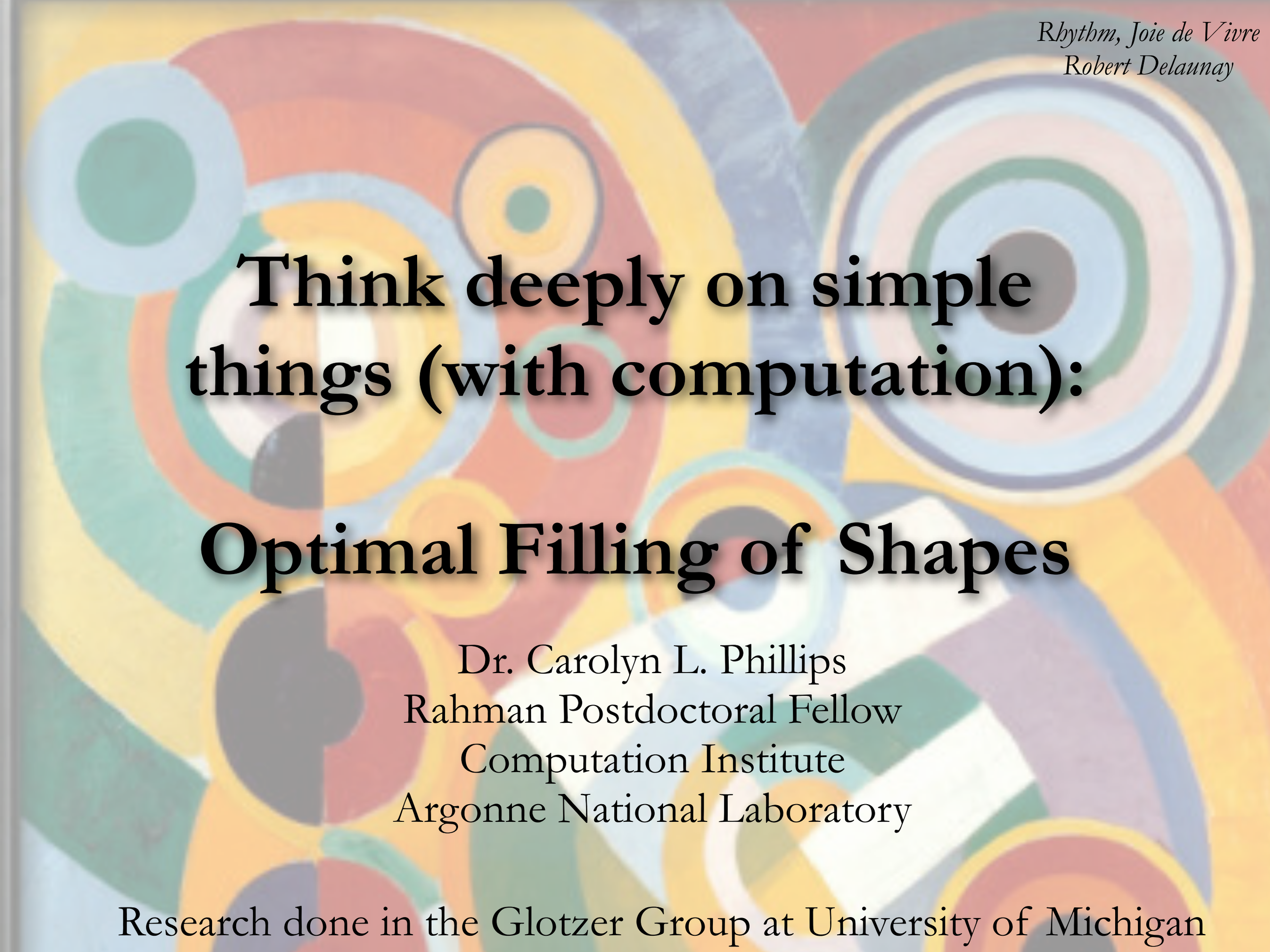


Think deeply on simple things (with computation):

Optimal Filling of Shapes

Dr. Carolyn L. Phillips
Rahman Postdoctoral Fellow
Computation Institute
Argonne National Laboratory

Research done in the Glotzer Group at University of Michigan

Babies are fascinated by shape

So are Physicists

Make everything as simple as possible,
but not simpler.

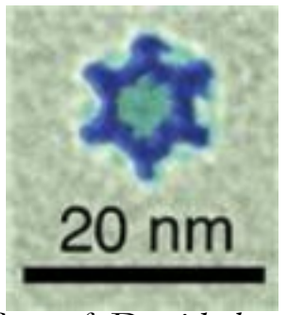
-Albert Einstein

by George W. Hart

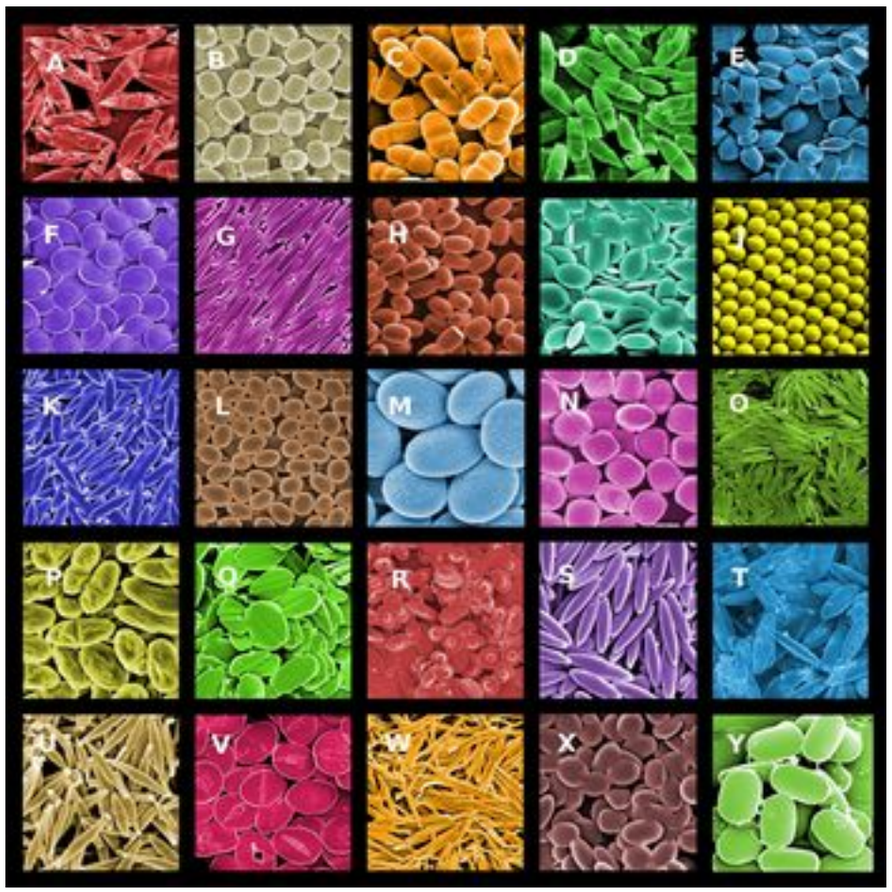
Lars Onsager (1903-1976)

The Brazil Nut Problem

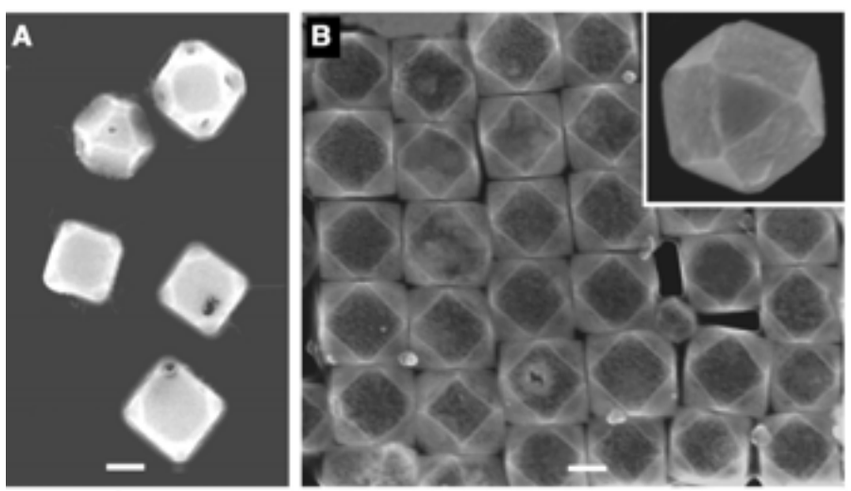
Shaped Nanoparticles



Star of David-shaped nanomaterial. (Credit: Image courtesy of Hebrew University of Jerusalem)

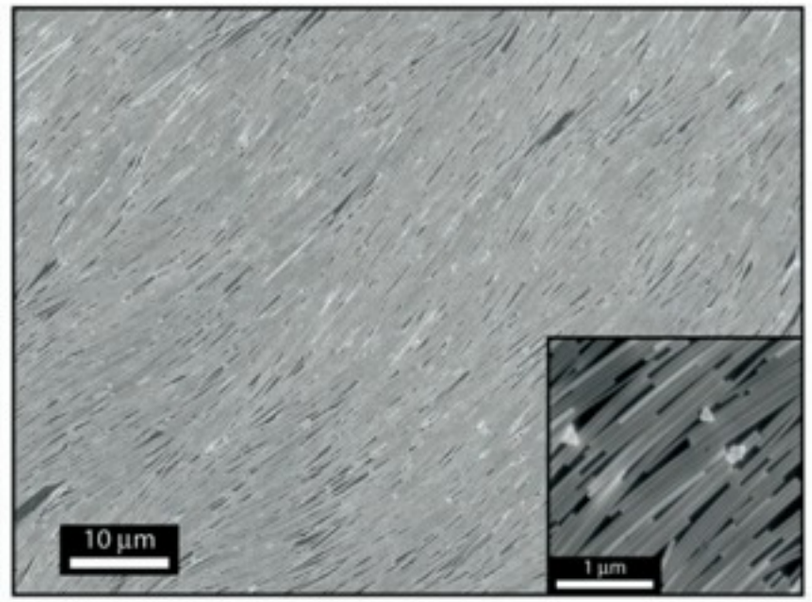


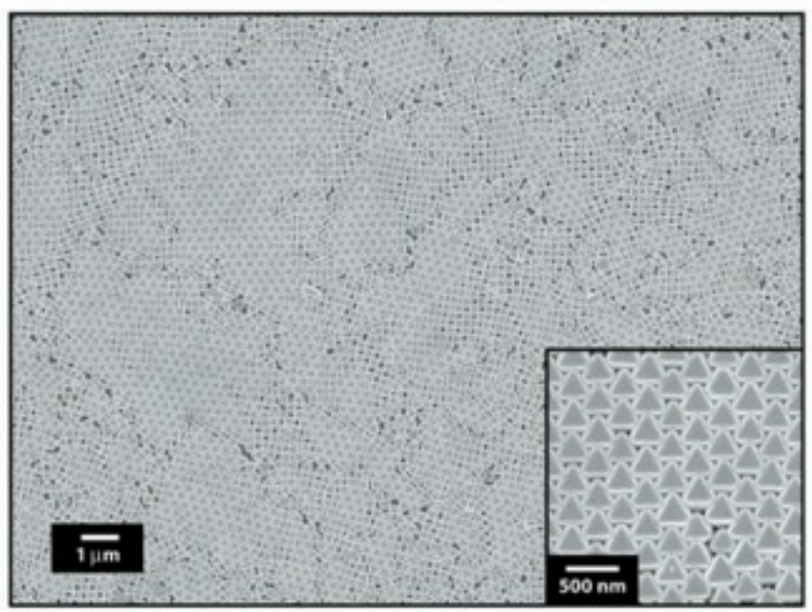
Champion, Katare, Mitragotri, PNAS, 2007



