Before we begin: A quick visit to the behavioral economics literature

Extraneous factors in judicial decisions

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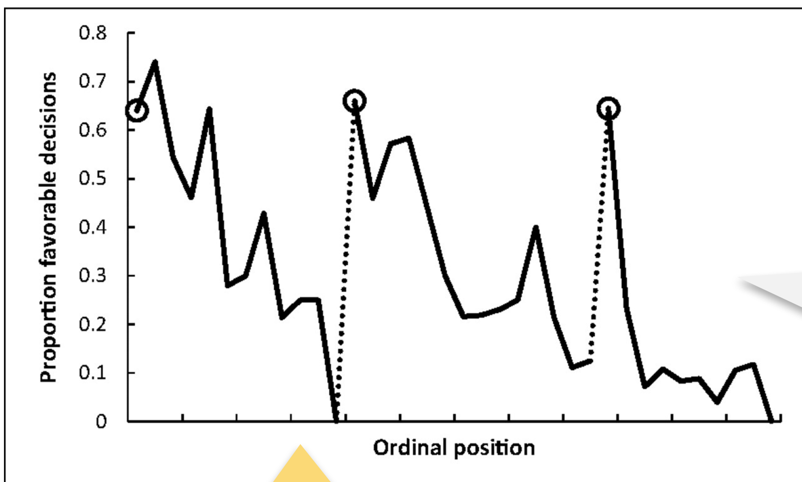
Edited* by Daniel Kahneman, Princeton University, Princeton, NJ, and approved February 25, 2011 (received for review December 8, 2010)



"Proportion of rulings in favor of the prisoners by ordinal position… **dotted line denotes food break**."

Time of this preliminary oral exam-- oops

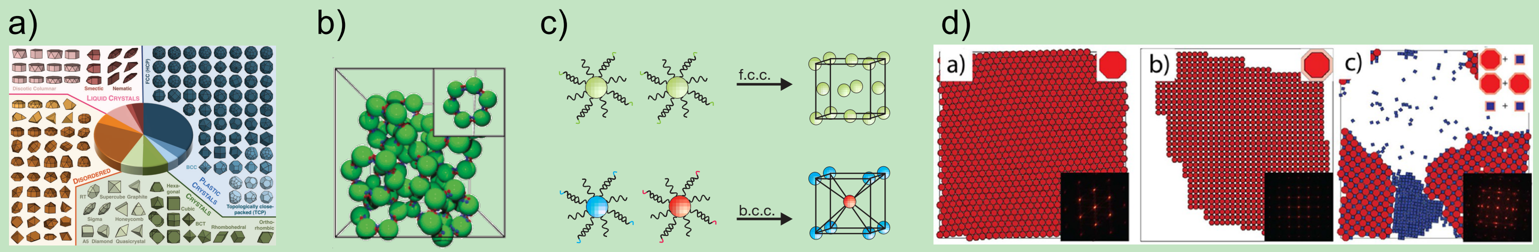
Designing an information-driven pathway approach for targeted self-assembly

Shannon Moran

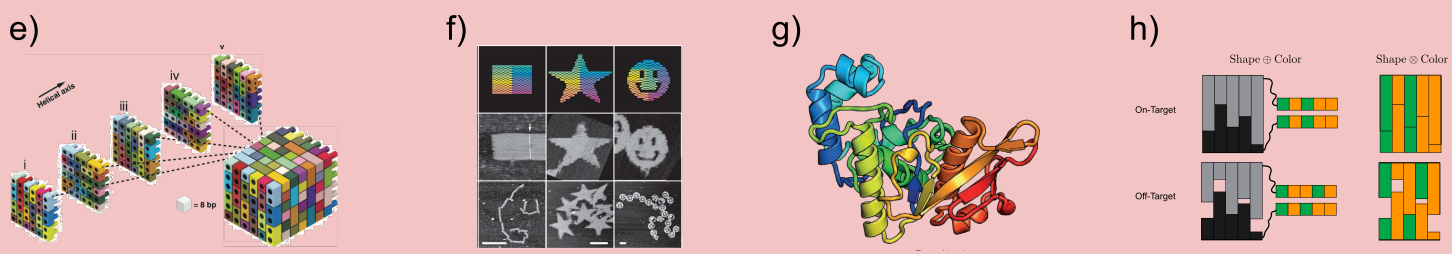
Research Proposal, Oral Presentation

February 21, 2018

Self-assembly: A challenge of specificity versus target complexity



Middle ground– minimizing instruction while maximizing complexity?



Source: (a) Damasceno et al, Science 2012; (b) Zhang et al, NanoLetters 2004; (c) Park et al, Nature 2008; d) Millan et al, 2014 ACS Nano; (e) Ke et al, Science 2014; (f) Rothemund et al, Nature 2006; (h) Huntley et al, PNAS 2016; ((g) Huang et al, Nature 2016

Understanding self-assembly: what approach to take?

"Different fields of science take different roads to understanding; each brings something to self-assembly.

Chemists and engineers tend to solve problems by designing and synthesizing (or fabricating, or building) new systems;

physicists observe existing systems;

biologists make modifications by mixing preexisting parts."

Self-Assembly at All Scales

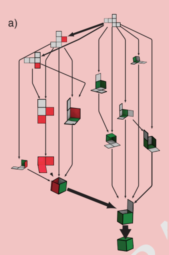
George M. Whitesides* and Bartosz Grzybowski

Source: Whitesides and Grzybowski, Science 2002

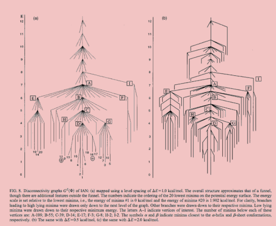
How can we tailor self-assembly?

Proposed work: What is the minimal set of instructions needed to achieve targeted, self-assembled complexity?

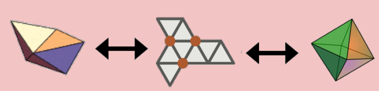
Project 1
Define measure of pathway information



Project 2
Develop energy landscapes for identifying kinetic barriers to assembly

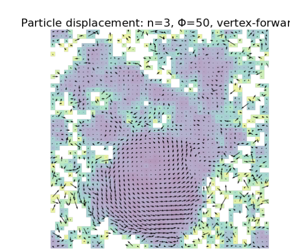


Project 3
Design pluripotent materials using minimal instructions



Prior work: How does shape impact assembly behavior in active systems?

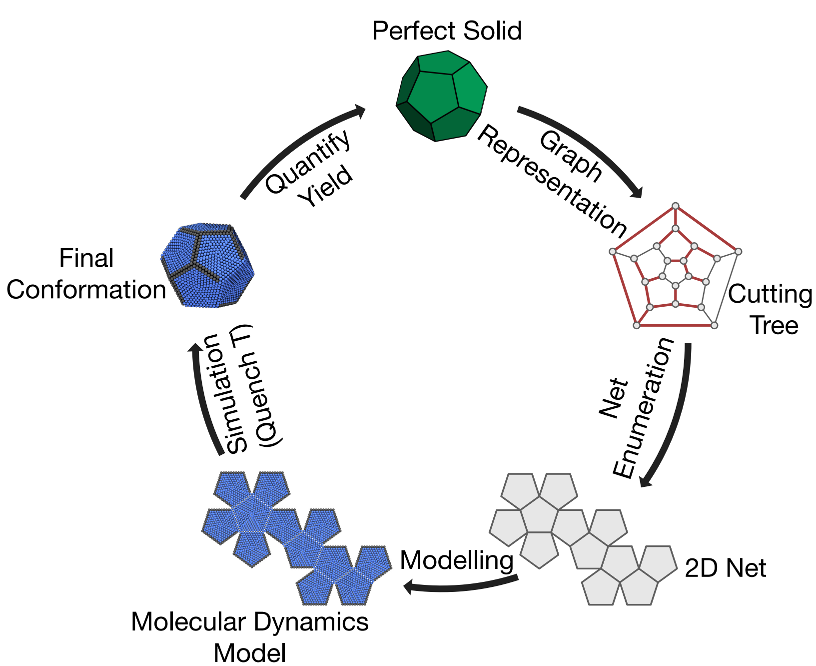
Project 0
Define role of particle anisotropy in a translationally-driven system



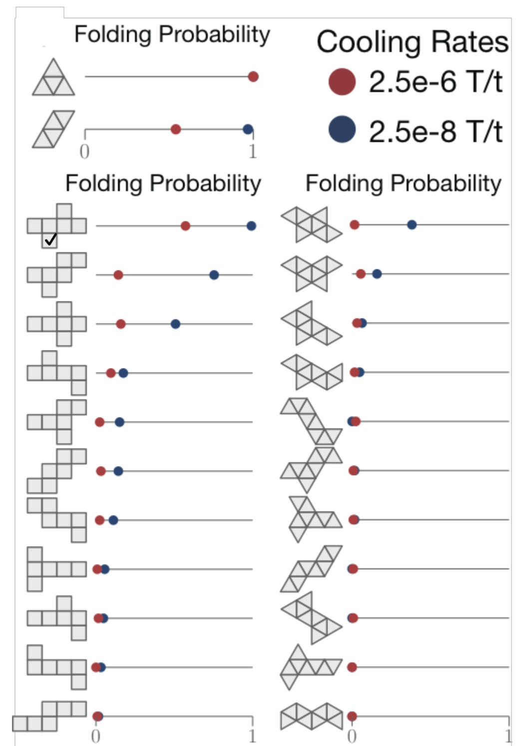
Source: Dodd et al, *in preparation* 2018

Proposed model: Nets of Platonic solids

Proposed system



Folding propensity of nets

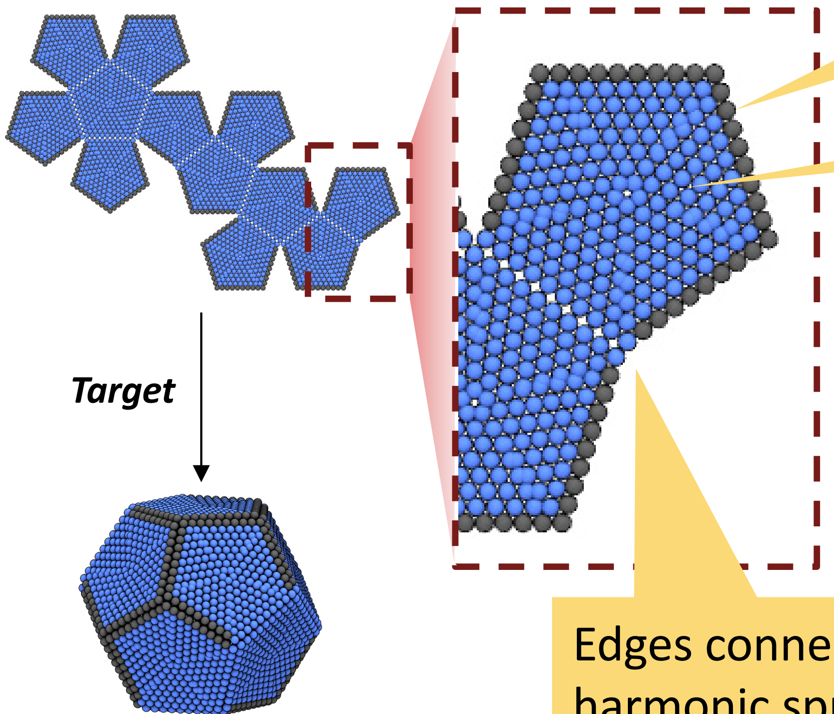


Compact, many leaves

Source: Dodd et al, *in preparation* 2018

Nets are modelled as rigid bodies

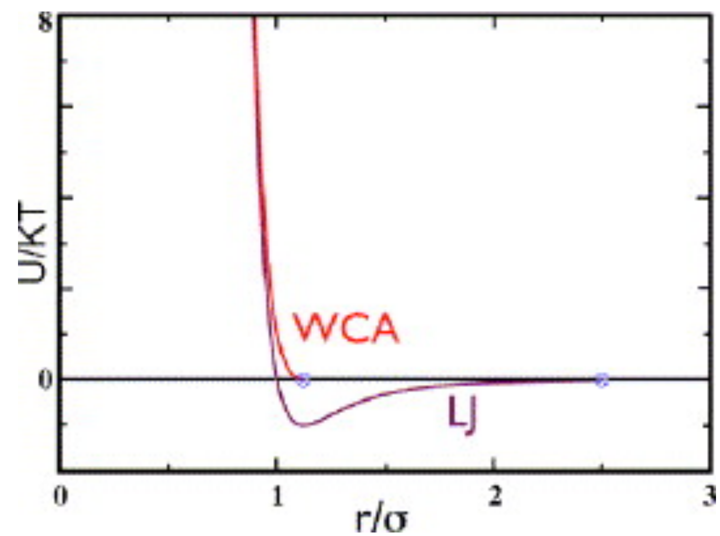
Rigid body faces connected by harmonic springs



