Packing tetrahedra and other figures using *Divide and Concur*

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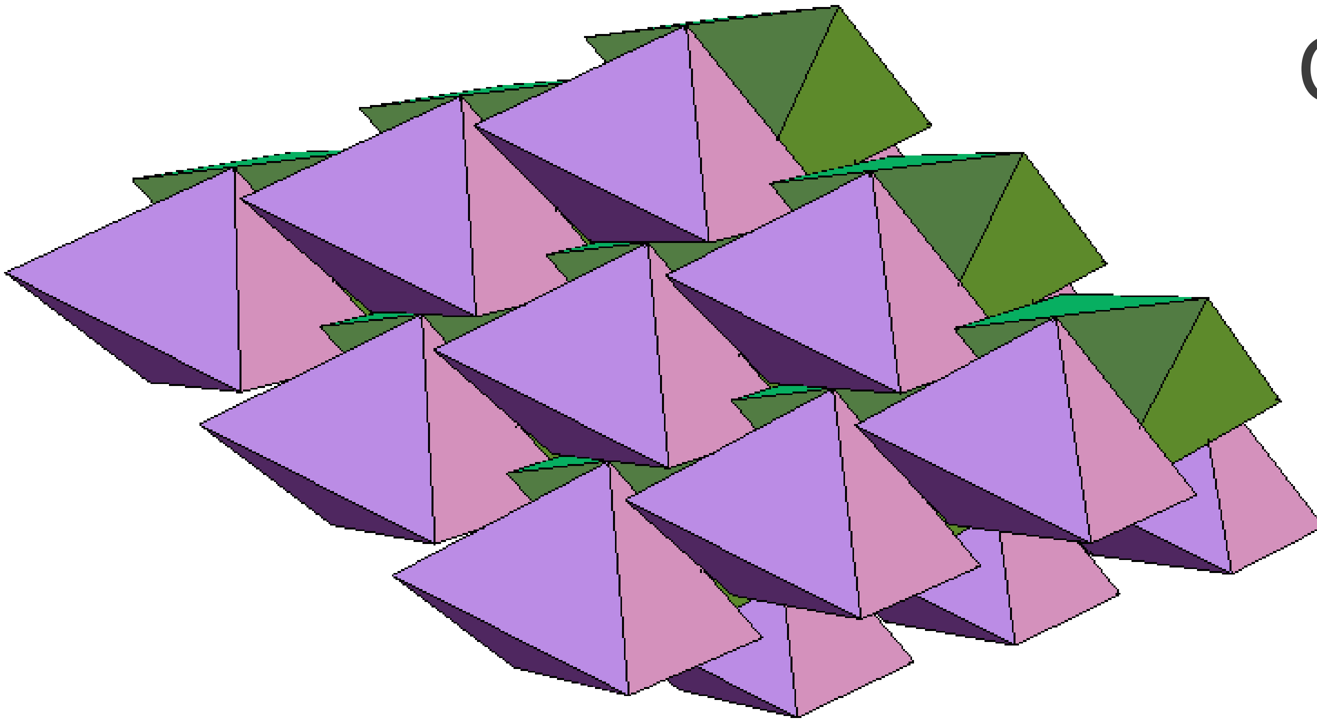
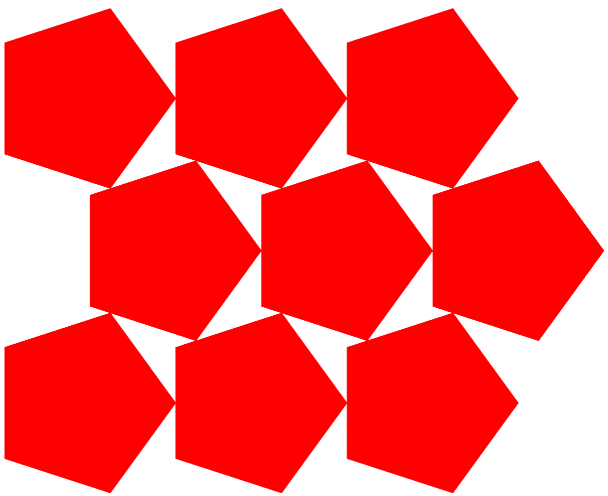


Widely applied math seminar
Harvard University
Nov. 1, 2010

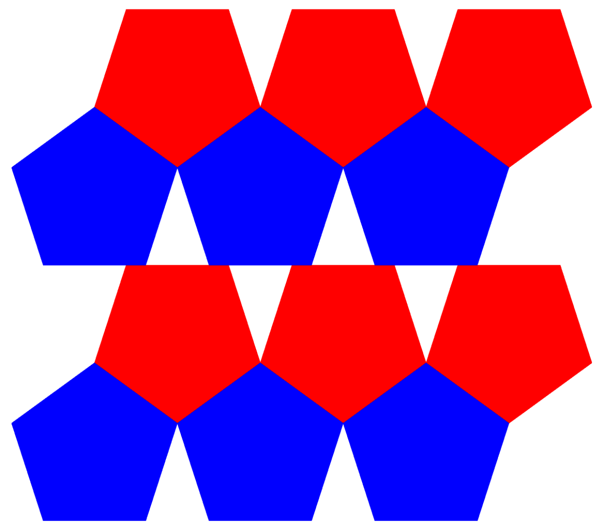
General packing problem

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

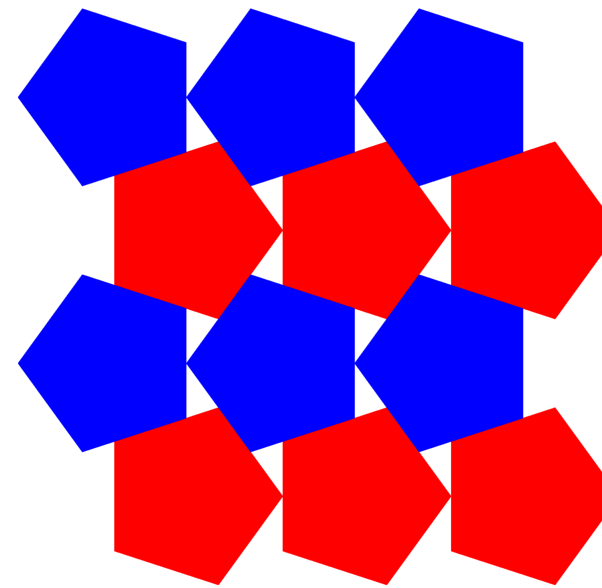
2D periodic examples:



$\varphi = 0.817$
N = 1



$\varphi = 0.854$
N = 2



$\varphi = 0.921$
N = 2

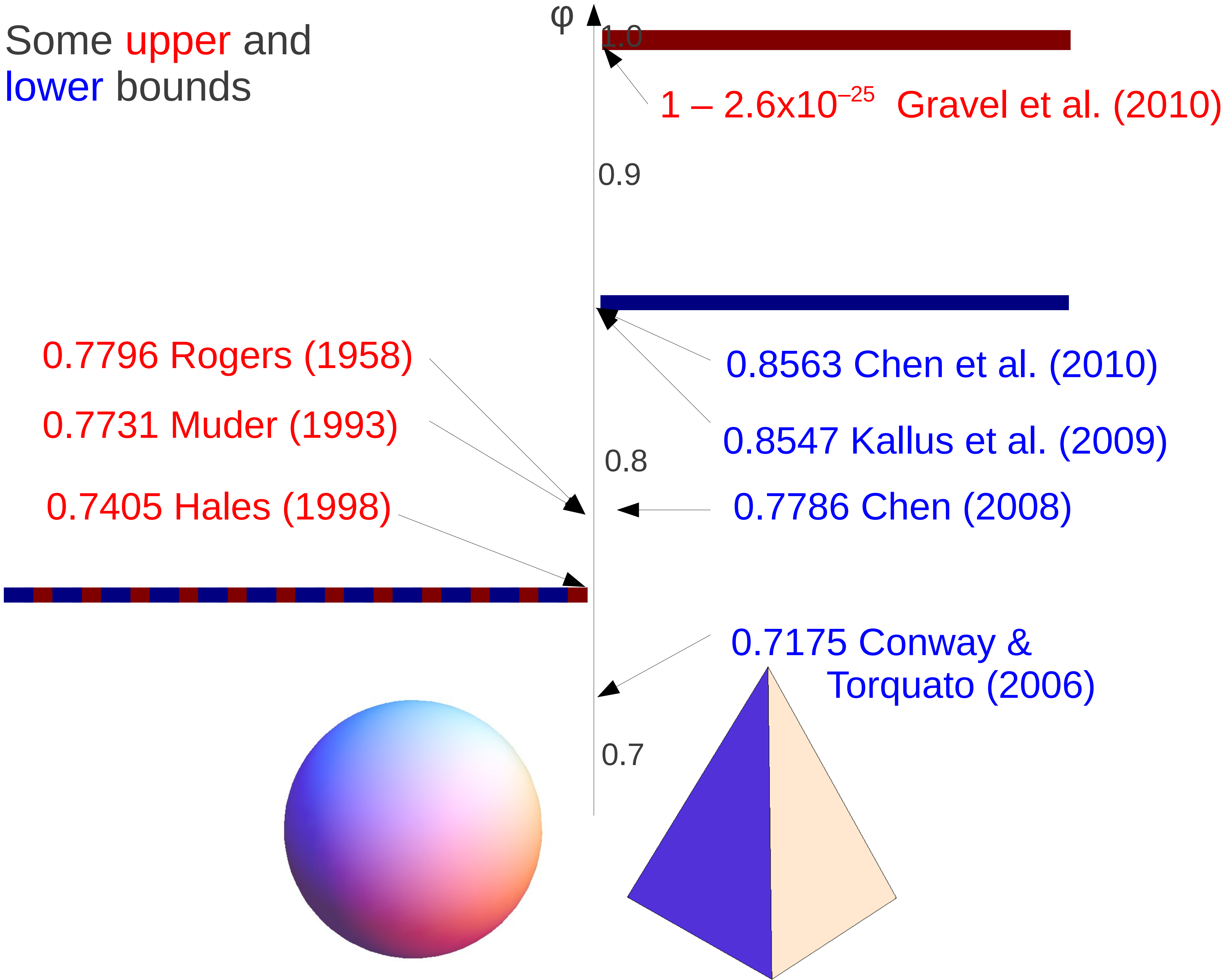
$\varphi_{max}(K)$ for d > 2 known only for spheres, space-filling solids.

From Hilbert's 18th problem:

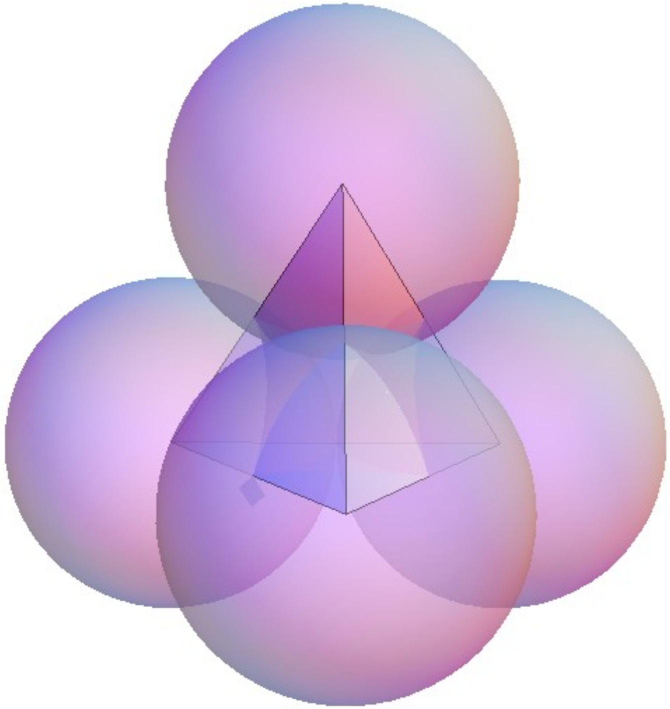
"How can one arrange most densely in space an infinite number of equal solids of a given form, e.g., ***spheres*** with given radii or ***regular tetrahedra*** with given edges (or in prescribed position), that is, how can one so fit them together that the ratio of the filled to the unfilled space may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

David Hilbert
(1862-1943)

