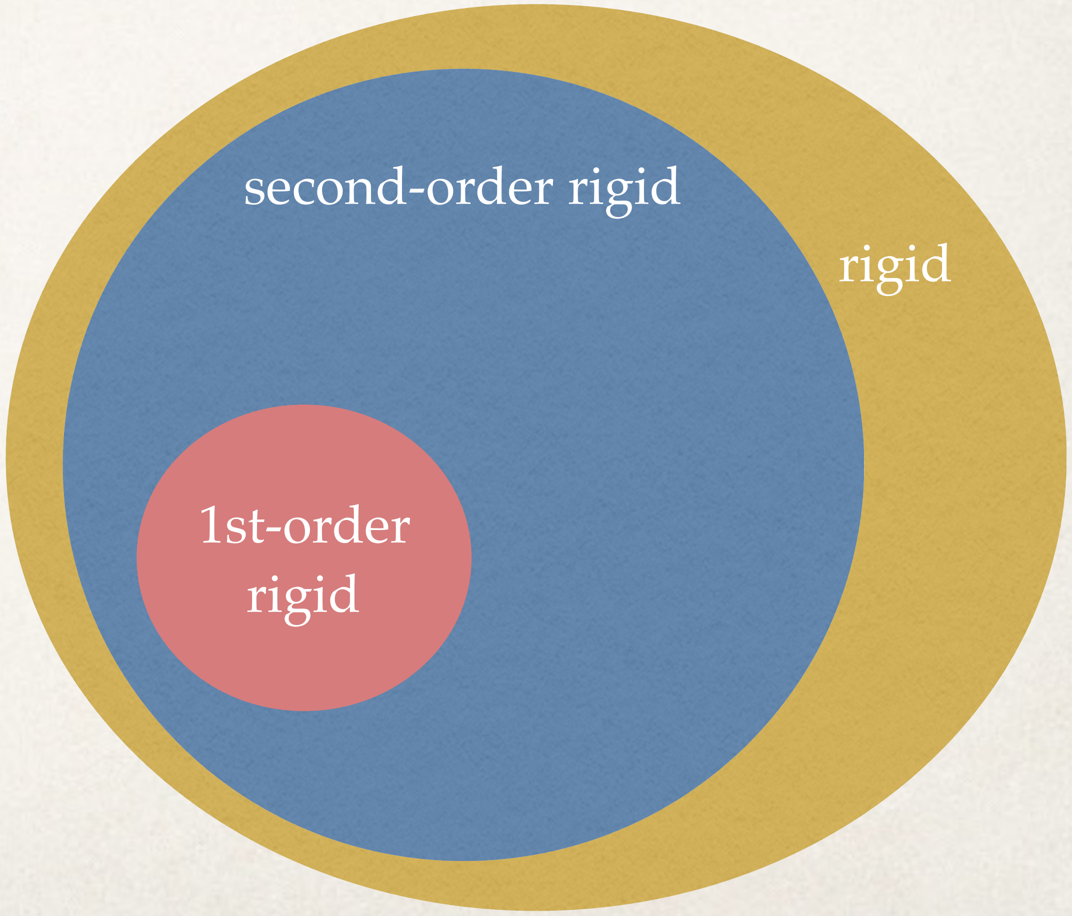
& Toys!!

Second-order rigid

- Take $d^2/dt^2|_{t=0}$ of $|x_i - x_j|^2 = d_{ij}^2$
- Result is $(x_i - x_j) \cdot (p_i'' - p_j'') = -(p_i' - p_j') \cdot (p_i' - p_j')$
- Write as

$$R(x)p'' = -R(p')p', \qquad R(x)p' = 0 \qquad (*2)$$

- A cluster is *second-order rigid* if there are no solutions (p′,p″) to (*2), except where p′ is trivial.
- **Theorem** (Connelly & Whiteley 1996):
  (x,A) is second-order rigid ⇒ (x,A) is rigid.



- Testing second-order rigidity is hard!
  No efficient method to do this.

Prestress stability

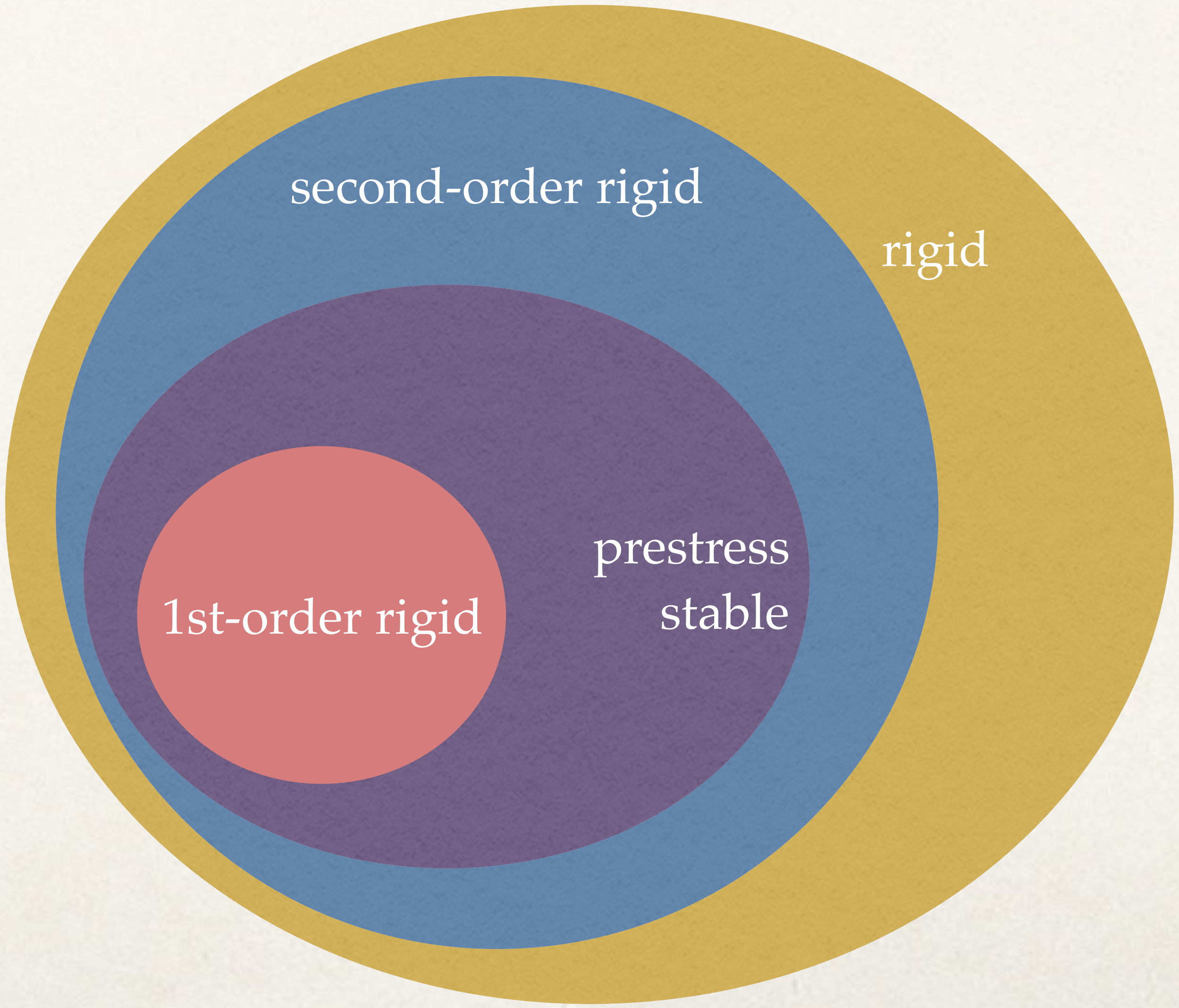
$$R(x)p'' = -R(p')p', \qquad R(x)p' = 0 \qquad (*2)$$

- (x,A) is *prestress stable* (PSS) if

$$\exists\, w \in \mathrm{Null}(R^T(x)) \quad \text{s.t.} \quad w^T R(p')p' > 0 \qquad \forall\, p' \in \mathscr{V},\ p' \neq 0 \qquad (\text{*pss})$$

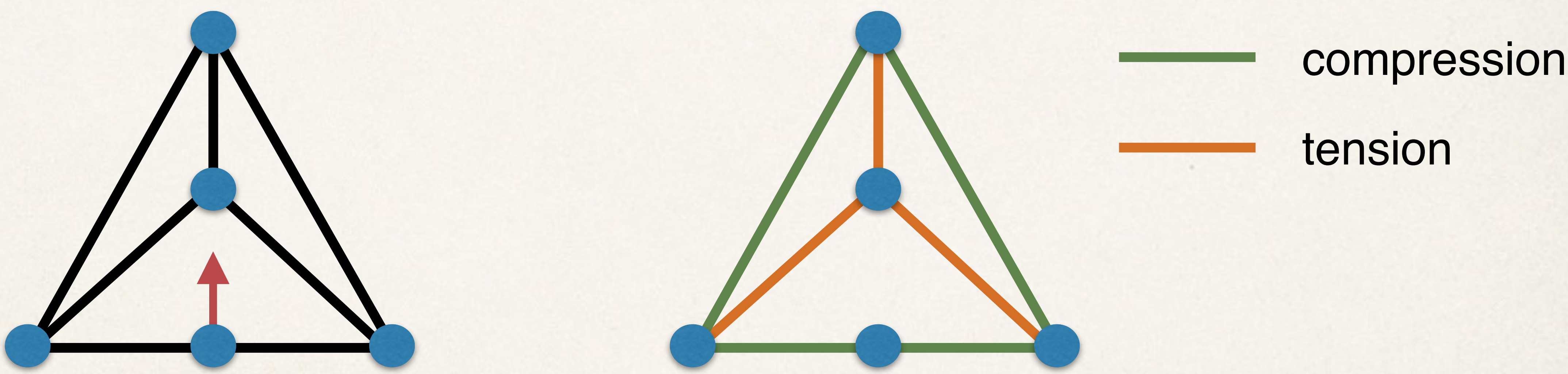
$\mathscr{V}$ = space of non-trivial flexes (solutions p′ to R(x)p′=0)

- (x,A) is PSS ⇒ (x,A) is second-order rigid ⇒ (x,A) is rigid



What is Null(R^T) physically?

- An element $w \in \mathrm{Null}(R^T(x))$ is a *self-stress*
- Physically a self-stress is a set of spring constants on edges to put them under tension or compression, so there is not net force on the system
- If deform with a flex, "energy" of this spring system increases.



Connelly & Whiteley (1996)

Sphere packings

What are all the rigid clusters of N identical spheres?

H.-C. (2016) *SIAM Review*

Previous approaches

(1) List all adjacency matrices with 3N-6 contacts

(2) For each adjacency matrix, solve (analytically or with computer) for the positions of the particles, or argue that no solution exists.

- N. Arkus, V. N. Manoharan, M. P. Brenner. *Phys. Rev. Lett., 103 (2009)*
- N. Arkus, V. N. Manoharan, M. P. Brenner. *SIAM J. Disc. Math., 25 (2011)*
- R. S. Hoy, J. Harwayne-Gindansky, C. O'Hern, *Phys. Rev. E*, 85 (2012)
- R. S. Hoy, *Phys. Rev. E*, 91 (2015)

Analytical: to N=10

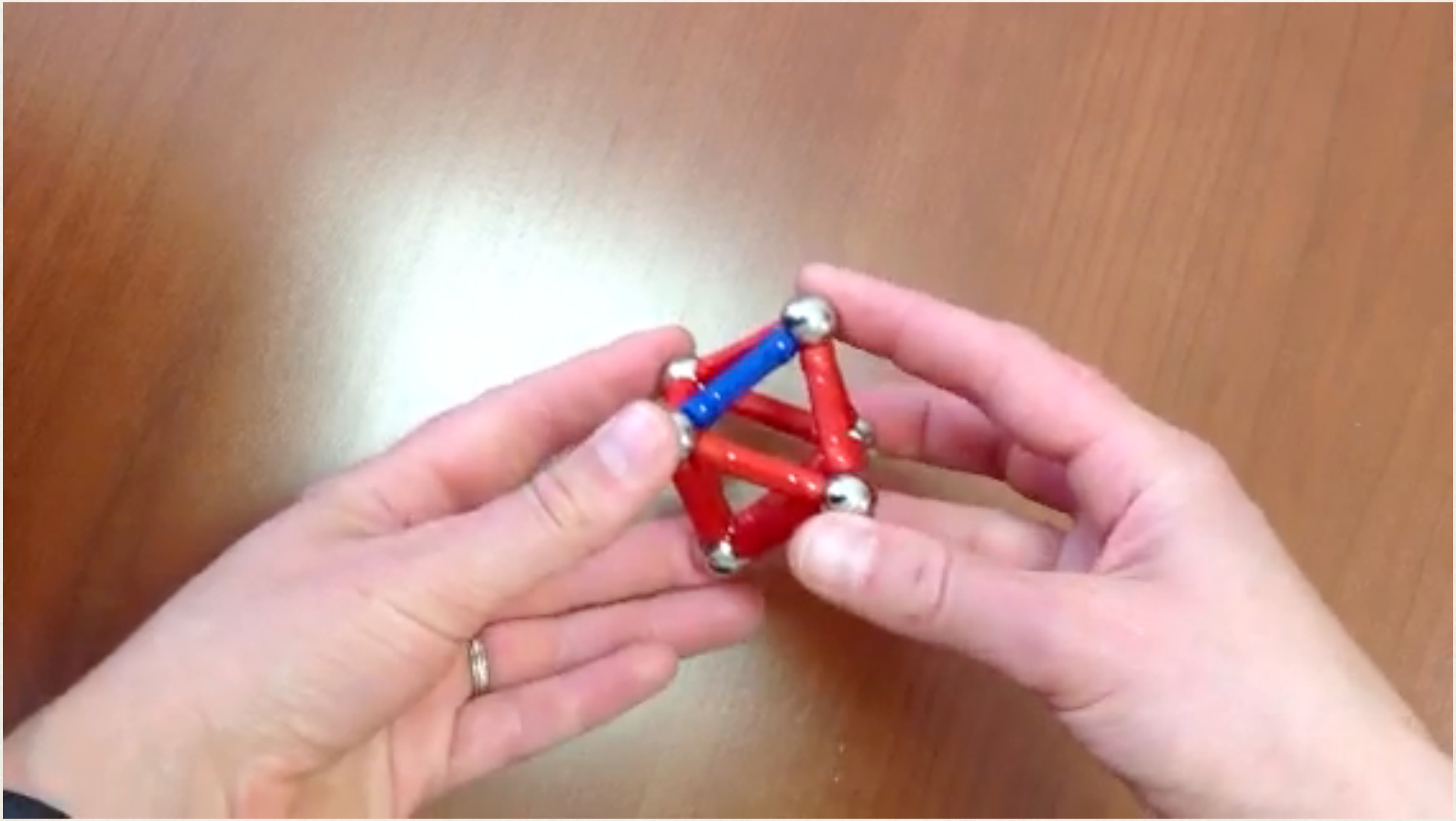
Computer: to N=13 (though many were missed)

Problems:

- LOTS of adjacency matrices: $\approx 2^{n(n-1)/2}$
- How to solve equations?
  - ✦ analytical — really hard
  - ✦ computer — can't guarantee found solutions
  - ✦ Degree of equations is VERY high ($\approx 2^{3N-6}$!)