Lennard-Jones potential on edges

Weeks-Chandler-Anderson (WCA) potential on faces

Edges connected by harmonic spring



Source: Dodd et al, *in preparation* 2018

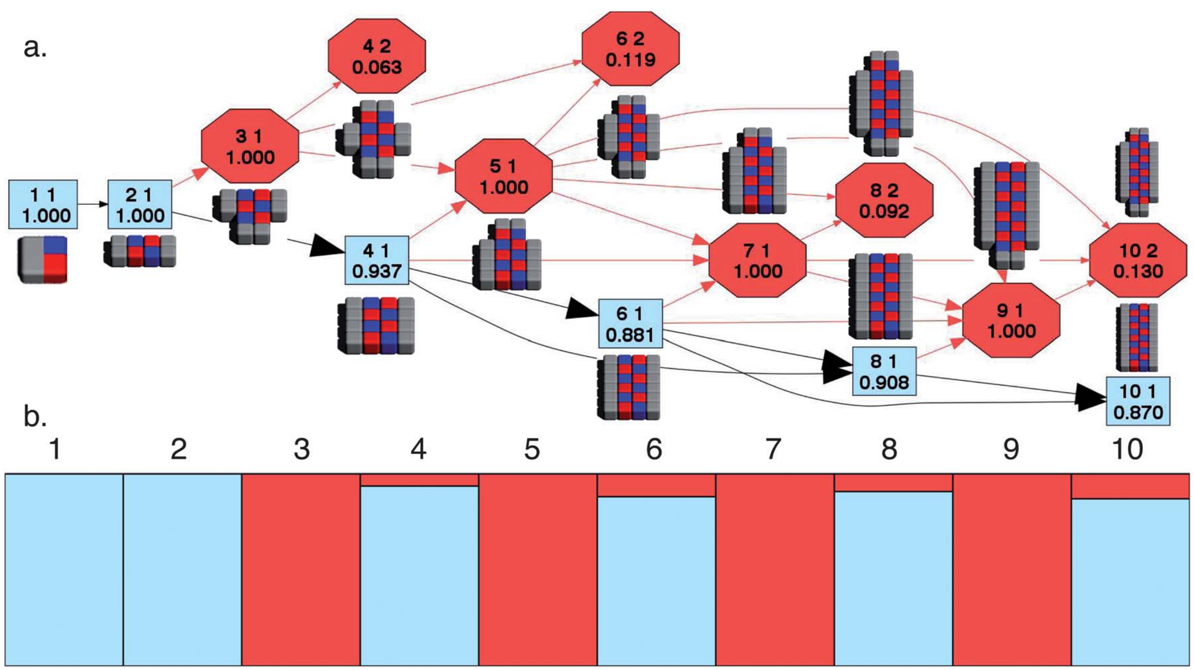
Project 1: Define measure of pathway information

	Task	Goal
1	**Define a measure of information for interactions in an assembly pathway (bonds on net)**	Measure correlation between an interaction and successful self-assembly to identify "critical bonds"
2	**Identify "critical bonds" in assembly pathway**	Use critical bonds to bias assembly towards target structures
3	**Demonstrate that poorly-folding nets fold with addition of *n* critical bonds**	Demonstrate approach works to tailor self-assembly

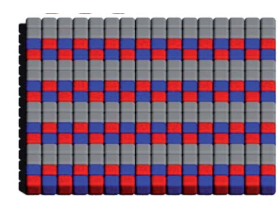
Transition state flux analysis to determine most important pathway intermediates

How compatible is an intermediate with assembly into a target pattern?

Self-assembly pathways



Target pattern



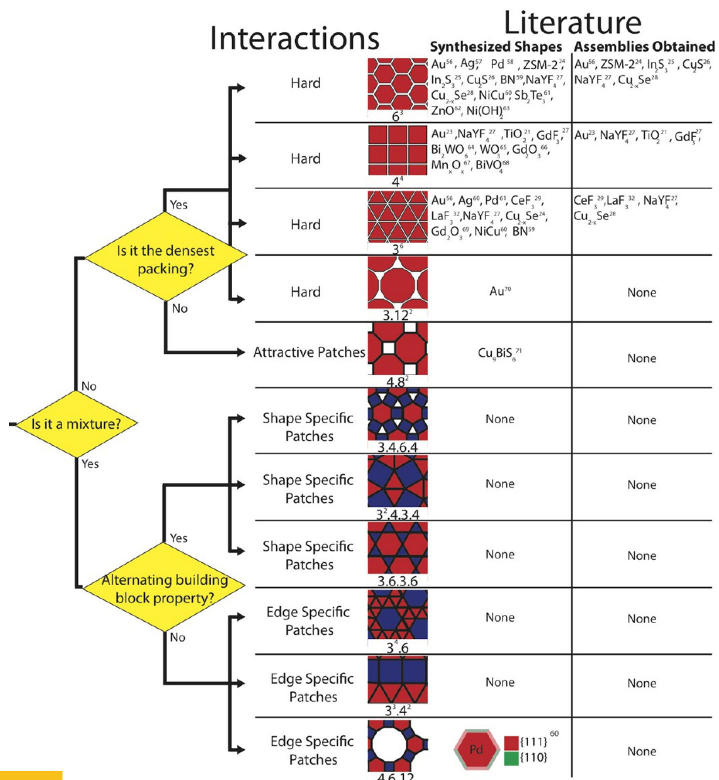
"Assembly fingerprint"

Citations: 35

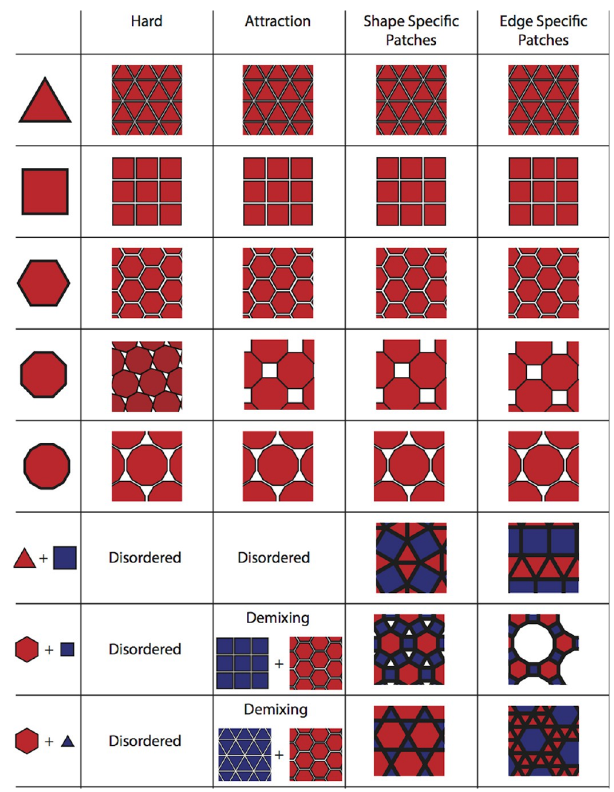
Sources: Jankowski and Glotzer, Soft Matter 2012

Hierarchical assembly of Archimedean tilings with increasingly specific instructions

Flow chart heuristic to assign interactions…



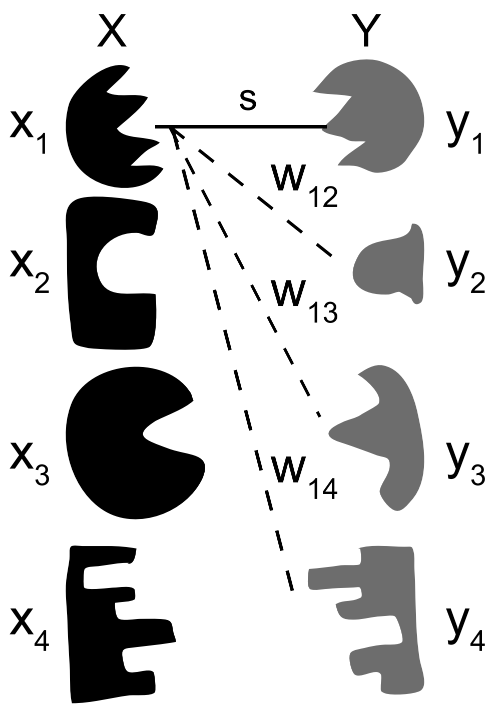
… increasing in instruction specificity and structure complexity



Citations: 41

Sources: Millan et al, ACS Nano 2014

Measuring mutual information in a lock and key pair (specificity)



$\Delta_{ij} = s - w_{ij}$

$E_{ij} \equiv E(x_i, y_j)$

How predictive is the identity of a lock x_i to the identity of a key y_j found bound to it?

Locks: $x_1, x_2, \ldots, x_N \in X$

Keys: $y_1, y_2, \ldots, y_N \in Y$

Probability of seeing x_i in a bound pair: $p(x_i)$

Probability of bound pair x_i, y_j: $p(x_i, y_j) = \frac{e^{-\beta E_{ij}}}{Z}$

$$I(X;Y) = \sum_{x_i \in X, y_j \in Y} p(x_i, y_j) \log_2 \frac{p(x_i, y_j)}{p(x_i)p(y_j)}$$

Citations: 7

Sources: Huntley et al, PNAS 2016

Quick primer on information theory

$$I(x_i, y_j) = p(x_i, y_j) \log_2 \frac{p(x_i, y_j)}{p(x_i)p(y_j)}$$

Input x_i → Channel (noise) → Output $y_j = x_i$ + noise

Communication theory *Claude Shannon*	Encoded message	Noise	Received message
Bond specificity *Huntley et al., PNAS 2016*	Identity of lock	Thermal fluctuations	Identity of key
Self-assembly pathway *Proposed work*	Presence of bond x_i	Thermal fluctuations	Yield of net y_j into target structure

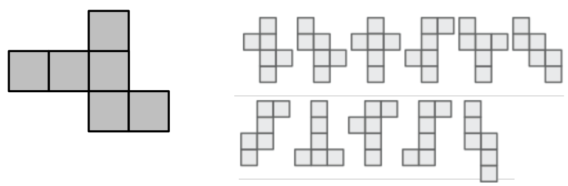
Task 1&2: Use transition pathways to measure which bonds are "most critical"

Enumerate states

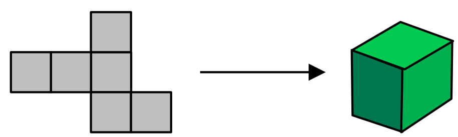
Measure probabilities

Define critical bonds

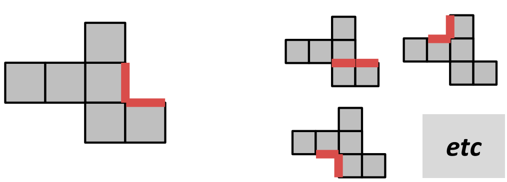
$y_j \in Y$



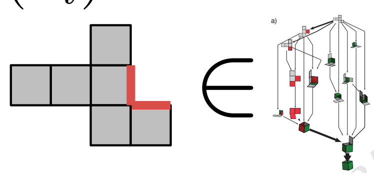
$p(y_j)$



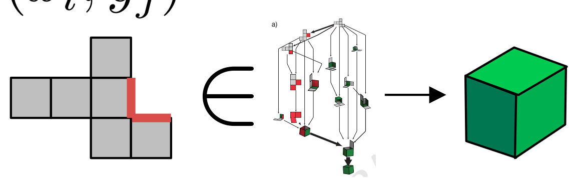
$x_i \in X$



$p(x_i)$



$p(x_i, y_j)$

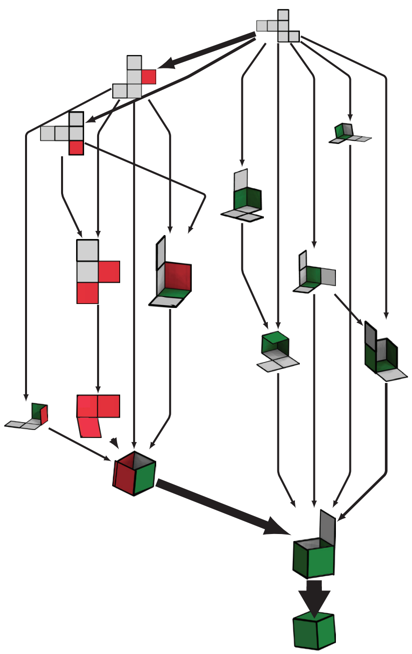


Define mutual information between each bond and target structure

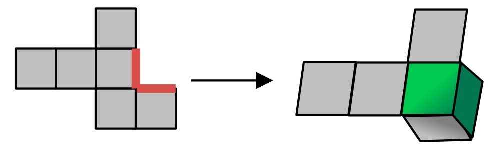
$$I(x_i, y_j) = p(x_i, y_j) \log_2 \frac{p(x_i, y_j)}{p(x_i)p(y_j)}$$

Hypothesis
"Most critical bonds" are those with the highest mutual information to the target state

<u>Task 3</u>: Demonstrating the role of critical bonds in enabling self-assembly



Can we seed the net with a bond that will reliably lead to formation of the target structure?