Sun, Xia Science, 2002

Tao, Habas, Yang, Small, 2008



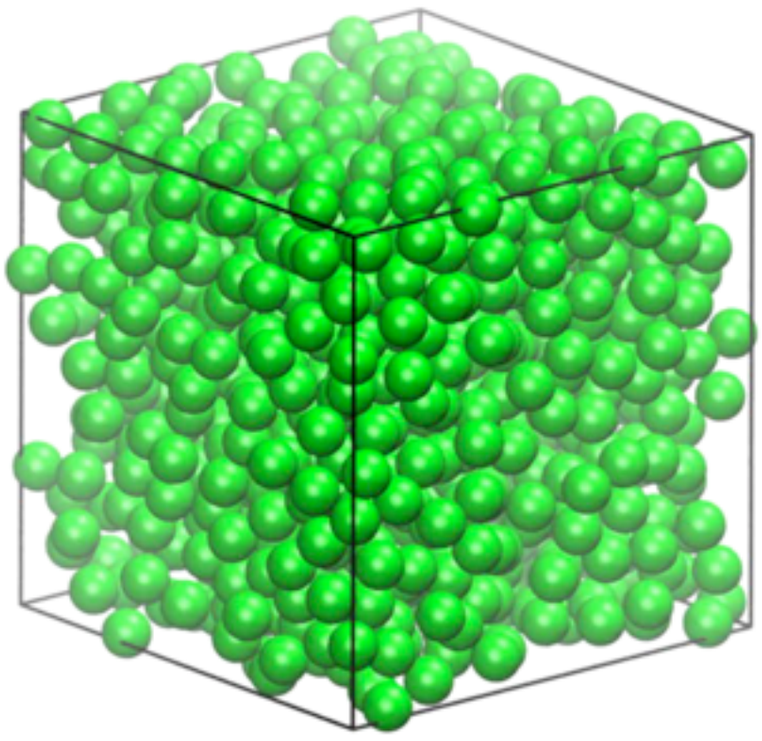


Shape in Computation

GPU Accelerated Many Particle Dynamics Code

www.codeblue.umich.edu/hoomd-blue

1 GPU ~ 30-100 CPUs with Infiniband

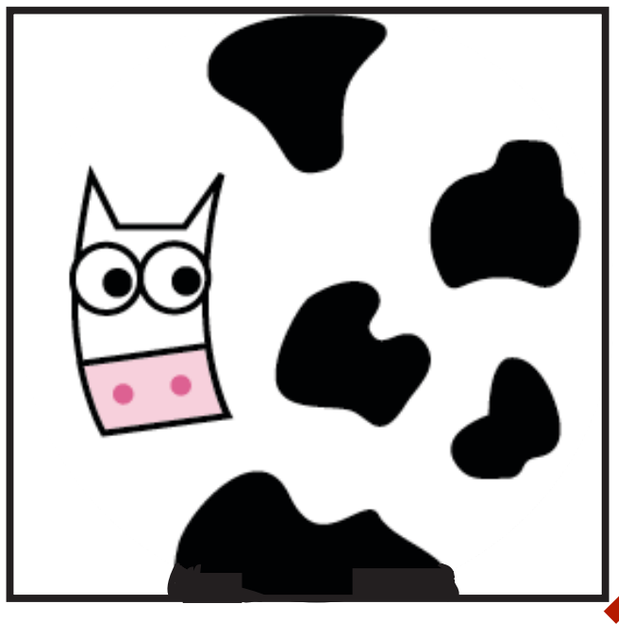


Molecular Dynamics (and especially HOOMD) is very good at:

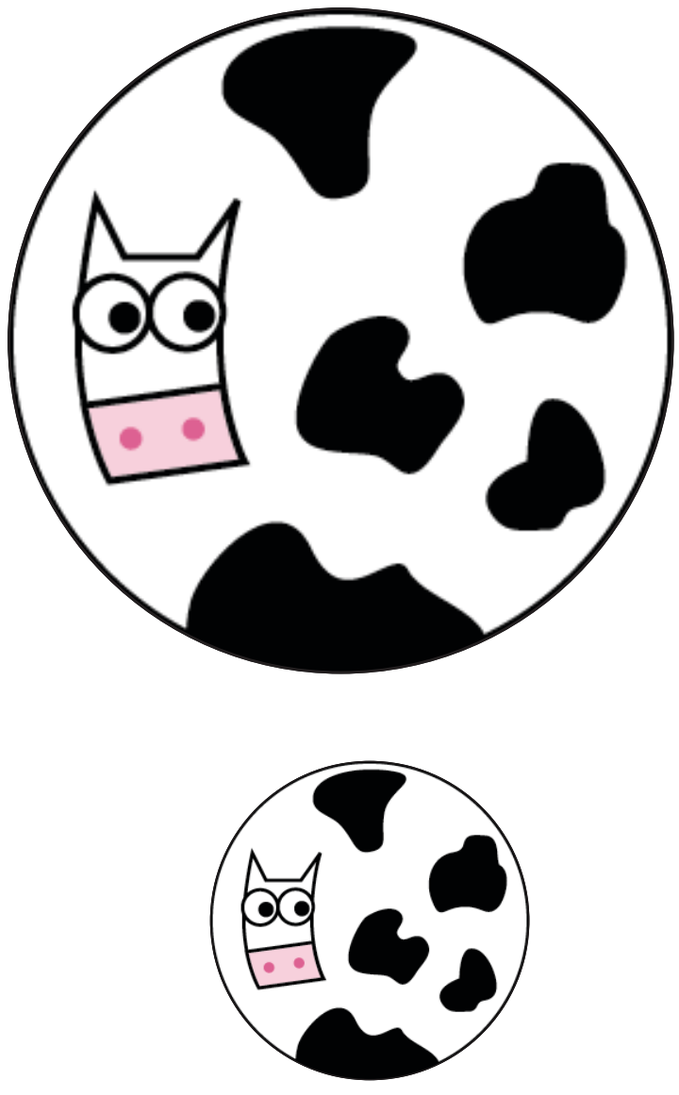
- Radially Shifted Isotropic Pair Potentials
- Rigid Body Integration

Nguyen, Phillips, Anderson, Glotzer, Journal of Computer Physics, 2011

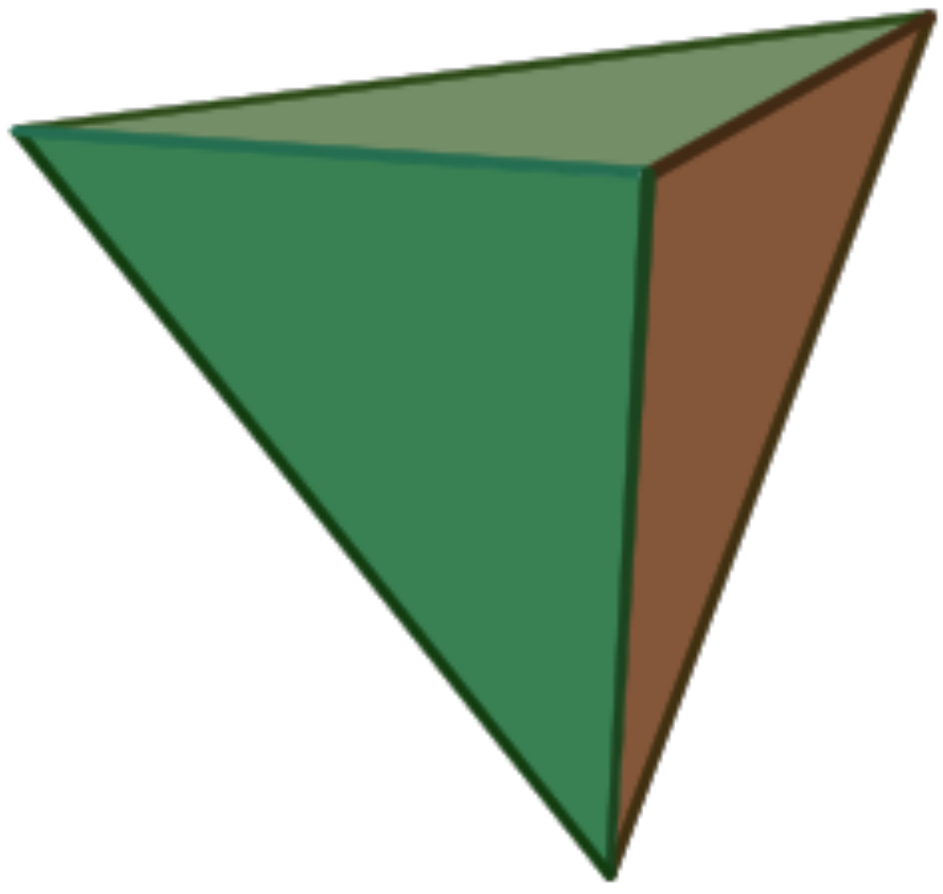
Assume a Spherical Cow.
Assume a Cubical Cow?



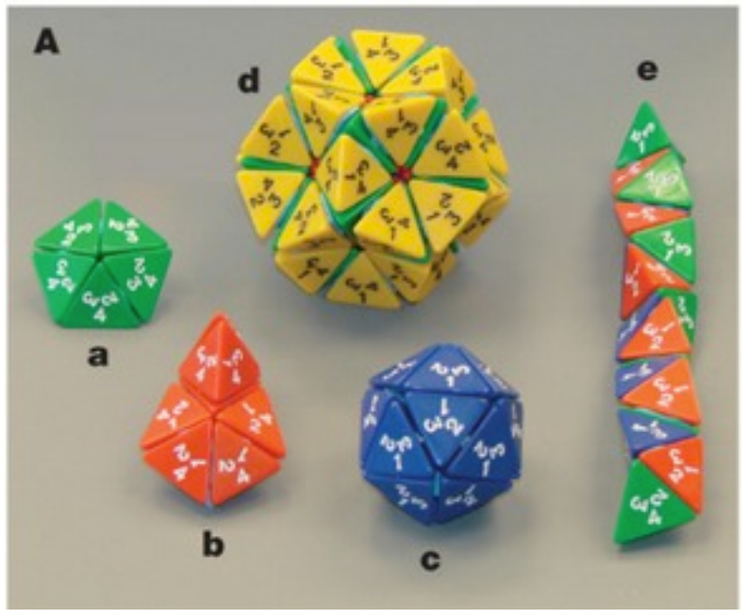
Assume MORE Spherical Cows.