A different algorithm

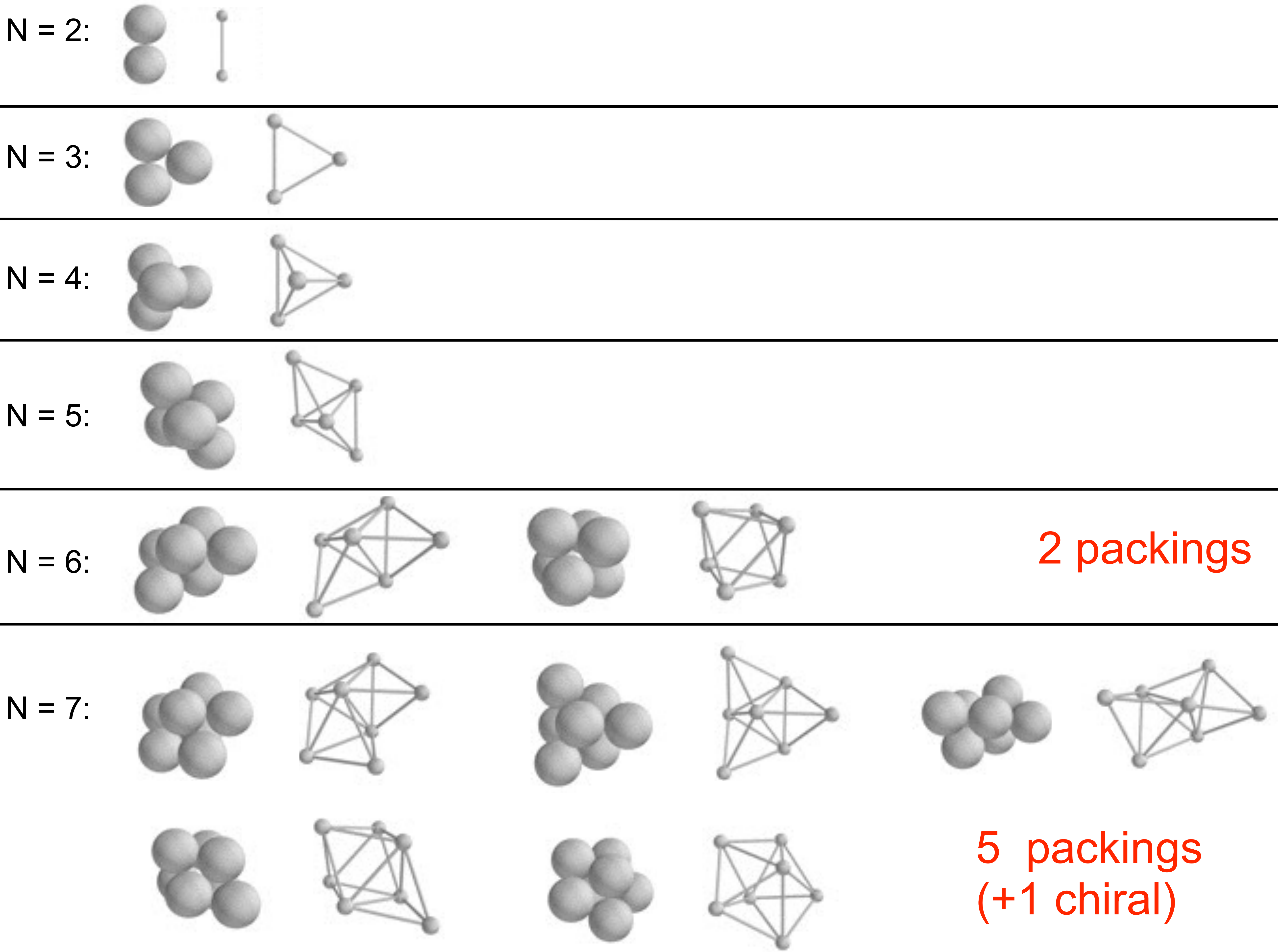
Move from cluster to cluster dynamically



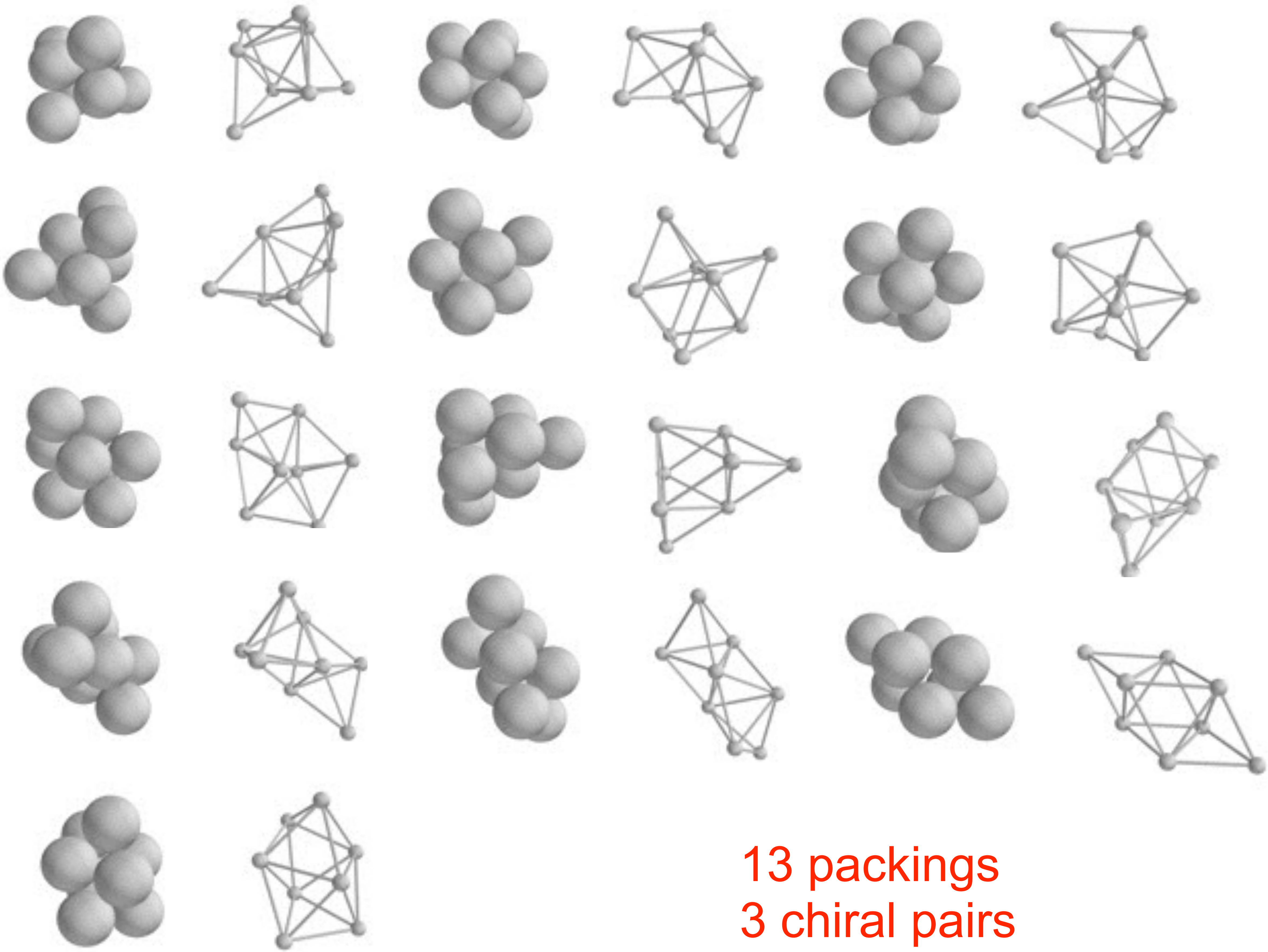
Algorithm

- Start with a single rigid cluster
- Break all subsets of bonds that give a cluster with one internal degree of freedom*.
- For each subset, move on this internal degree of freedom until another bond is formed.
- If resulting cluster is rigid (pss), add to list.
- Repeat for all clusters in list. Stop when reach end of list.

* Testing for one dof is hard.

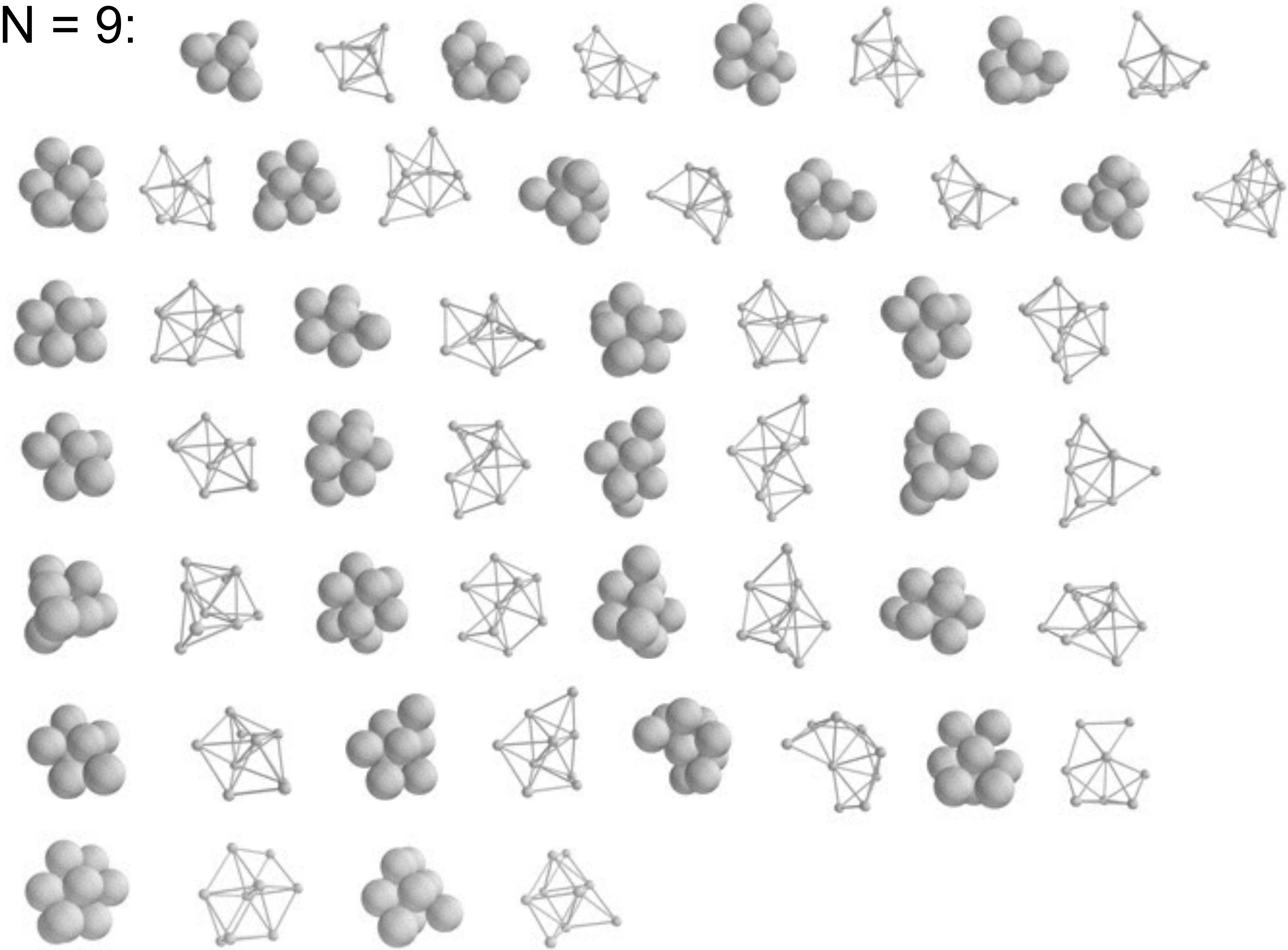

N = 2:
N = 3:
N = 4:
N = 5:
N = 6:
2 packings
N = 7:
5 packings
(+1 chiral)

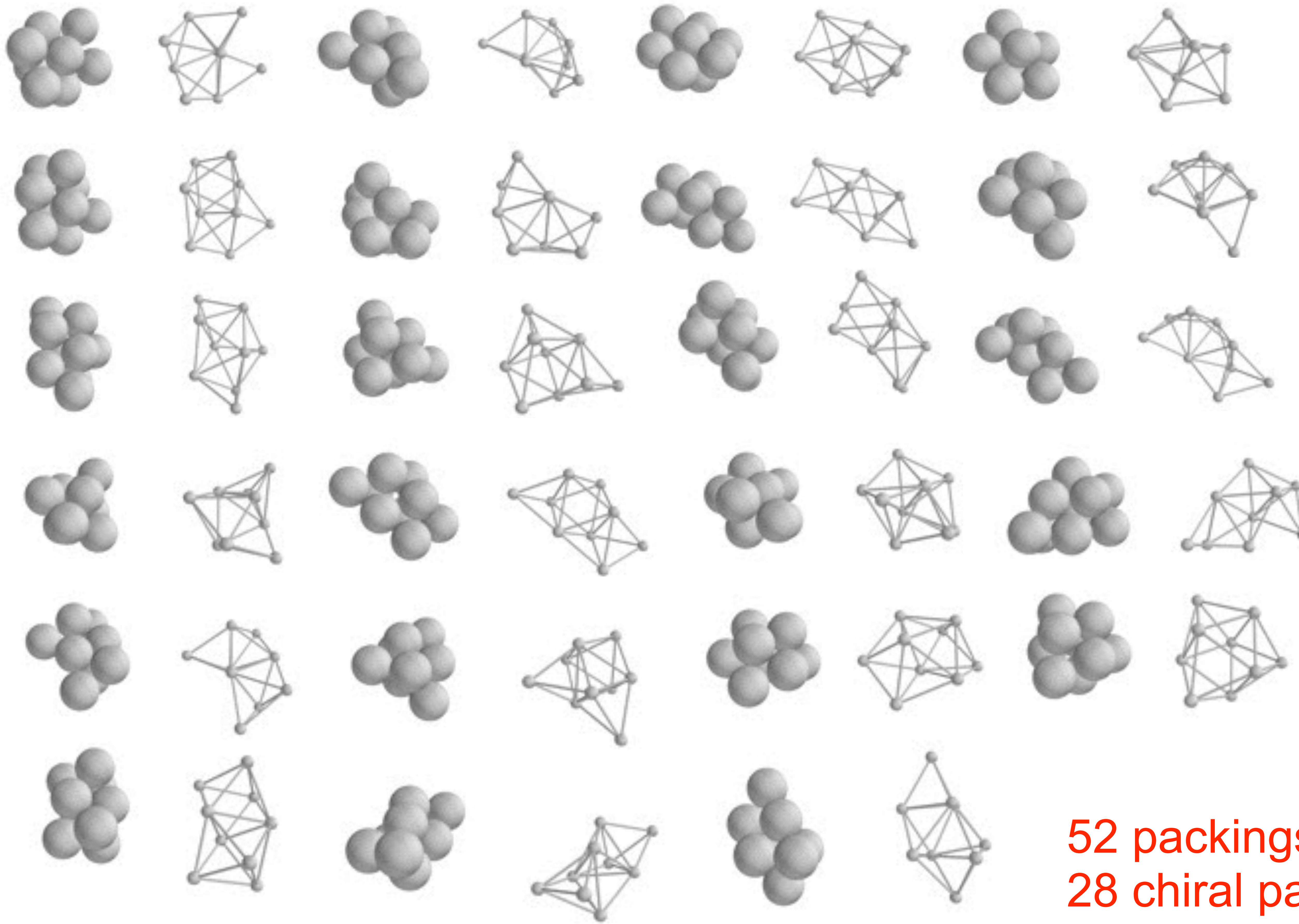
N = 8:



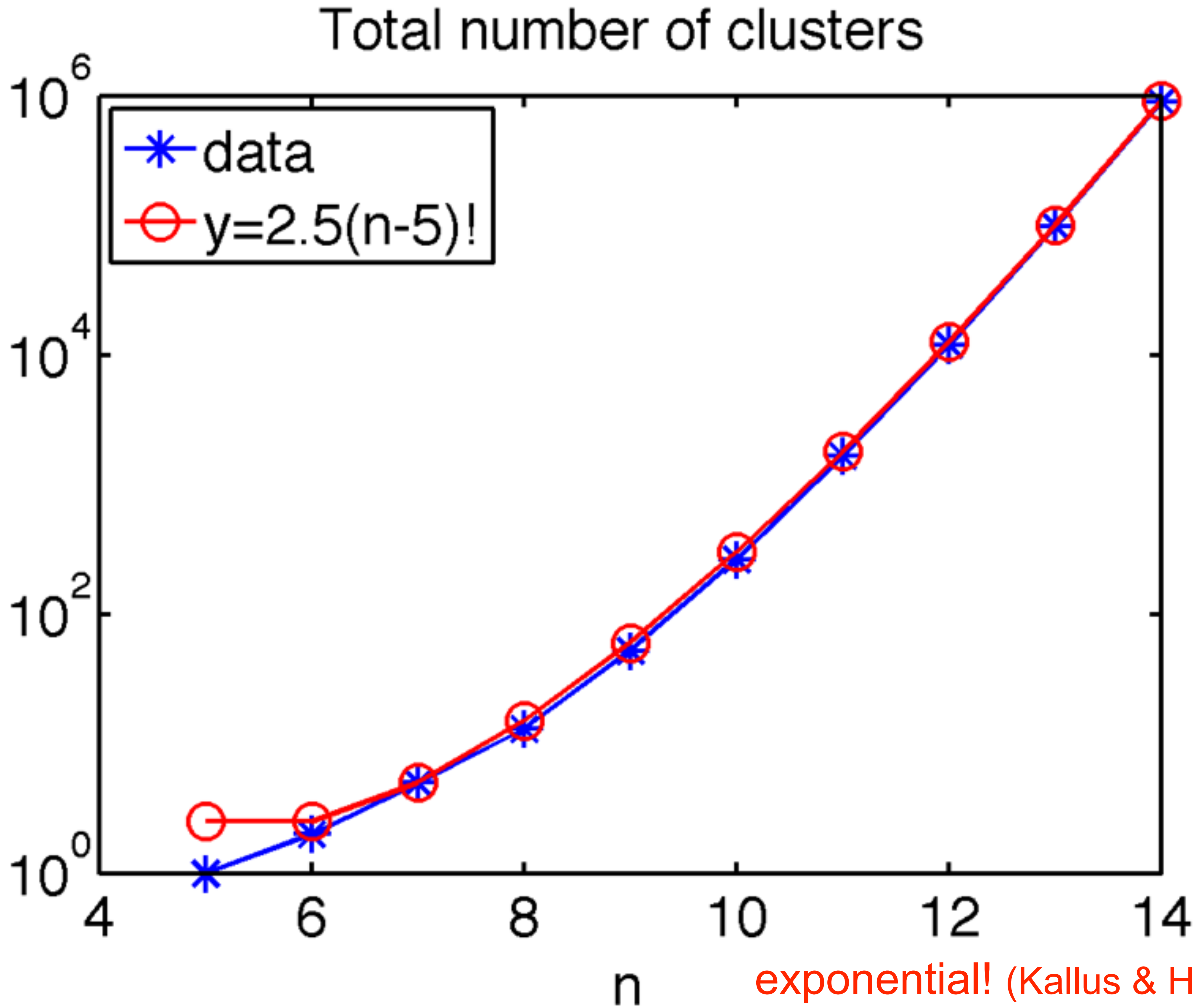
13 packings
3 chiral pairs

N = 9:





52 packings
28 chiral pairs



exponential! (Kallus & H.C., In Prep.)

~~Total grows as ≈ 2.5(N - 5)!~~ ~~FASTER than exponential~~ —> non-extensive?

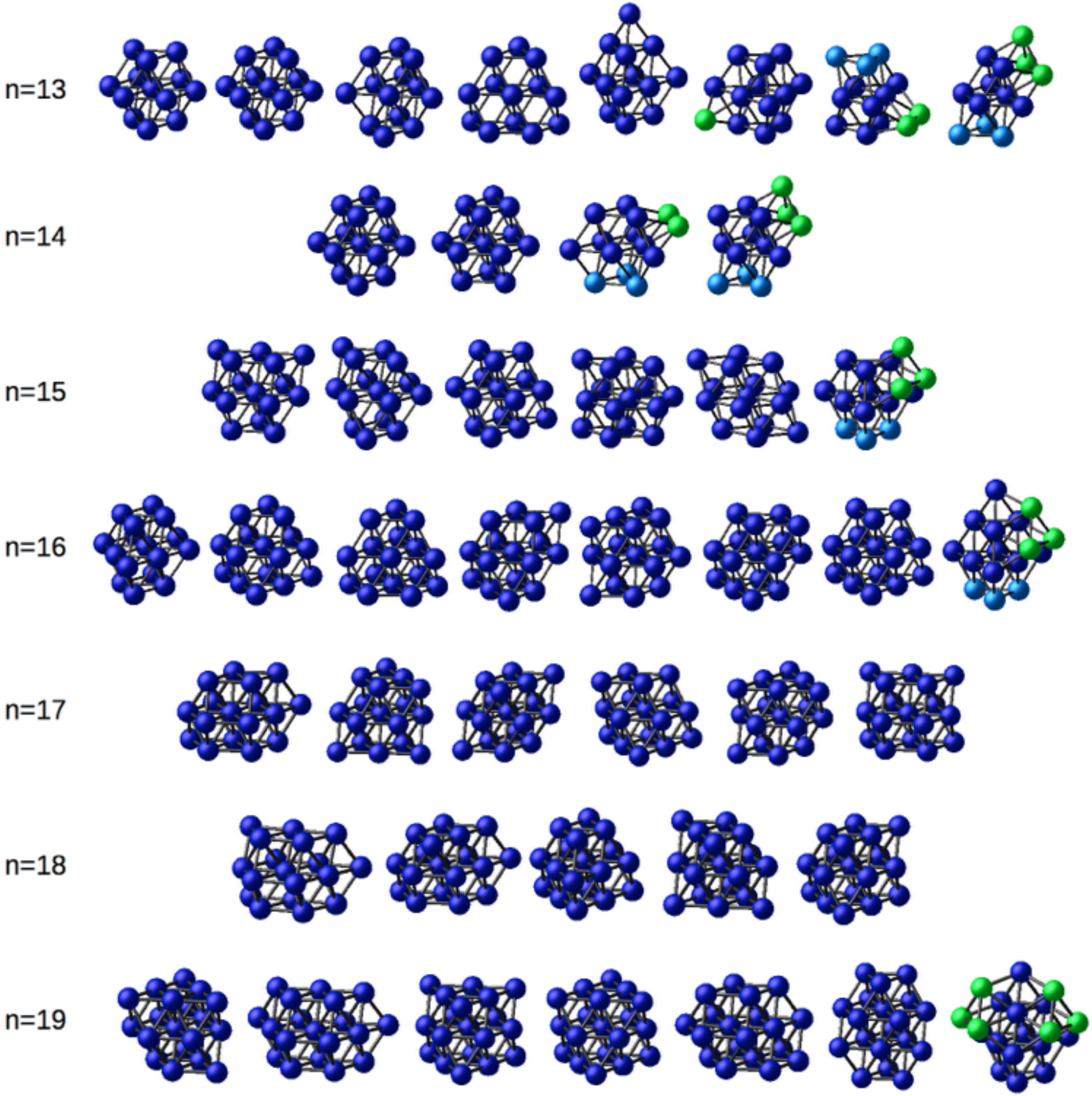
~~(why? is this provable/disprovable?)~~ e.g. Stillinger ~~(1984,1995)~~, Frenkel (2014), etc.

Total number of clusters computed

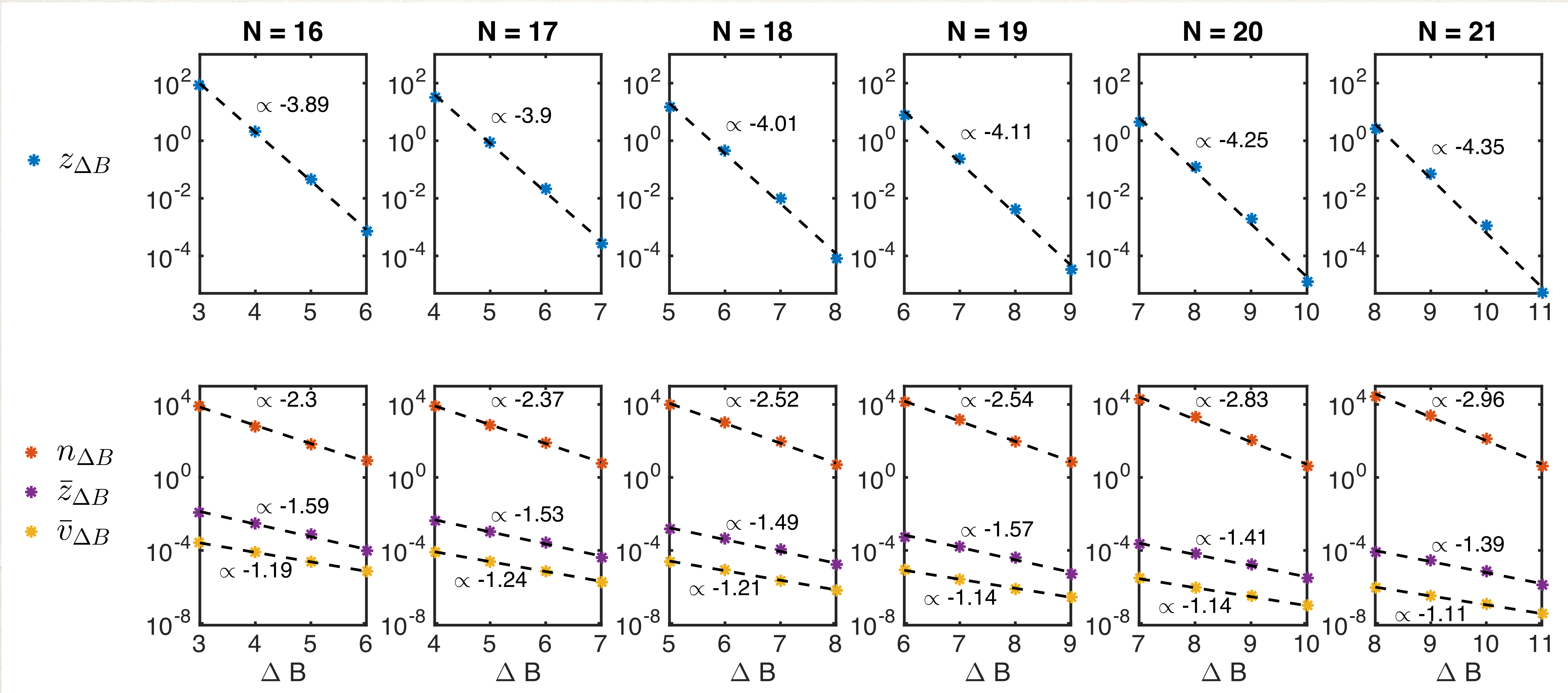
n	number of contacts								
	$3n-9$	$3n-8$	$3n-7$	$3n-6$	$3n-5$	$3n-4$	$3n-3$	$3n-2$	Total
5				1					1
6				2					2
7				5					5
8				13					13
9				52					52
10			1	259	3				263
11		2	18	1618	20	1			1659
12		11	148	11,638	174	8	1		11,980
13		87	1221	95,810	1307	96	8		98,529
14	1	707	10,537	872,992	10,280	878	79	4	895,478
	$3n-4$	$3n-3$	$3n-2$	$3n-1$	$3n$	$3n+1$	$3n+2$		
15	7675	782	55	6					(9×10^6 est.)
16		7895	664	62	8				(1×10^8 est.)
17			7796	789	85	6			(1.2×10^9 est.)
18				9629	1085	91	5		(1.6×10^{10} est.)
19					13,472	1458	95	7	(2.2×10^{11} est.)

(N=20,21 also; data not shown)

hyperstatic


n=13
n=14
n=15
n=16
n=17
n=18
n=19

Some scaling laws



Why all these exponential scaling laws?

Do the exponents approach a common value as N→∞ ?

can explain using geometry, combinatorics, random matrix theory, …?

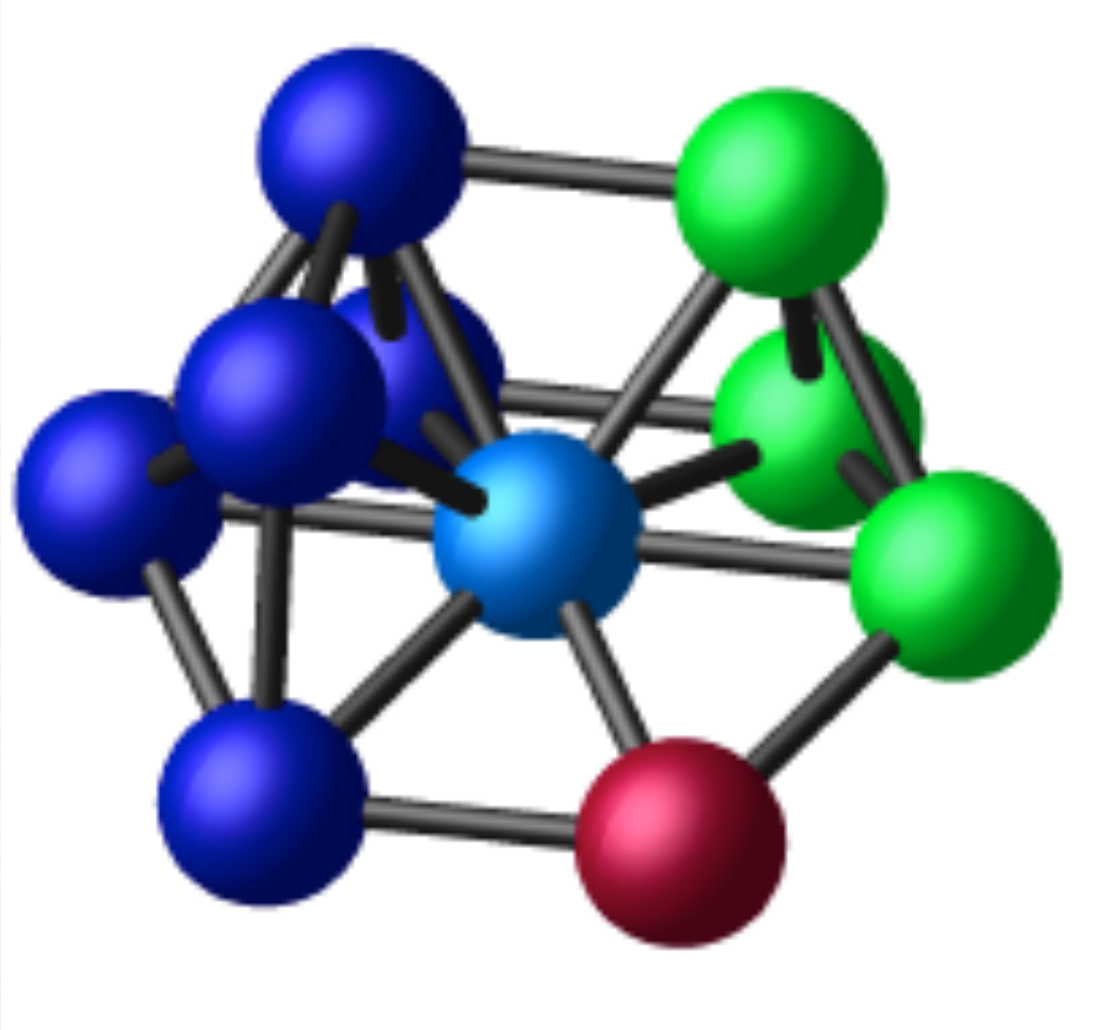
Total number of clusters computed

n	number of contacts								
	$3n-9$	$3n-8$	$3n-7$	$3n-6$	$3n-5$	$3n-4$	$3n-3$	$3n-2$	Total
5				1					1
6				2					2
7				5					5
8				13					13
9				52					52
10			1	259	3				263
11		2	18	1618	20	1			1659
12		11	148	11,638	174	8	1		11,980
13		87	1221	95,810	1307	96	8		98,529
14	1	707	10,537	872,992	10,280	878	79	4	895,478
	$3n-4$	$3n-3$	$3n-2$	$3n-1$	$3n$	$3n+1$	$3n+2$		
15	7675	782	55	6					(9×10^6 est.)
16		7895	664	62	8				(1×10^8 est.)
17			7796	789	85	6			(1.2×10^9 est.)
18				9629	1085	91	5		(1.6×10^{10} est.)
19					13,472	1458	95	7	(2.2×10^{11} est.)