Some upper and lower bounds



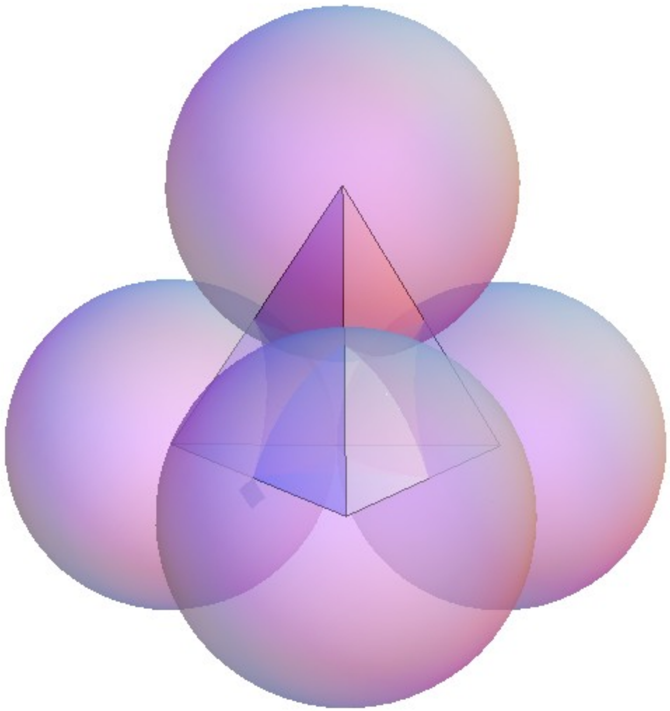
Rogers bound



$\varphi(B) \leq 0.7796$

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

Rogers bound



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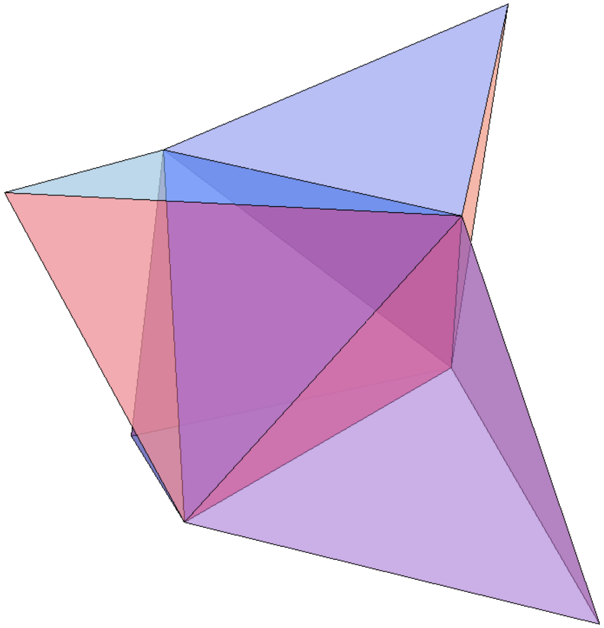
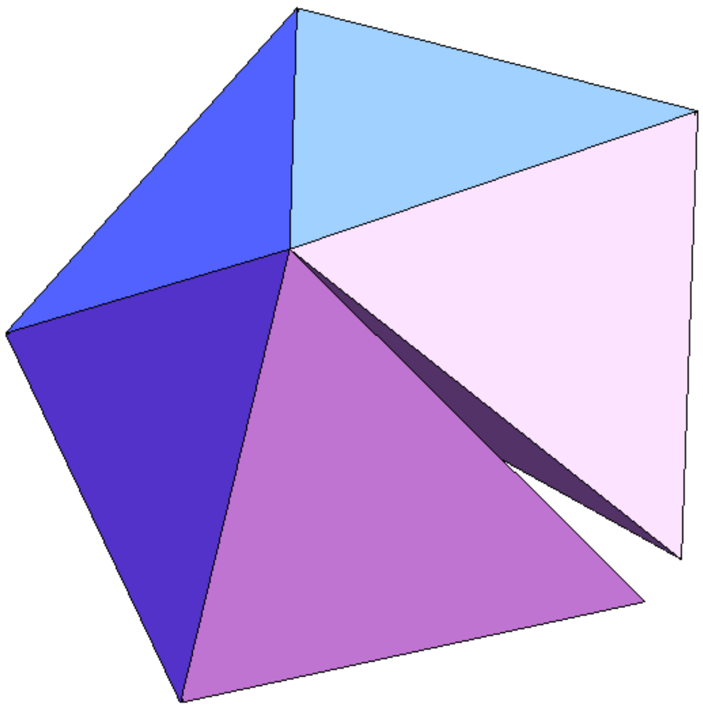


The tetrahedron can easily fill its Voronoi region

Regular tetrahedra do not fill space



Missing angle: 7.4º

Therefore, $\varphi(T) < 1$

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

Tetrahedron packing upper bound

Optimization challenge:

1. Prove $\varphi \leq 1 - \varepsilon$, where $\varepsilon > 0$
2. Maximize ε

Tetrahedron packing upper bound

Optimization challenge:

1. Prove $\varphi \leq 1 - \varepsilon$, where $\varepsilon > 0$

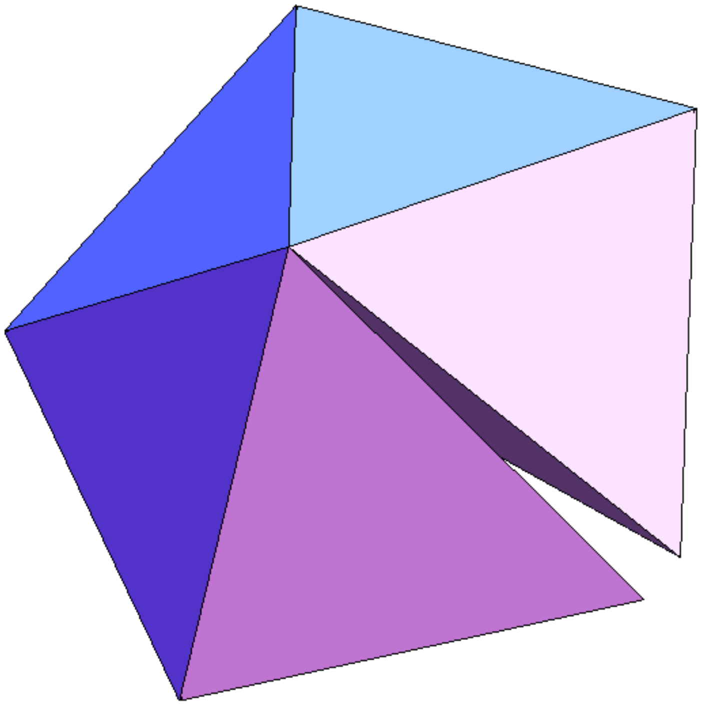
~~2. Maximize ε~~

2'. Minimize length of proof

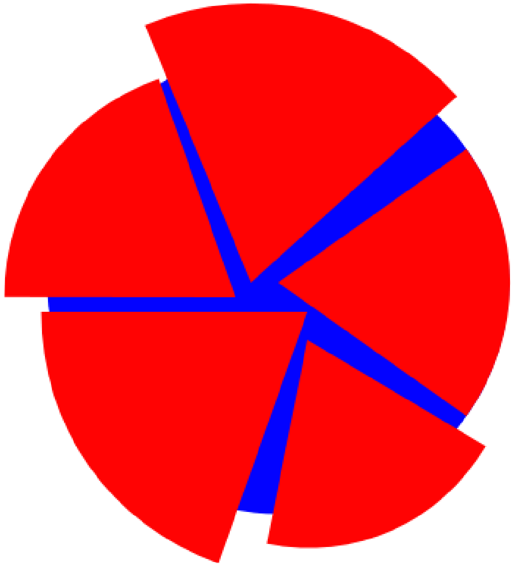
Solution: $\varepsilon = 2.6... \times 10^{-25}$ (15 pages)

Gravel, Elser, & Kallus, Discrete and Computational Geometry (2010)

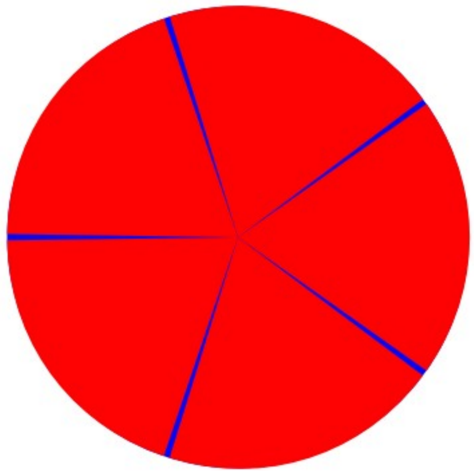
Bound from angle mismatch



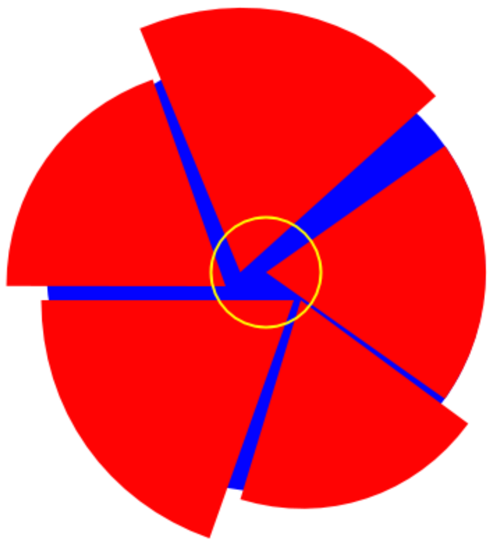
“Wedge”