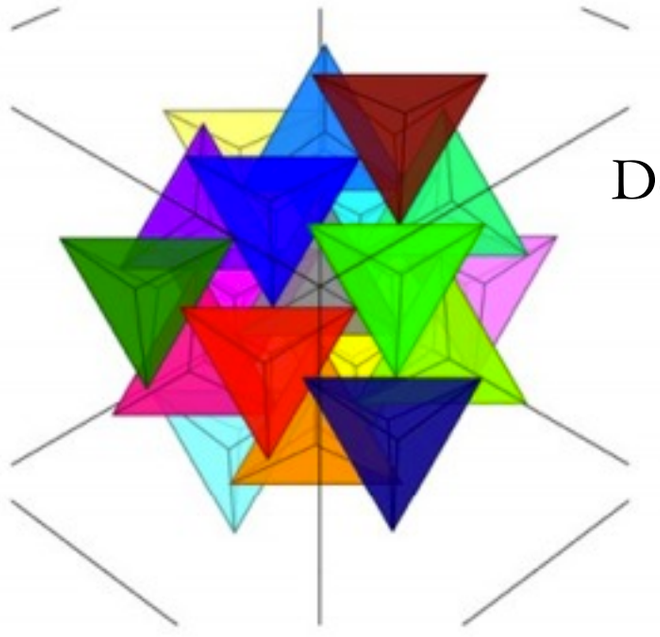


Tetrahedron

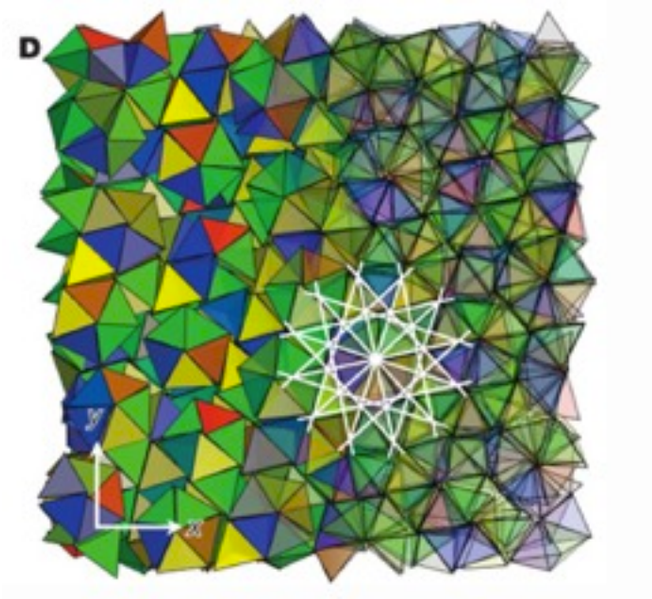


Glotzer Group Research in Tetrahedra

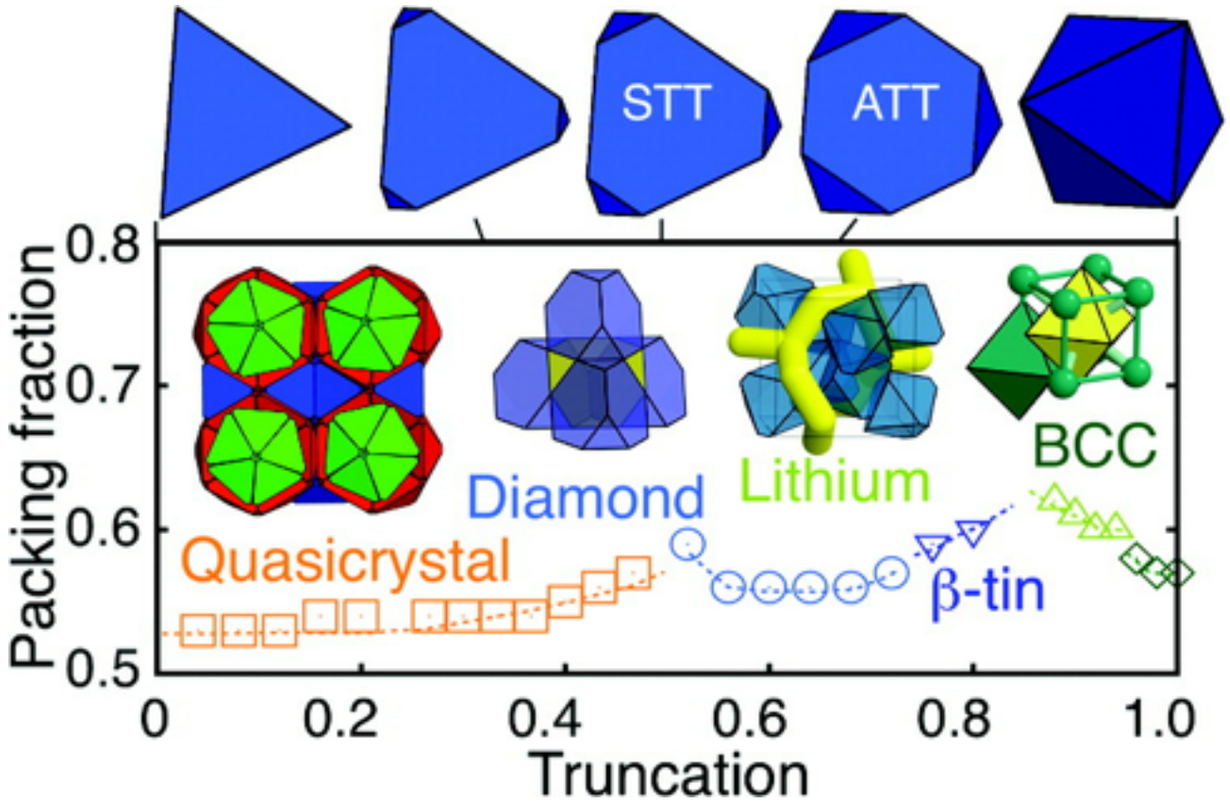




Dense crystalline dimer packing of regular tetrahedra, *Chen, Engel, Glotzer, Discrete Computational Geoemtery, 2010*

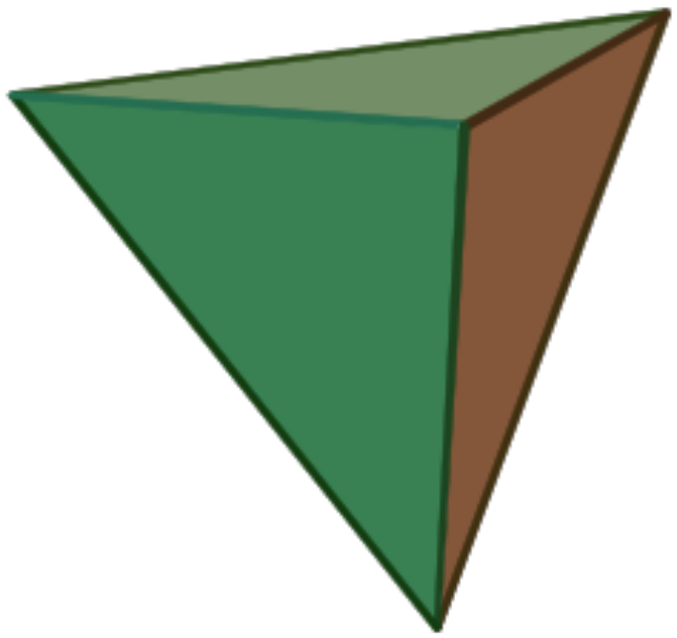


Packing Tetrahedra to form a quasi-crystal, *Haji-Ackbari, Engel, Glotzer, Nature, 2009*



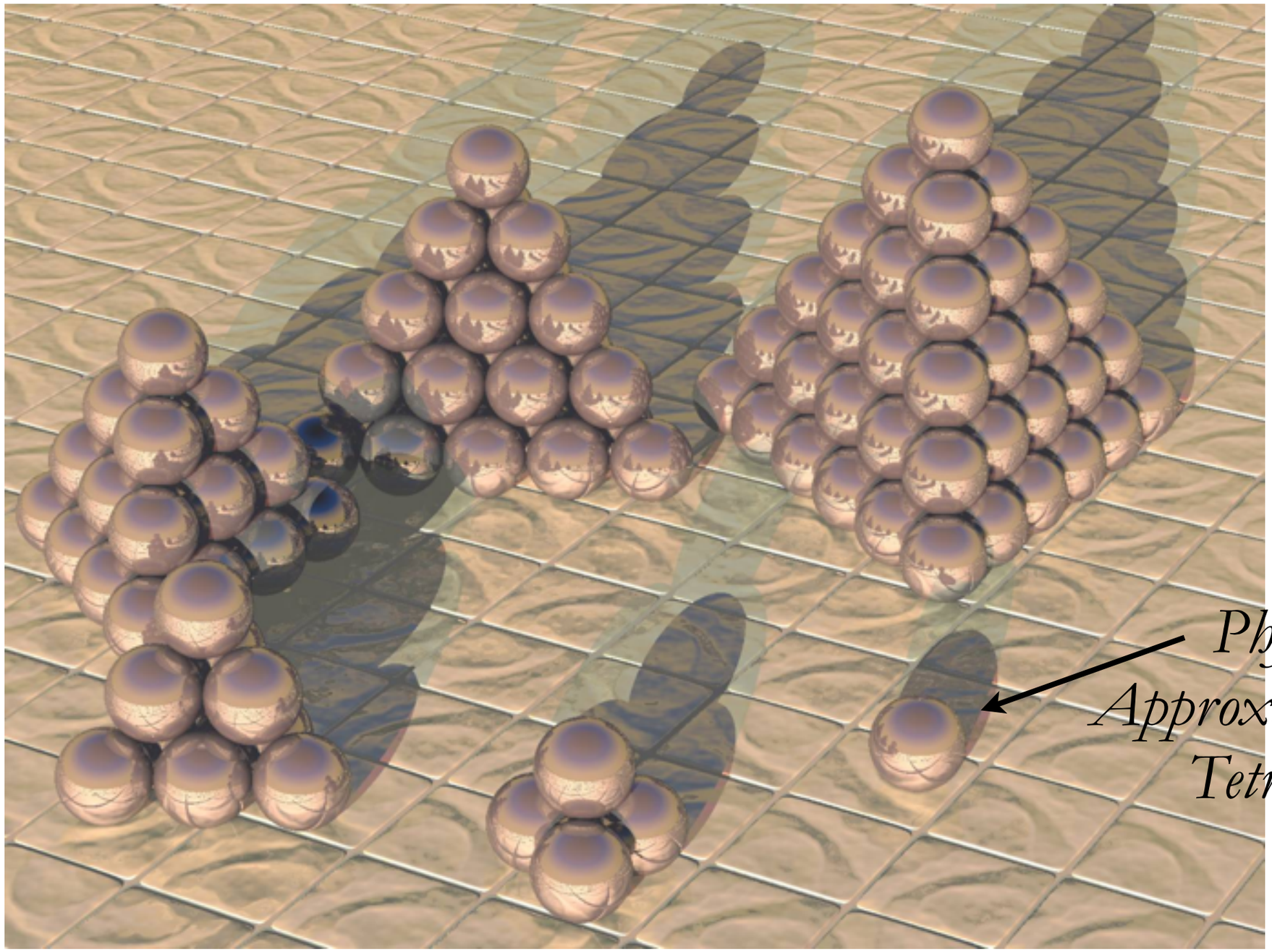
Damasceno, Engel, Glotzer, ACS Nano, 2012

How do I make this



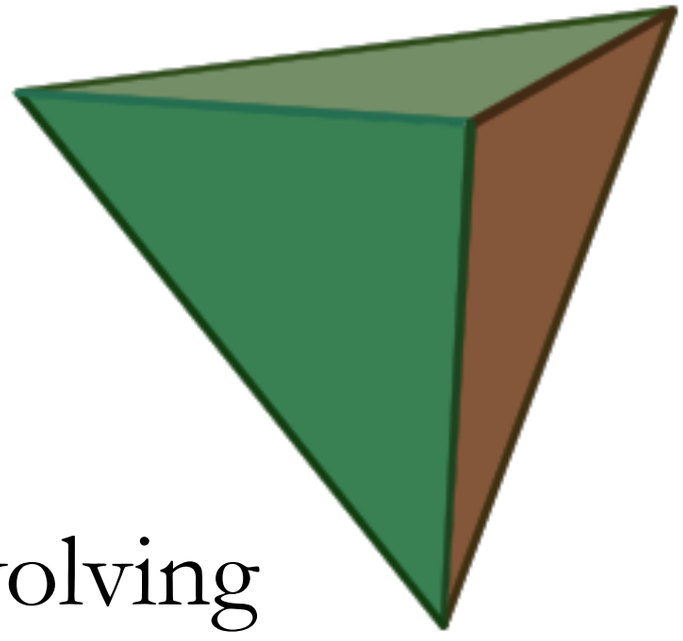
from the smallest number of these

Not the Answer!



NEW

Filling

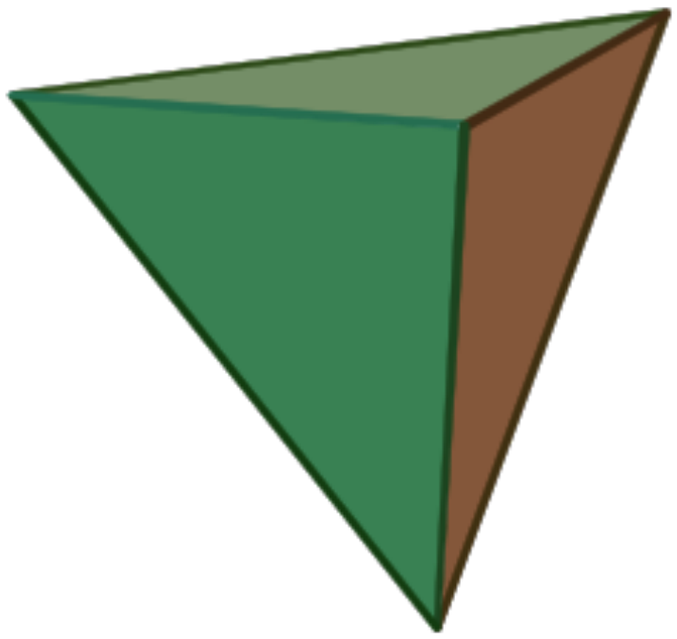


- A class of optimization problems involving *packing* simple objects inside a container, where the objects are permitted to overlap each other without restriction.
- The aim is to find the maximal *coverage* of the interior of the container.
- Our simple object are n-balls with varying diameters.