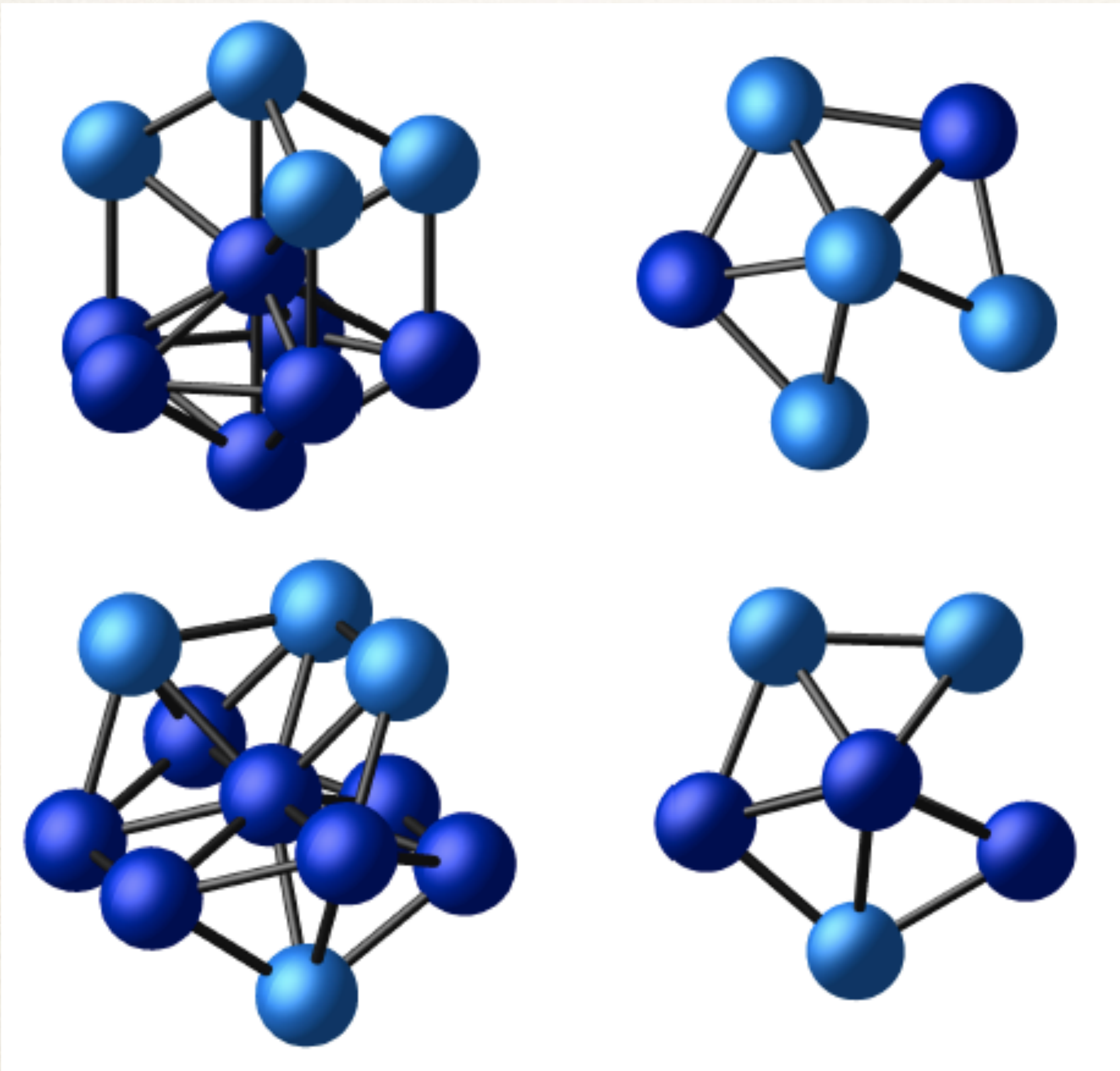
(N=20,21 also; data not shown)

