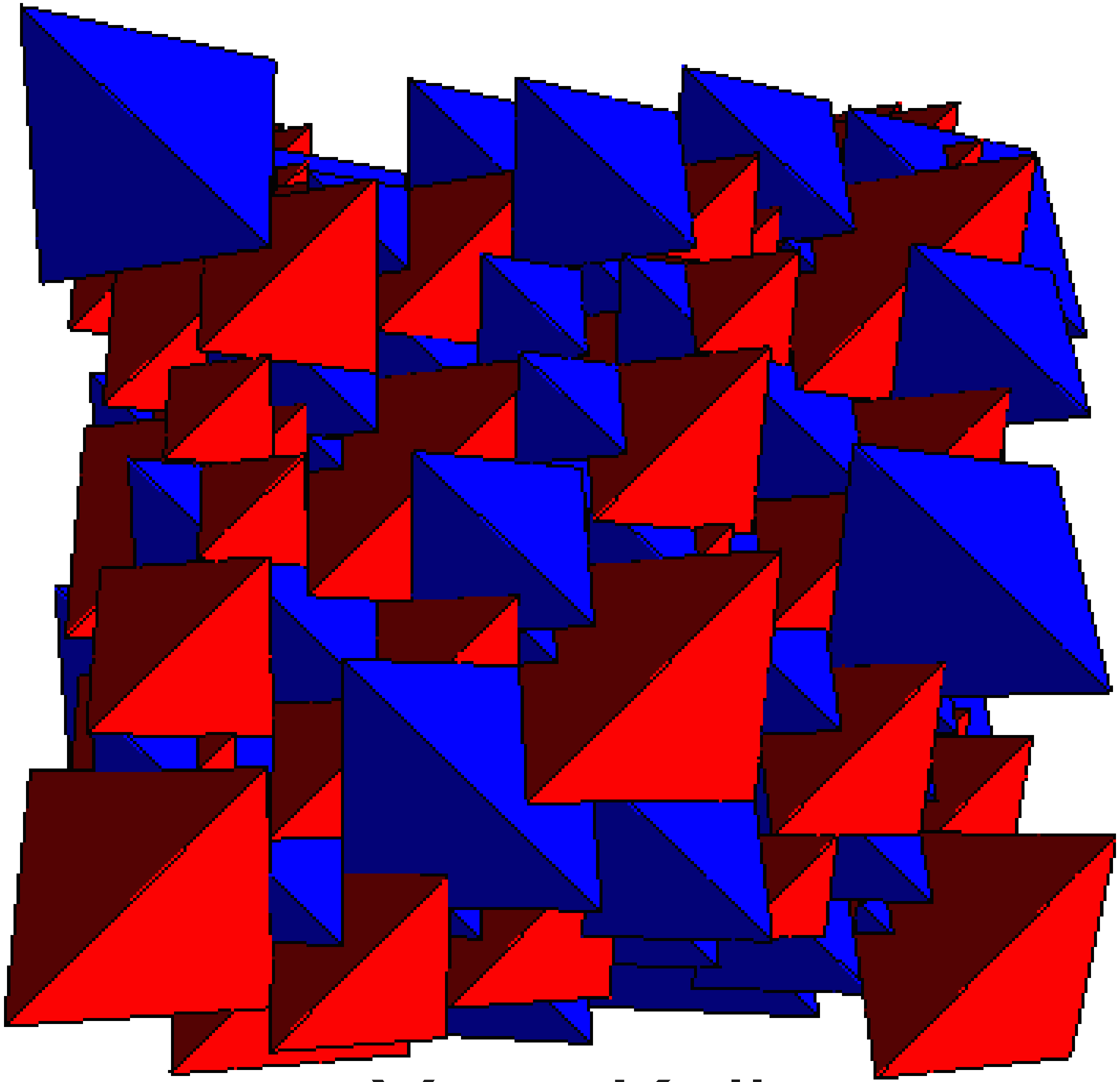
Tetrahedron Packing



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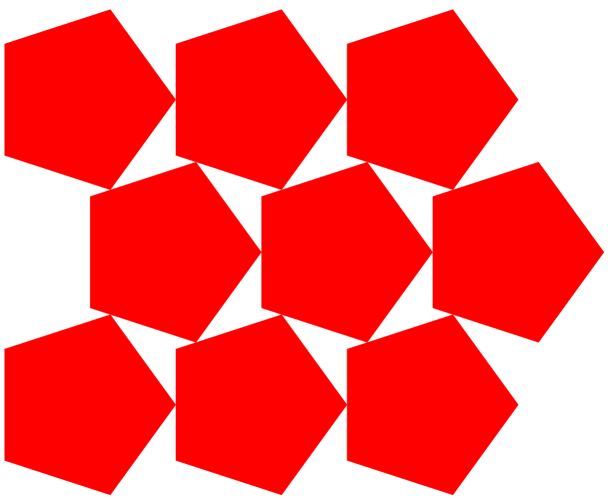
Geometry Seminar
Courant Institute
February 9, 2010

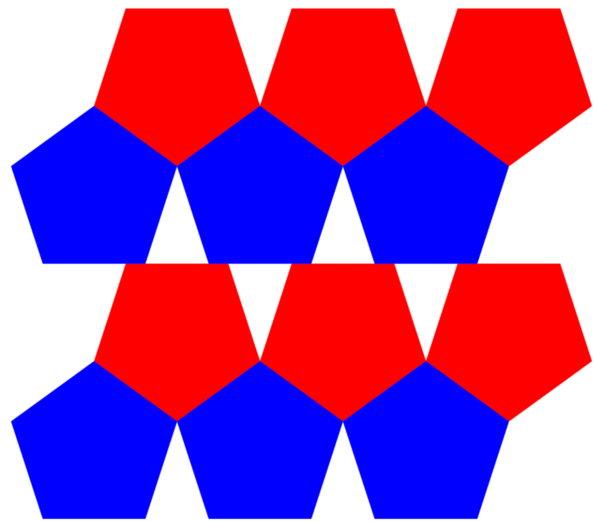
General packing problem

Let φ_{max} (K) be the highest achievable density for packings of convex d-dimensional body K.

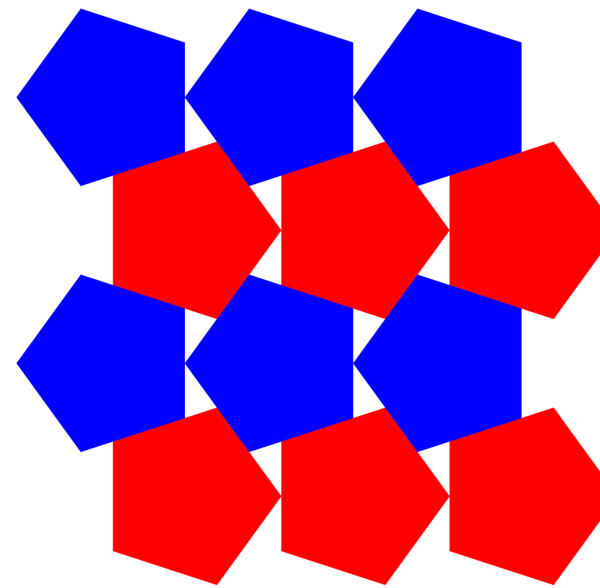
2D periodic examples:



$\varphi = 0.817$
N = 1



$\varphi = 0.854$
N = 2



$\varphi = 0.921$
N = 2

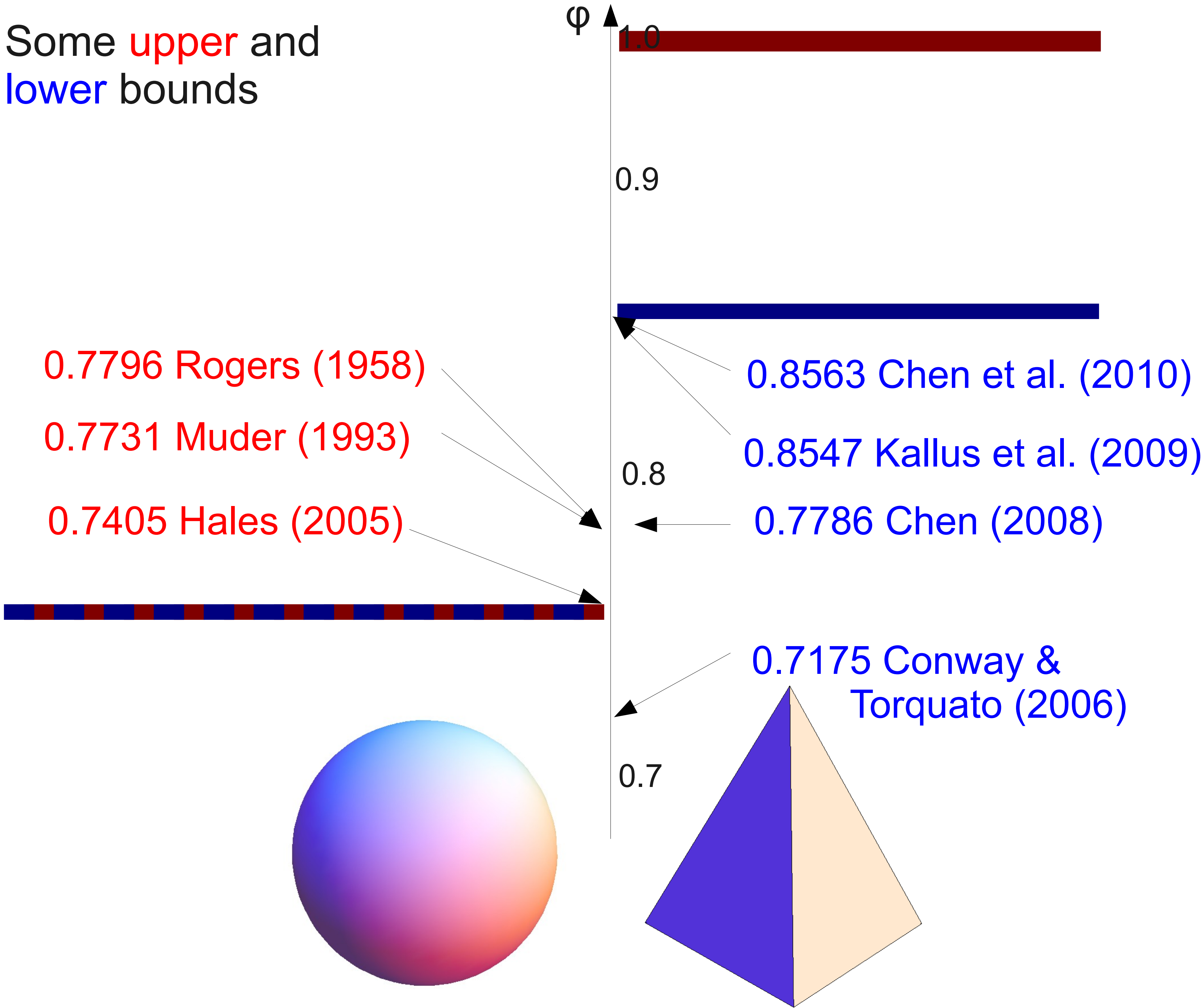
φ_{max} (K) for d > 2 known only for spheres, space-filling solids.

From Hilbert's 18th problem:

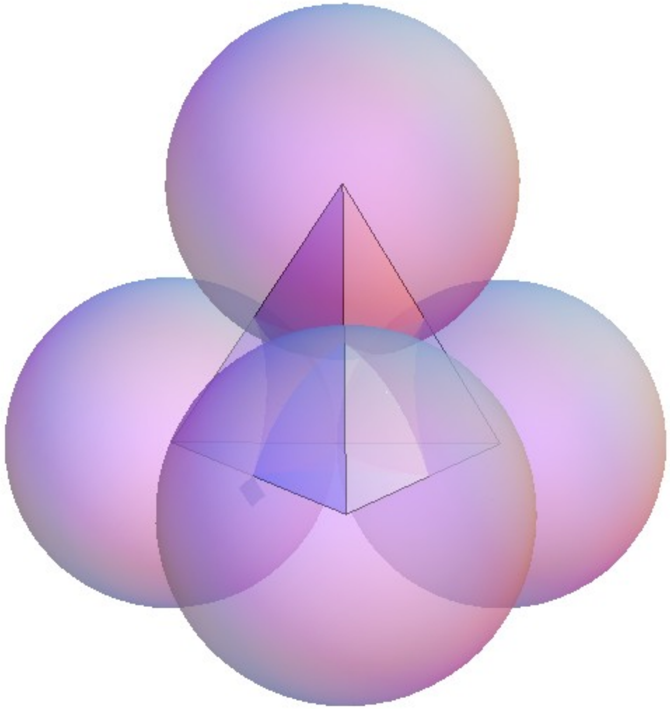
"How can one arrange most densely in space an infinite number of equal solids of a given form, e.g., ***spheres*** with given radii or ***regular tetrahedra*** with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as large as possible?"

David Hilbert
(1862-1943)