Phillips, Anderson, Huber, Glotzer, Optimal Filling of Shapes, PRL, 2012

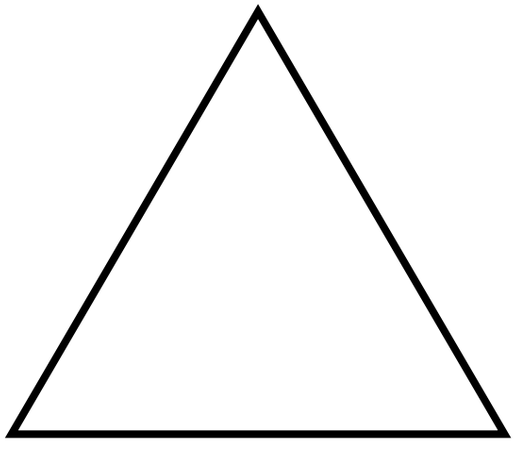
The problem (make it simpler)

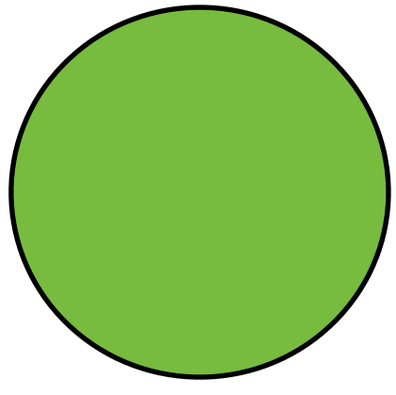
How do I make this

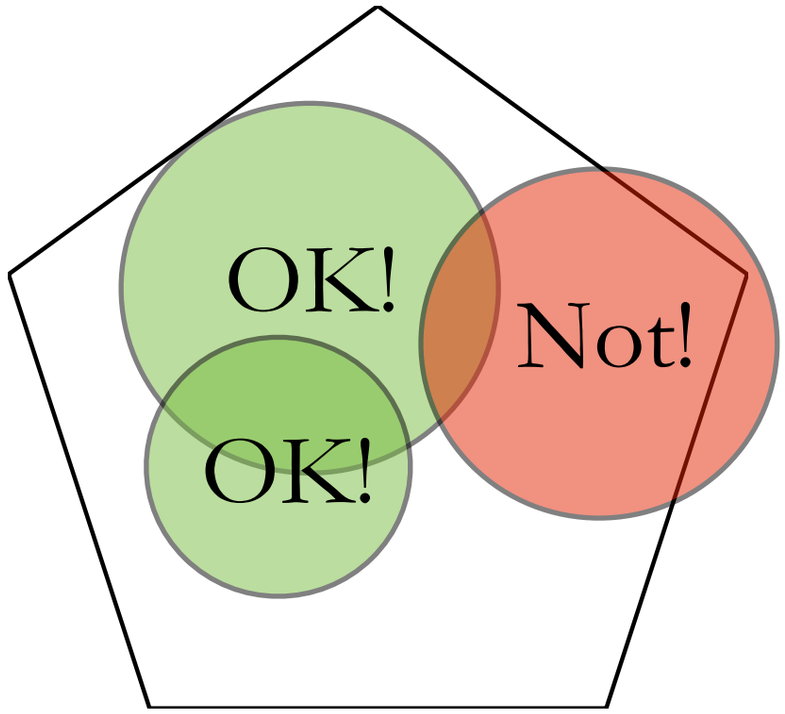


from the smallest number of these

!!! Let's drop a dimension !!!



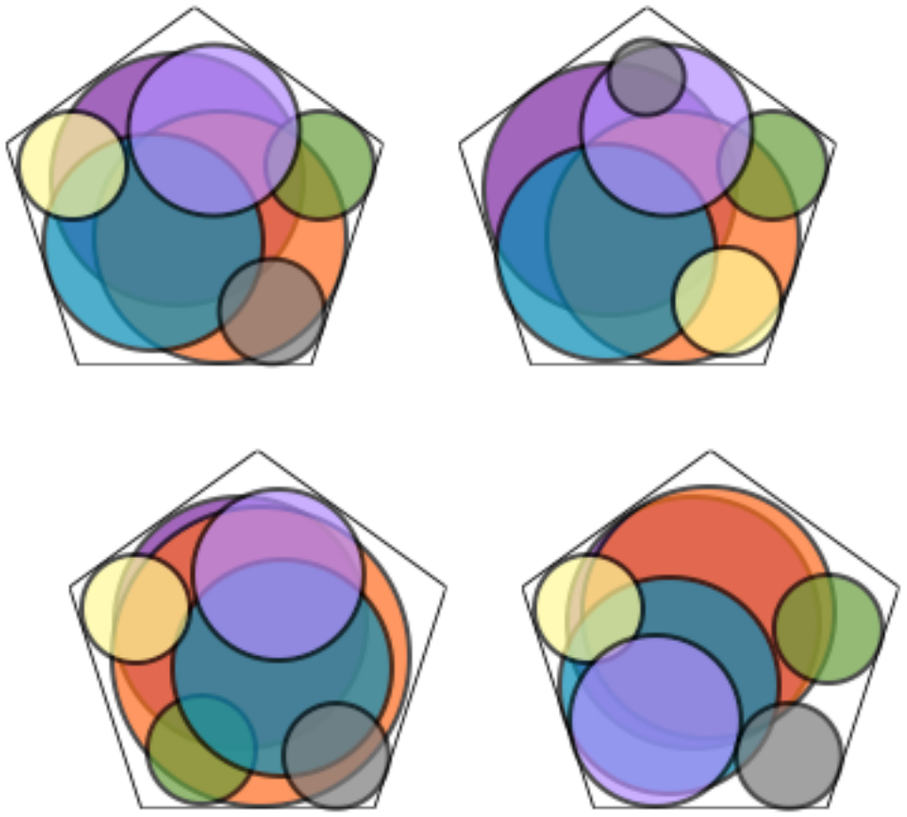



OK!
Not!
OK!

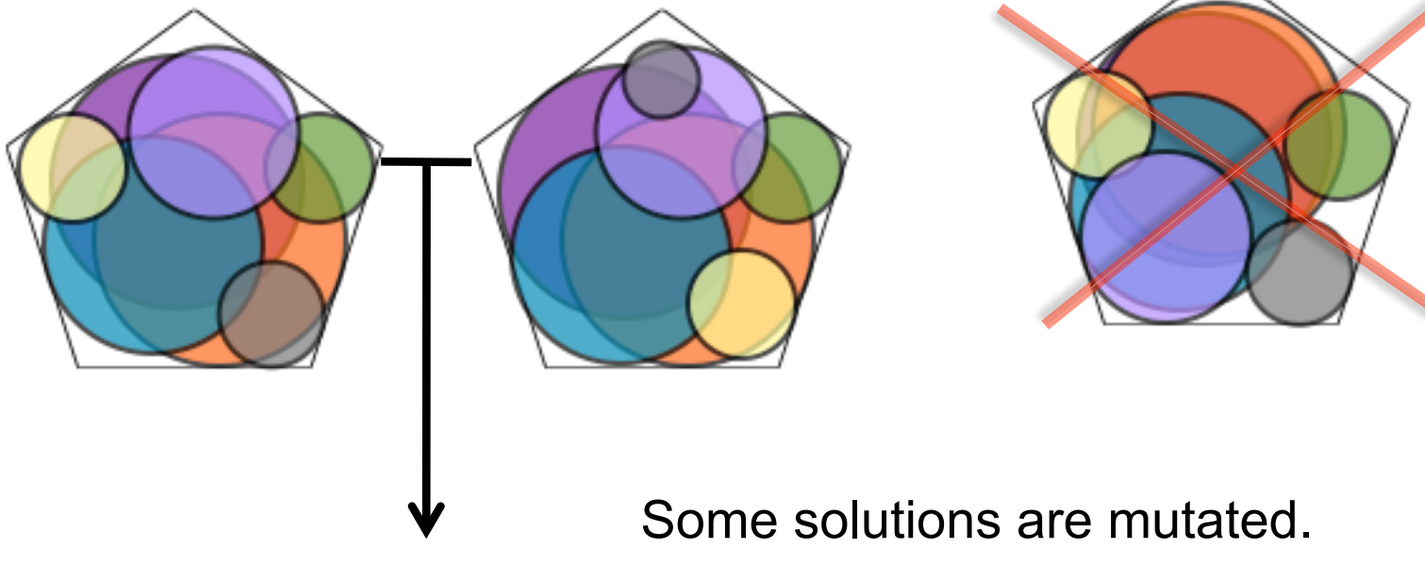
Ben Schultz

Genetic Algorithm

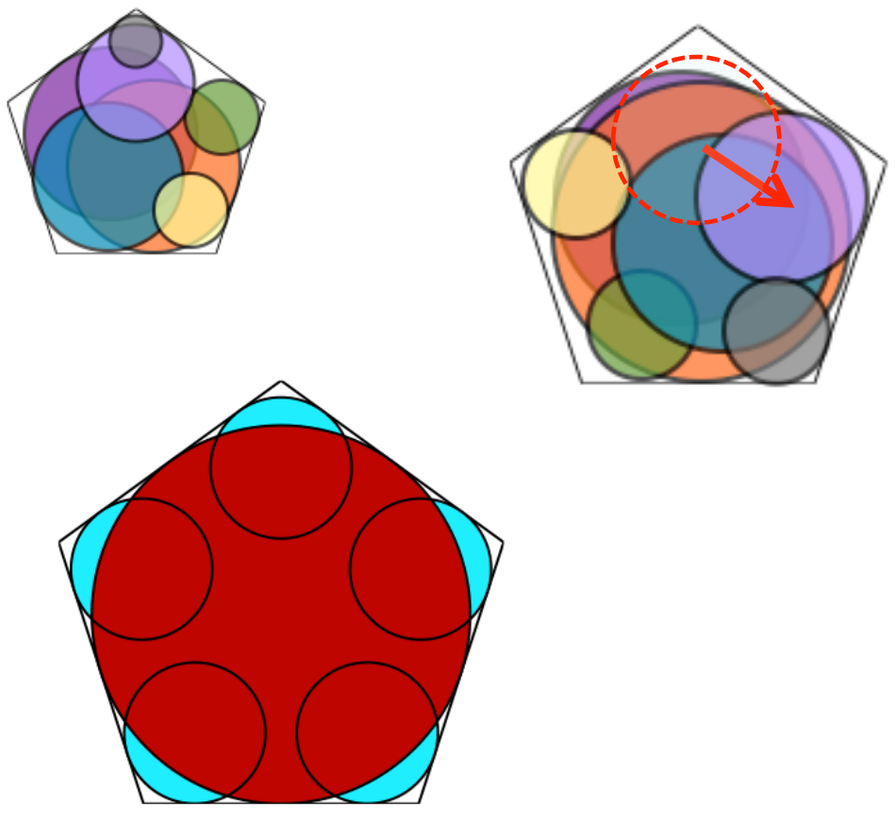
We create a population of random solutions. Each solution has a genome {x1,y1,,r1, x2,y2,r2,…}



The best solutions are “mated” to make children solutions. The worst are thrown away.

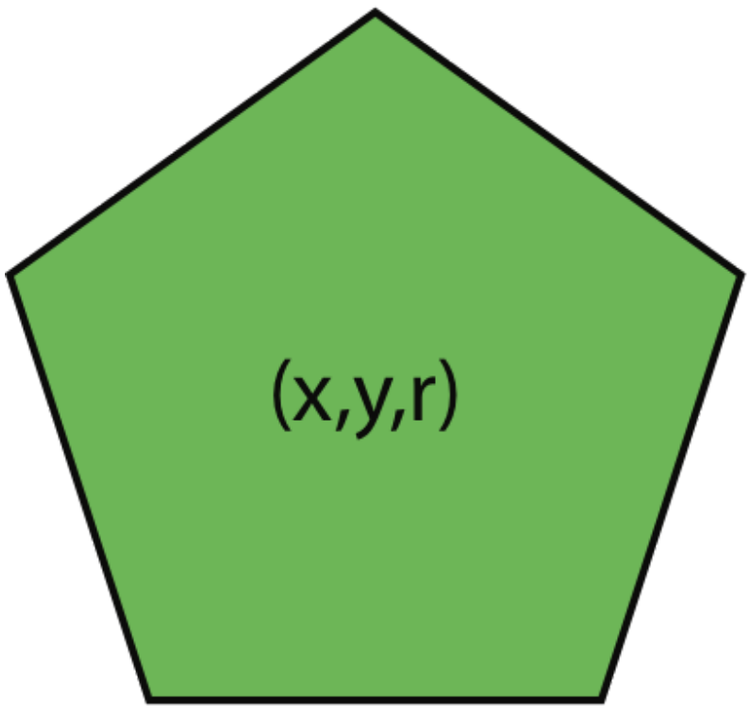


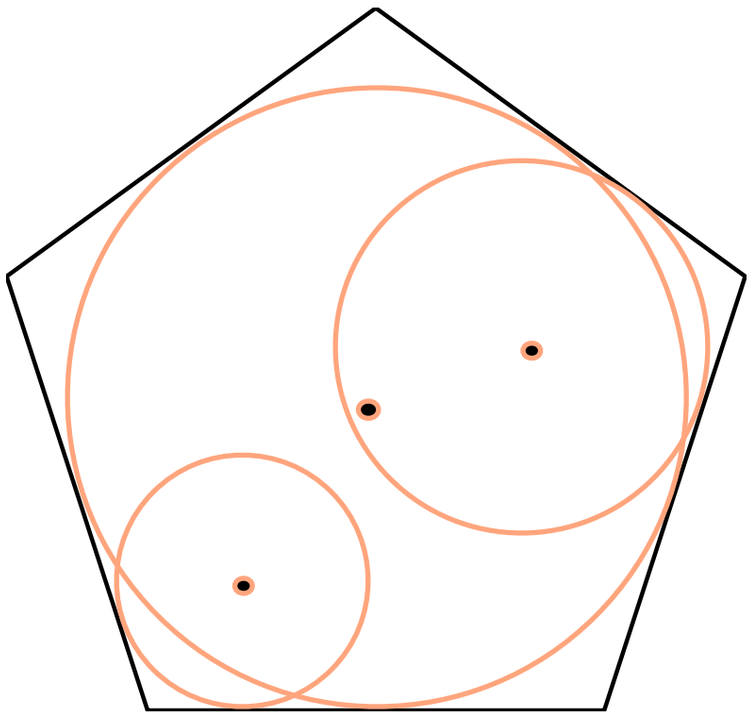
Some solutions are mutated.