hypostatic

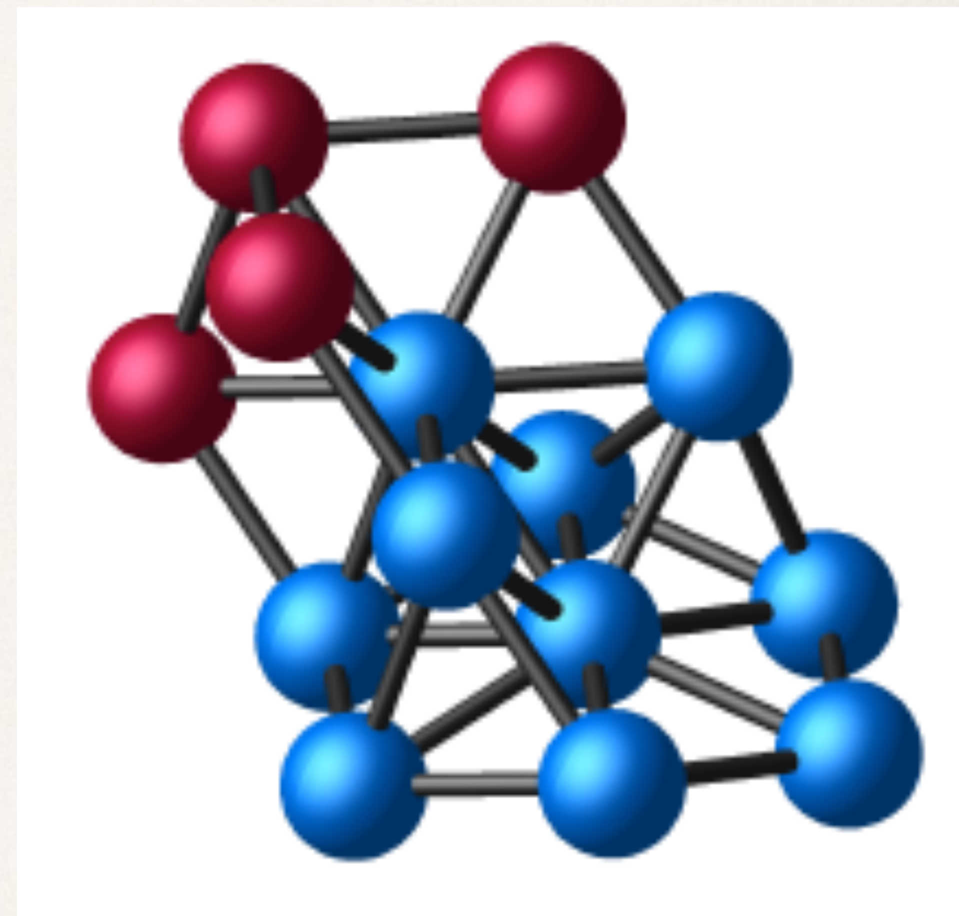
A cluster “missing” one contact, N=10



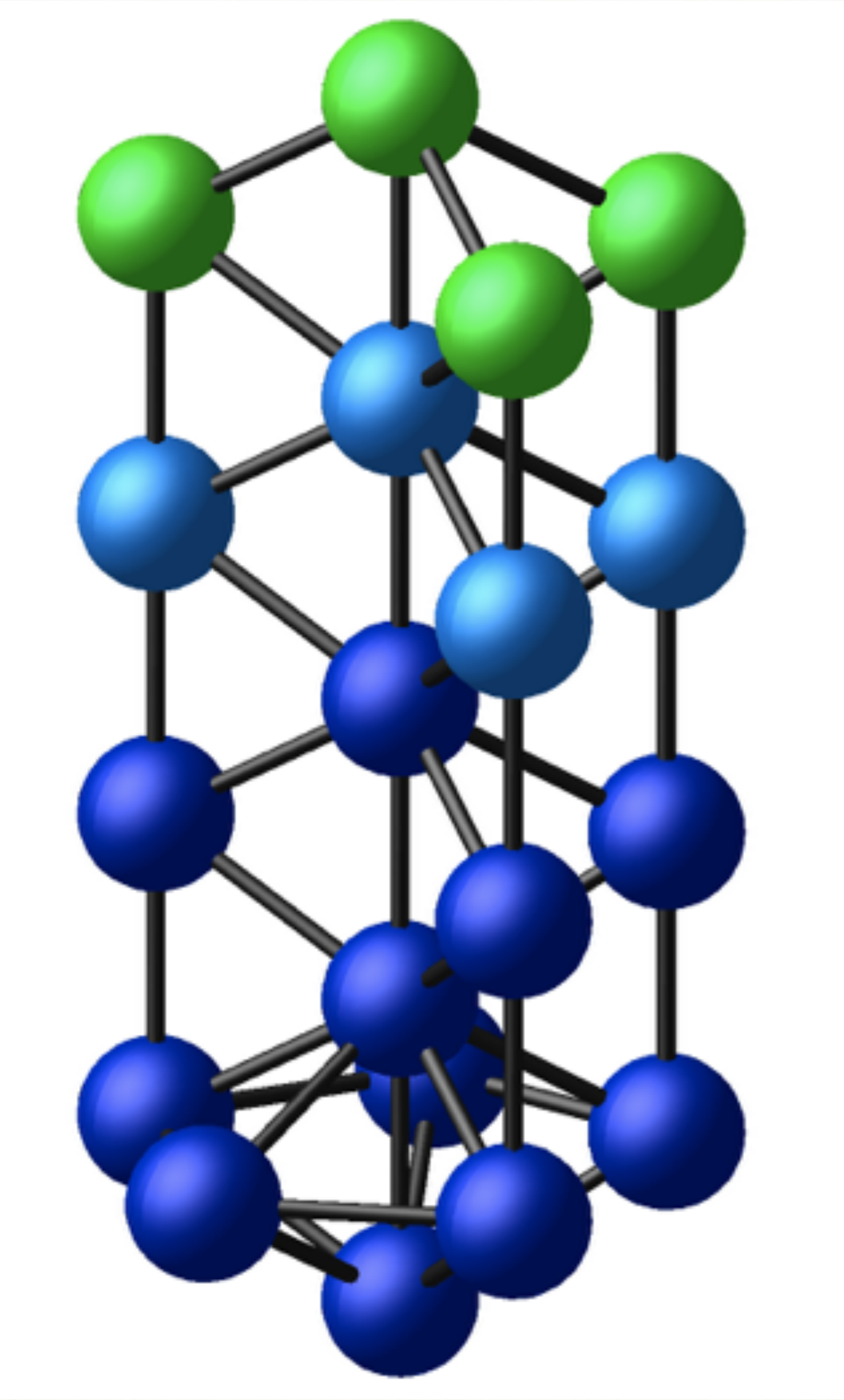
clusters missing two contacts, N=11



cluster missing three contacts, N=14

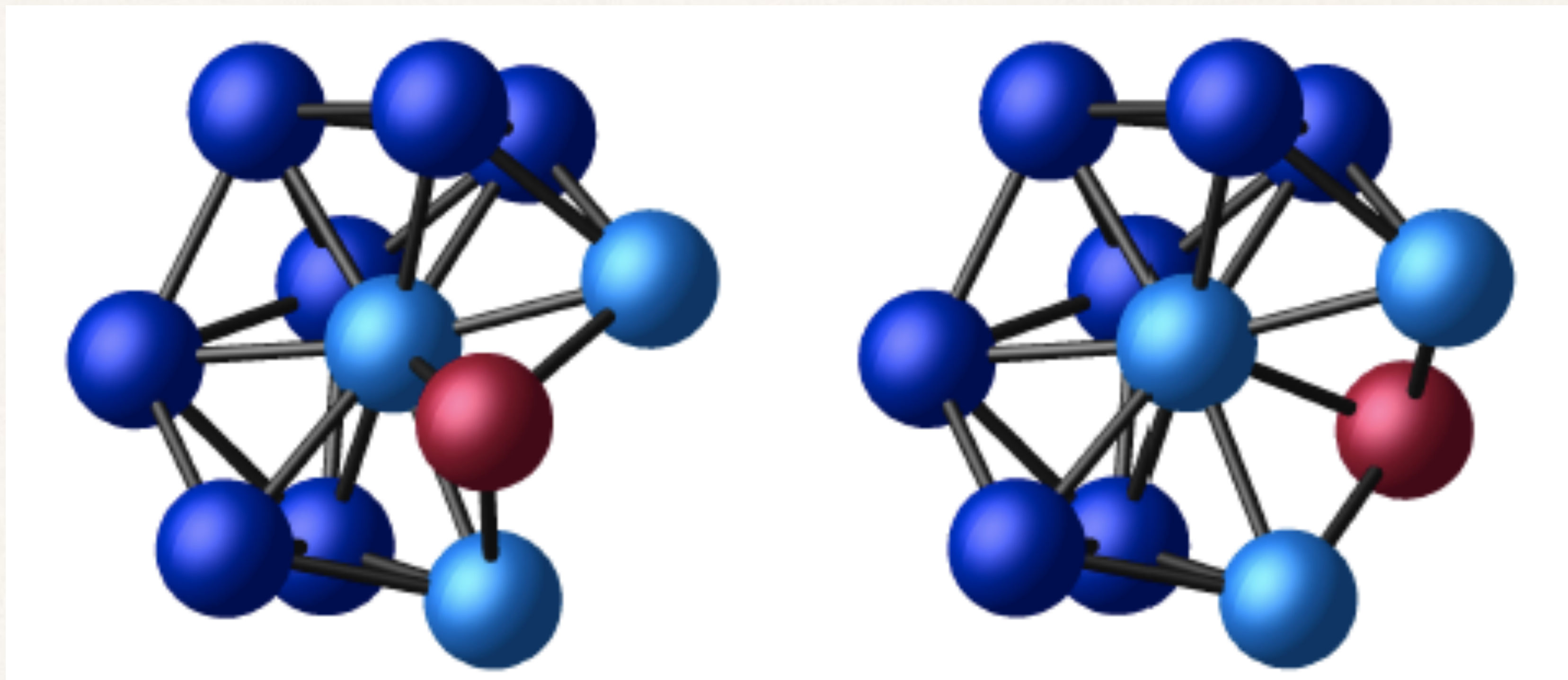


cluster missing arbitrarily many contacts

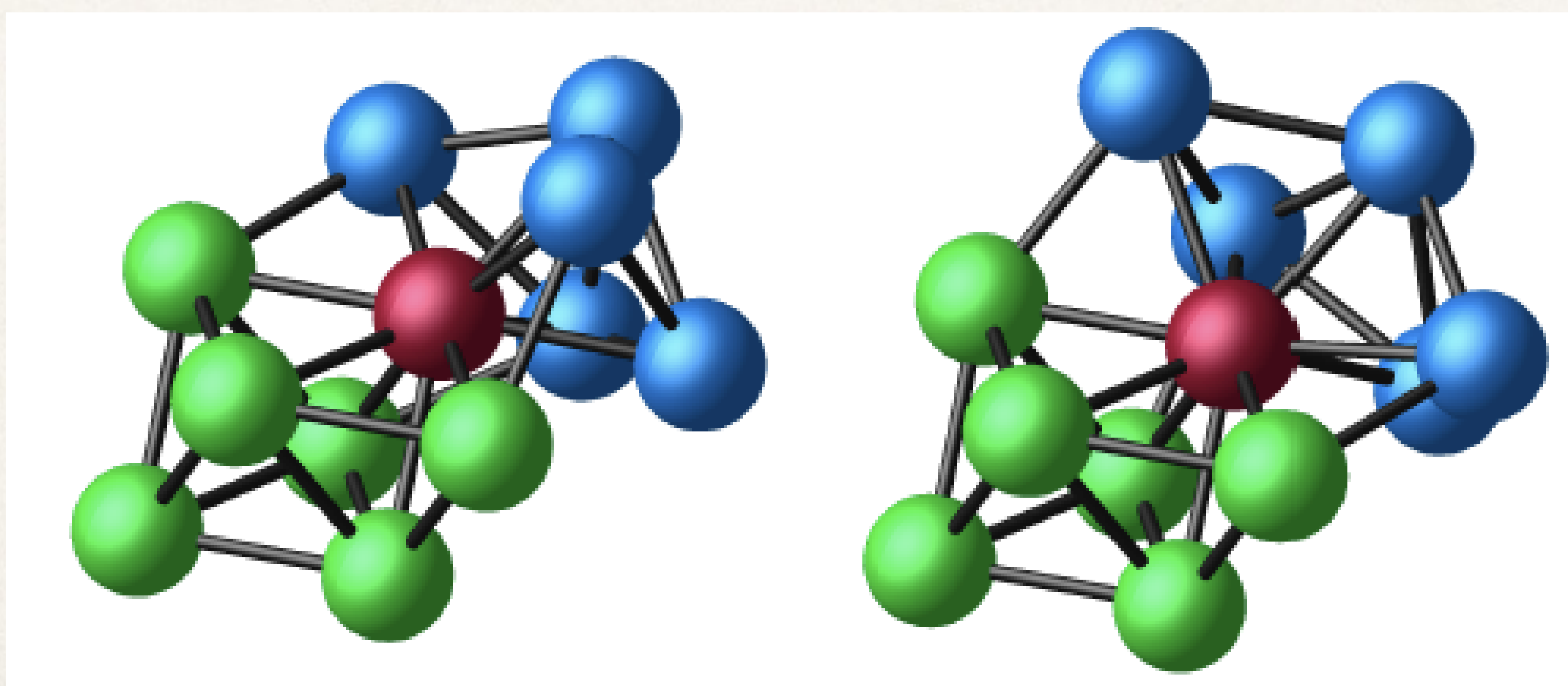


# of contacts ~ 2N when N large

Clusters with the same adjacency matrix

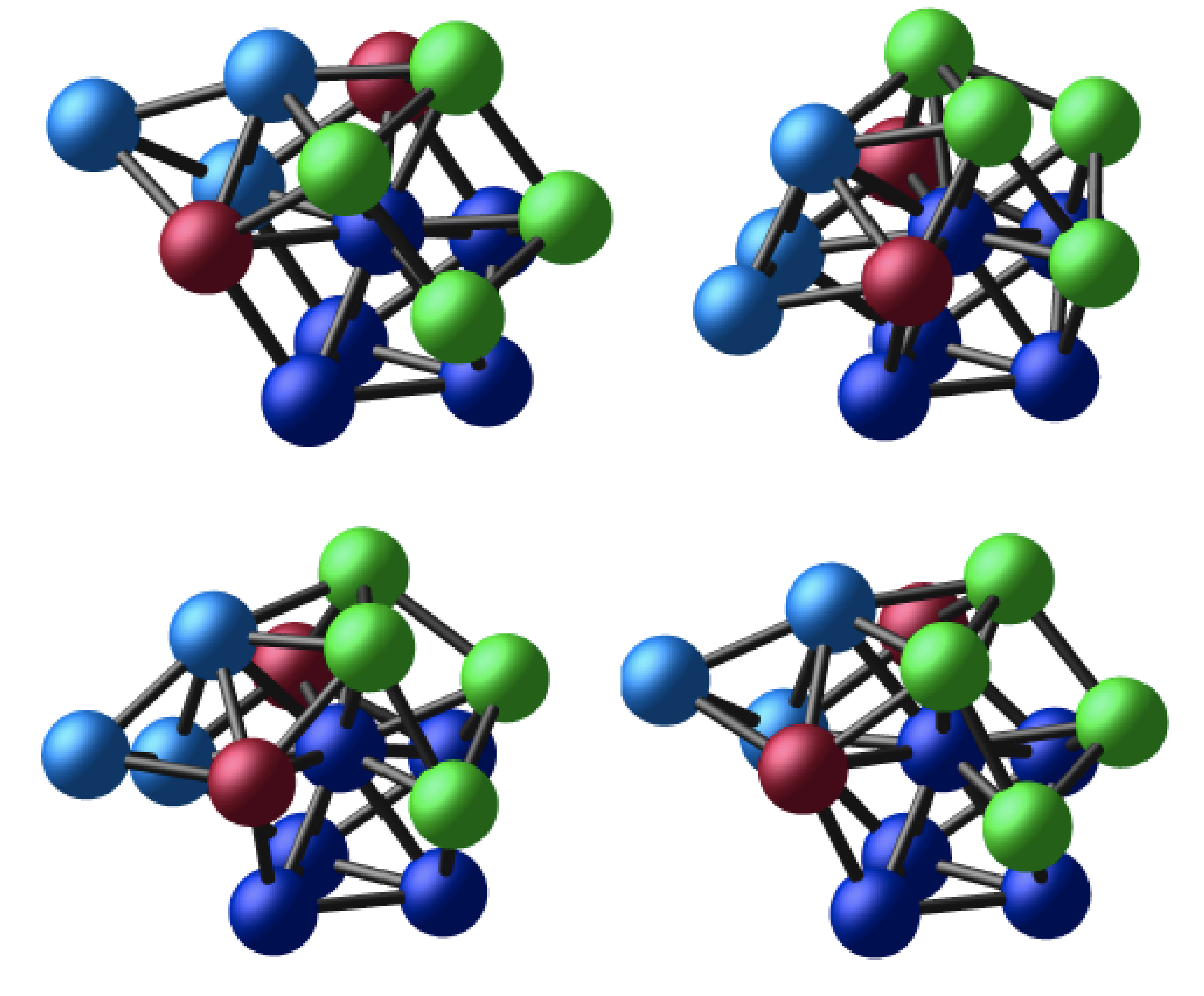


N=11



N=12

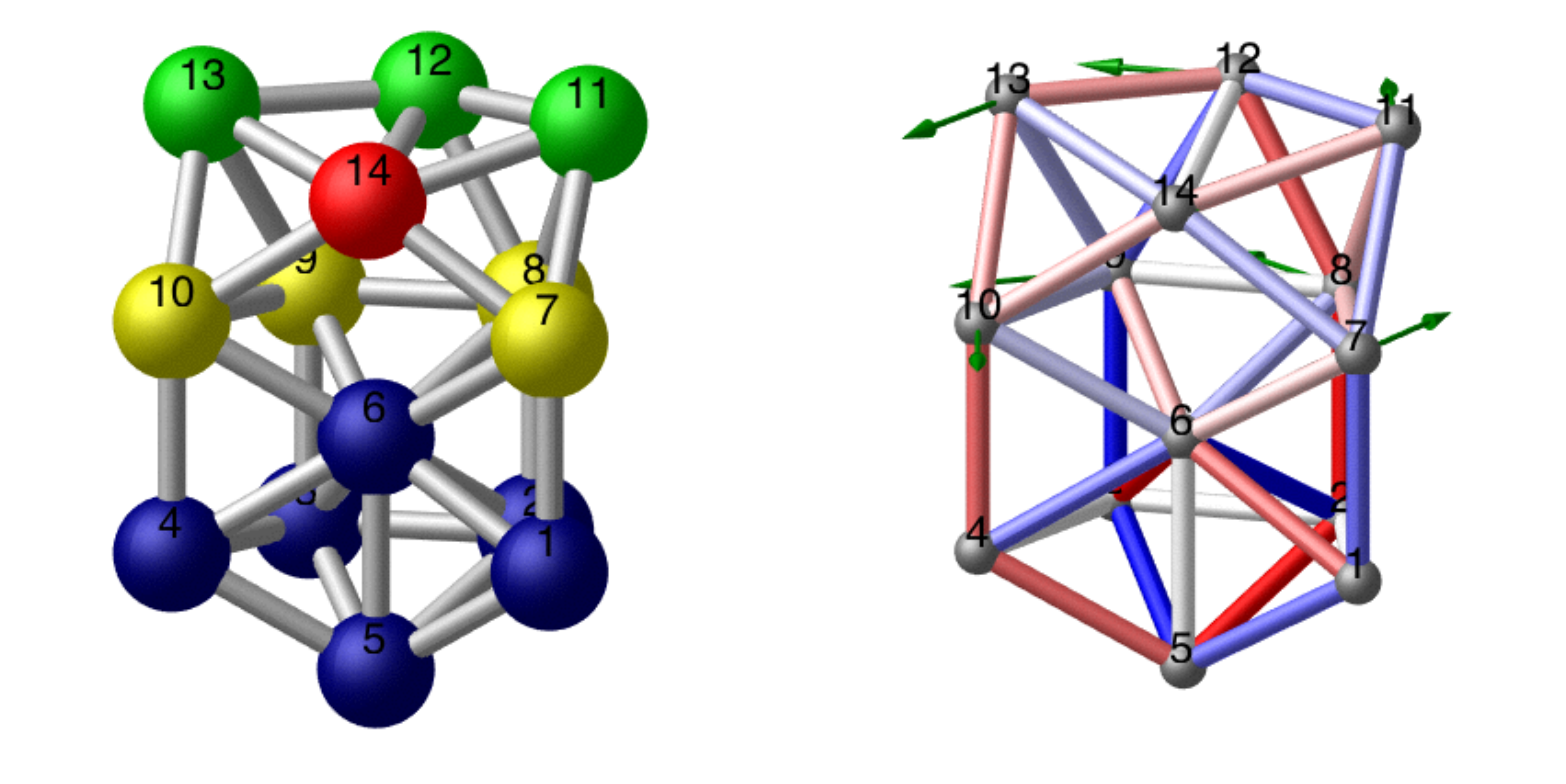
4 clusters with the same adjacency matrix (N=14)



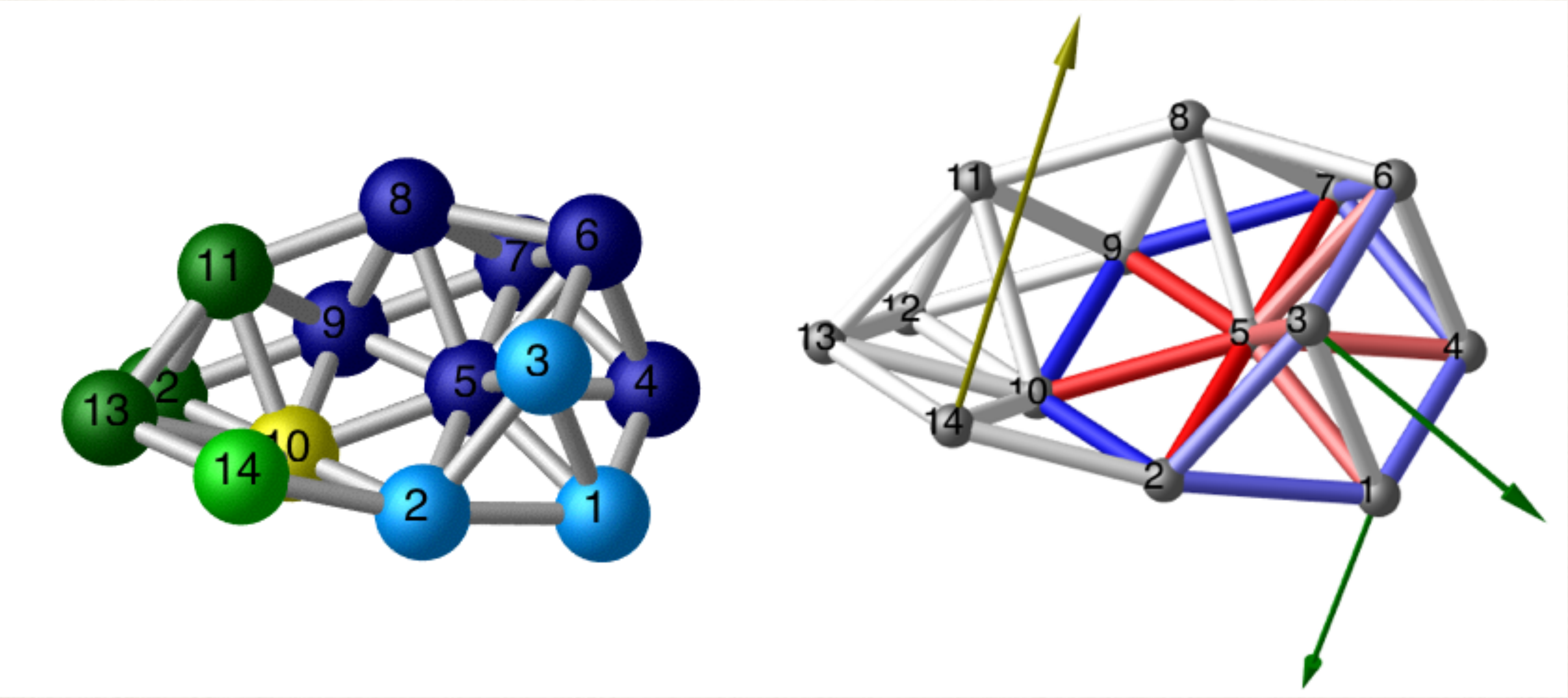
adj. matrices with multiple copies: N=11 (1), N=12 (23), N=13 (474), N=14 (6672)

with Bob Connelly,
Jonathan Hauenstein

A "Third-order rigid" cluster (algebraic multiplicity = 3)