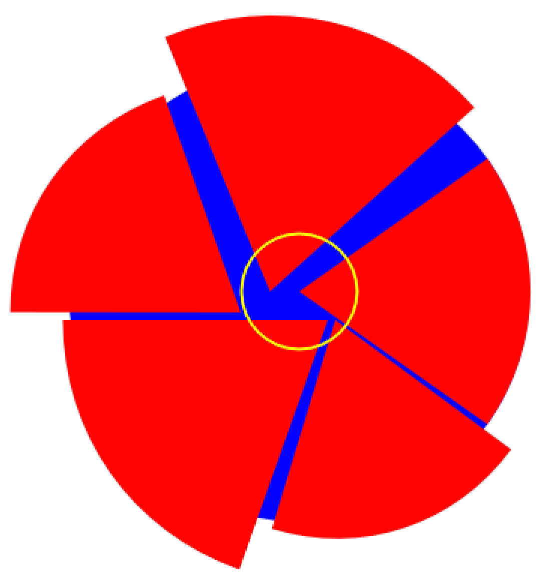
If we can put a lower bound the amount of uncovered space in a unit ball with five non-overlapping wedges, we can get a non-trivial upper bound on the density of a tetrahedron packing.



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



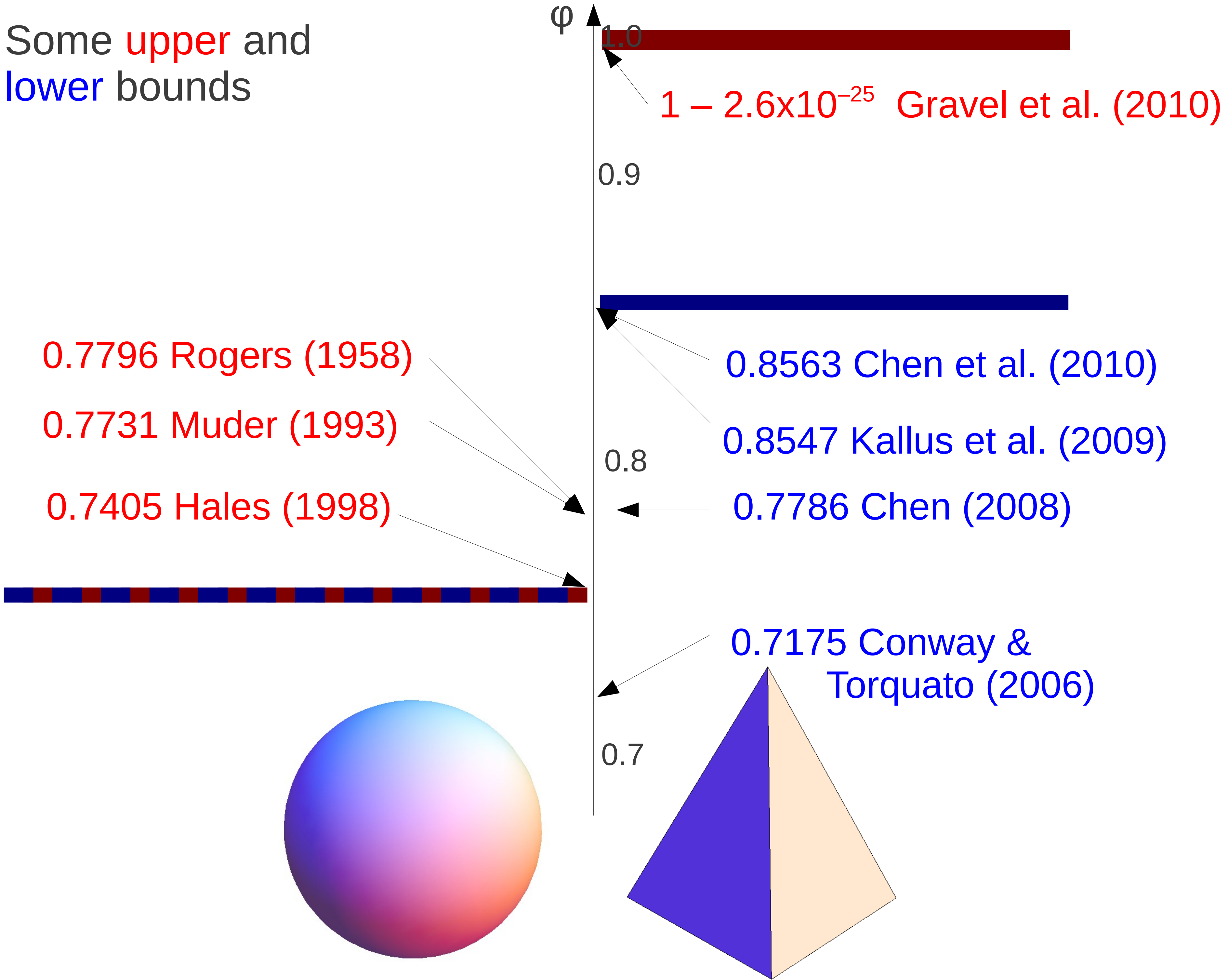
Still, if all wedge edges pass within a given distance of the center, we can still easily calculate a bound on the uncovered volume.



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.

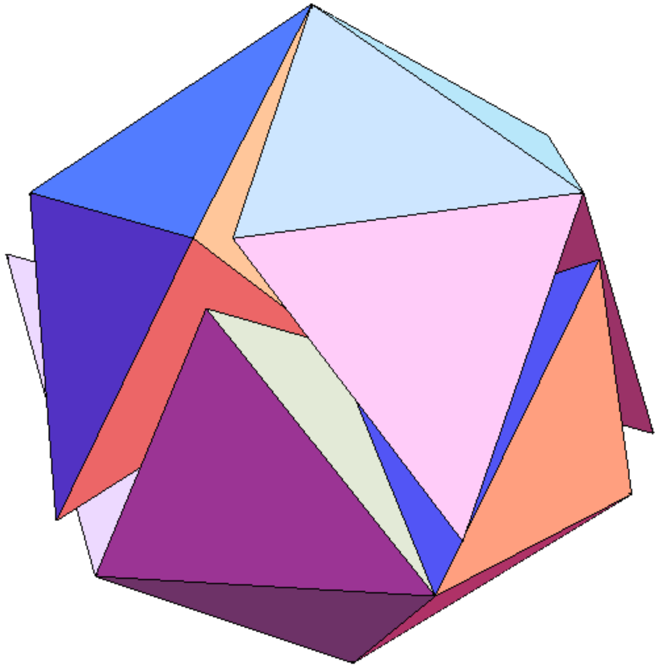
By applying this argument iteratively: $\varphi(T) \leq 1 - (2.6\ldots) \times 10^{-25}$

Some upper and lower bounds



Lower bounds (densest known packings)