Some nets may need more than one bond to fold properly– can we define an ***efficiency*** metric?

$$\eta = \frac{\text{instruction added}}{\text{target yield}}$$

How are these critical bonds related to the energetic landscape of the assembly?

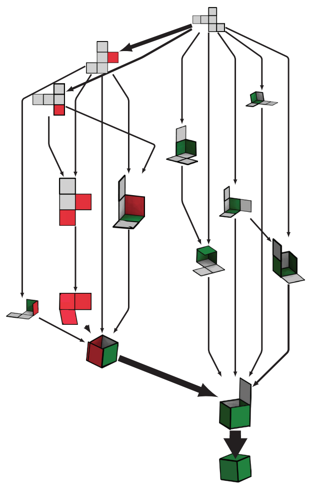
Project 2: Develop energy landscapes for identifying kinetic barriers to assembly

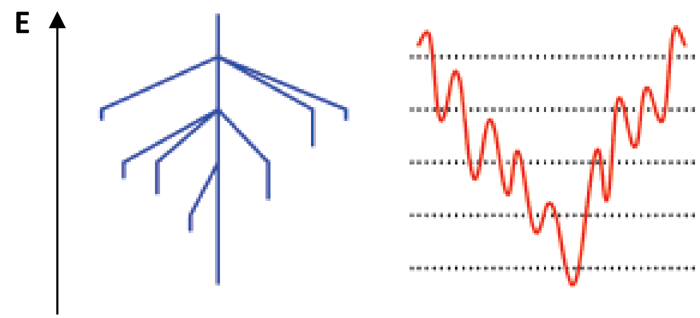
	Task	Goal
1	**Develop disconnectivity graphs for folding pathways**	Visualize and understand the energetics of system folding
2	**Study favorable pathways identified from disconnectivity graphs**	Identify commonalities between favorable paths (we expect that critical bonds would help assembly avoid kinetic traps)
3	**Identify which characteristics of a nets correspond to a narrower energetic funnel**	Determine whether characteristics that correlate to higher yield (great leaves, compactness) correlate with narrower energetic funnel

Task 1: Develop free energy disconnectivity graphs for folding pathways

Folding pathways with transition states…

… Mapped onto disconnectivity graph





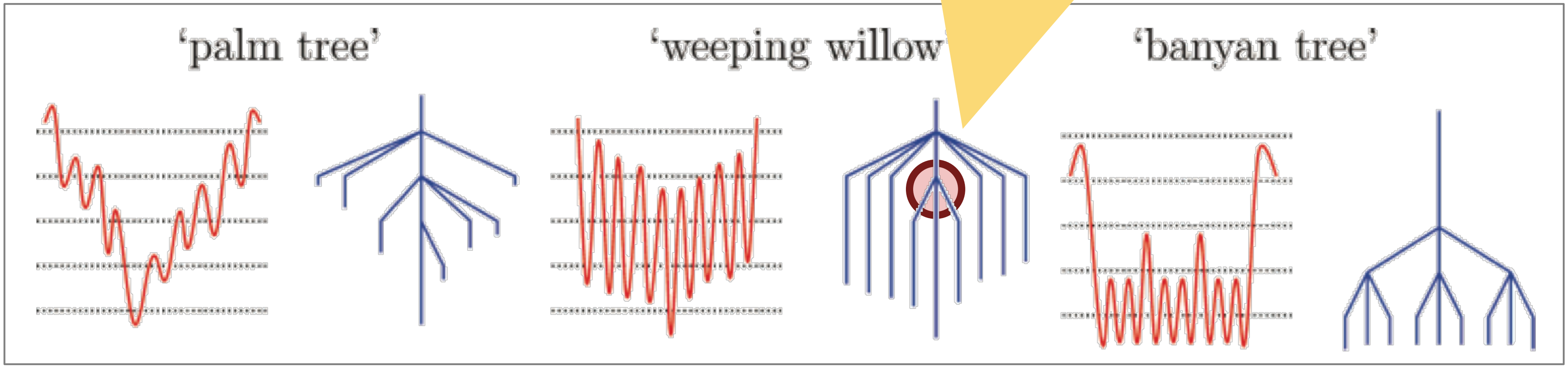
Calculate energy for each transition state

Will require significantly adapting existing code or writing our own methods for this

Source: Dodd *et al.*, in preparation 2018; Wales et al, Journal of Chemical Physics B 2006

Tasks 2&3: What characteristics of a net correspond to a narrower energetic funnel?

Hypothesize that critical bonds prevent exploration of local minima



Can we find features of nets that make their energies look like this…

… Rather than this?

Knowing the energy landscape, can we hop from one minimum to another?

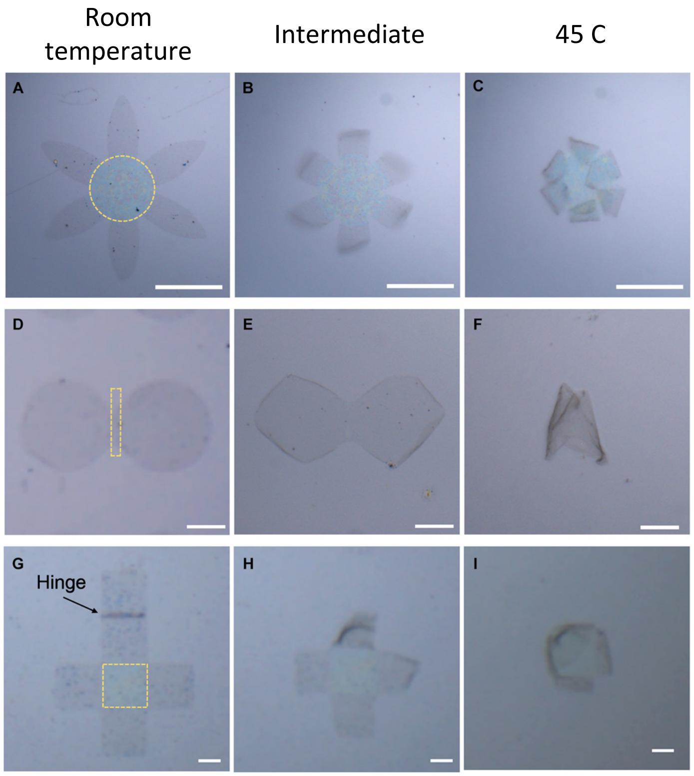
Source: Wales et al, Journal of Chemical Physics B 2006

Project 3: Design pluripotent materials from minimal instructions

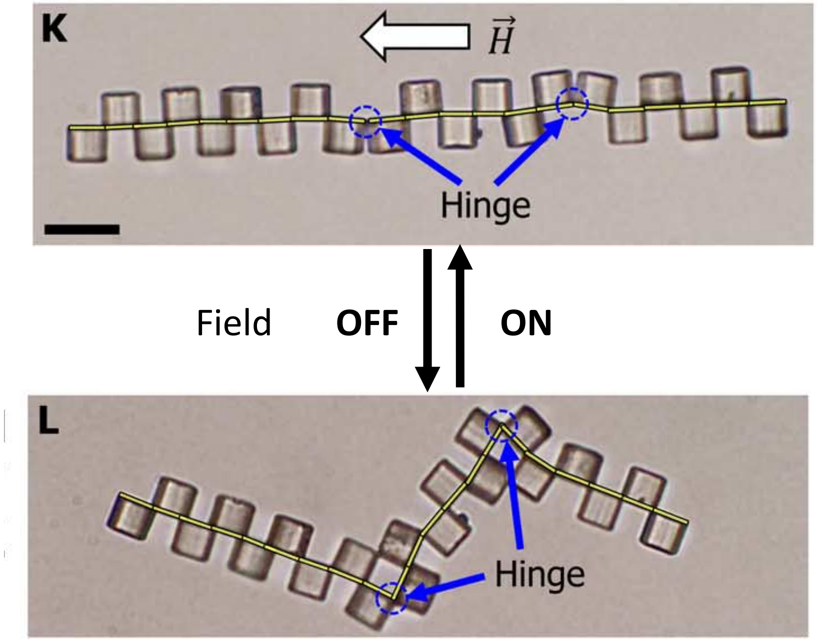
	Task	Goal
1	**Identify set of nets to test (multiple local minima of interest)**	Assemble system into one local minima, then another, based on minimal programmed interactions
2	**Develop minimal set of instructions (“critical bonds”) to fold into each**	Apply approach from Project 1 to identifying critical bonds for a given target structure
3	**Seed pluripotent materials (nets) with critical bonds for target structure and test assembly**	Demonstrate that minimal instructions can be used to enable pluripotency

Folding is a demonstrated method of embedding pluripotency at microscale

Thermo-responsive self-folding graphene sheets



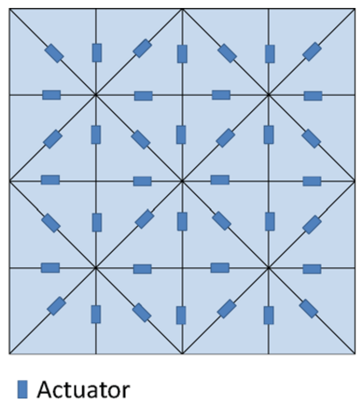
Patchy magnetic cubes

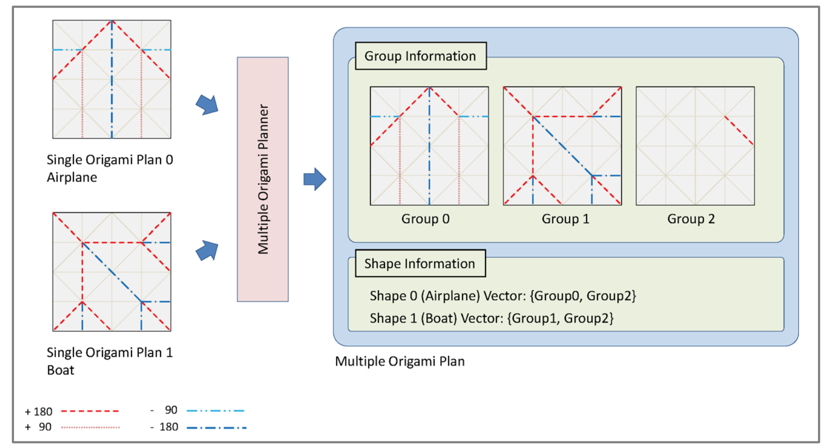


Source: Xu et al, Science Advances 2017; Han et al, Science Advances 2017

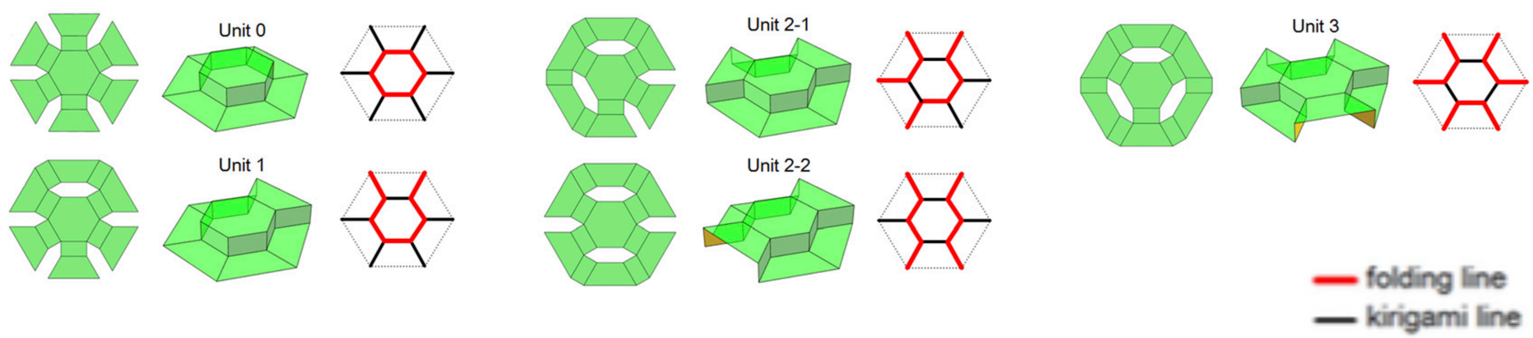
Macroscale folding pluripotency has been studied in origami, kirigami systems