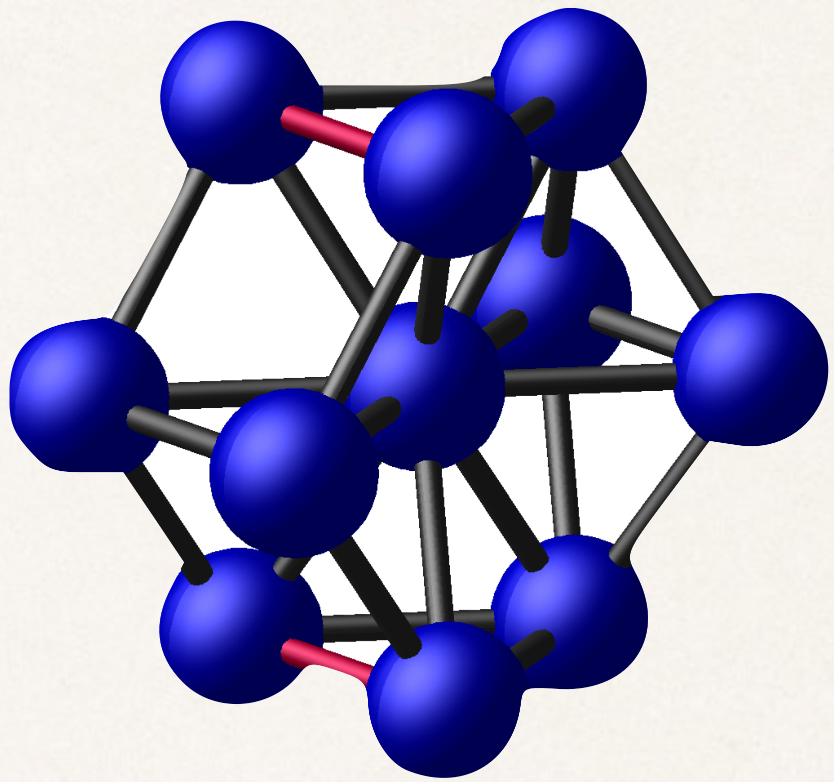


Another higher-order rigid cluster



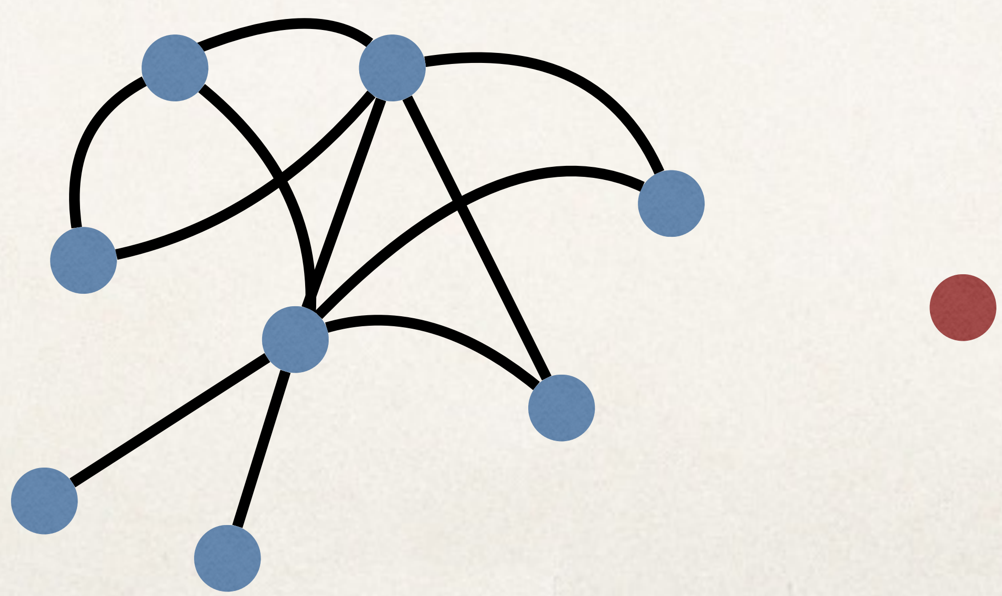
Does the algorithm find everything?

No……… here's an example:



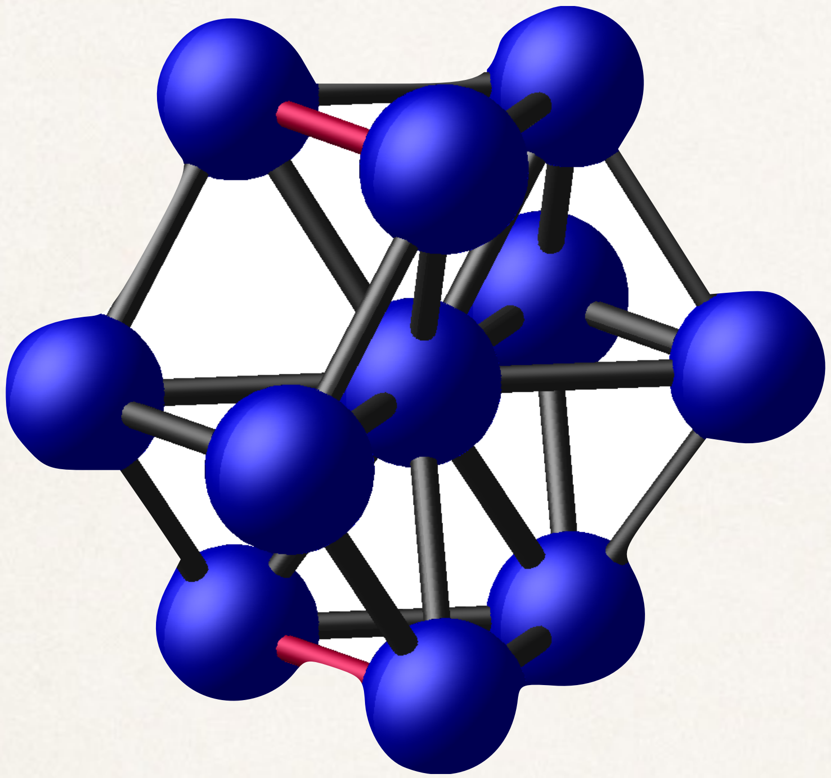
N=11
hypostatic
3N-7 contacts
hcp fragment

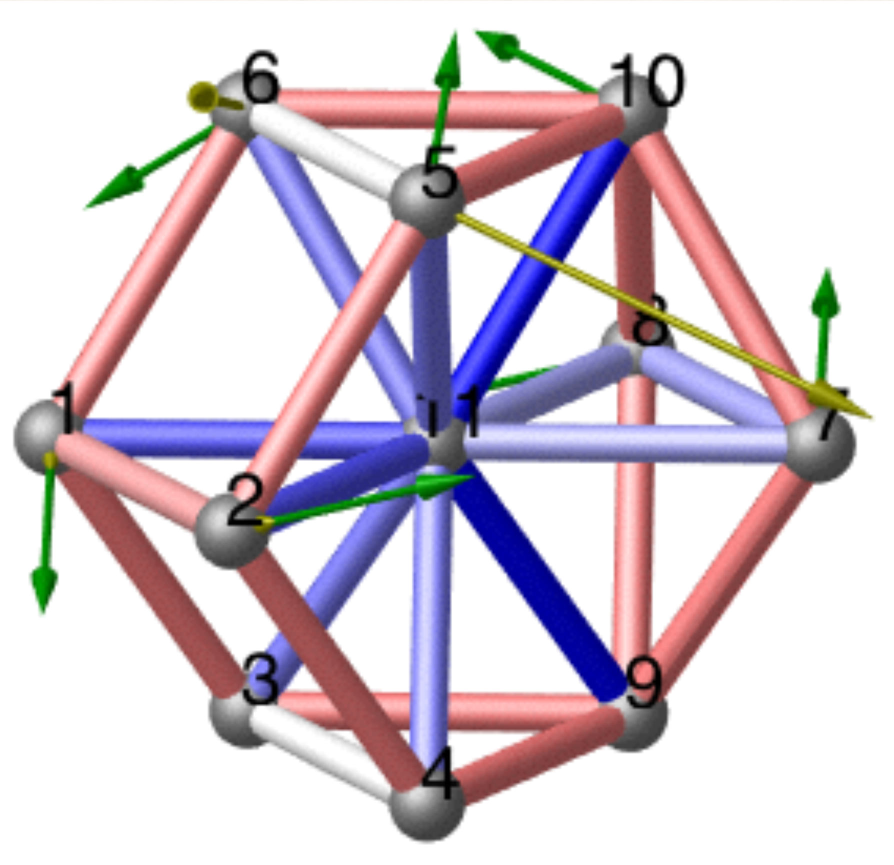
Cluster landscape looks like:



Question:
Is the landscape ever connected (by 1 dof motions), under additional assumptions?
e.g. clusters are regular, isostatic, have random diameters, ….

A peek into why we can't find it (thanks to Louis Theran)



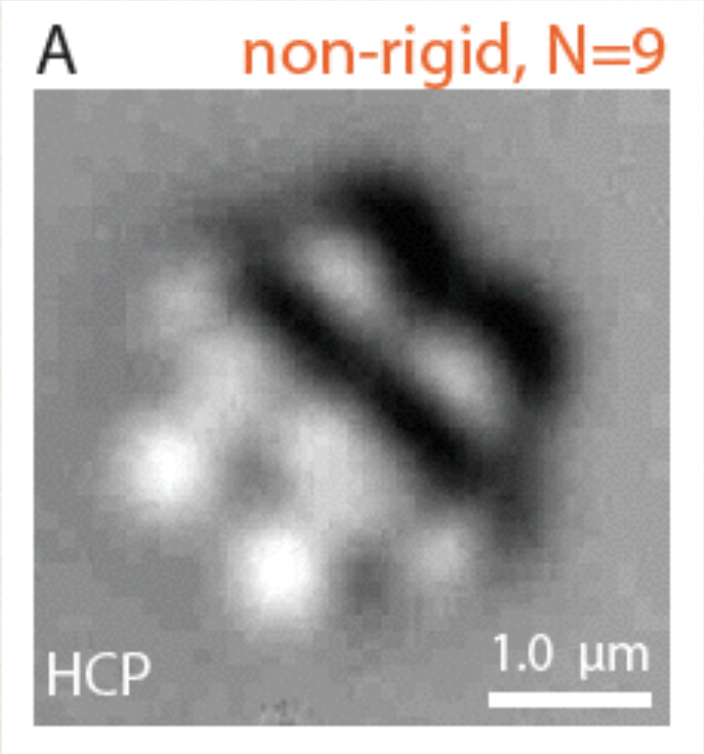


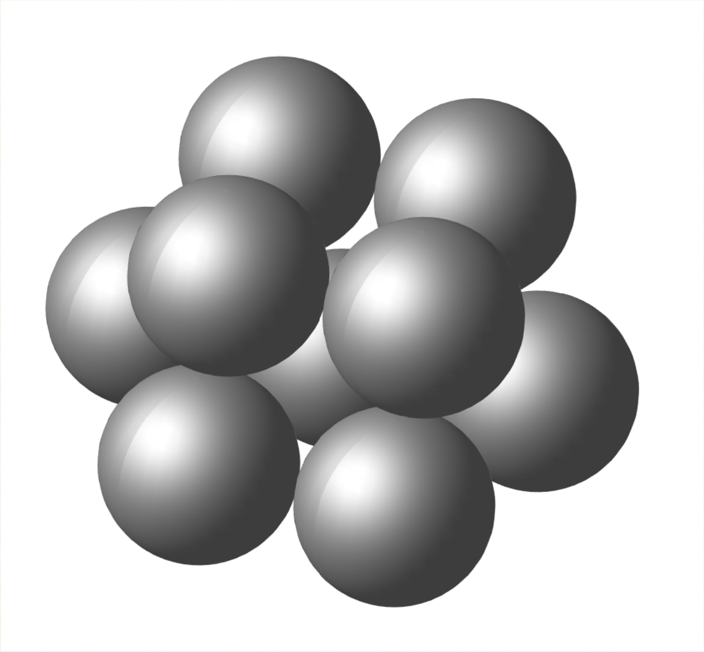
- Recipe for making a cluster the algorithm can't find (L. Theran):
  Make a cluster which is
  - hypostatic
  - has a stress supported on all edges
- Cut the stress —> cluster becomes regular, hence > 1 d.o.f.

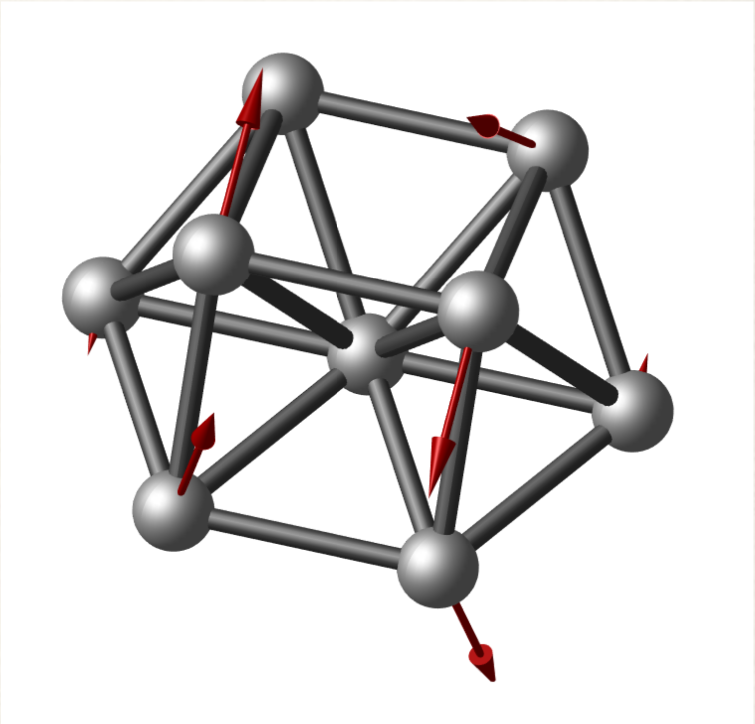
Data contains lots of singular clusters

Singular cluster: rigid but not first-order rigid
This is a *nonlinear* notion of rigidity.