1. Conway & Torquato (2006)



Icosahedral packing: $\varphi = 0.7166$

N=20

“Welsh” packing: $\varphi = 0.7175$

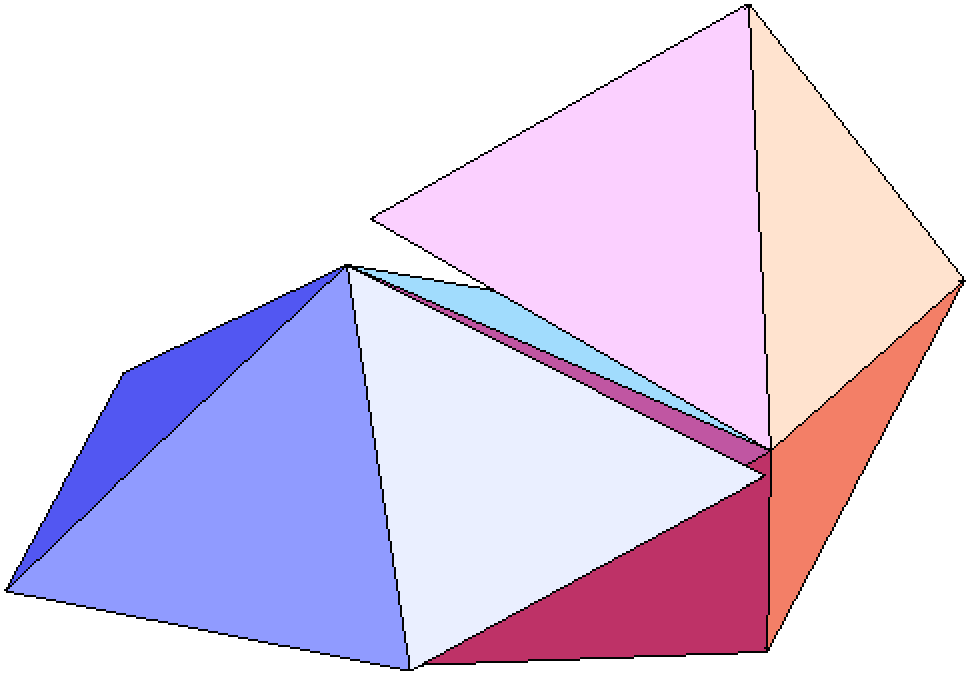
N=34

Conjecture: $\varphi_{max}(T) < \varphi_{max}(B)$

PNAS (2006)

Densest known packings

2. Chen (2008)



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

N=18

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

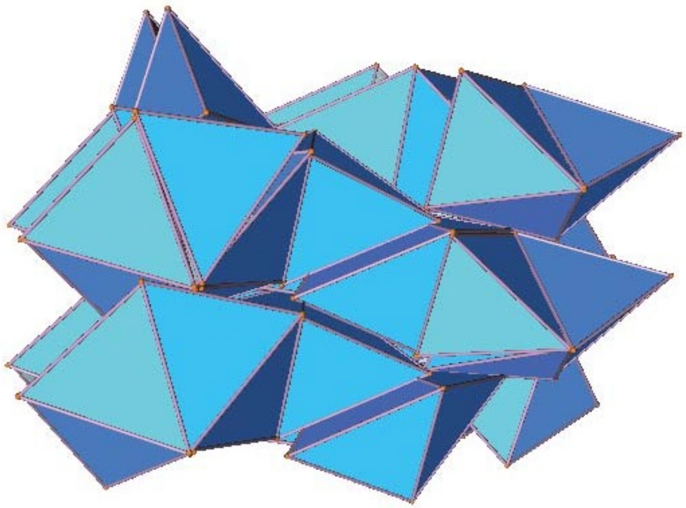
Discrete & Compu. Geom. (2008)

Densest known packings

3. Torquato & Jiao (2009)

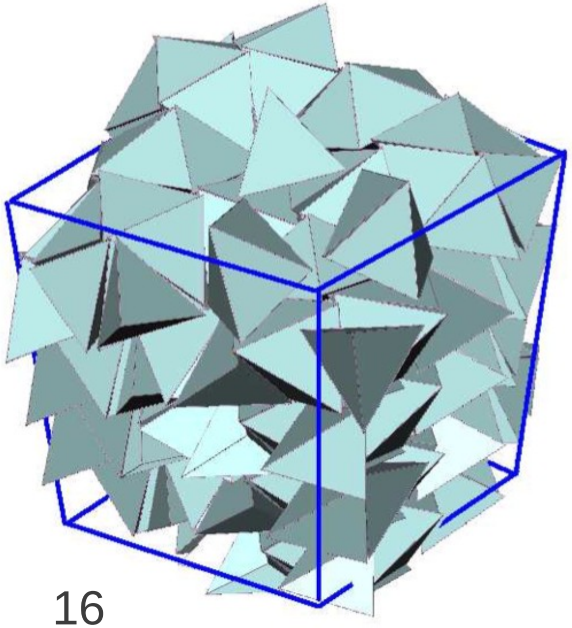
Challenge for numerical search: highly frustrated optimization problem

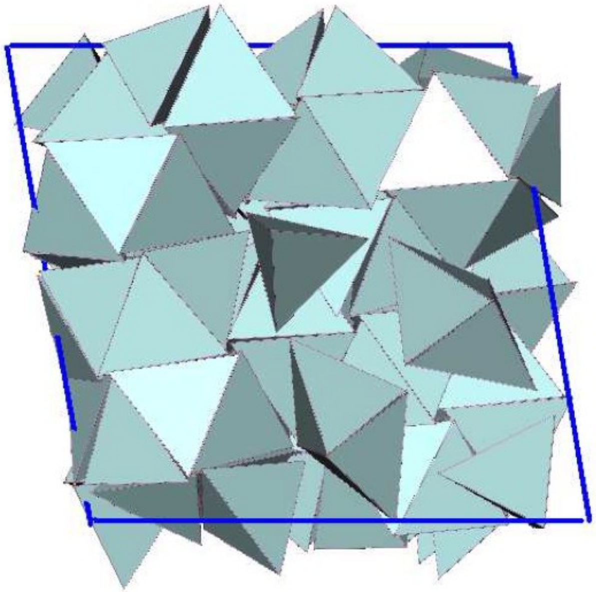
Search often got stuck at local optima



φ = 0.7820
N = 72

Nature (2009)