Some upper and lower bounds



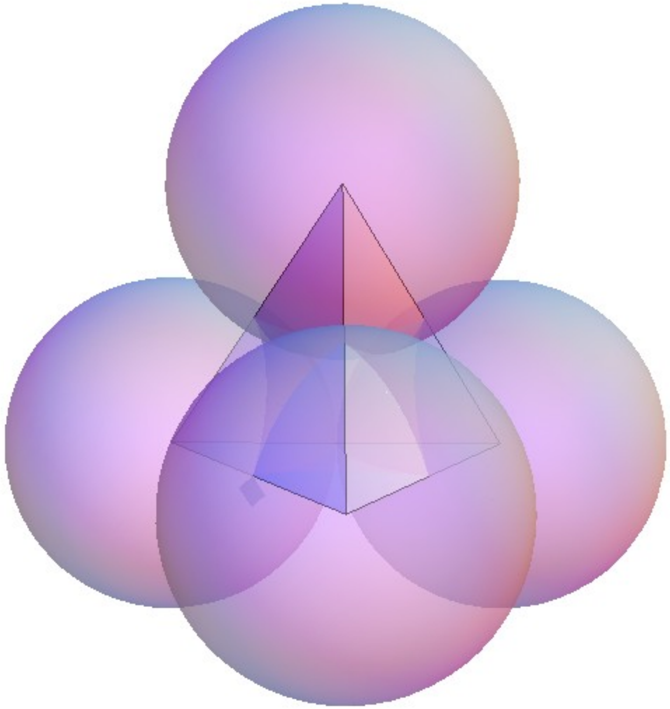
Rogers bound



$\varphi(B) \leq 0.7796$

Argument: the sphere cannot fill its Voronoi region, a polyhedron

Rogers bound



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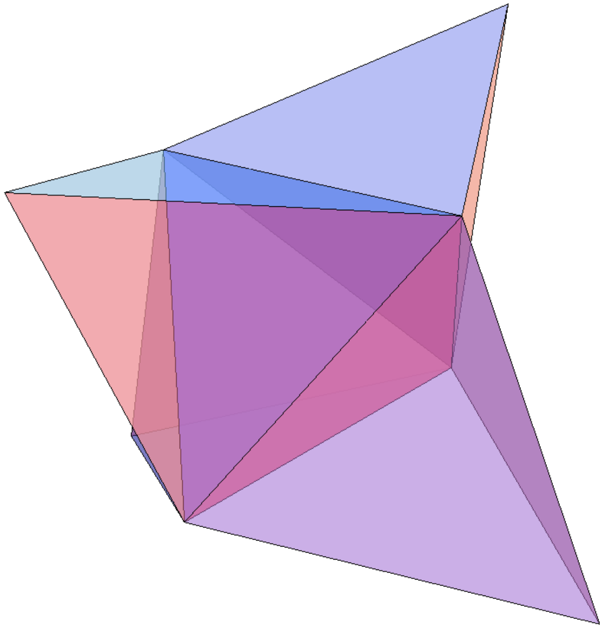
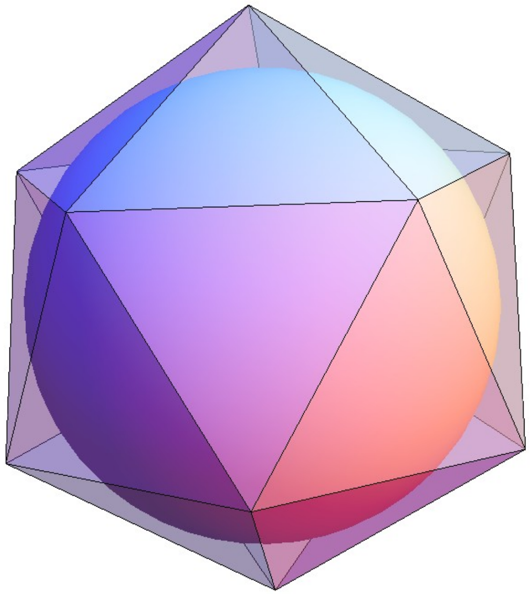


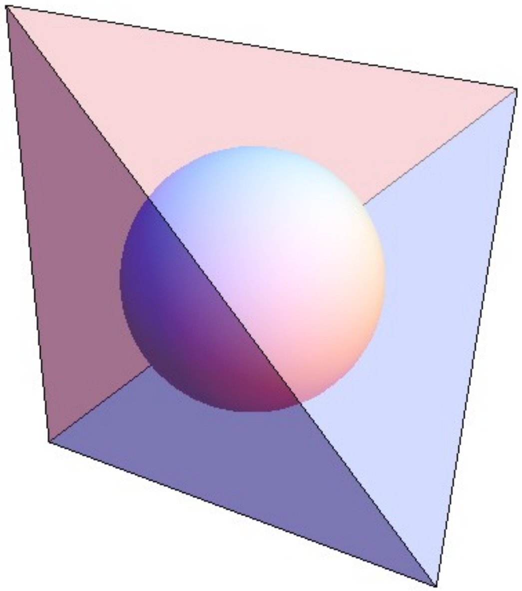
The tetrahedron can easily fill its Voronoi region

Bound from inscribed spheres



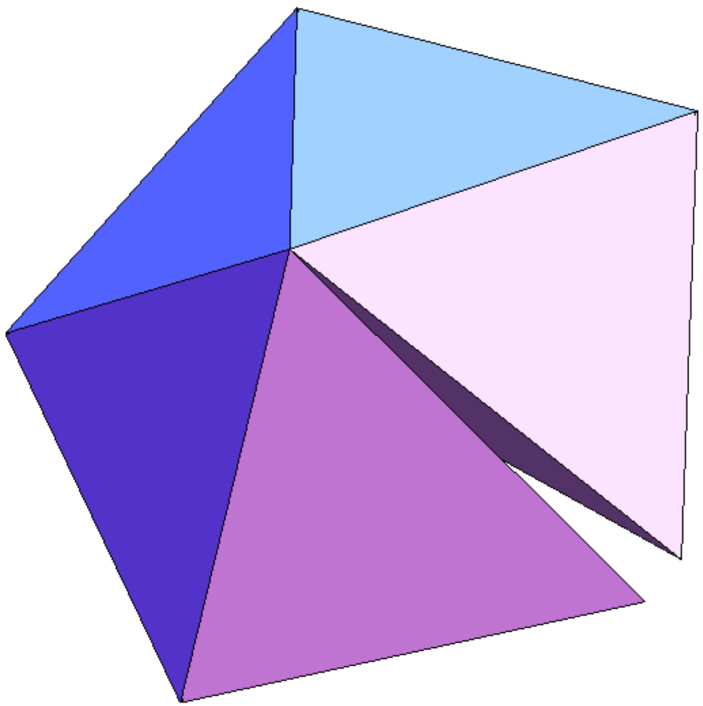
φ(I) ≤ 0.8934

Compare to lower bound: φ(I) ≥ 0.8364



φ(T) ≤ 2.449

Regular tetrahedra do not fill space



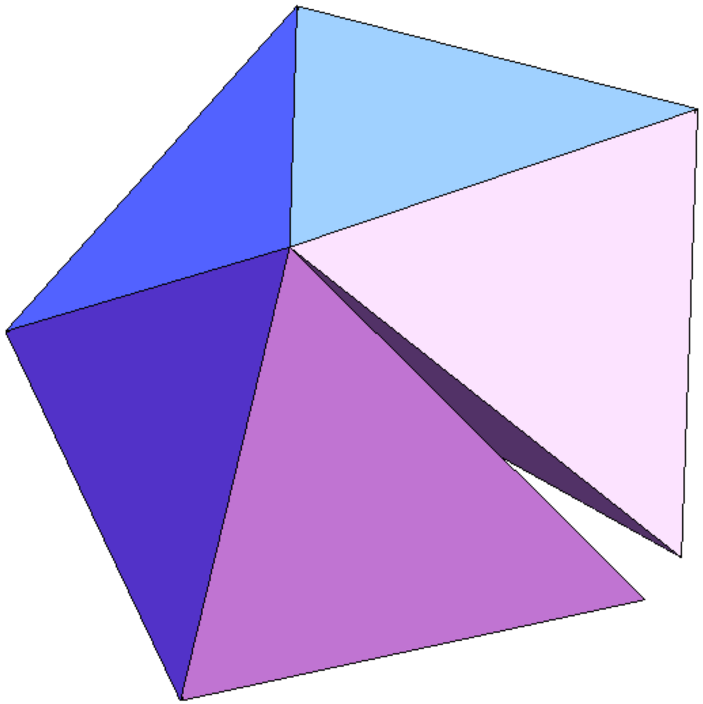
Missing angle: 7.4º

Therefore, $\varphi(T) < 1$

But can we find $\varphi^U < 1$ such that $\varphi(T) \leq \varphi^U$?

We believe we have come up with an argument giving the first non-trivial upper bound on the packing density of tetrahedra, but we feel kind of silly reporting it:

Regular tetrahedra do not fill space



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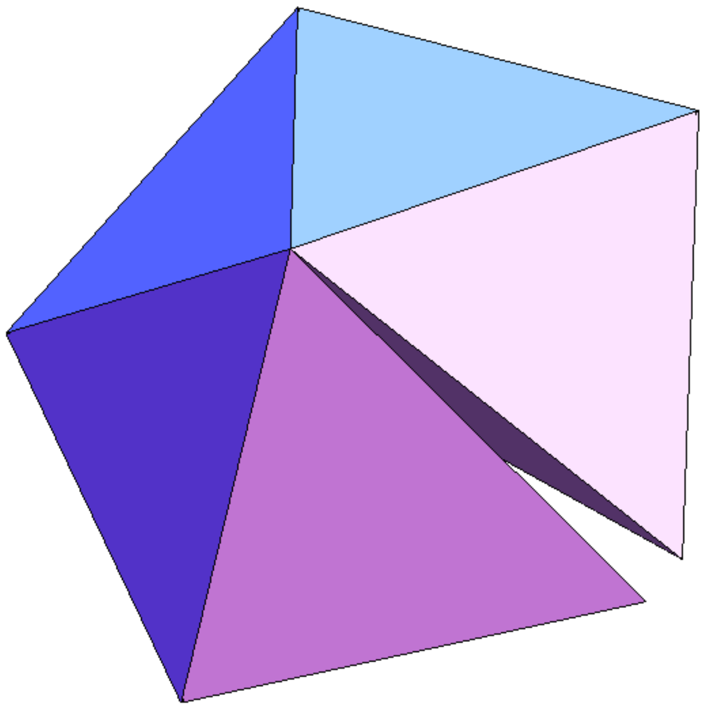
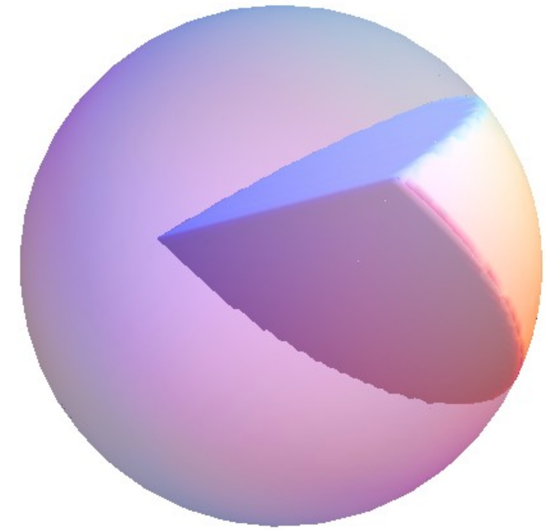
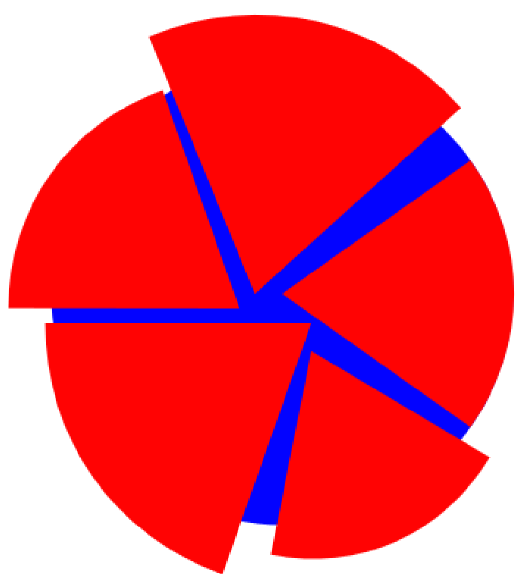
$$\varphi(T) \leq 1 - (2.6...) \times 10^{-28}$$

Bound from angle mismatch?

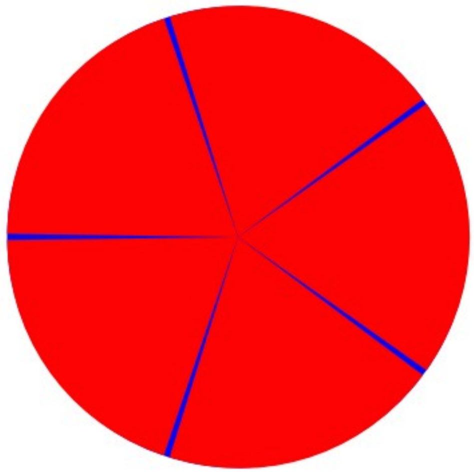




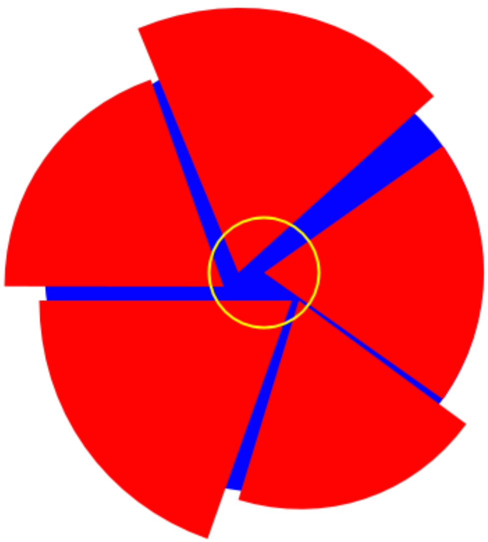
“Wedge”



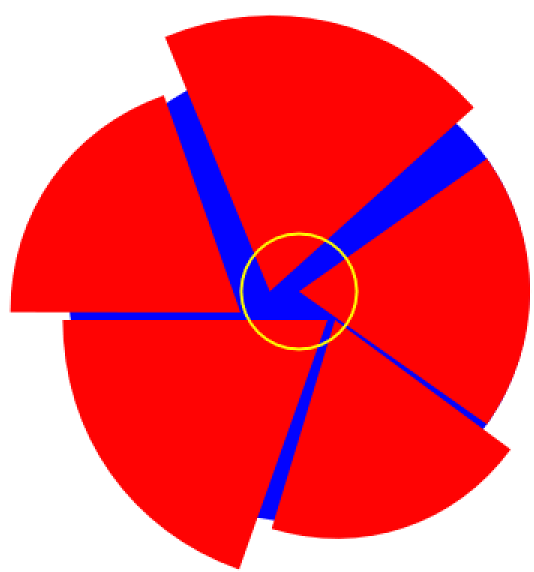
If we can put a lower bound the amount of uncovered space in a unit ball with five non-overlapping wedges, we can get a non-trivial upper bound on the density of a tetrahedron packing.



If all wedge edges pass through the center, we can easily calculate the uncovered volume. Unfortunately, this isn't given.



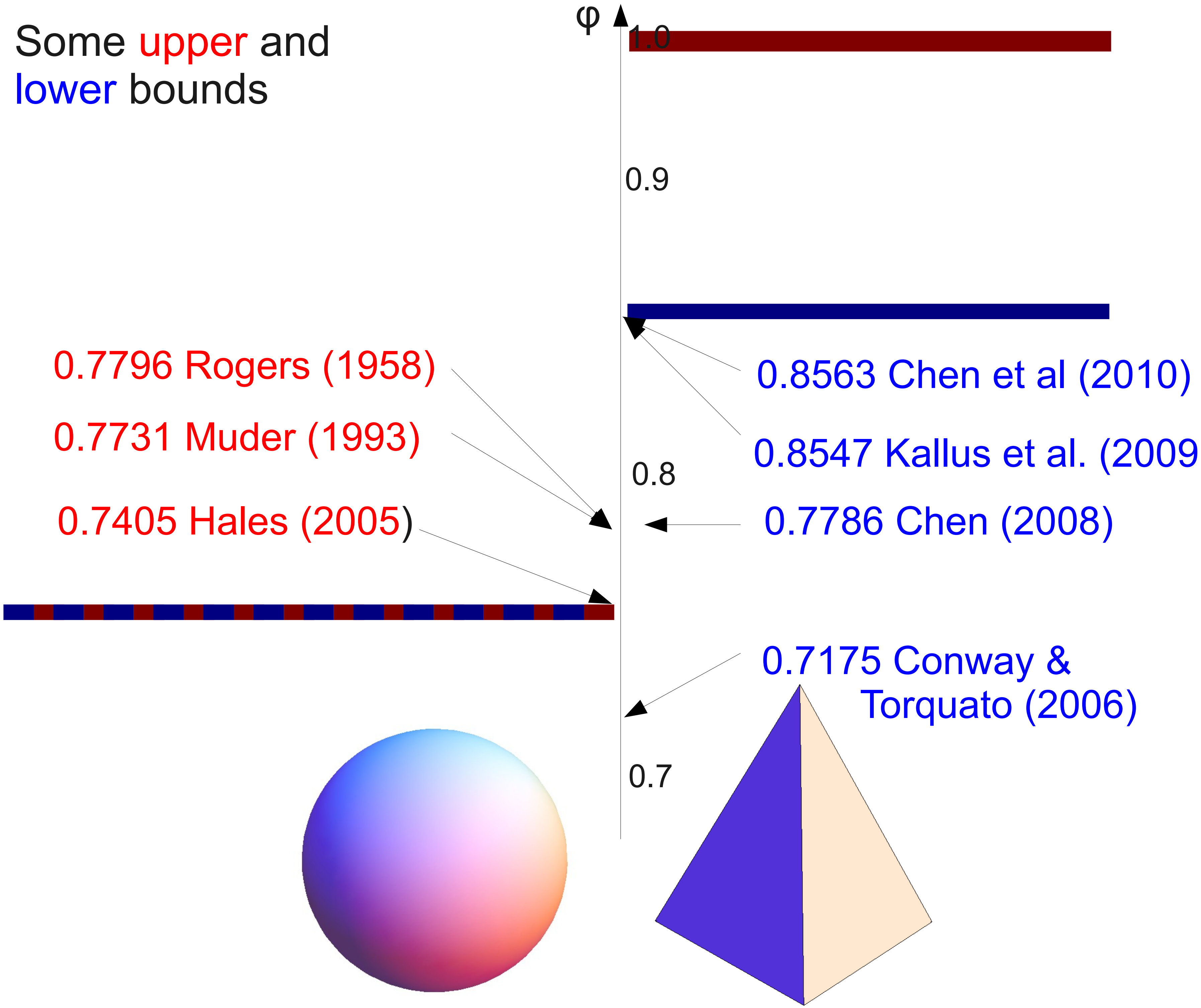
Still, if all wedge edges pass within a given distance of the center, we can still easily calculate a bound on the uncovered volume.