Origami





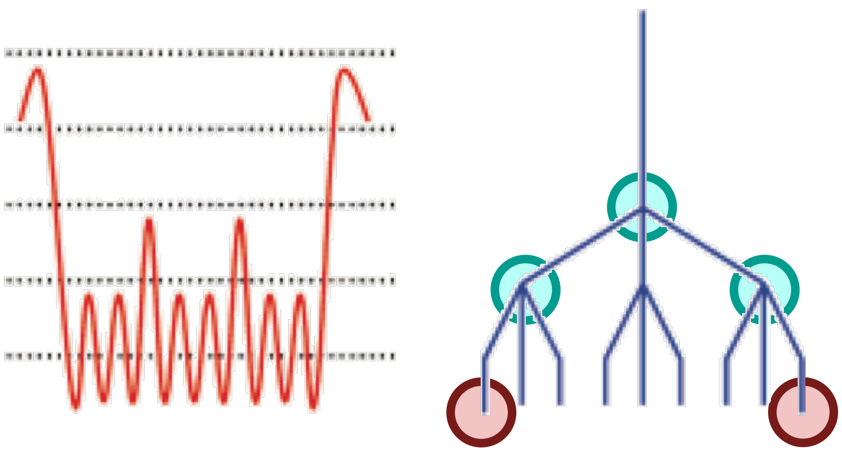
Kirigami



Source: An et al, Robotica 2011; Sussman et al, PNAS 2015

Task 1&2: Identify target structures, critical bonds on disconnectivity graphs

Disconnectivity graph



Patchy magnetic cubes

Identify two target states (Project 2)

Find critical bonds to get to each (Projects 1&2)

Find minimum set of interactions that need to be programmed to push material into either

Example: Move between local minima in the energetic landscape of an octahedron

Poly-tetrahedron

Octahedron

Lower free energy, higher rotational entropy

Higher free energy, lower rotational entropy

Source: Meng et al, Science 2010

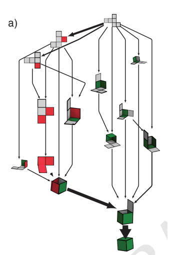
How can we tailor self-assembly?

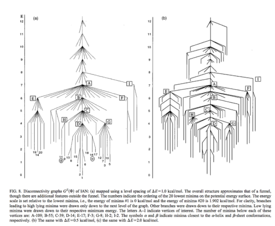
Proposed work: What is the minimal set of instructions needed to achieve targeted, self-assembled complexity?

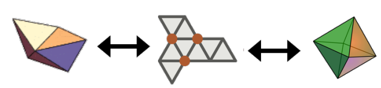
Project 1
Define measure of pathway information

Project 2
Develop energy landscapes for identifying kinetic barriers to assembly

Project 3
Design pluripotent materials using minimal instructions

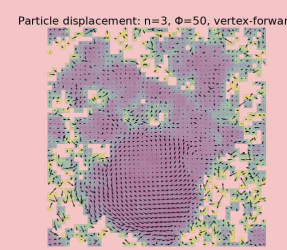






Prior work: How does shape impact assembly behavior in active systems?

Project 0
Define role of particle anisotropy in a translationally-driven system

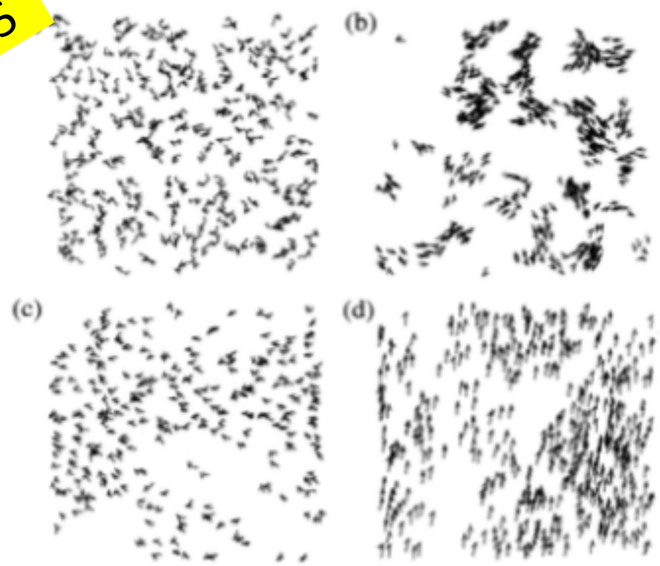


Source: Dodd et al, *in preparation* 2018

Active matter has been *active* for 20+ years, but the field is still establishing the basics

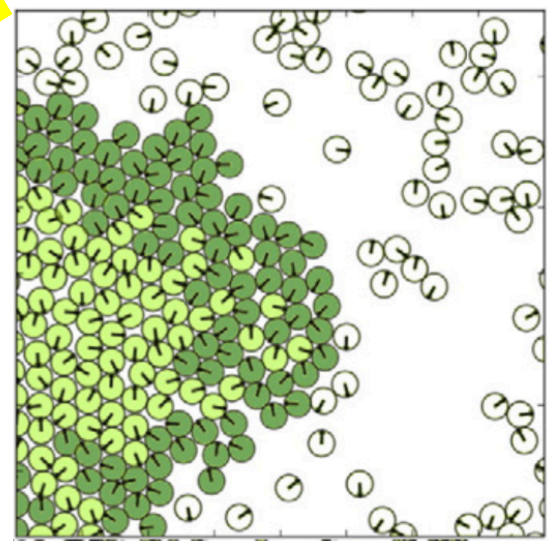
Particles with explicit alignment rules

1995



Isotropic particles

2016

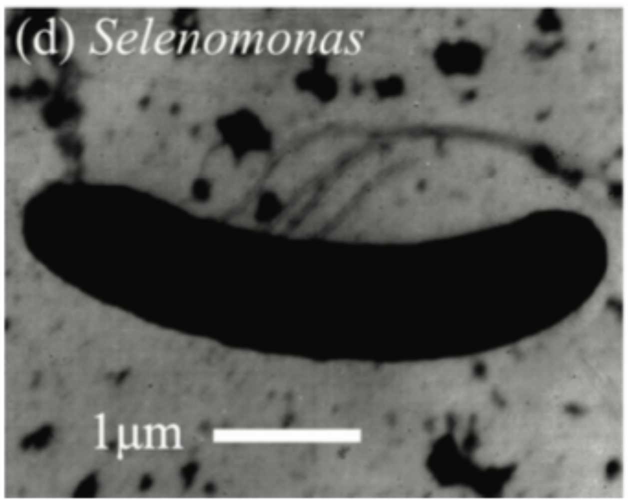


In nature, “particles” aren’t isotropic– that’s the exception rather than the norm

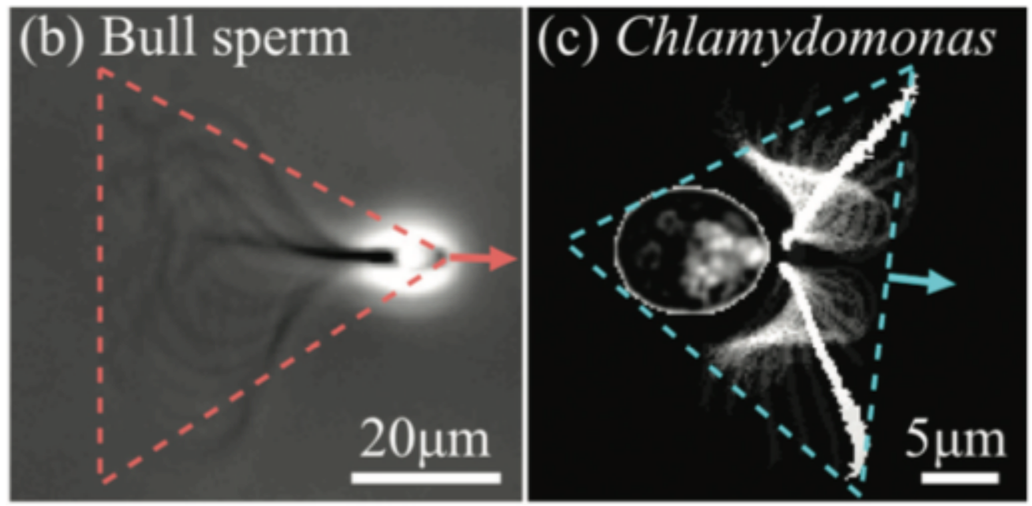
Source: Vicsek et al, PRL 1995; Marchetti et al, Current Opinion in Colloid & Interface Science 2016

In nature, active *particle* anisotropy manifests itself two primary ways

Shape



Force direction

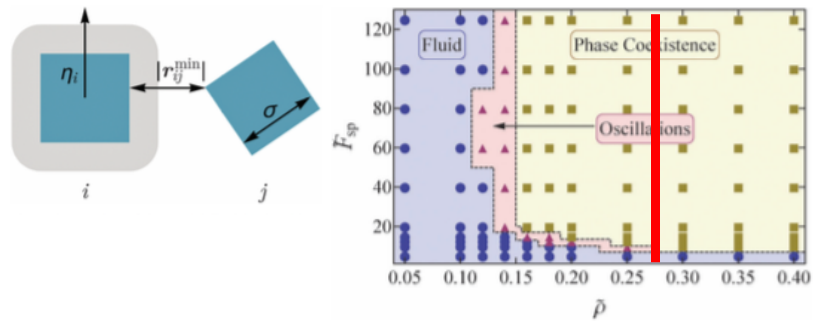


Source: Wensink et al, PRE 2014

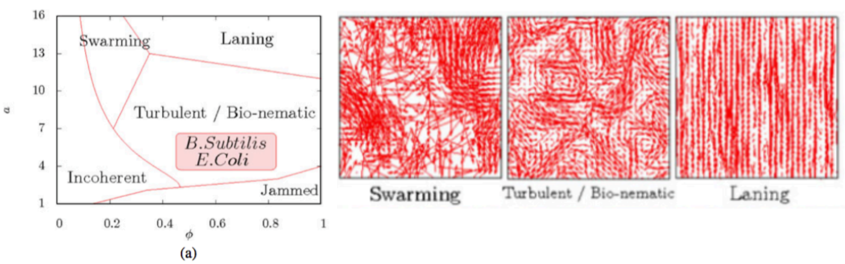
The active matter community has also begun to study anisotropy in one-off experiments

Shape

Critical density

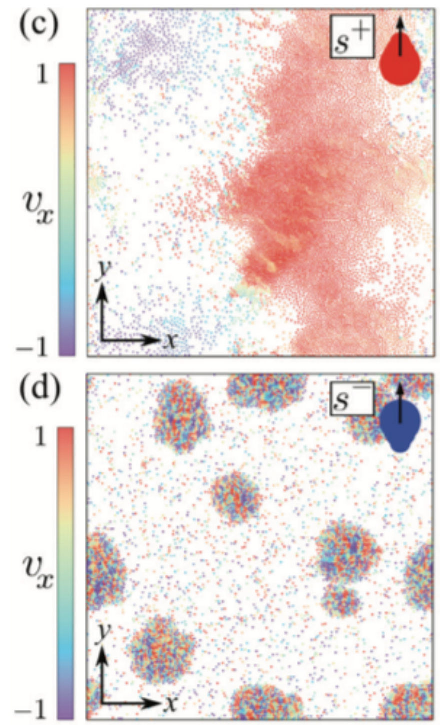


Collective behavior



Force direction

Collective behavior



Source: Prymidis et al, Soft Matter 2016; Wensink et al, EPJ 2013; Wensink et al, PRE 2014

Large open question: How/why does anisotropy allow for these different types of critical/collective behavior?

More targeted question: Can we explain why anisotropy leads to different critical and collective behaviors in a specific system?