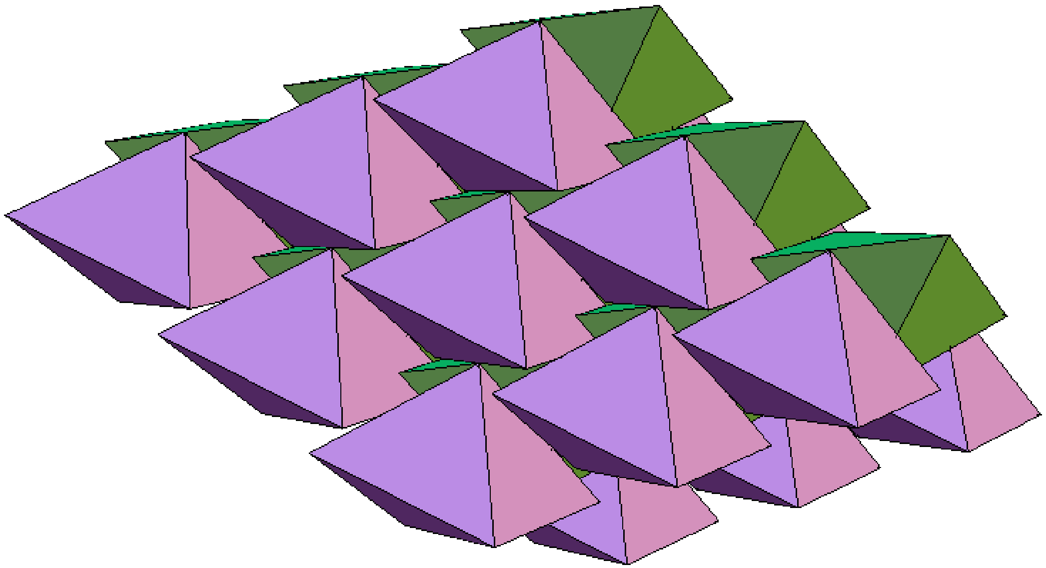
φ = 0.8226
N = 314

Phys. Rev. E (2009)

Densest known packings

4. Kallus et al. (2009)

Method: “divide and concur”



φ = 0.8547
N = 4 (!)

All tetrahedra equivalent
(tetrahedron-transitive packing)

Discrete & Compu. Geom. (2010)

5. Chen et al. (2010)

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

Discrete & Compu. Geom. (2010)

Computational approach to packing problems:

Optimization: given a collection of figures, arrange them without overlaps as densely as possible.

Feasibility: find an arrangement of density > φ

Possible approaches:

- Complete algorithm
- Specialized incomplete (heuristic) algorithm
- General purpose incomplete algorithm

  e.g.: simulated annealing, genetic algorithms, etc.

Divide and Concur belongs to the last category

Two constraint feasibility

$$x \in A \cap B$$

Example:

A = permutations of "`acgiknp`"

B = 7-letter English words

Two constraint feasibility

$$x \in A \cap B$$

Example:

A = permutations of "`acgiknp`"

B = 7-letter English words

x = "`packing`"

More structure

A, B are sets in a Euclidean configuration space Ω

simple constraints:
easy, efficient **projections** to A, B

$$P_A(x) = y \in A \quad \text{s.t.} \quad ||x - y|| \text{ is minimized}$$

Brief (incomplete) history of

$$x_{i+1} = x_i + P_B(2P_A(x_i) - x_i) - P_A(x_i)$$

J. Douglas and H. H. Rachford, *On the numerical solution of heat conduction problems in two or three space variables*, Trans. Am. Math. Soc. 82 (1956), 421–439.

splitting scheme for numerical PDE solutions

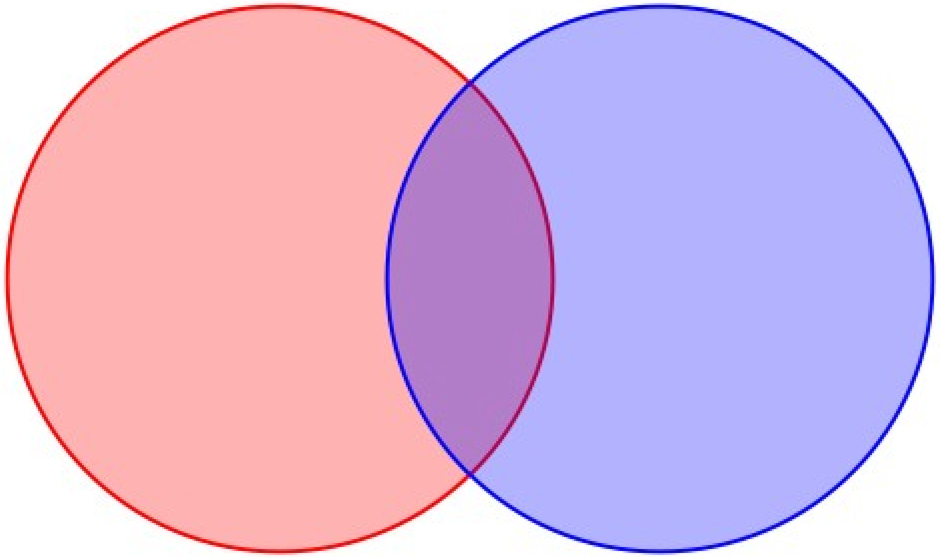
J.R. Fienup, Phase retrieval algorithms: a comparison, Applied Optics 21 (1982), 2758-2769.

rediscovery, control theory motivation, phase retrieval

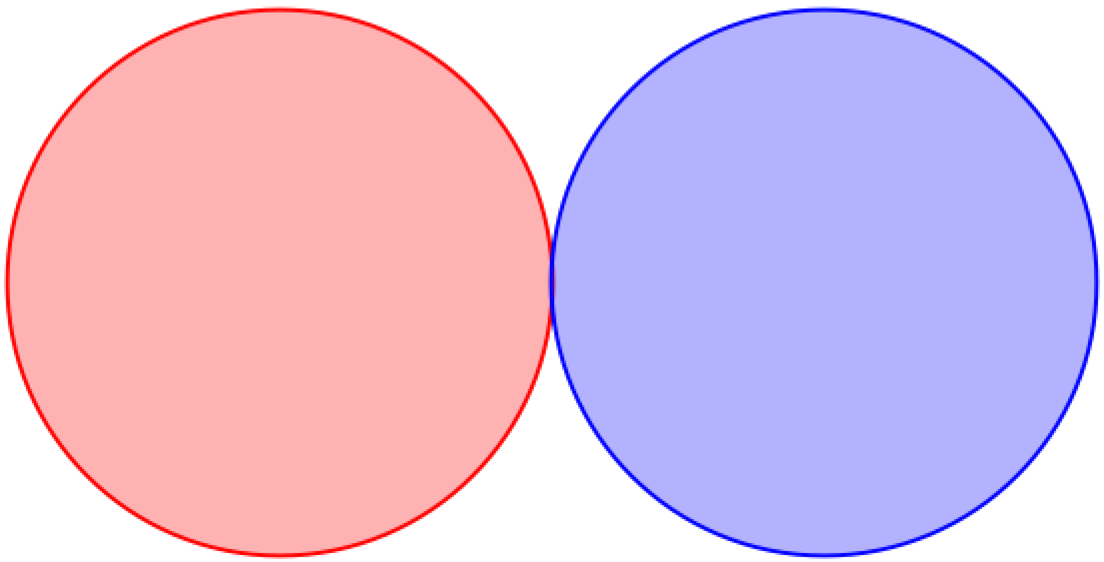
V. Elser, I. Rankenburg, and P. Thibault, Searching with iterated maps, PNAS 104, (2007), 418-423.

generalized form, applied to hard/frustrated problems:
spin glass, SAT, protein folding, Latin squares, etc.