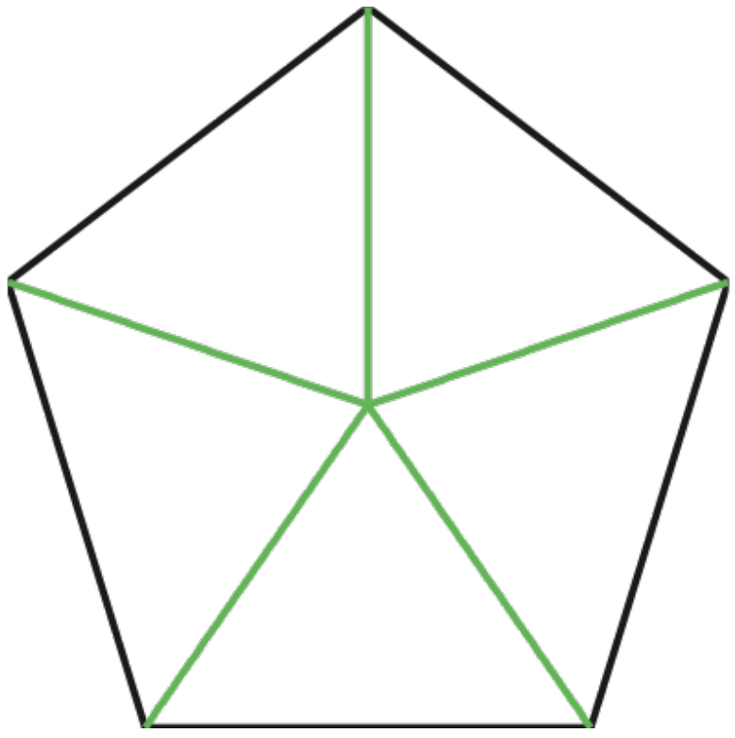
We repeat until the process has converged

centers + radius



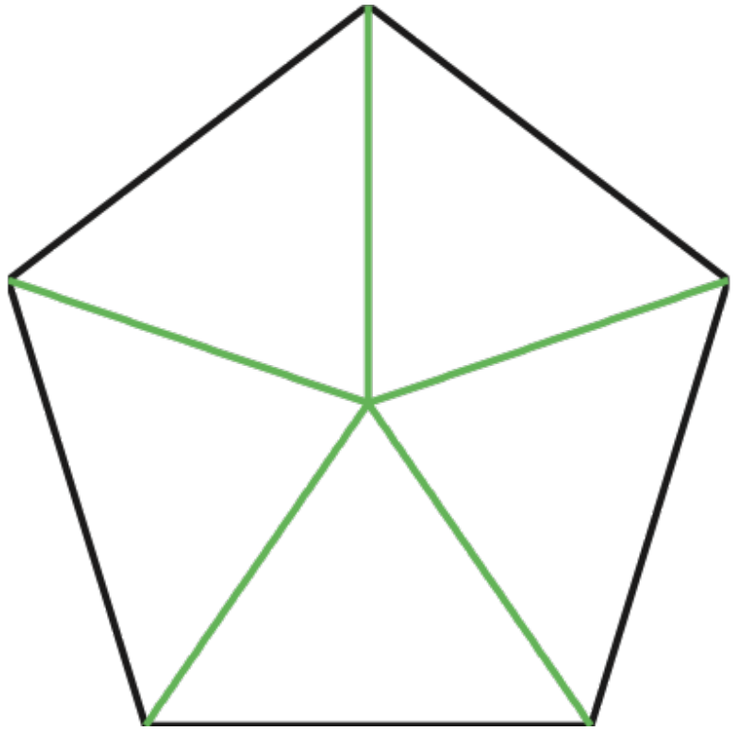


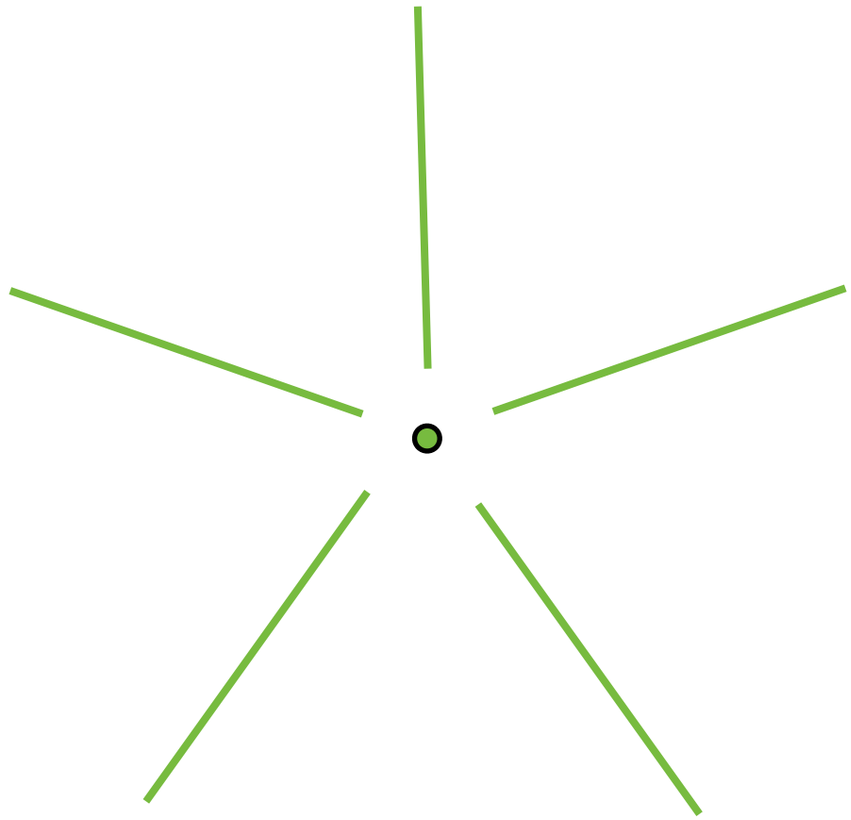
maximal discs



medial axis

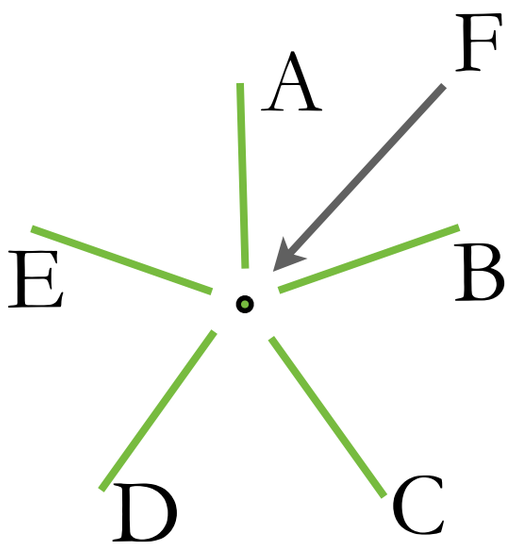
Blum 1967, 1971,1978





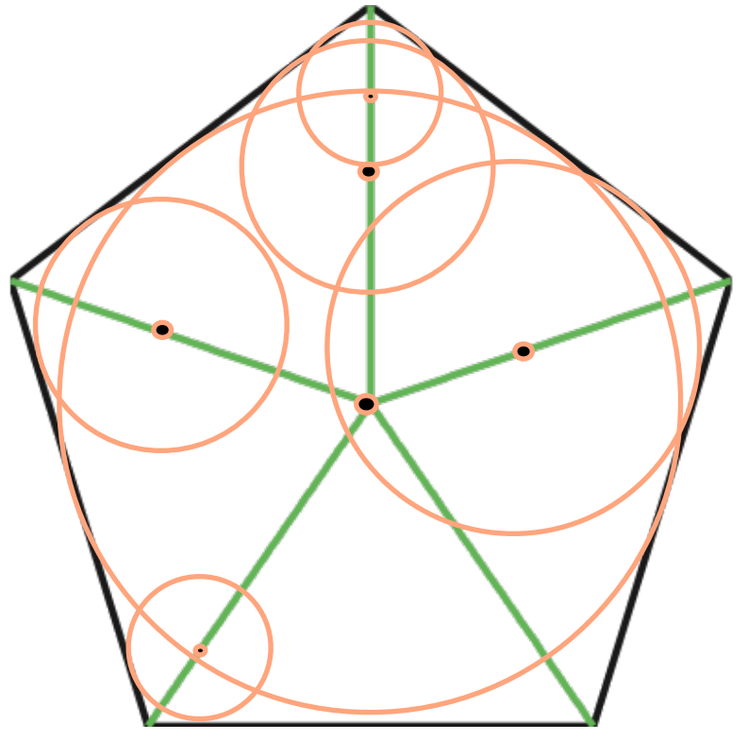
Conjecture: There is only at most, one local maximum per way of partitioning N discs over the pieces

Number of searches for local maxima ~ $O(N^{K-J-1})$

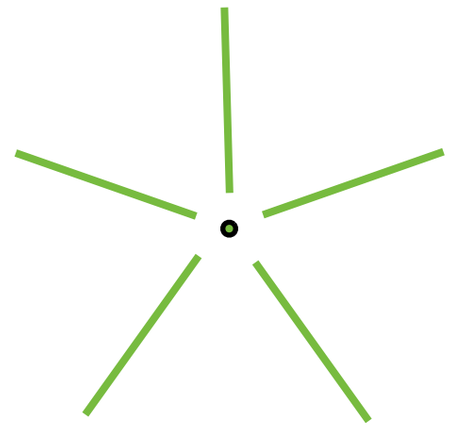


2 1 0 1 1 1

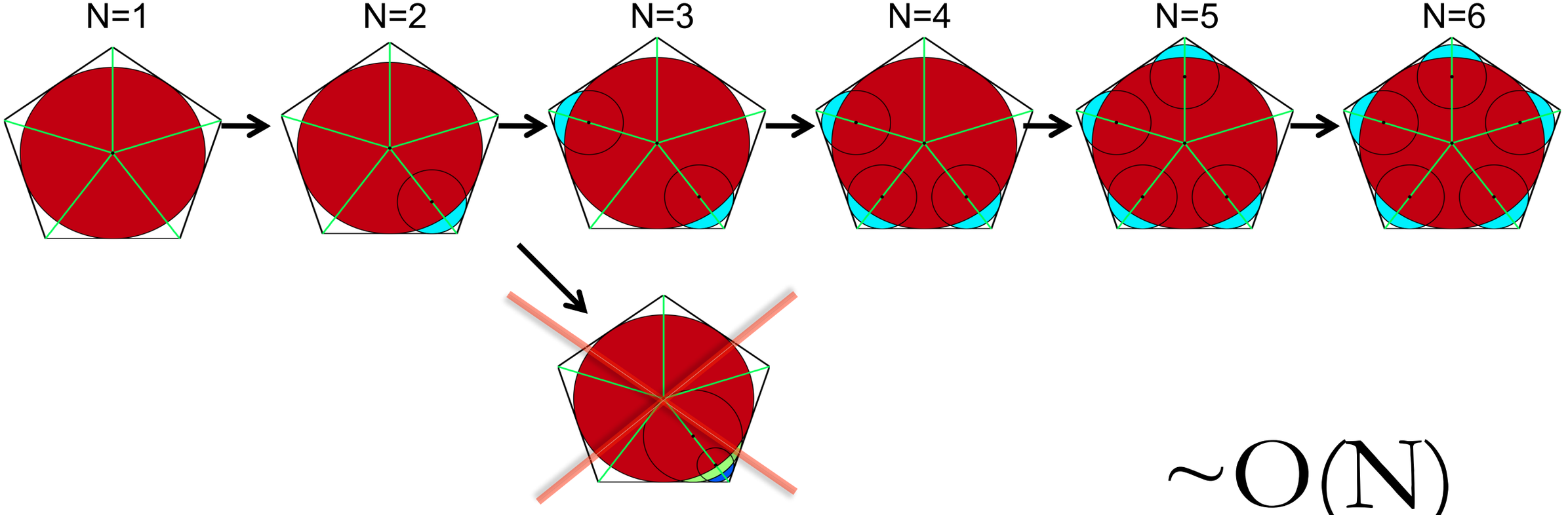
A B C D E F



$O(N^4)$



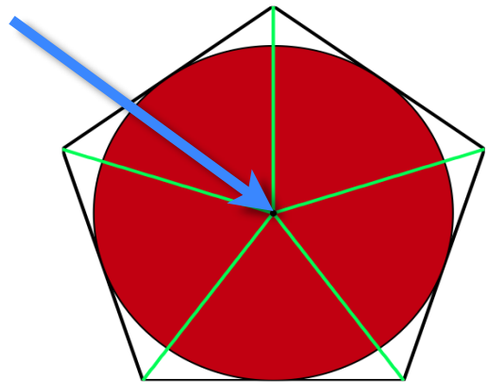
Assume the best way to partition N discs over the pieces is *near* the best way of partitioning N-1 discs