Smallest singular cluster: N=9

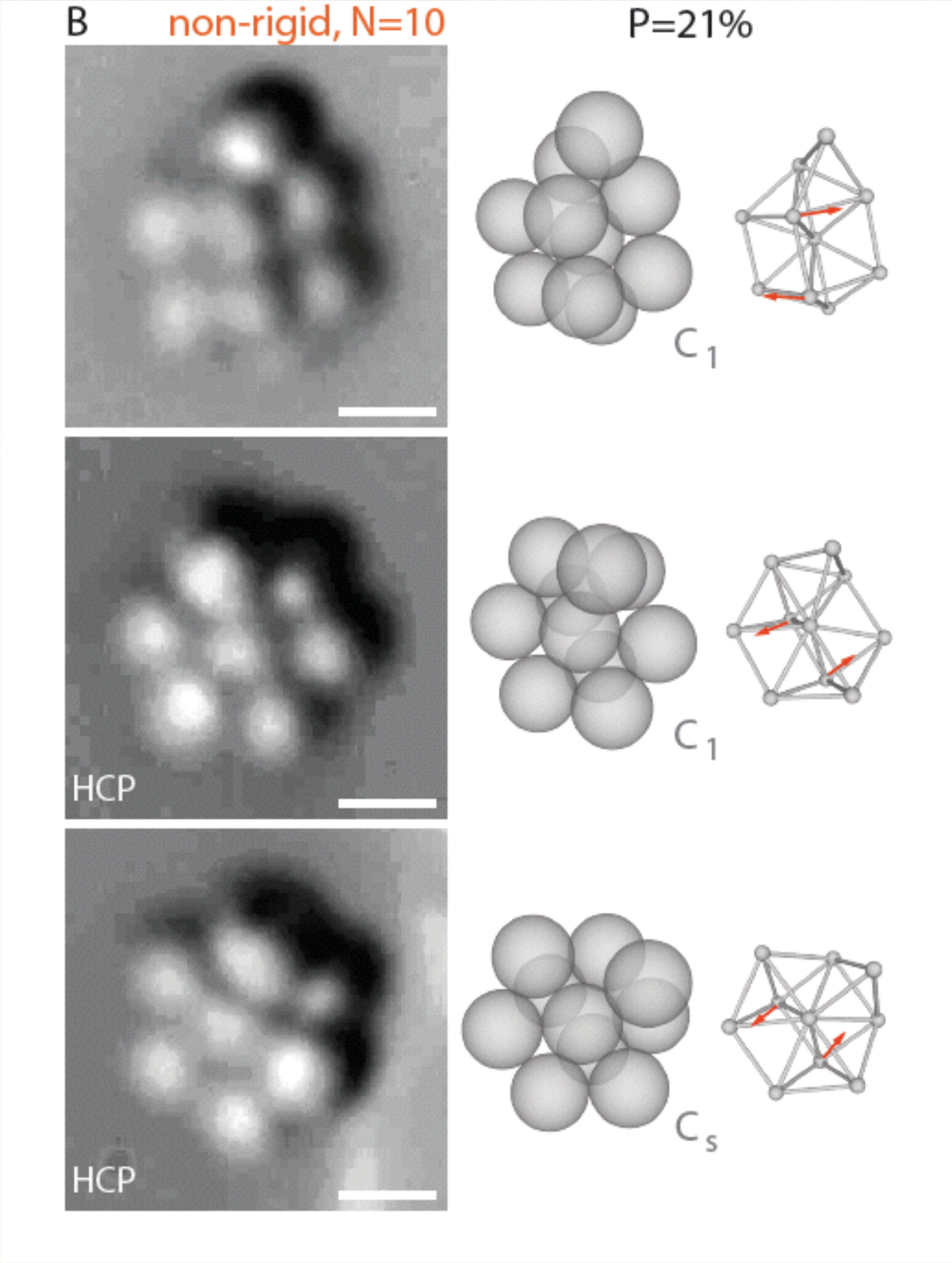






G. Meng, N. Arkus, M. P. Brenner, V. N. Manoharan, Science 327 (2010)

Probability 11% in experiments! (out of 52 clusters total)



N=10:
singular 21%,
hyperstatic 12%
despite > 250 total clusters!

Is there a competition between singular, hyperstatic clusters as N increases?

—> not symmetry number that matters, rather degree of singularity / hyperstaticity?

Singular clusters

N	%
11	3%
12	2.9%
13	2.7%
14	2.5%

Close-packing fragments

N	%
10	17%
11	7.2%
12	3.6%
13	1.6%
14	0.63%

H.-C. (2016) *SIAM Review*

Statistical Mechanics

What is the probability of a cluster x in the sticky-sphere (short-ranged interaction) limit?

M. H.-C., S. Gortler, M.P.Brenner, PNAS (2013)
Y. Kallus, M. H.-C., Phys. Rev. E (2017)

Probability(cluster x) ∝ Partition function Z_x

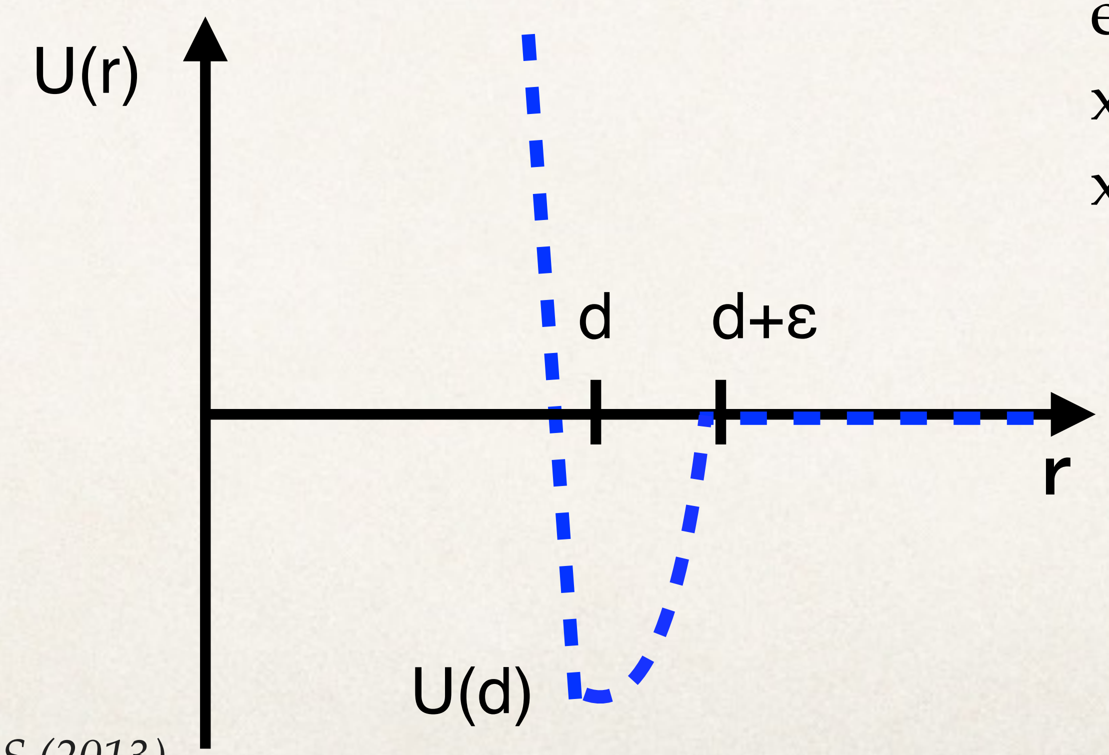
$$Z_x = \int_{N(x)} e^{-\beta V(x')} dx'$$

V(x) = energy of configuration x, $\beta = 1/k_B T$ = inverse temperature
N(x) = neighbourhood of x, including translations, rotations, permutations, and bonds with lengths ∊ (d - ε, d + ε)

energy of a pair = $U(|x_i - x_j|)$
x_i=center of i^{th} sphere,
$x=(x_1,x_2,\ldots,x_N)$

Sticky-sphere limit:

- Range ε « d
- Depth U(d) » 1



$$V(x) = \sum_{i \neq j} U(|x_i - x_j|)$$

M. H.-C., S. Gortler, M.P. Brenner, PNAS (2013)
Y. Kallus, M. H.-C., Phys. Rev. E (2017)

“Geometry” of the calculation

Asymptotically as ε —> 0:

B = # of bonds

$$Z_x \sim e^{-\beta B U(d)} \int_{\{-\epsilon \leq y_k(x) \leq \epsilon\}_{k=1}^{B}} dx$$

constraints ``fattened” by ε

$y_k(x) = |x_{i_k} - x_{j_k}| - 1$ = excess bond distance between spheres i_k, j_k

$\{x : y_k(x) = 0\}$ is hypersurface where sphere i_k touches sphere j_k

Z_x ≈ Exp(# of contacts) * Volume(constraint intersection region)

$\to \infty$ “energy” $\to 0$ “entropy”

Example (regular)

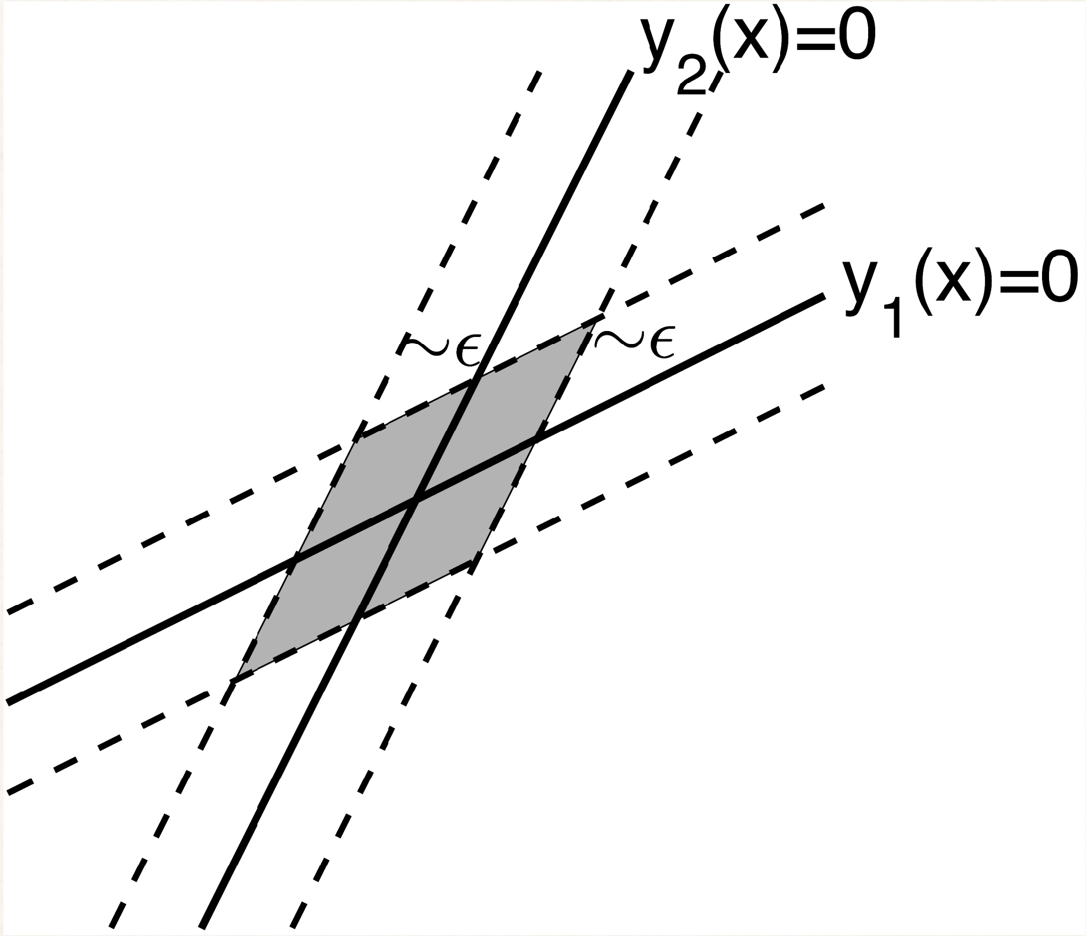
$x \in R^2$

$y_1(x) = v_1 \cdot x = 0$

$y_2(x) = v_2 \cdot x = 0$

Want volume of region

$M = \{ -\varepsilon < y_1(x), y_2(x) < \varepsilon \}$



$$\mathrm{Vol}(M) = 4 \, | \, v_1 \times v_2 \, |^{-1} \, \varepsilon^2$$

"Regular" constraints should have volumes that scale as

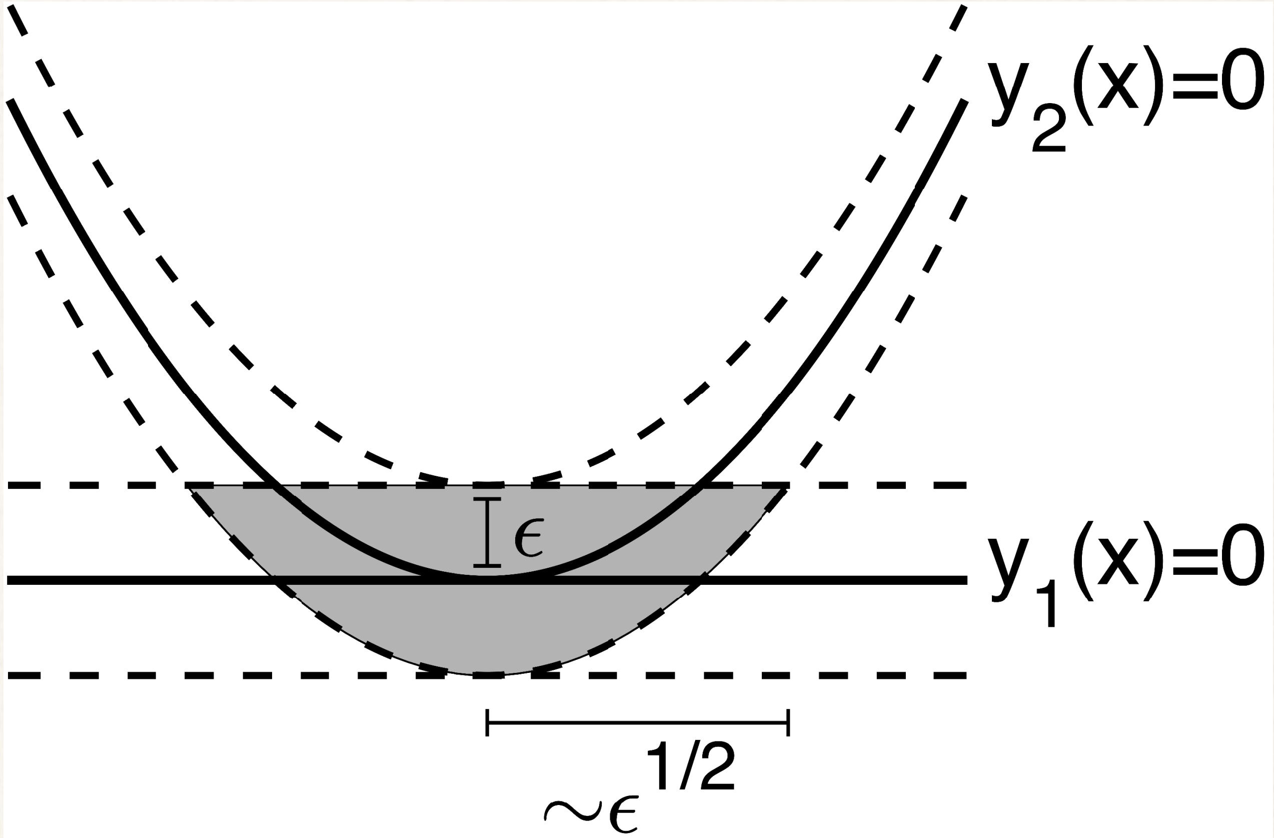
$\varepsilon^{\text{dimension of intersection set}}$

Example (singular)

$x \in R^2$

$y_1(x) = x_2$

$y_2(x) = (x_1)^2 - x_2$



Change variables:

$Y_1 = y_1 / \varepsilon$

$Y_2 = y_2 / \varepsilon^{1/2}$

$$\frac{\partial Y}{\partial x} = 2\epsilon^{-3/2}\sqrt{Y_1 + Y_2}$$

$$\mathrm{Vol} = \epsilon^{3/2} \iint_{\substack{-1 \leq Y_1 \leq 1 \\ -1 \leq Y_2 \leq 1}} \frac{1}{2\sqrt{Y_1 + Y_2}} dY_1 dY_2 = \boxed{\epsilon^{3/2}} \cdot O(1)$$

$$\frac{\text{Vol(Example 2)}}{\text{Vol(Example 1)}} \sim \frac{1}{\epsilon^{1/2}} \qquad \nearrow \infty \quad \text{as } \epsilon \to 0$$

—> Free energy of singular clusters should dominate that of regular clusters (with the same number of contacts), in the sticky-sphere limit.

Physically, they have more ***entropy***.