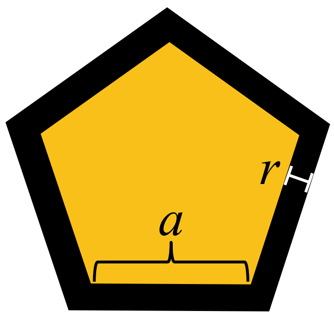
Methods: Excluded-volume particle interactions in the Brownian regime

Particle model

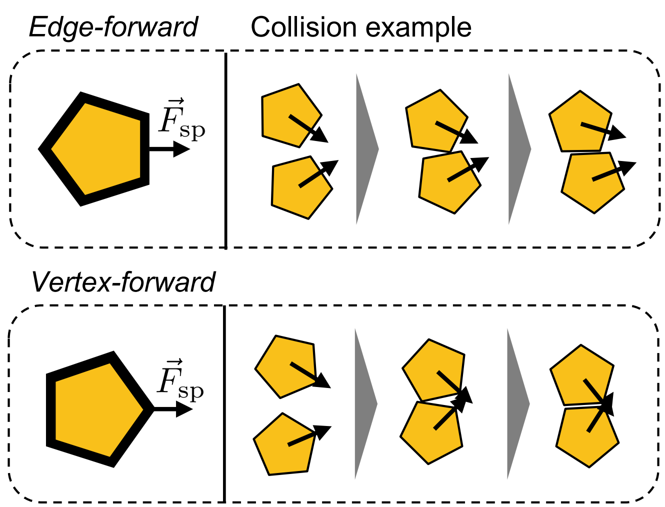
Shape

$$n = [3, 4, 5, 6, 7, 8]$$

$$0.9 = \frac{n \cdot a}{2\pi r}$$



Force director



Weeks-Chandler-Anderson (WCA) inter-particle potential, simulated using the Discrete Element Method (DEM)

Langevin dynamics

$$m\frac{d\vec{v}}{dt} = \vec{F_C} - \gamma \cdot \vec{v} + \vec{F_R}$$

$$\langle \vec{F_R} \rangle = 0$$

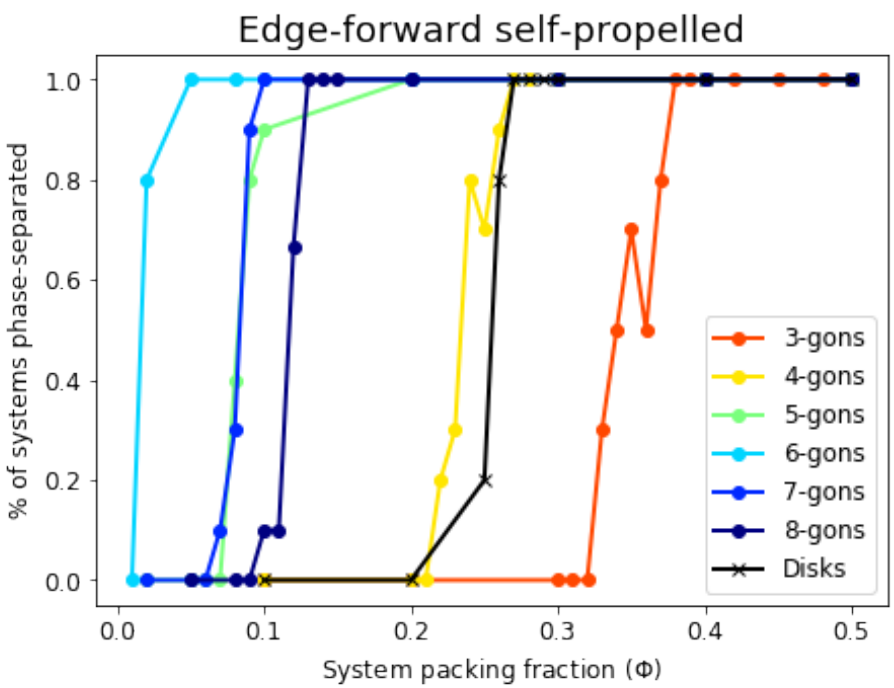
$$\langle |\vec{F_R}|^2 \rangle = 2dkT\gamma/\delta t$$

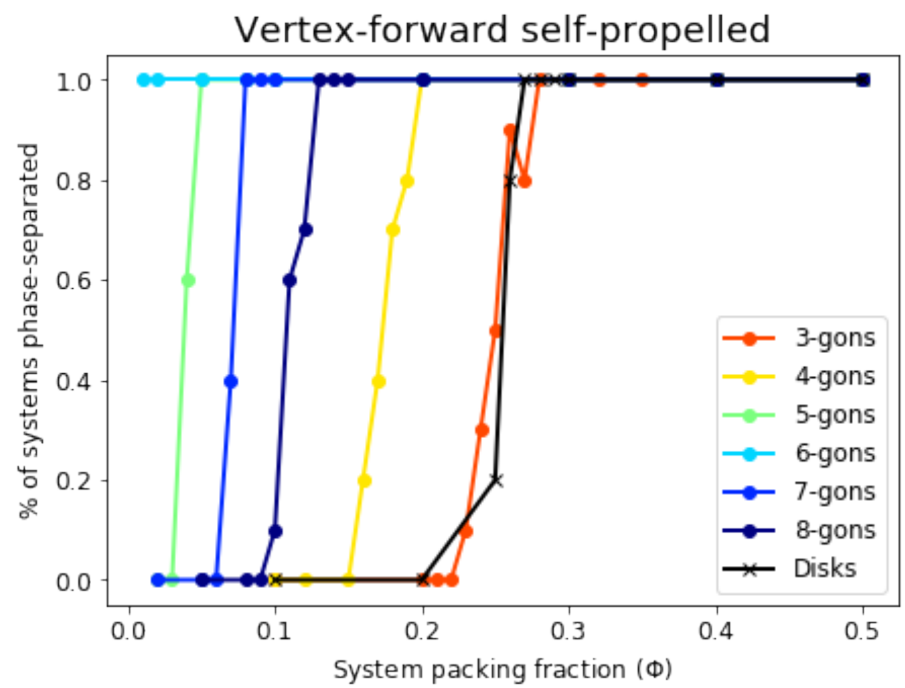
Set mass equal to 1e-2 to approximate Brownian dynamics

Project 0: Outline and hypotheses

Topic	Questions	Hypotheses
Critical density *Phase separation*	**How** does shape/force offset impact the critical density?	Anisotropy should depress critical density relative to that seen in disks
	Why does shape/force offset impact the critical density at all?	Should have **“more effective”** collisions– e.g. able to align with neighbors
Collective behavior *Nucleation*	**How** does shape/force offset impact nucleation behavior?	*TBD*
	Why does shape/force offset impact nucleation behavior?	Steric interactions between anisotropic particles are known to allow **translation** and **rotation** of clusters

Phase separation: Observe change in critical density, though not linearly with shape



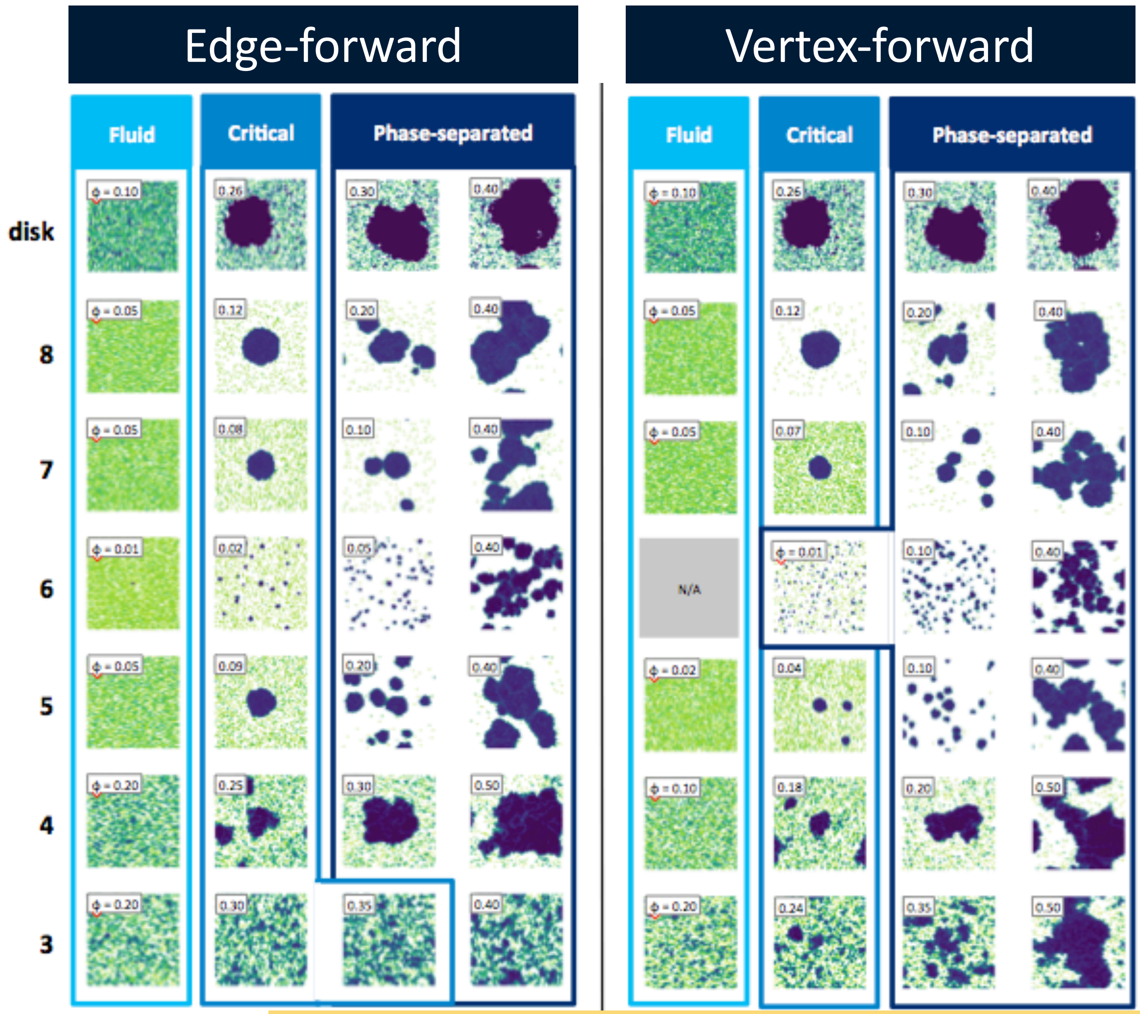


6 > 5/7 > 8 > 4 > disks > 3

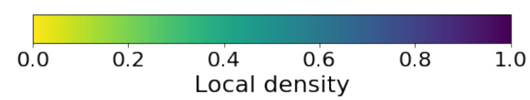
6 > 5 > 7 > 8 > 4 > 3/disks

Notes: Phase separation determined by looking at local density histograms (looking for two density peaks) over 10 replicates– different from other studies, which have used “fraction of system in largest cluster”

Nucleation: Large clusters of shapes form through combinations from smaller clusters



We don't see any qualitative difference in nucleation with force offset



Videos and displacement field images available in back-up material, if there's interest

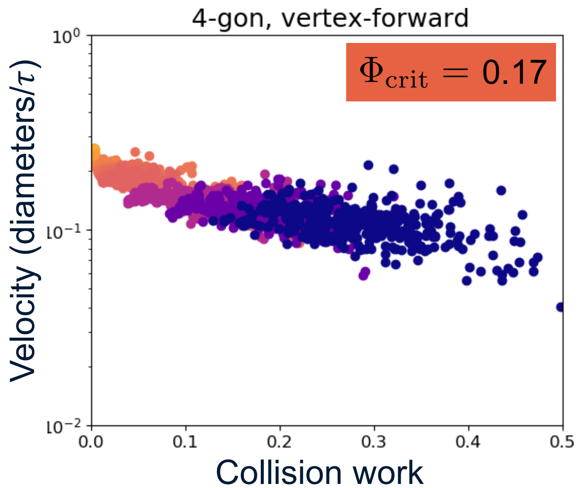
Other active matter theories don't work well to explain the behavior we see here

Theory	Schematic
Kinetic theory *Redner et al, PRL 2013*	Based on the assumptions that: • Particles can diffuse and escape clusters (WRONG) • System forms one large cluster which nucleates and` grows (WRONG)
Motility-induced phase separation (MIPS) *Tailleur and Cates, PRL 2008*	We can extend this to say: • "More effective" collisions are those that are more effective at slowing particles down→ **i.e. some shapes have more efficient collisions than others** • <u>**Novel**</u>: Explanation that shape can be used to tune phase separation by increasing "effectiveness" of interactions
Collision theory *Bruss and Glotzer, arxiv 2017*	Based on free time, triangles should phase separate most easily (highest cross section to area ratio) **→ Reinforces that our observations must be explained by collision time-scale!**

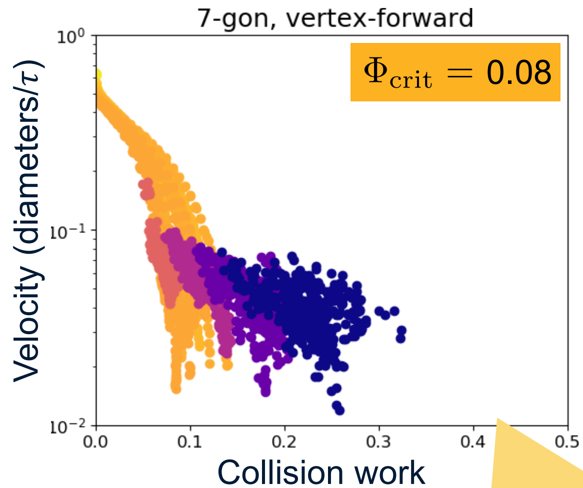
Source: Redner et al, PRL 2016; Bruss and Glotzer, arxiv 2017; "Elementary Reactions" from *An Introduction to Chemical Kinetics*, isbn 978-1-6817-4664-7