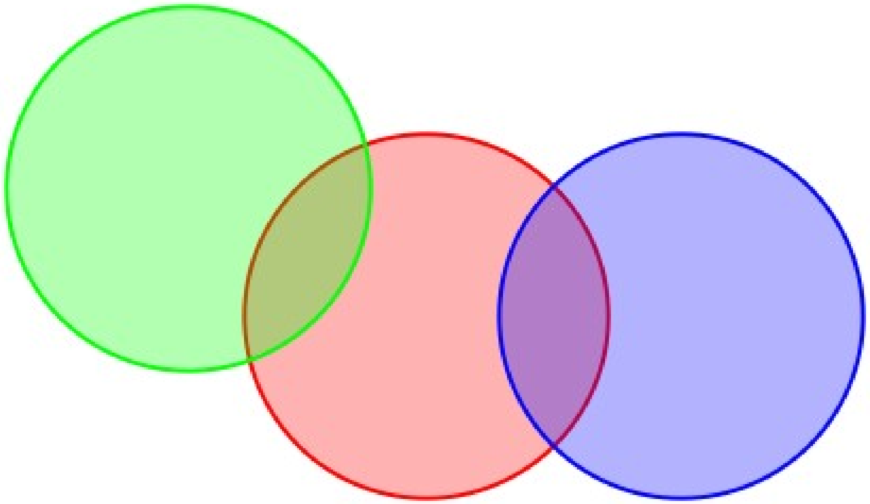
Projection to the packing (no overlaps) constraint



Projection to the packing (no overlaps) constraint



Dividing the Constraints



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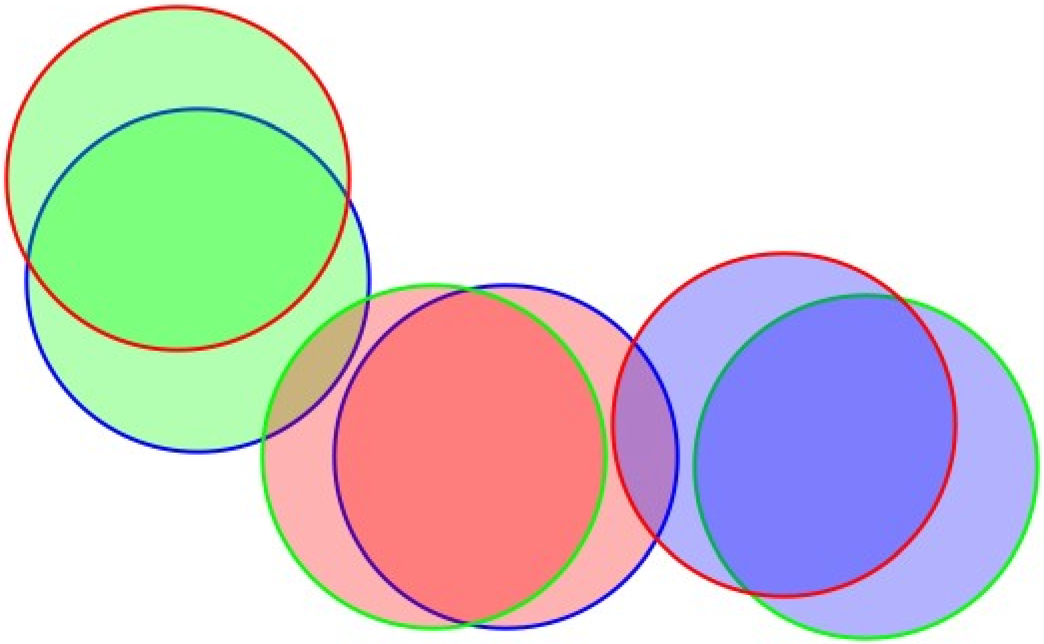

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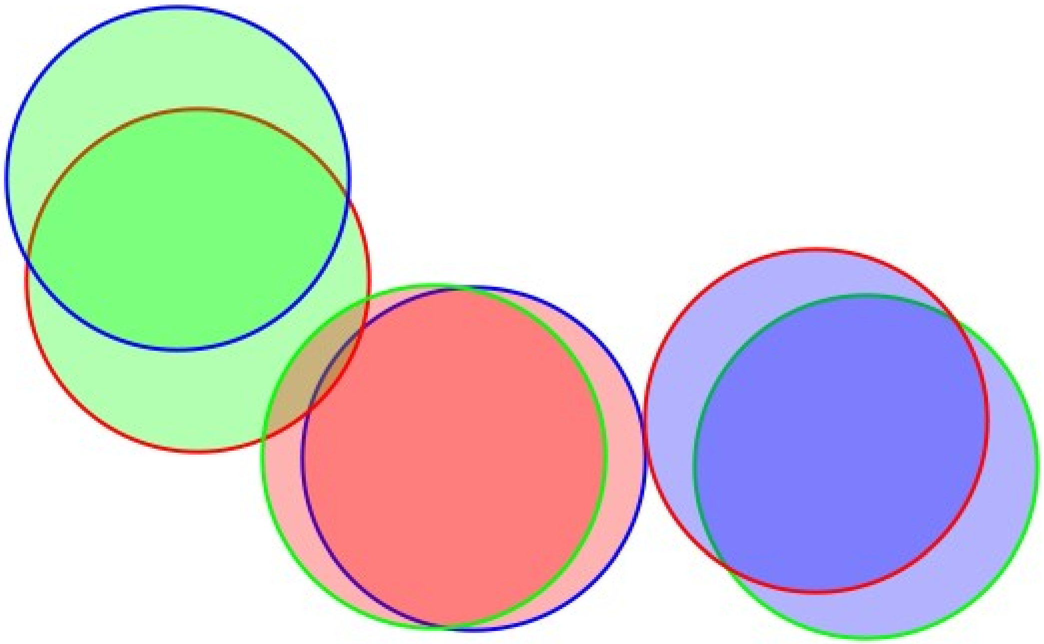
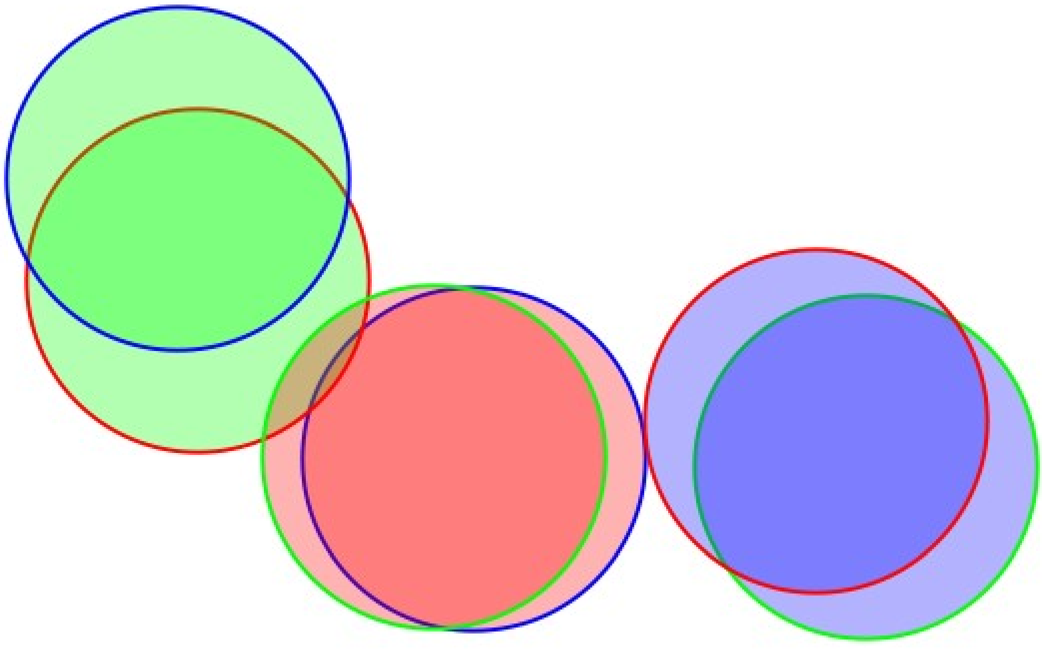
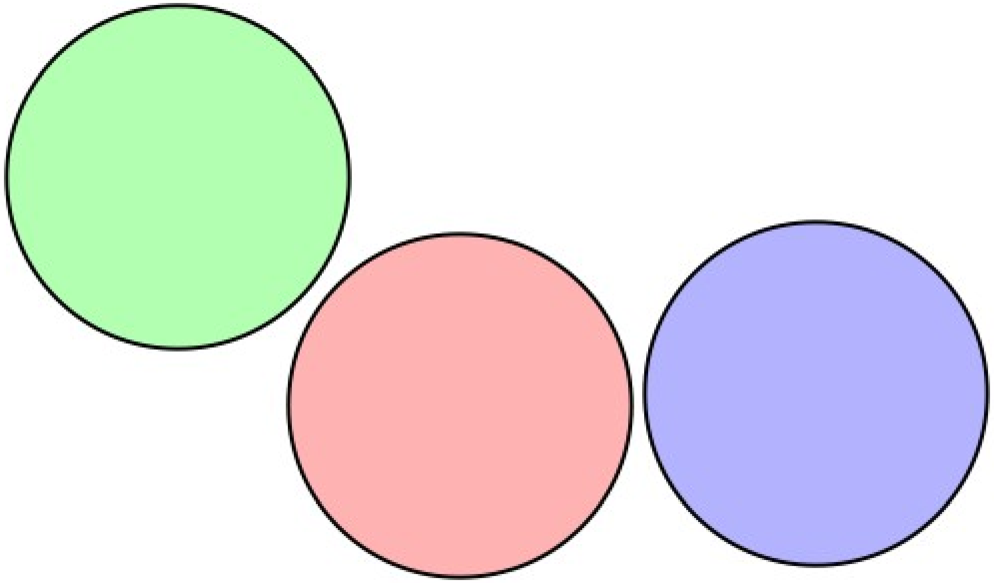