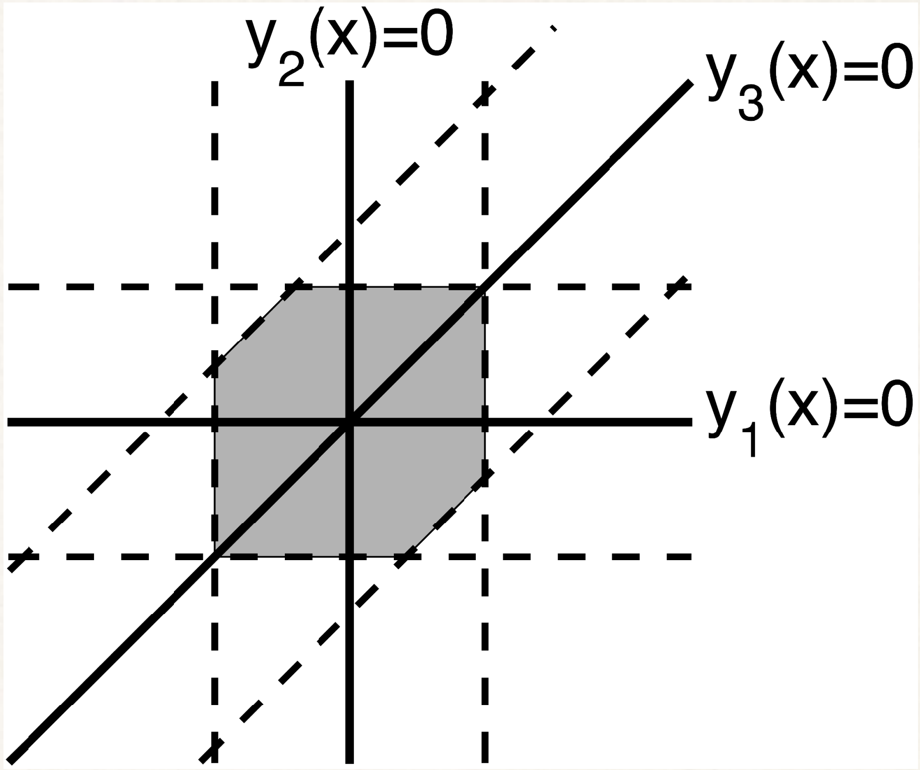
Example (hyperstatic)

$x \in R^2$

$y_1(x) = v_1 \cdot x$

$y_2(x) = v_2 \cdot x$

$y_3(x) = v_3 \cdot x$



$\mathrm{Vol} \propto \varepsilon^2$ $\qquad Z_x \propto e^{-3\beta U(d)} \epsilon^2$

$Z_x \approx$ Exp(# of contacts) * Volume(constraint intersection region)

$$\frac{Z_x(\text{hyperstatic example})}{Z_x(\text{regular example})} \propto e^{-\beta U(d)} \quad \to \infty \quad \text{as } U(d) \to -\infty$$

—> Free energy of hyperstatic clusters should dominate that of regular clusters, in the sticky-sphere limit.

Physically, they have lower ***energy***.

Who wins: singular clusters or hyperstatic clusters, as N $\to\infty$?

General case

How does the free energy of singular clusters scale with ε?

Algebraic geometry:

$$\mathrm{Vol} \sim \epsilon^q (\log \epsilon)^k, \qquad q \in \mathbb{Q}, \quad k \in \mathbb{Z}$$

q,k related to the algebraic nature of the singularity, i.e. what it looks like once it is "resolved"

IGUSA INTEGRALS AND VOLUME ASYMPTOTICS
IN ANALYTIC AND ADELIC GEOMETRY

ANTOINE CHAMBERT-LOIR

Université de Rennes 1 and Institut universitaire de France,
IRMAR–UMR 6625 du CNRS, Campus de Beaulieu,
35042 Rennes Cedex, France
antoine.chambert-loir@univ-rennes1.fr

YURI TSCHINKEL

Courant Institute, NYU, 251 Mercer St.
New York, NY 10012, USA
tschinkel@cims.nyu.edu

Received 24 December 2009
Revised 11 October 2010

We establish asymptotic formulas for volumes of height balls in analytic varieties over local fields and in adelic points of algebraic varieties over number fields, relating the Mellin transforms of height functions to Igusa integrals and to global geometric invariants of the underlying variety. In the adelic setting, this involves the construction of general Tamagawa measures.

Keywords: Heights; Poisson formula; Manin's conjecture; Tamagawa measure.

AMS Subject Classification: 11G50 (11G35, 14G05)

Our approach

$$Z_x = \int_{N(x)} e^{-\beta V(x')} dx'$$

- Taylor-expand the potential V(x) = $\sum_{i \neq j} U(|x_i - x_j|)$
- Evaluate integral using Laplace asymptotics
- Asymptotically the same scaling as square-well potential:
  $\log(Z_{square}) \sim \log(Z_x)$ as $\varepsilon \to 0$, $U(d) \to \infty$ (Kallus & H.-C., Phys Rev E (2017))

M. H.-C., S. Gortler, M.P.Brenner, PNAS (2013)
Y. Kallus, M. H.-C., Phys. Rev. E (2017)

Partition function for second-order rigid cluster

of bonds beyond 3N-6

# of singular directions

$$Z_x = \gamma^{\Delta B} \alpha^{d_X} z_x$$

Exp(depth)

width$^{-1/2}$

where the geometrical part is

$$z_x = (\text{const}) \cdot \frac{\sqrt{I(x)}}{\sigma} \prod_{\lambda_i \neq 0} \lambda_i^{-1/2}(x) \int_X e^{-Q(\tilde{\mathbf{x}})} d\tilde{\mathbf{x}}$$

parameters are

$$\gamma = e^{-\beta U(d)}$$
$$\alpha = (U''(d)\beta d^2)^{1/4}$$

Only TWO parameters needed!

geometry-dependent variables are

ΔB = # of bonds beyond isostatic (=B-(3N-6))

d_X = # of singular directions

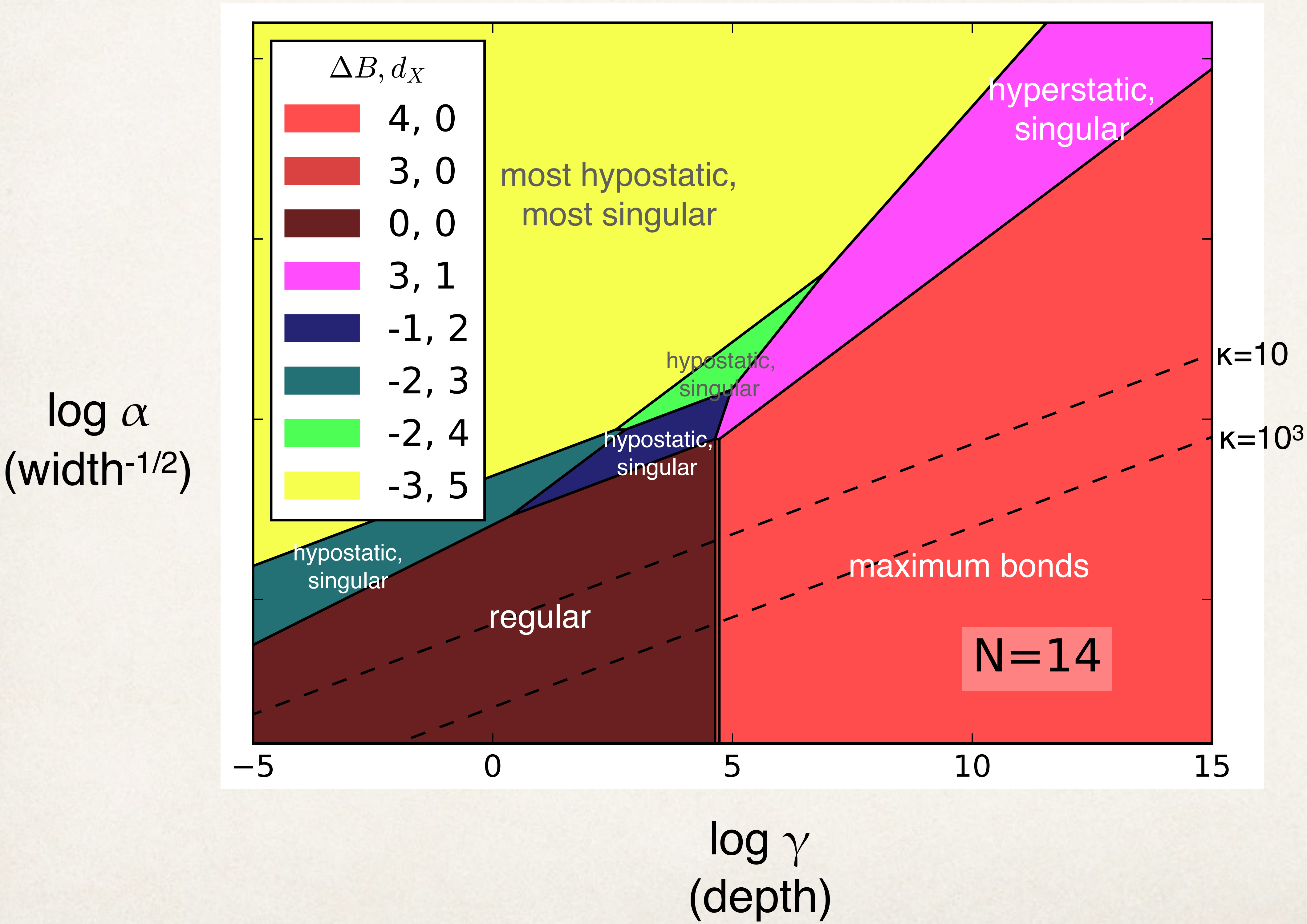
I(x) = determinant of moment of inertia tensor

σ = symmetry number

$\boldsymbol{\lambda}_i(x)$ = eigenvalues of $\nabla\nabla V = R(x)R^T(x)$

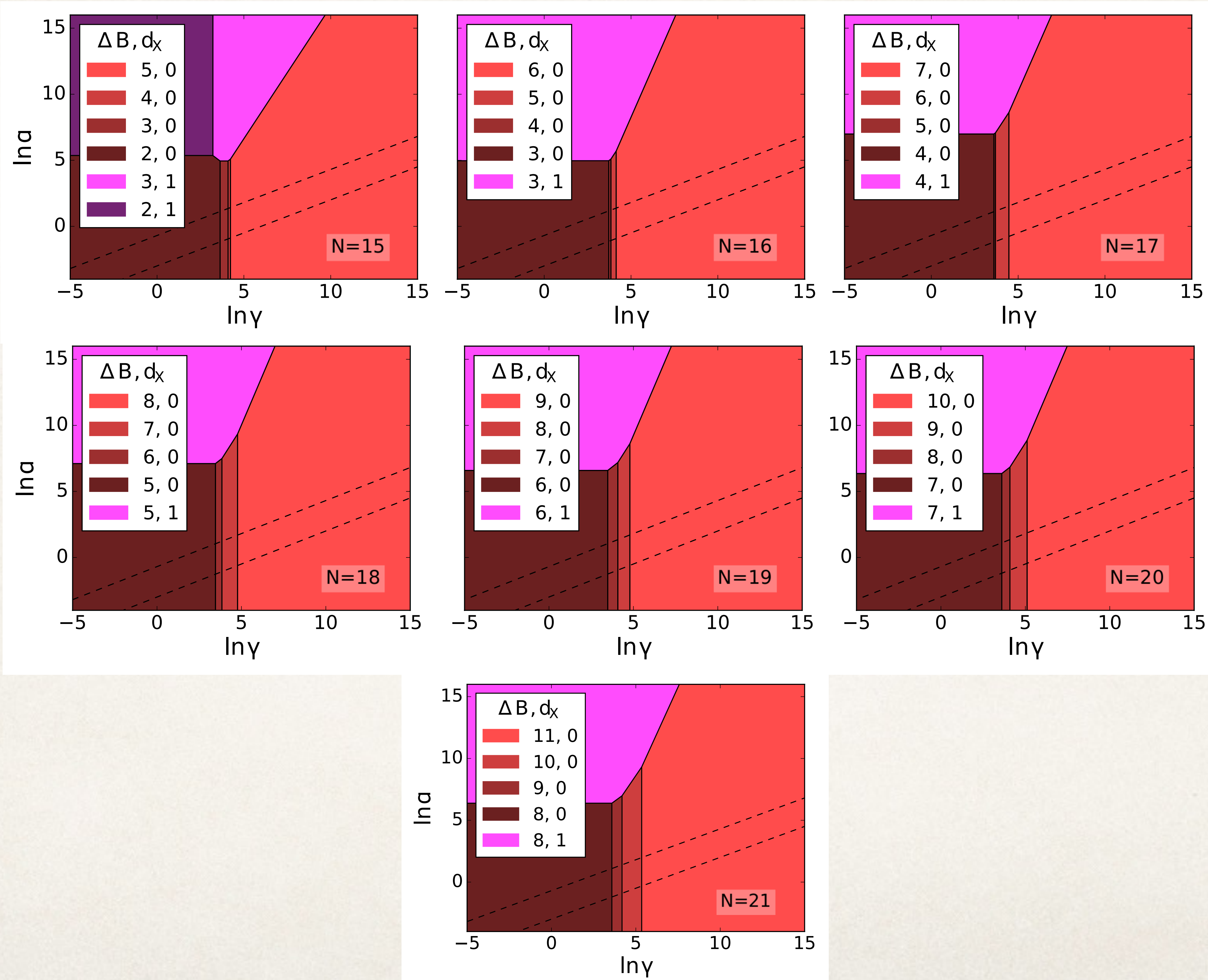
Q(x) = quartic function on space X of singular directions

N=14



$\Delta B, d_X$
4, 0
3, 0
0, 0
3, 1
-1, 2
-2, 3
-2, 4
-3, 5
most hypostatic,
most singular
hyperstatic,
singular
hypostatic,
singular
hypostatic,
singular
hypostatic,
singular
regular
maximum bonds
N=14
κ=10
κ=10^3
−5
0
5
10
15
log α
(width$^{-1/2}$)
log γ
(depth)

N=15-21



ΔB, d_X
5, 0
4, 0
3, 0
2, 0
3, 1
2, 1
N=15
ΔB, d_X
6, 0
5, 0
4, 0
3, 0
3, 1
N=16
ΔB, d_X
7, 0
6, 0
5, 0
4, 0
4, 1
N=17
ΔB, d_X
8, 0
7, 0
6, 0
5, 0
5, 1
N=18
ΔB, d_X
9, 0
8, 0
7, 0
6, 0
6, 1
N=19
ΔB, d_X
10, 0
9, 0
8, 0
7, 0
7, 1
N=20
ΔB, d_X
11, 0
10, 0
9, 0
8, 0
8, 1
N=21
lnα
lnγ
−5
0
5
10
15

Conclusions / Outlook

- Hyperstatic > Singular (empirically*, for identical spheres) *(no floppy)
  - Why? ∃ underlying geometric, or statistical, reason?
  - High temperature —> disorder. Critical temperature predicted by geometry.
  - Do other systems favour singular, or hypostatic structures (e.g. non-identical spheres, ellipses, ….?)
- Computational challenges still remain
  - Efficiently determining rigidity, in the presence of "noise" (numerical error)
  - Efficiently determining "floppiness": degrees of freedom, and "true" tangent space
- Algorithm gives us (leading-order) Transition Rates!
  - Predictions agree with our experiments

    (R. W. Perry, M. H.-C., M. P. Brenner, V. N. Manoharan, PRL (2015))