"More efficient" shape collisions slow velocity more with less work done by collisions

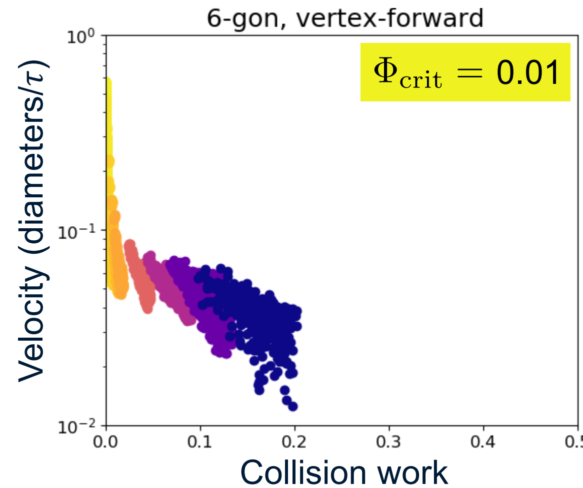
3 and 4-gons



5/7/8-gons

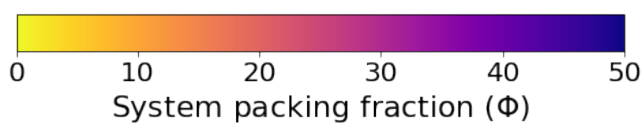


6-gons



$$W = \frac{1}{2}\sum_i \sum_{j \neq i} \vec{F}_{ij} \cdot \vec{r}_{ij}$$

Currently working to clarify behavior in critical regime



Near-term next steps

- Project 0: Particle anisotropy in active system
  - Solidify "collision efficiency" metric
  - Finalize and submit paper for publication
- Project 1: Pathway information
  - Analyzing data already available from in-preparation paper on folding nets
  - How accurate is the first approximation at a mutual information between edge bonds and net folding?
- Project 2: Energy landscapes
  - Restart collaboration between Wales group alum and Glotzer lab

Thank you in advance for your questions and feedback!

How can we tailor self-assembly?

Proposed work: What is the minimal set of instructions needed to achieve targeted, self-assembled complexity?

Project 1
Define measure of pathway information

Project 2
Develop energy landscapes for identifying kinetic barriers to assembly

Project 3
Design pluripotent materials using minimal instructions

Prior work: How does shape impact assembly behavior in active systems?

Project 0
Define role of particle anisotropy in a translationally-driven system

Reference slides

Integration methods

- Langevin implemented using a velocity verlet algorithm (same as the NVE)
- Brownian: Nose Hoover, have to solve for using predictor corrector method (slower, have to use smaller time step)

Planned timeline

			2017				2018				2019				2020	
Project	**Status**	**Description**	**Q1**	**Q2**	**Q3**	**Q4**	**Q1**	**Q2**	**Q3**	**Q4**	**Q1**	**Q2**	**Q3**	**Q4**	**Q1**	**Q2**
Project 0	100%	Data collection	■	■	■	■										
Active shapes	90%	Analysis		■	■	■	■									
	75%	Writing				■	■									
	0%	Submit, revisions					■	■								
Project 1	0%	Data collection					■	■	■							
Information metrics	0%	Analysis					■	■	■	■						
	0%	Writing							■	■						
	0%	Submit, revisions								■	■					
Project 2	0%	Develop code							■	■						
Energy landscapes	0%	Data collection								■	■	■				
	0%	Analysis									■	■				
	0%	Writing										■	■			
	0%	Submit, revisions										■	■			
Project 3	0%	Data collection										■	■			
Pluripotent materials	0%	Analysis											■	■		
	0%	Writing											■	■		
	0%	Submit, revisions												■	■	
Thesis	0%	Data meeting													■	
	0%	Defense														■

While info. theory struggles to catch on in assembly, in non-eq stat mech it is gaining

nature physics

INSIGHT | REVIEW ARTICLES

PUBLISHED ONLINE: 3 FEBRUARY 2015 | DOI: 10.1038/NPHYS3230

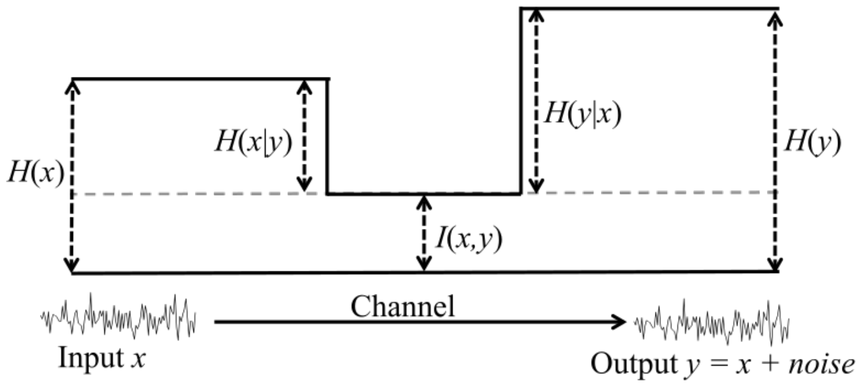
Thermodynamics of information

Juan M. R. Parrondo[1*], Jordan M. Horowitz[2] and Takahiro Sagawa[3]

By its very nature, the second law of thermodynamics is probabilistic, in that its formulation requires a probabilistic description of the state of a system. This raises questions about the objectivity of the second law: does it depend, for example, on what we know about the system? For over a century, much effort has been devoted to incorporating information into thermodynamics and assessing the entropic and energetic costs of manipulating information. More recently, this historically theoretical pursuit has become relevant in practical situations where information is manipulated at small scales, such as in molecular and cell biology, artificial nano-devices or quantum computation. Here we give an introduction to a novel theoretical framework for the thermodynamics of information based on stochastic thermodynamics and fluctuation theorems, review some recent experimental results, and present an overview of the state of the art in the field.

Citations: 292

Quick primer on information theory (cont.)

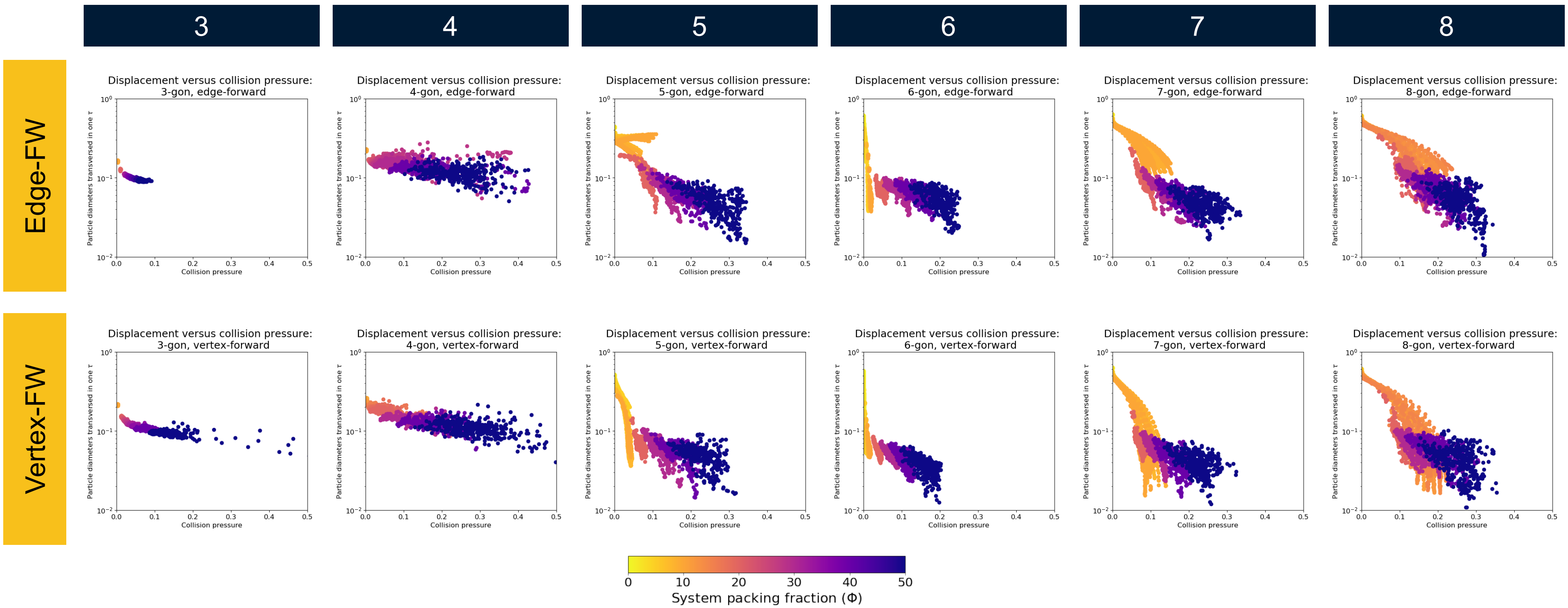


$$H(X) = -\sum_{x} p(x) \log_2 p(x)$$

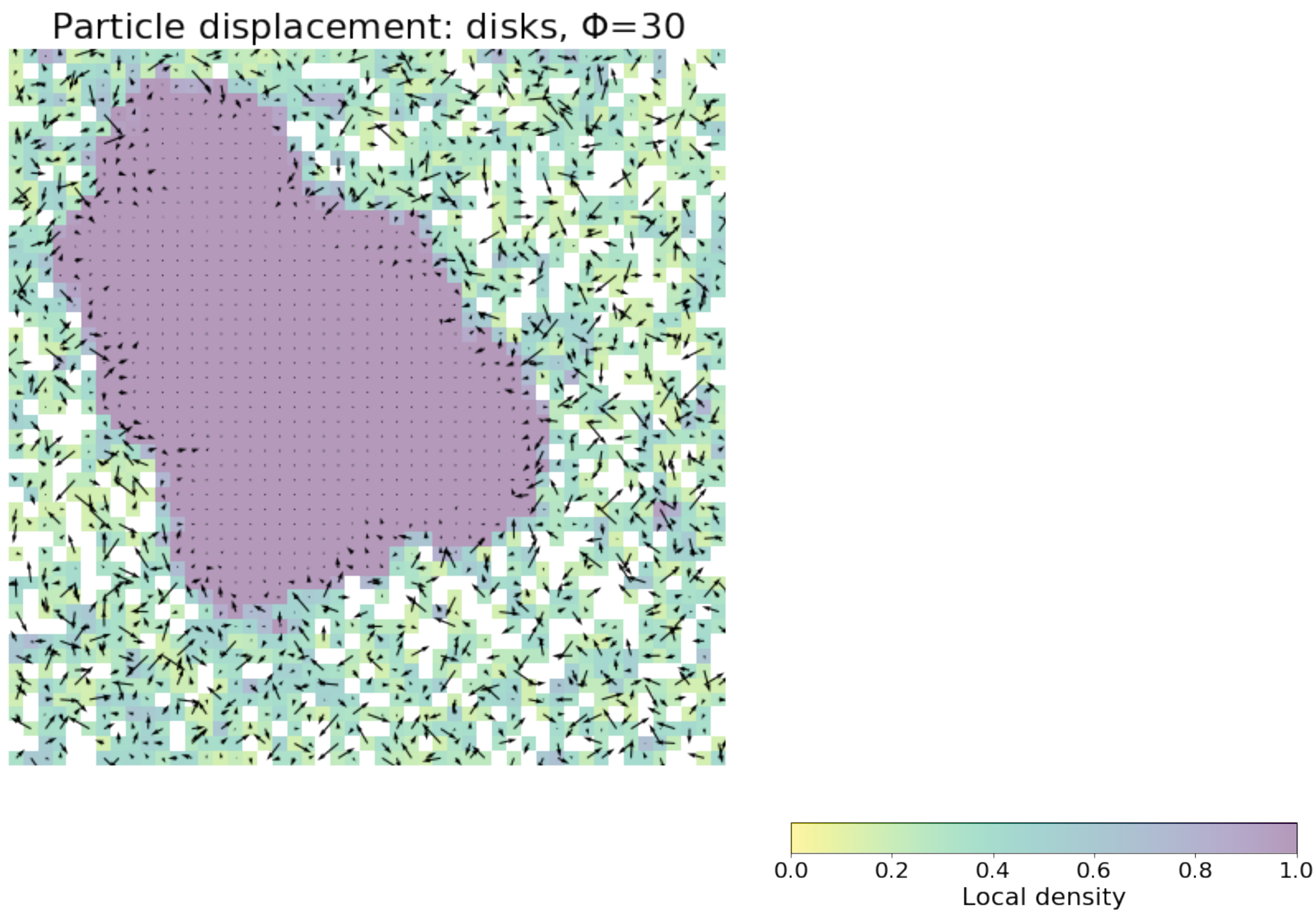
$$I(X;Y) = H(X) + H(Y) - H(X,Y)$$

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) \\ &= H(Y) - H(Y|X) \end{aligned}$$