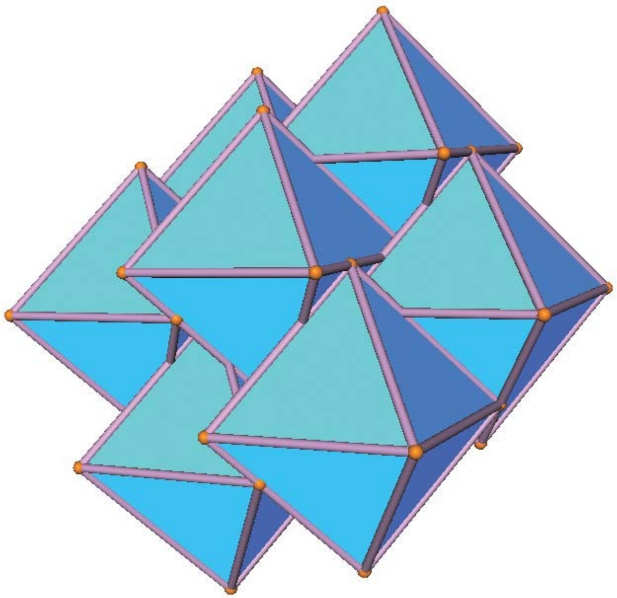
And if one or more edge wedges fall outside the yellow sphere, we are left with a simpler configuration inside the yellow sphere, and we can try to put a bound on the uncovered volume inside it.

By applying this argument iteratively, we get a bound on the unfilled space in the original sphere, but that bound is very small.

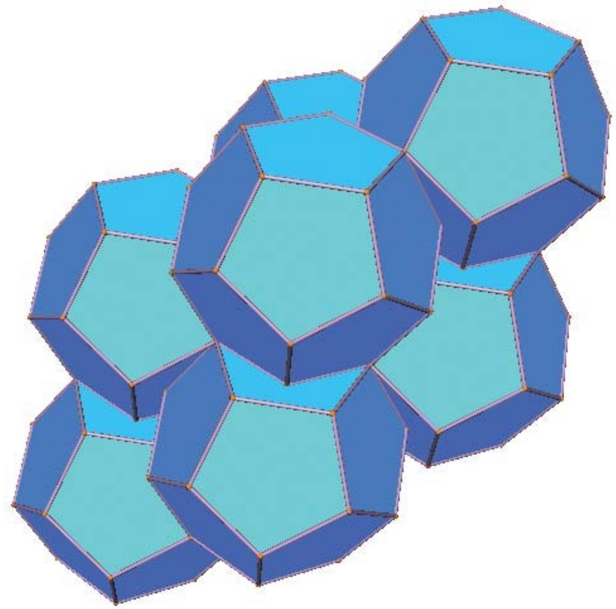
Some upper and lower bounds



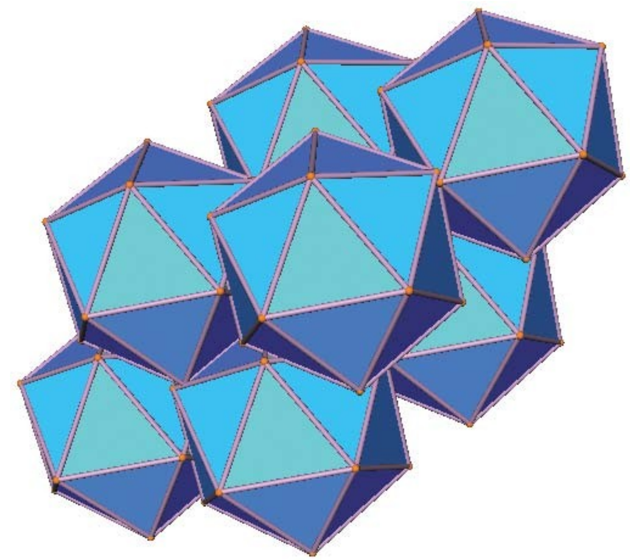
Densest known packings of the Platonic solids



$\varphi = 0.9474$



$\varphi = 0.9045$

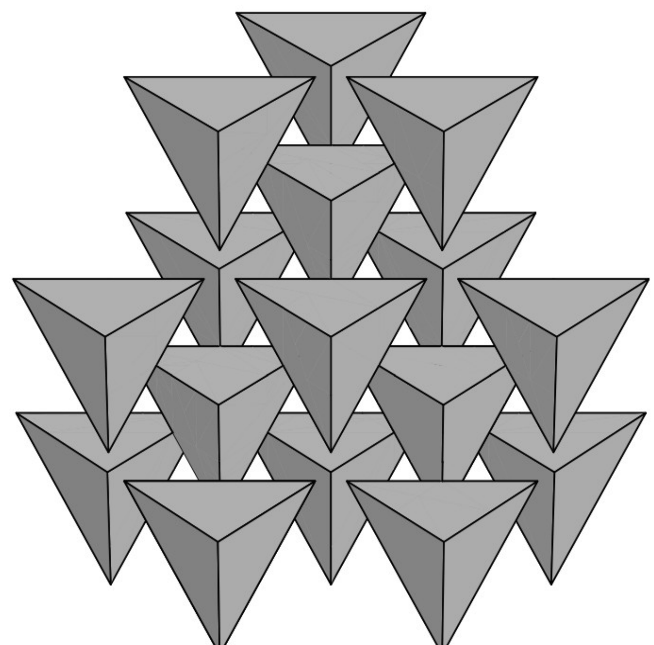


$\varphi = 0.8364$

All are lattice packings (N=1)

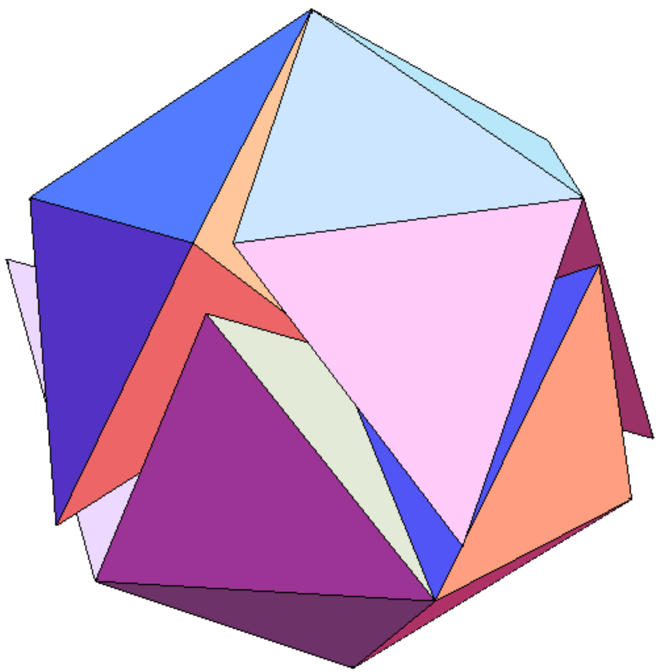
Compare with densest lattice packing of regular tetrahedra:

$\varphi = 0.3673$



Lower bounds (densest known packings)

1. Conway & Torquato (2006)



Icosahedral packing: $\varphi = 0.7166$

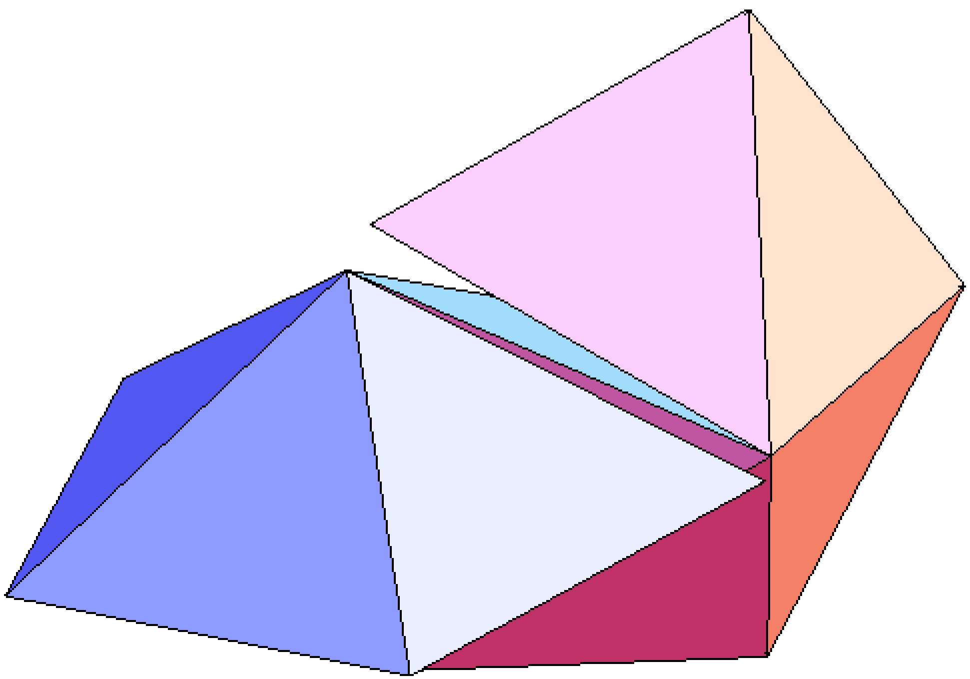
N=20

"Welsh" packing: $\varphi = 0.7175$

N=34

Densest known packings

2. Chen (2008)



“wagon wheels” packing: $\varphi = 0.7786$

N=18

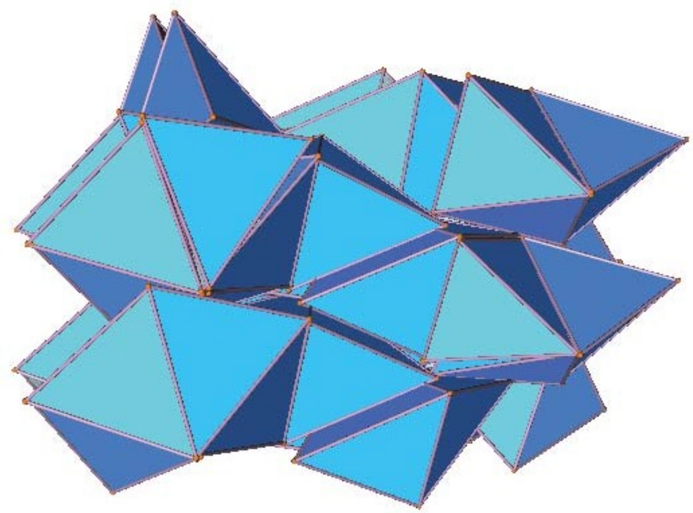
$\varphi > \varphi_{max}$ (B)

Densest known packings

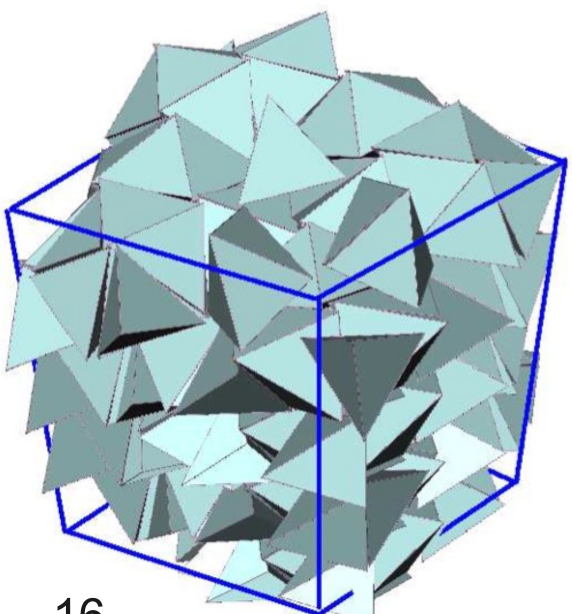
3. Torquato & Jiao (2009)

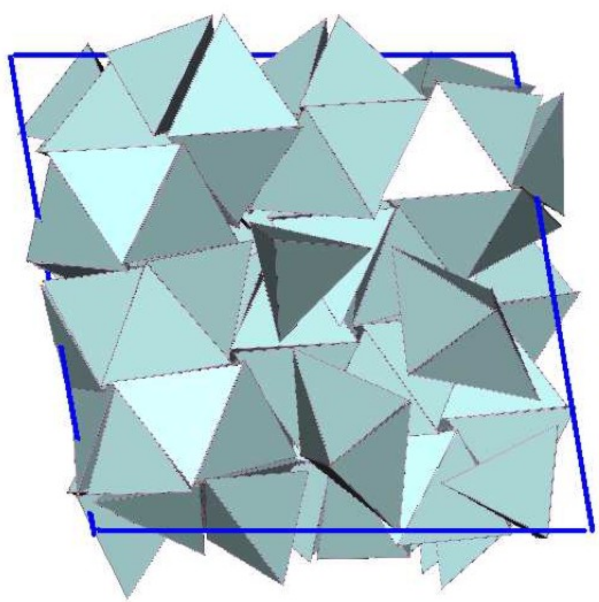
Challenge for numerical search: highly frustrated optimization problem

Search often got stuck at local optima



φ = 0.7820 (April)
N = 72



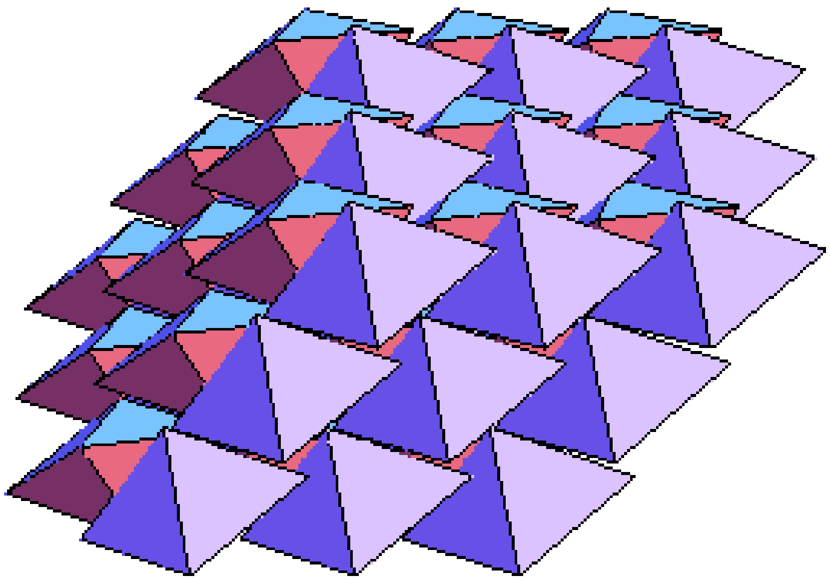


φ = 0.8226 (July)
N = 314

Densest known packings

4. Kallus et al. (2009)

Method: “divide and concur”, designed for highly frustrated problems



$\varphi = 0.8547$
$N = 4$ (!)