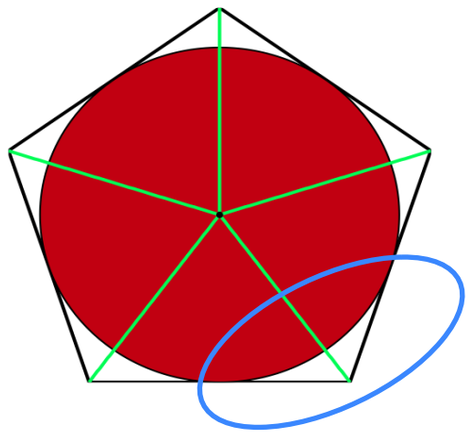
$\sim O(N)$

A few more tricks

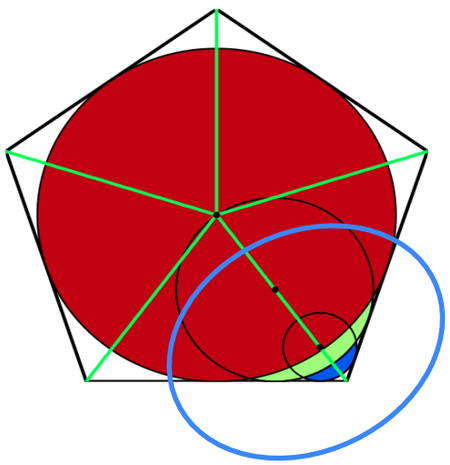
- As N gets large, junctions stay occupied



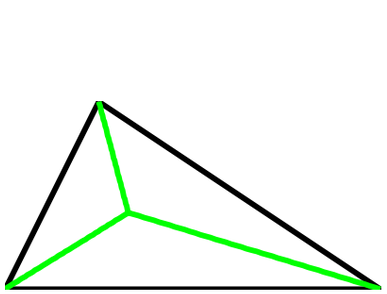
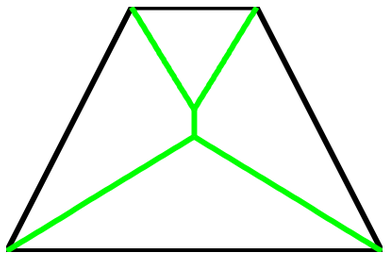
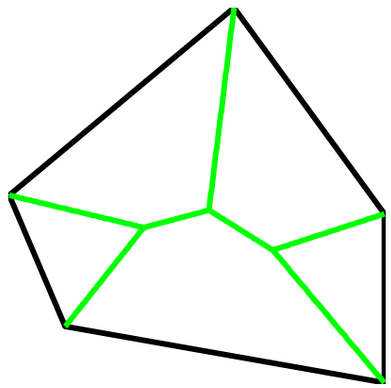
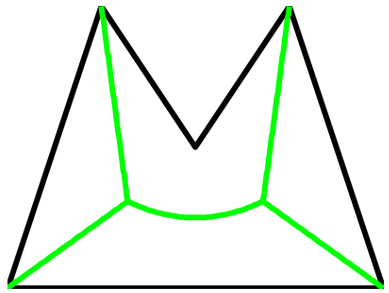
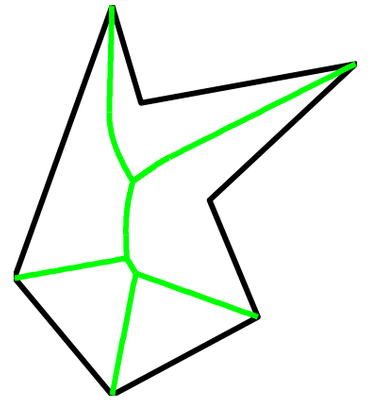
- Occupied junctions divide filling space into smaller independent spaces

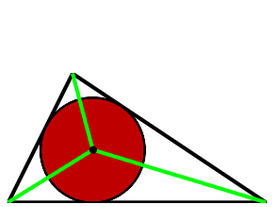


- Cache solved sub-problems



~O(N) with a coefficient of 1 !!!



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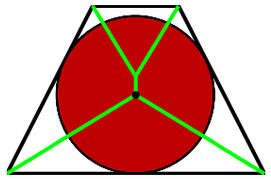

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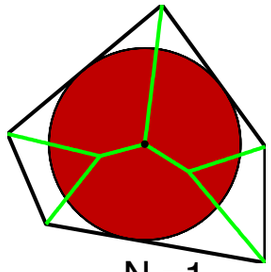

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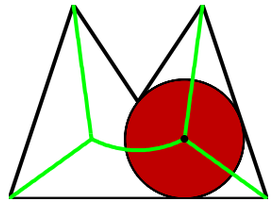
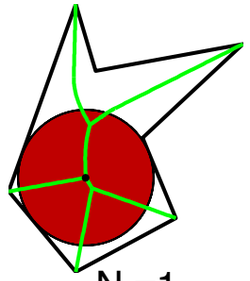
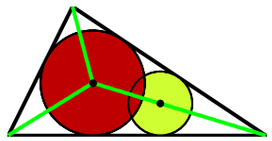


N =1



N =1



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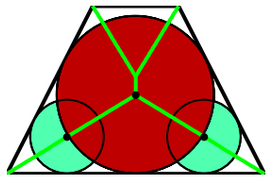

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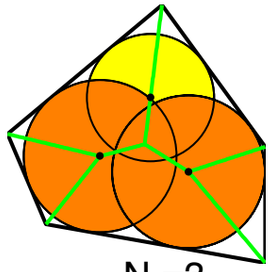

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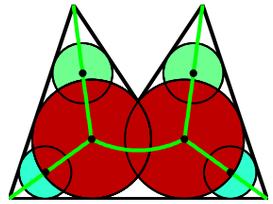
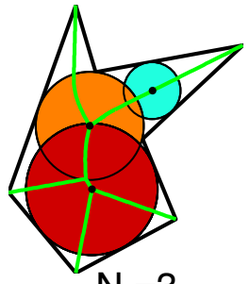


N =6



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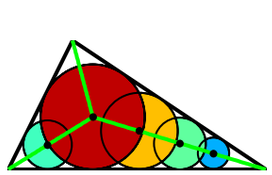

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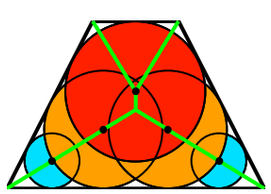

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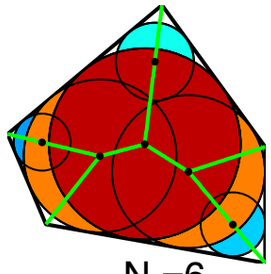

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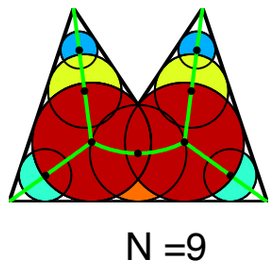

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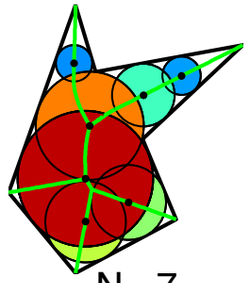

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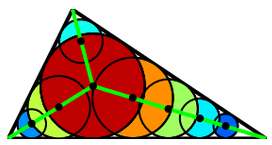

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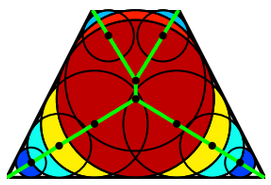

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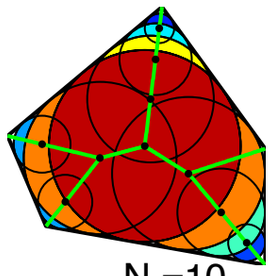

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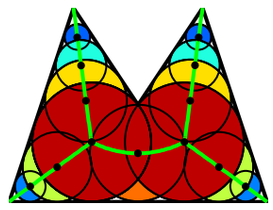

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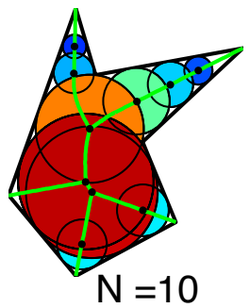

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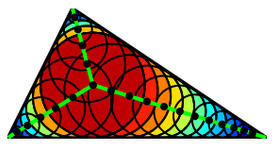

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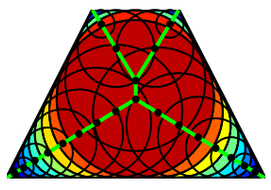

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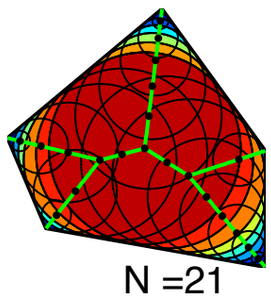

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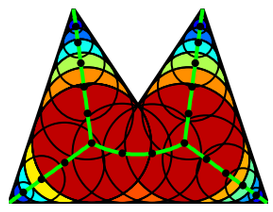

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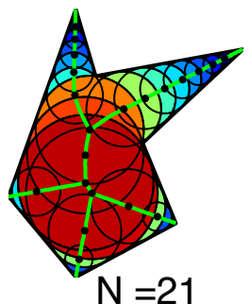