Shapes with lower critical densities have steeper change in velocity versus pressure

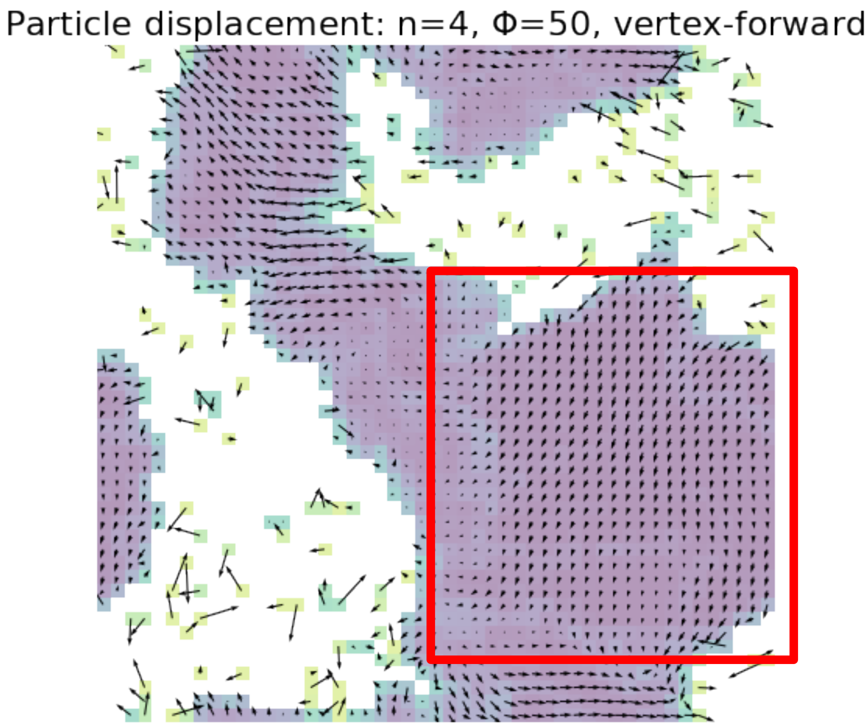


Clusters of disks do not have translational or rotational motion

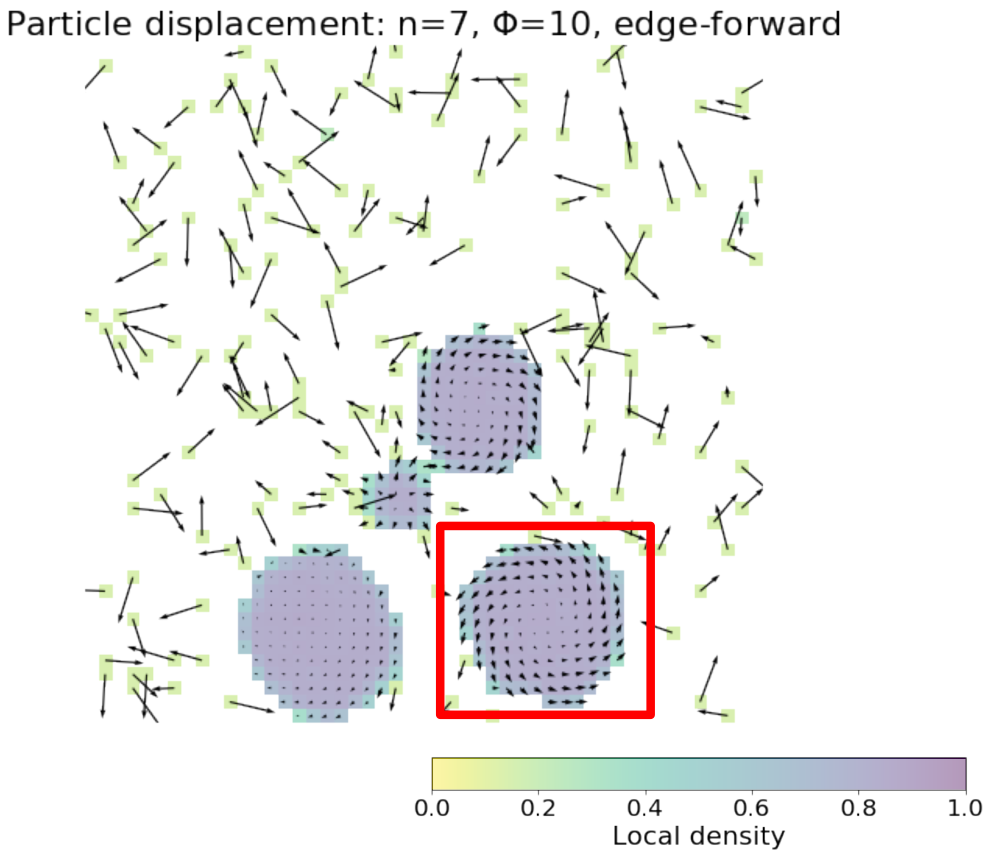


Clusters of shapes can sustain both translational and rotational motion

Example: Translational motion

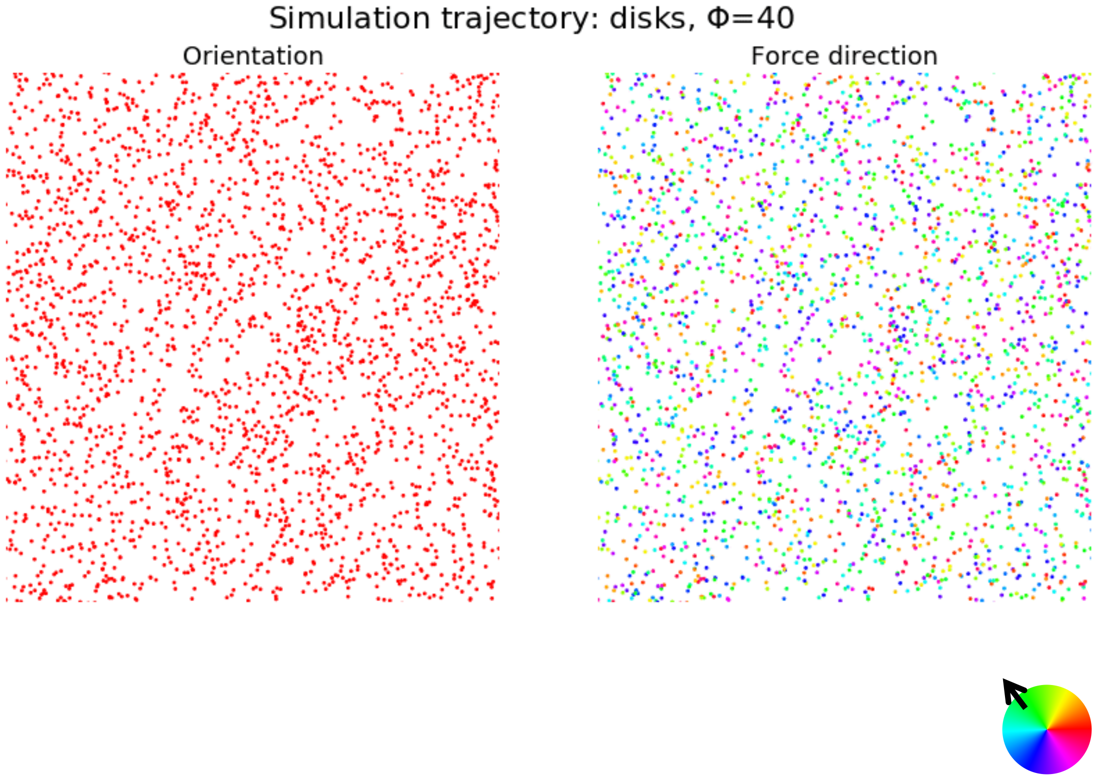


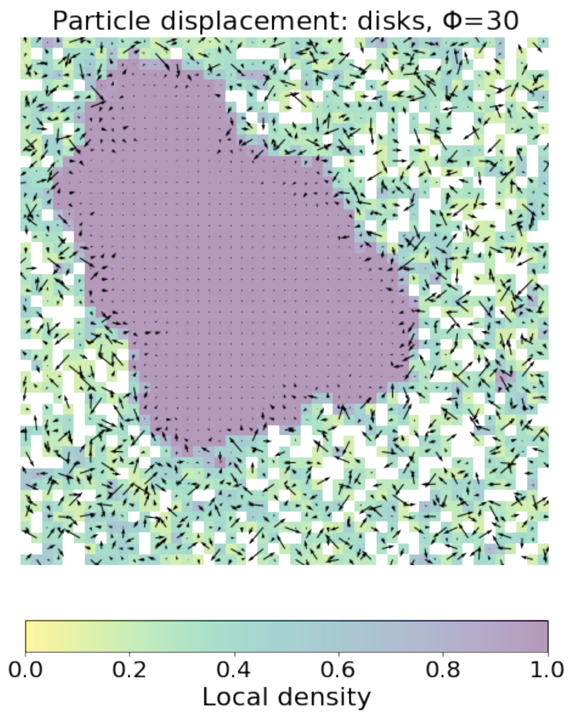
Example: Rotational motion



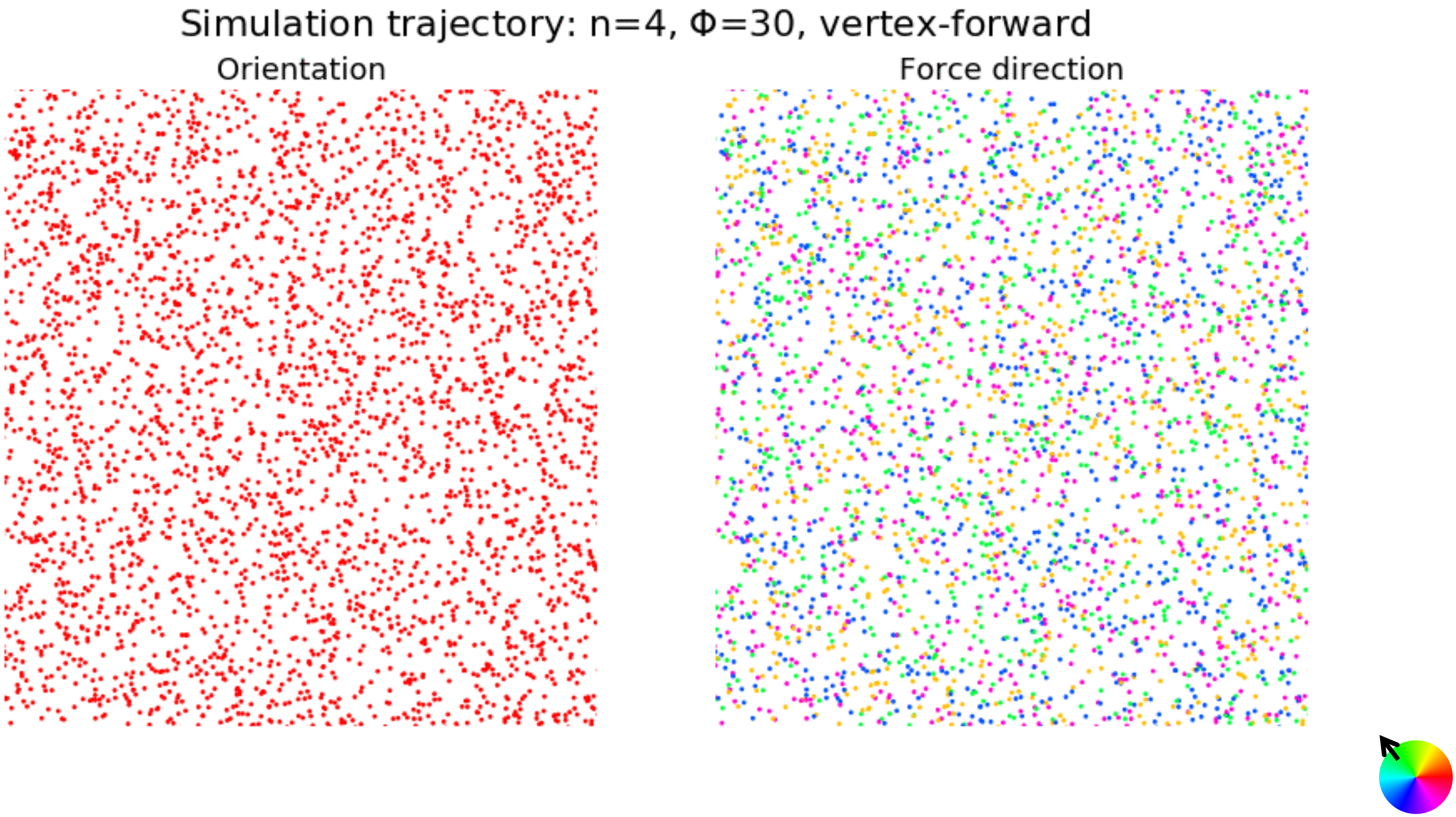
In disks, large clusters form via ***merging***, rather than colliding)