All tetrahedra equivalent
(tetrahedron-transitive packing)

5. Chen et al. (2010)

Slight analytical improvement to the above structure: $\varphi = 0.8563$
(New, denser, packing is no longer tetrahedron-transitive)

Dimer double lattice

G. Kuperberg & W. Kuperberg (1990):
Any convex planar body can be packed with density at least .866 by a double lattice.

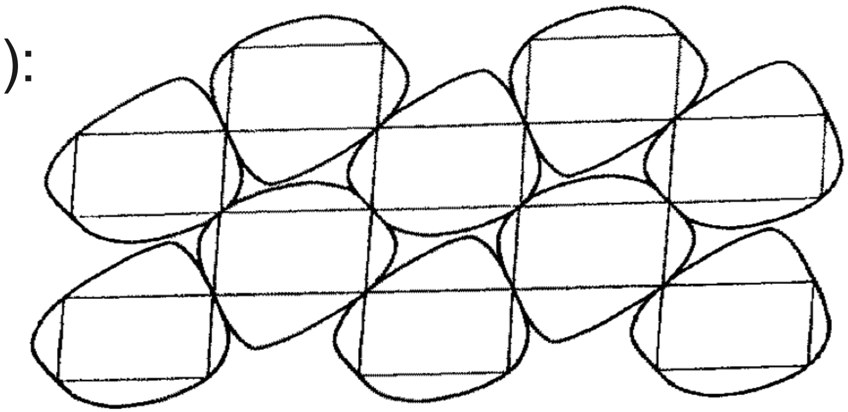
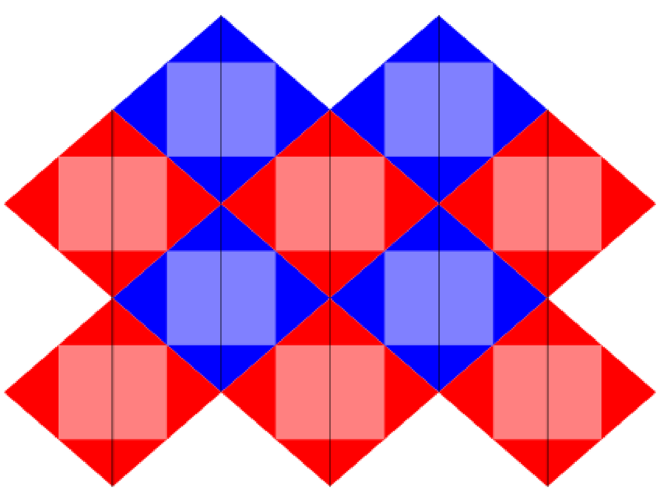
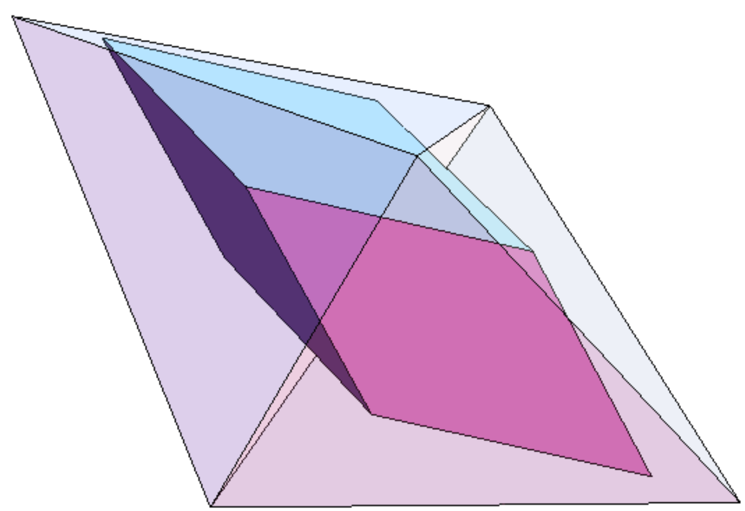


Fig. 4. **Double-lattice packing generated by an extensive parallelogram.**

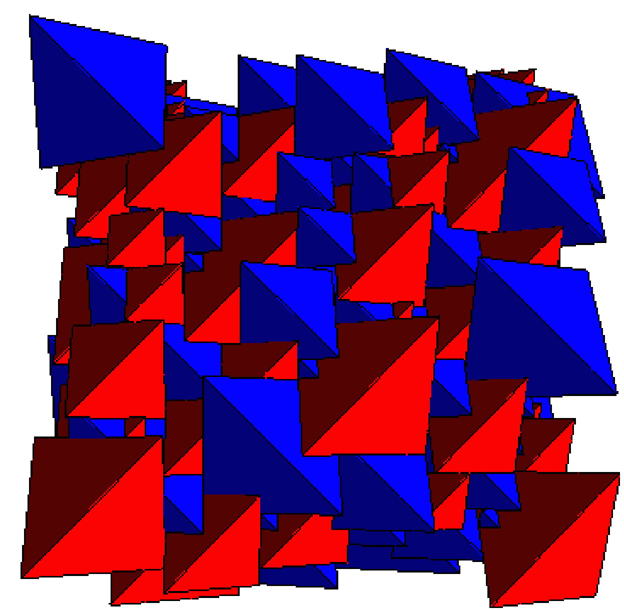
2D



3D



4D?



Hard Tetrahedron Fluid

Large system of hard tetrahedra defined by the thermodynamic ensemble:

$$\text{Prob.} \sim \exp(-P\,V / k_B T)$$

Densest packing corresponds to ground state ($k_B T / P = 0$).

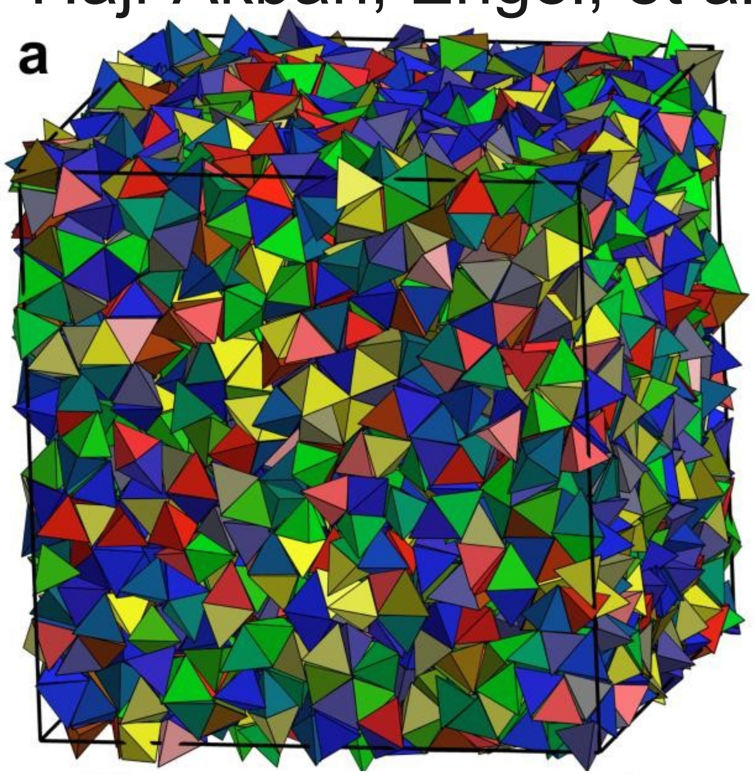
Ordering transitions in hard particle systems:

e.g. spheres: fluid → crystal
cylinders: fluid → nematic → crystal

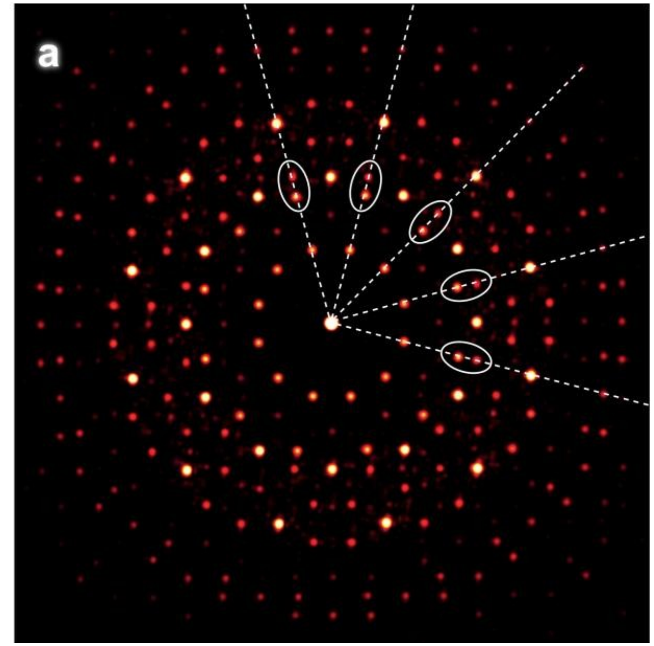
Kolafa & Nezbeda (1994): “there may be a close similarity between the structural properties of the hard tetrahedron fluid and another 'anomalous' fluid, namely, water”

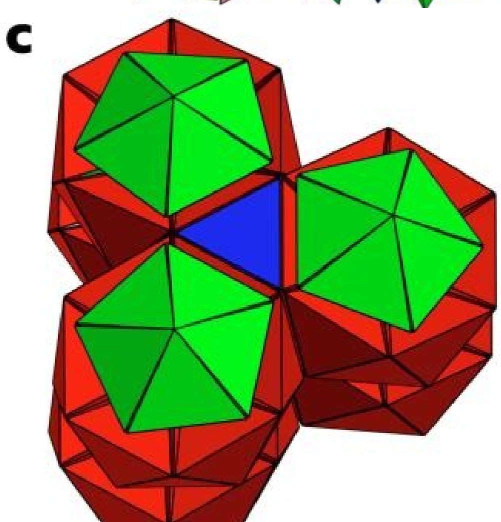
Hard Tetrahedron Fluid – quasicrystal transition

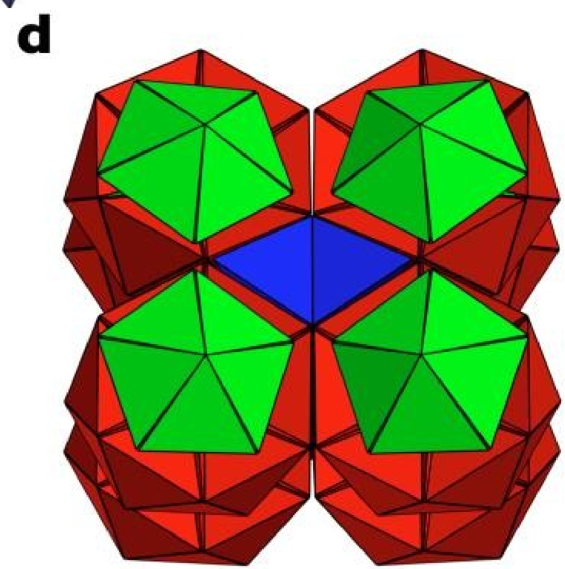
Haji-Akbari, Engel, et al. (2009)

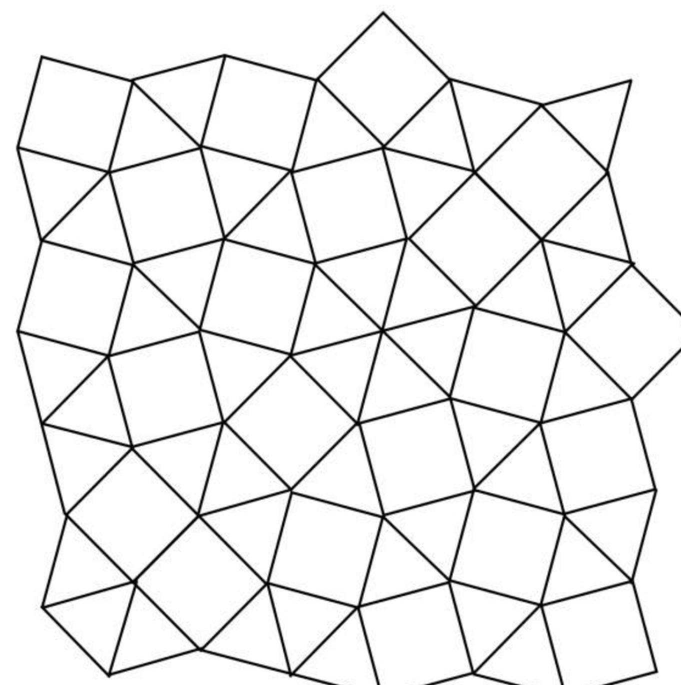


$\varphi = 0.8503$









Hard Tetrahedron Fluid – quasicrytal transition

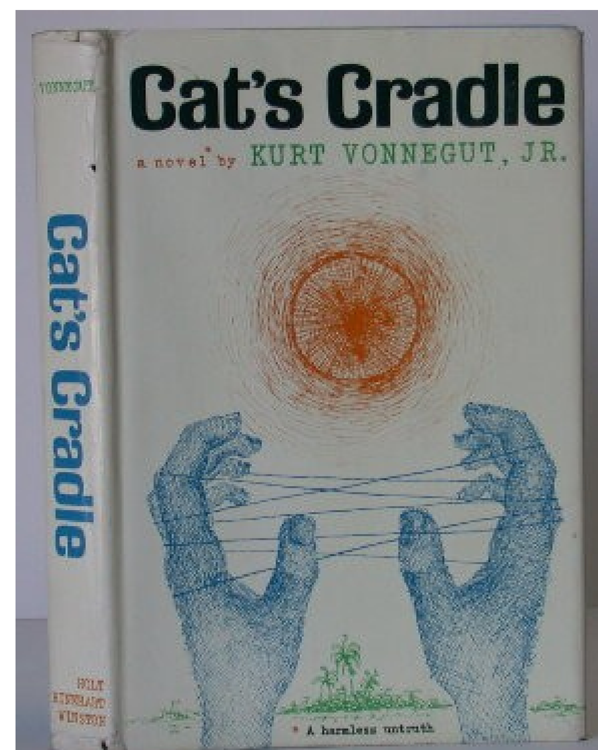
Why doesn't the hard tetrahedron fluid form the dimer double lattice crystal under pressure?

- The tetrahedra know something we don't

  i.e. there is a yet undiscovered quasicrystalline packing denser than the crystal packing

- We know something that the tetrahedra don't

  An “ice-nine” hard tetrahedron phase?



Summary:

• Tight upper bound is hard to achieve.

• Dense packings (lower bounds) are hard to search for, due to a “rugged” optimization landscape.

• Hard tetrahedron fluid exhibits unexpected and anomalous behavior.