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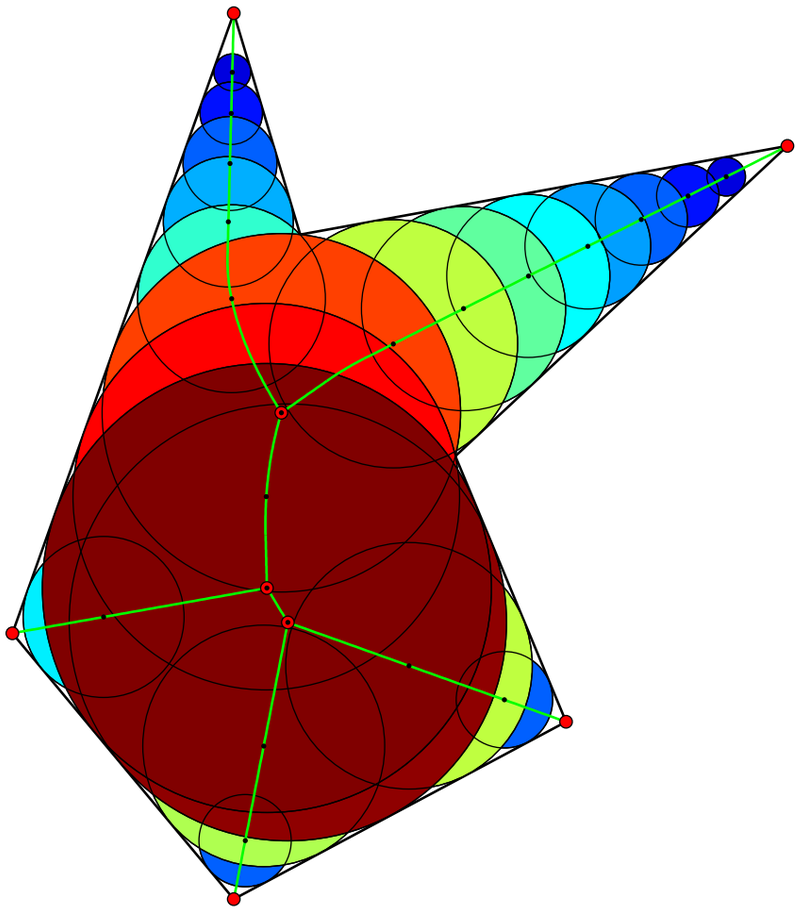
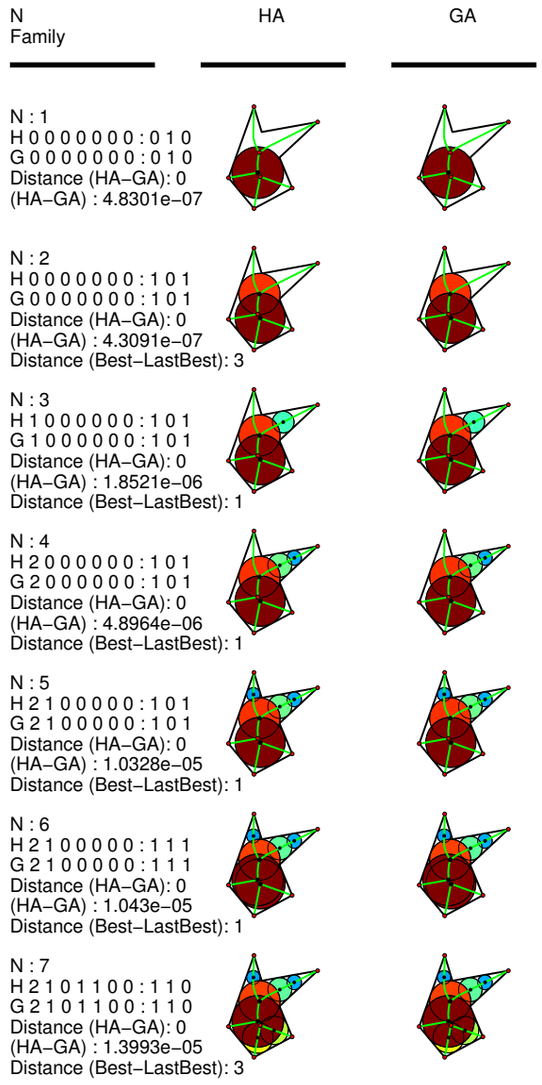
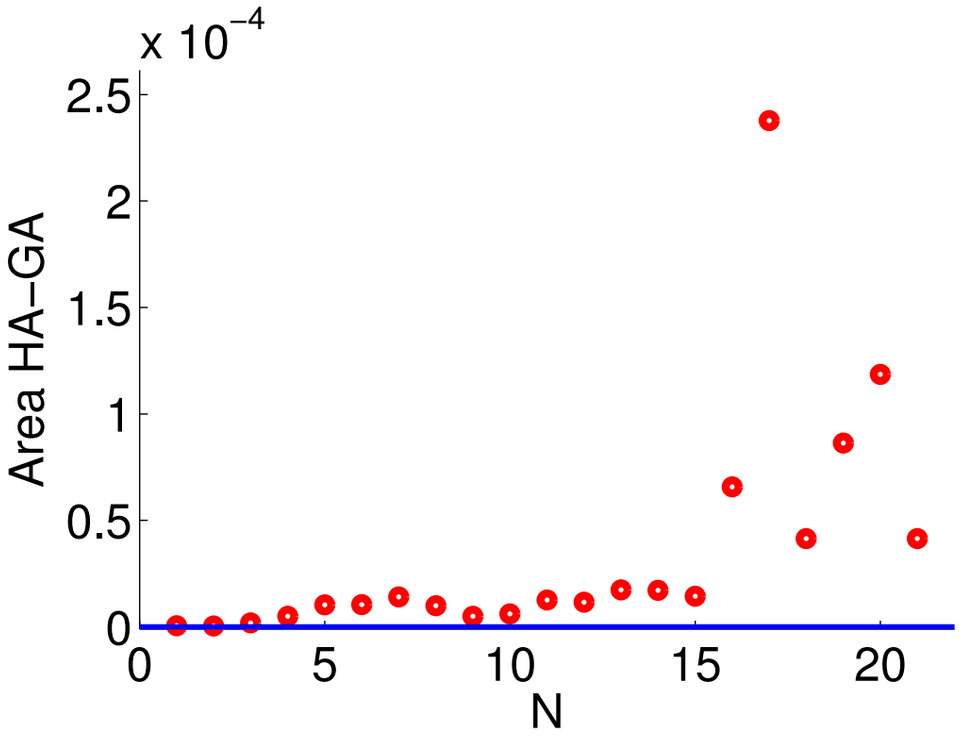
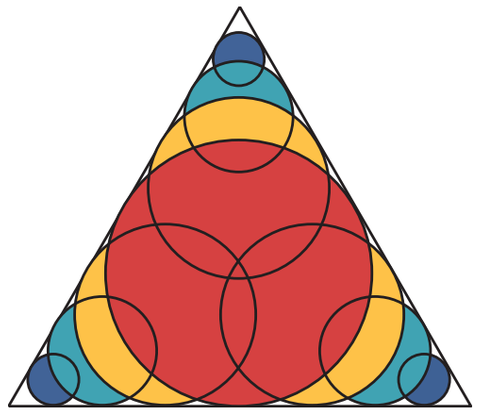






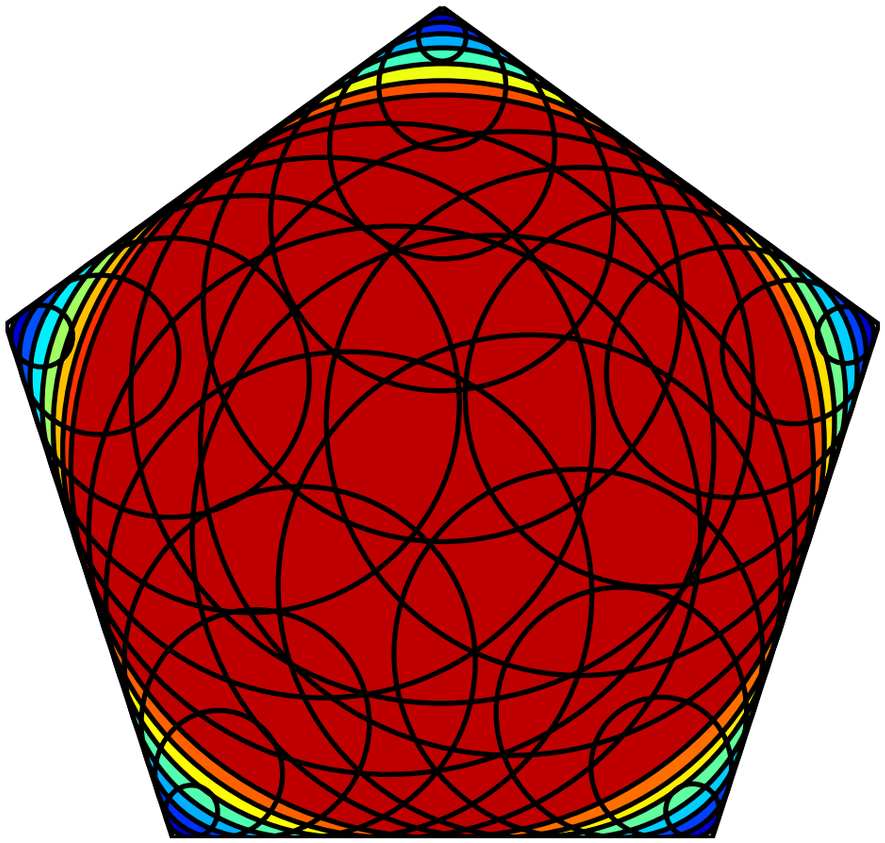
	HA and GA Way Match	Best Way: HA	Best Way: GA	Best ϕ : HA
Convex	98.1%	1.9%	0%	100%
Concave	92.97%	3.4%	3.63%	96.37%



Filler

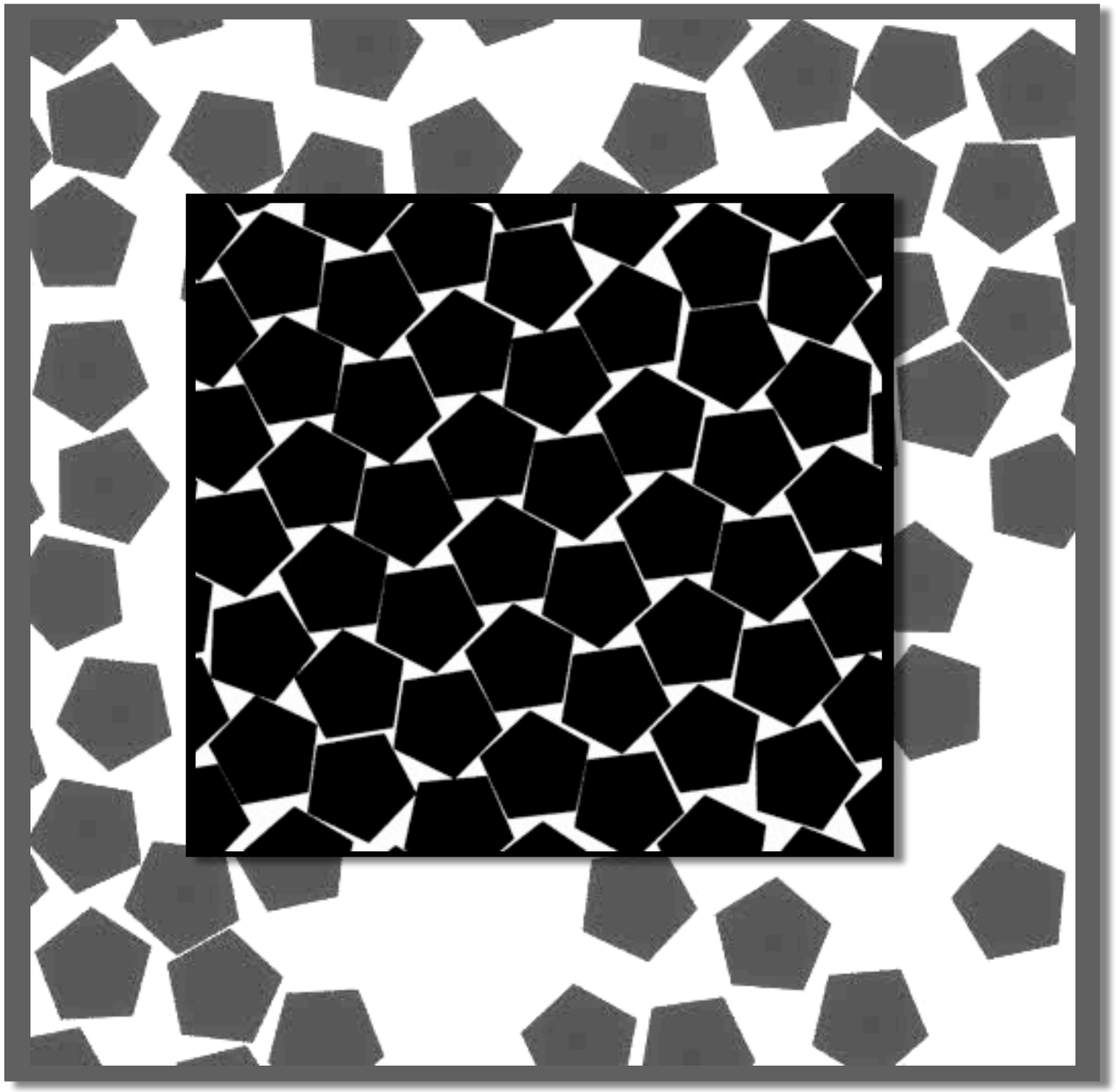
A freely distributed code for generating optimal filling solutions for convex and concave polygons.