Disks

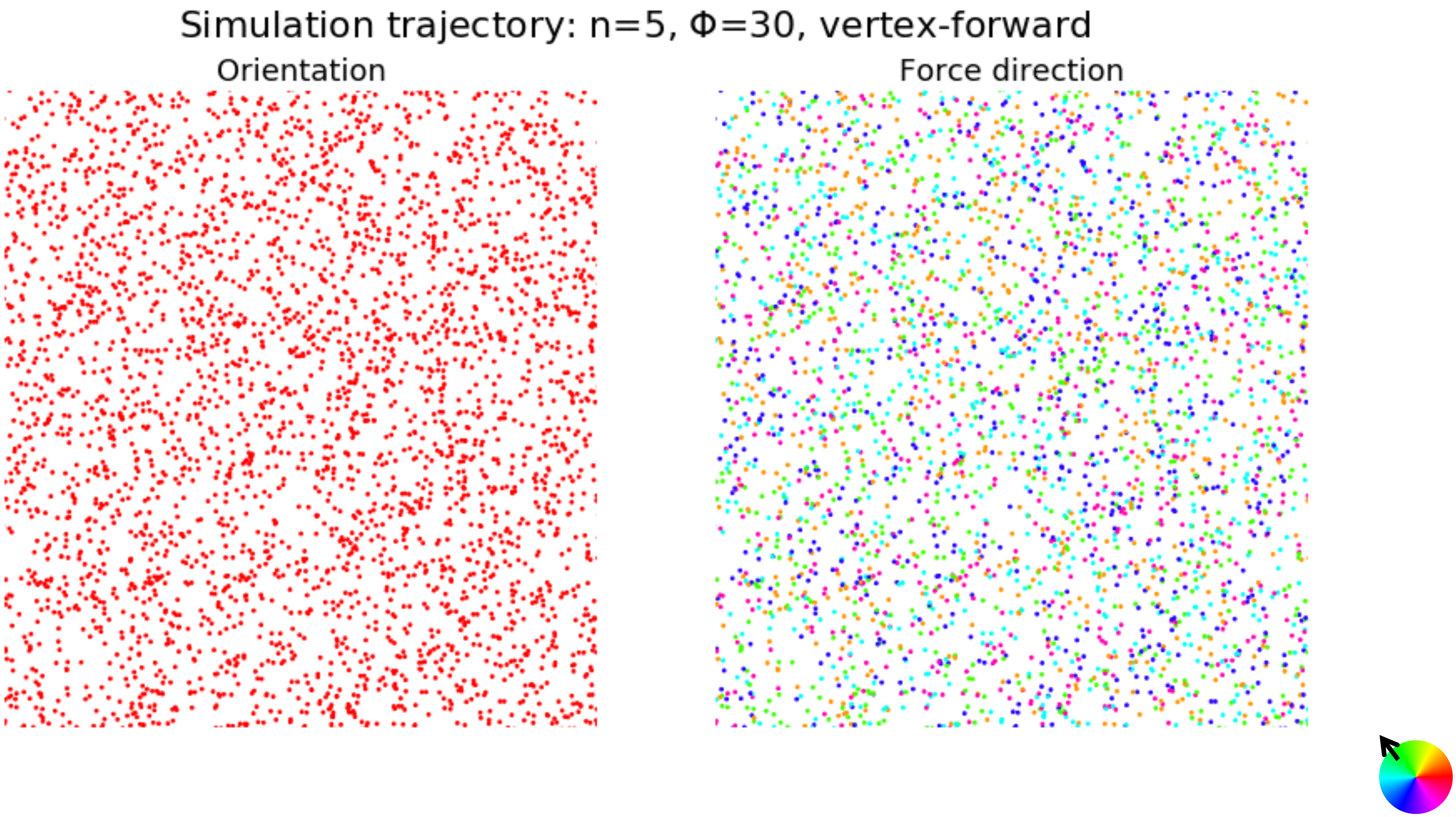




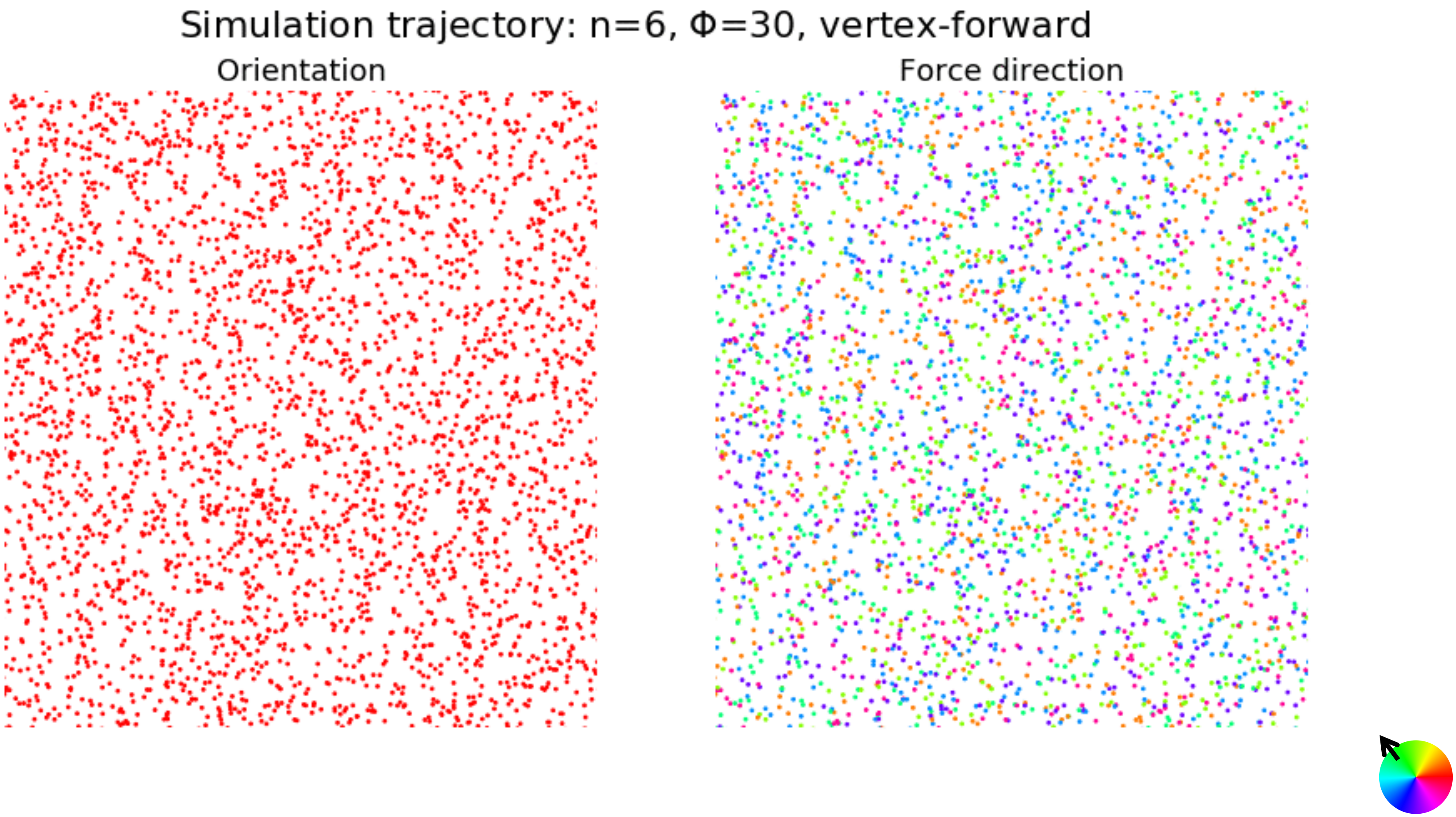
Video: 3 and 4-gons have shear planes, can't stabilize stresses



Video: 5/7/8-gons pack, but not perfectly



Video: 6-gons tile space



Could envision modeling a 4-fold pentile to test whether the density of the packing/lack of shear planes matters

In conclusion: Shape matters

Topic		Questions	Findings
Critical density *Phase separation*	1	**How** does shape/force offset impact the critical density?	Shape can enable lower (or higher!) critical densities than disks
	2	**Why** does shape/force offset impact the critical density at all?	Shape and force offset can work together to change the efficiency of collision, i.e. the change in velocity due to collision
Collective behavior *Nucleation*	3	**How** does shape/force offset impact nucleation behavior?	Shapes cluster through an initial arrested phase separation (?) then combination/relaxation, rather than a cluster percolation model (disks)
	4	**Why** does shape/force offset impact nucleation behavior?	Steric interactions between anisotropic particles allow **translation** and **rotation** of clusters; ability of densest packing can stabilize shear may come into play

Statistical mechanics

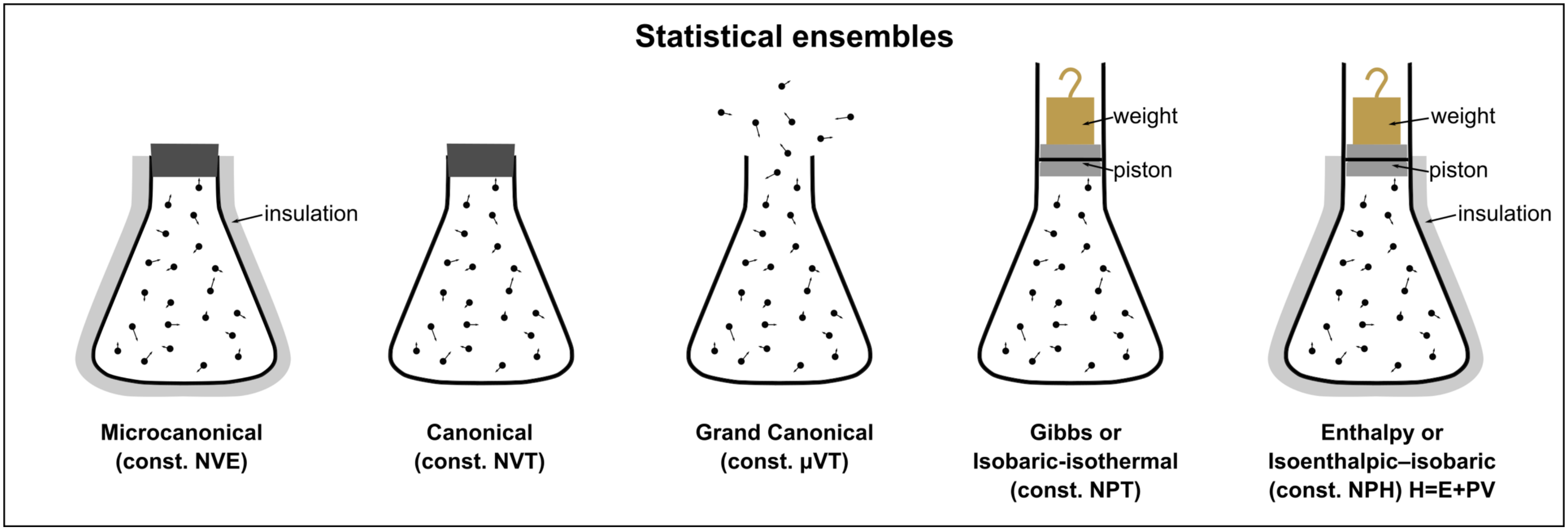
Boltzman distribution law:

$$p_i = \frac{e^{-\beta E_i}}{Z}$$

Partition function:

$$Z = \sum_{i=1}^{N} e^{-\beta E_i}$$

Ensembles


Statistical ensembles
insulation
weight
piston
weight
piston
insulation
Microcanonical
(const. NVE)
Canonical
(const. NVT)
Grand Canonical
(const. µVT)
Gibbs or
Isobaric-isothermal
(const. NPT)
Enthalpy or
Isoenthalpic–isobaric
(const. NPH) H=E+PV