Simulating shaped particles with MD

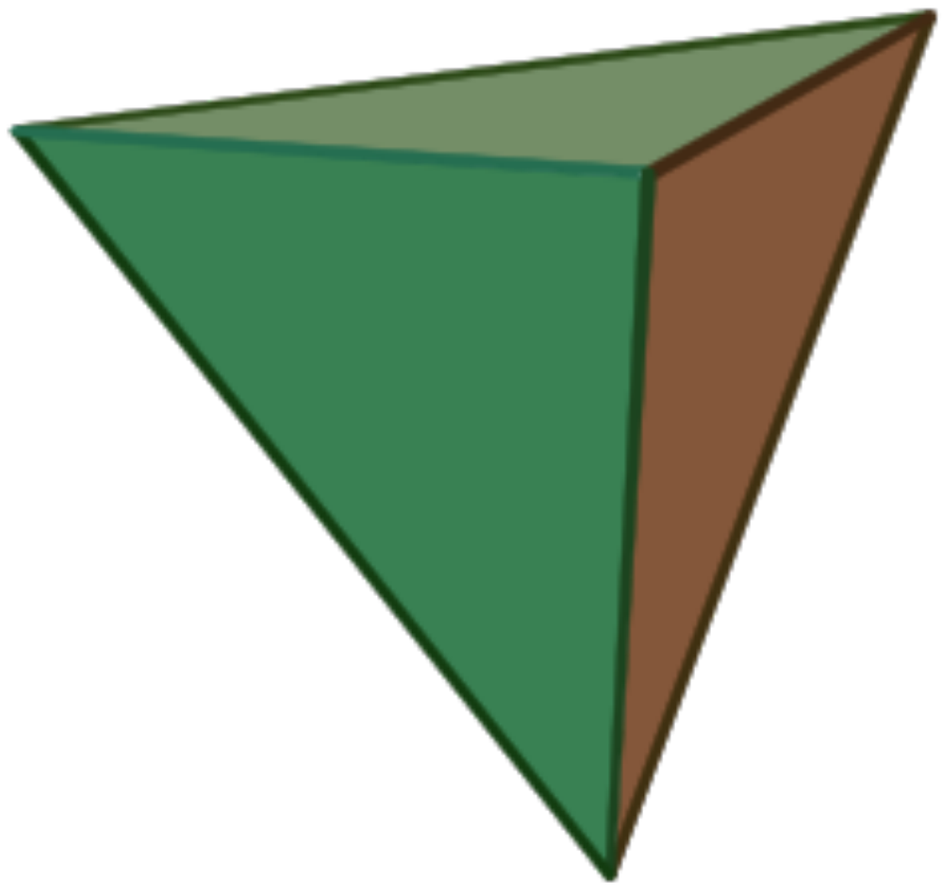


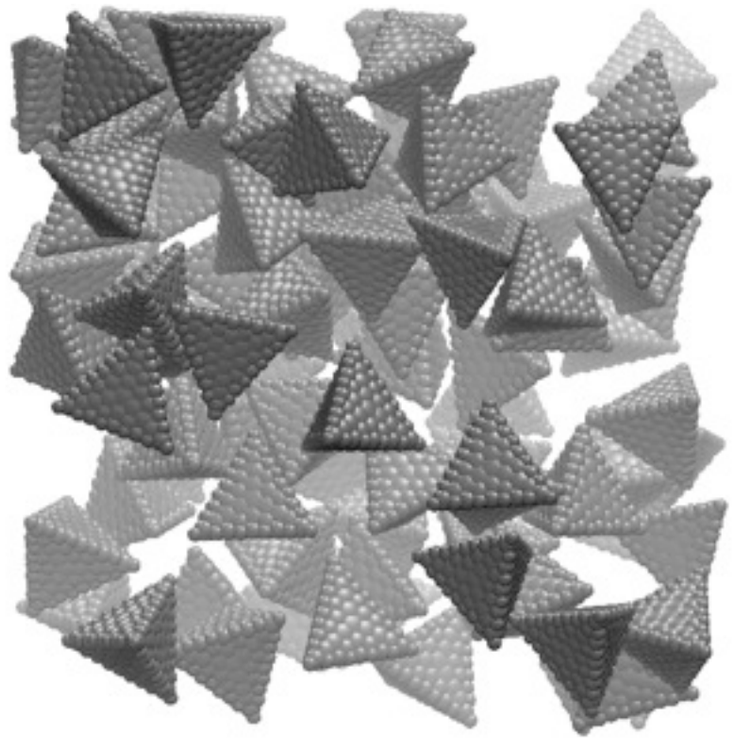
N=31

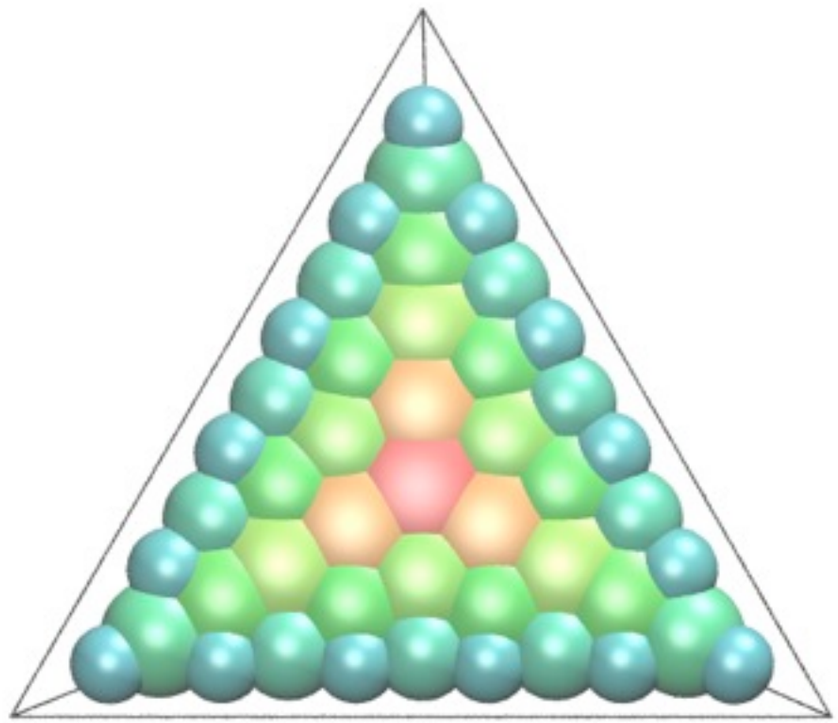
In this picture, there is only circles...



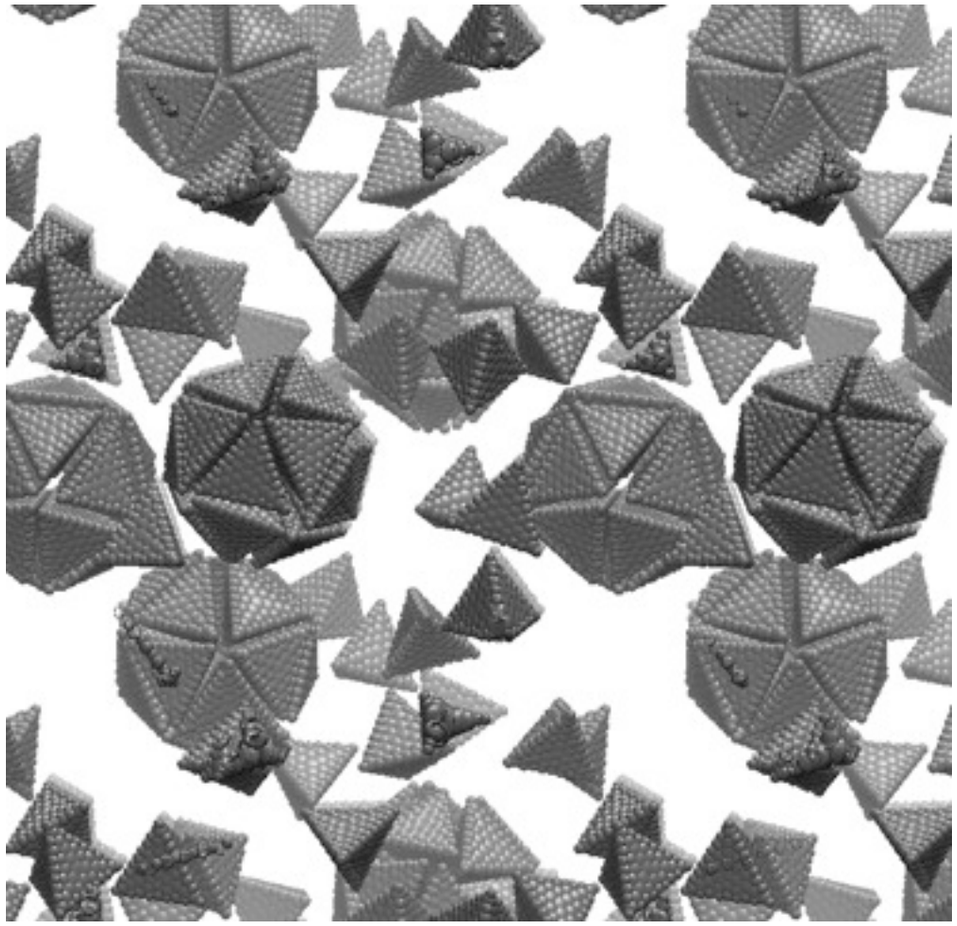
Tetrahedron







$N = 81$



Other Applications

- Designing colloidal particles
- Compact data representation
- Designing shaped wave fronts
- Material removal (lasers with tunable beams)

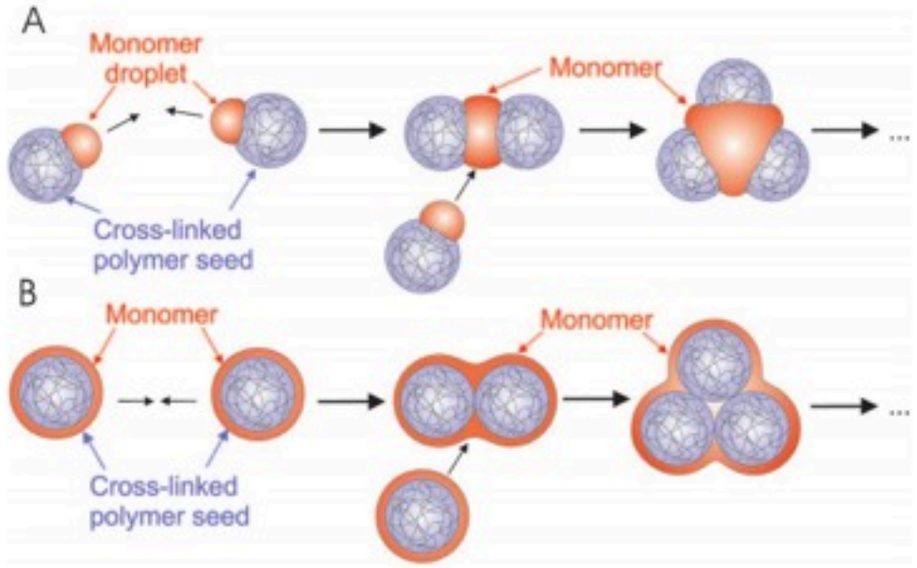
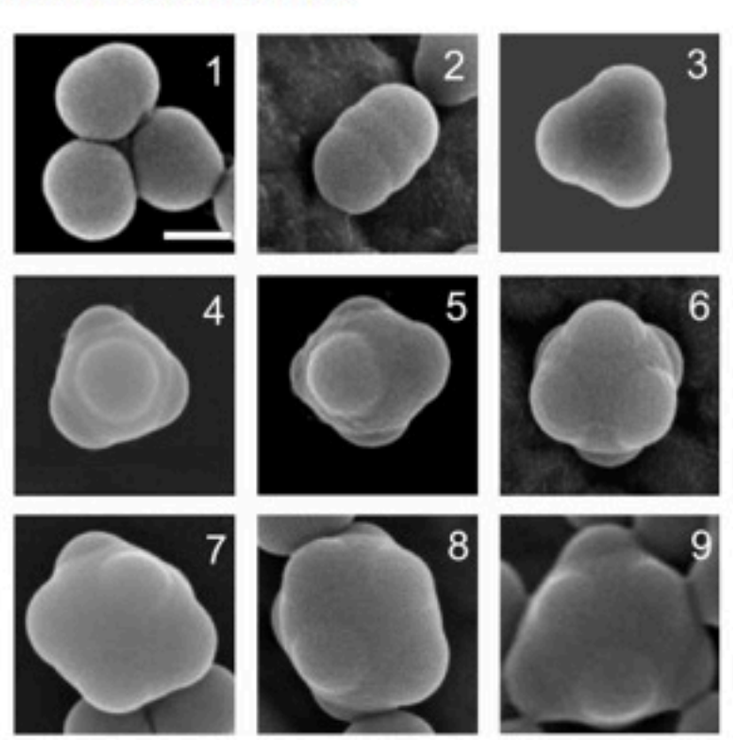


Figure 1. Schematic of merging of (A) liquid protrusions or (B) wetting layers, yielding colloidal molecules.



Kraft, Vlug, van Kats, van Blaaderen, Imhof, Kegel ,Self-Assembly of Colloids with Liquid Protrusions. JACS., 2009, 131 (3), 1182-1186

Acknowledgements

In Memory of Dr. Sally Ride
1951-2012

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Prof. Sharon Glotzer and the Glotzer Lab and useful discussions with Beth Chen, Amir Haji-Akbari, Michael Engel

The Cartooning Genius of Ben Schultz

http://codeblue.umich.edu/hoomd-blue/

http://www.ks.uiuc.edu/Research/vmd/