Projection to concurrence constraint



Projection to concurrence constraint



Divide and Concur scheme

___A_____	___B_____
No overlaps between designated replicas	All replicas of a particular figure concur
"divided" packing constraints	"concurrence" constraint

What can we do with projections?

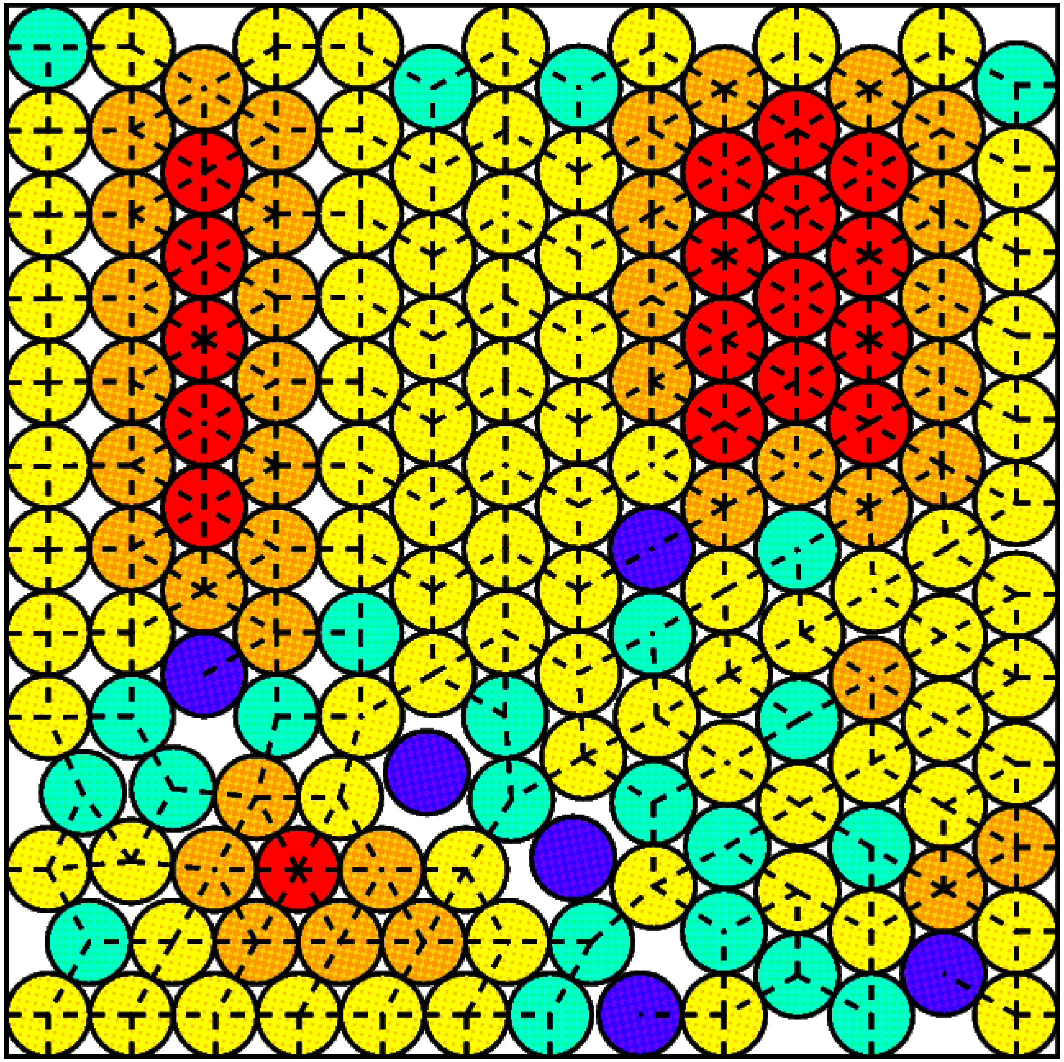
- alternating projections:

$$x_i' = P_A(x_i); \quad x_{i+1} = P_B(x_i')$$

- Douglas-Rachford iteration (a/k/a difference map):

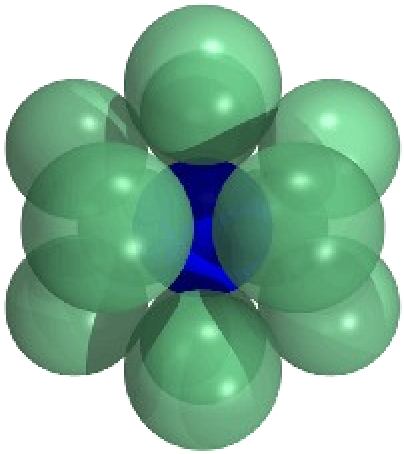
$$x_{i+1} = x_i + P_B(2P_A(x_i) - x_i) - P_A(x_i)$$

Finite packing problems

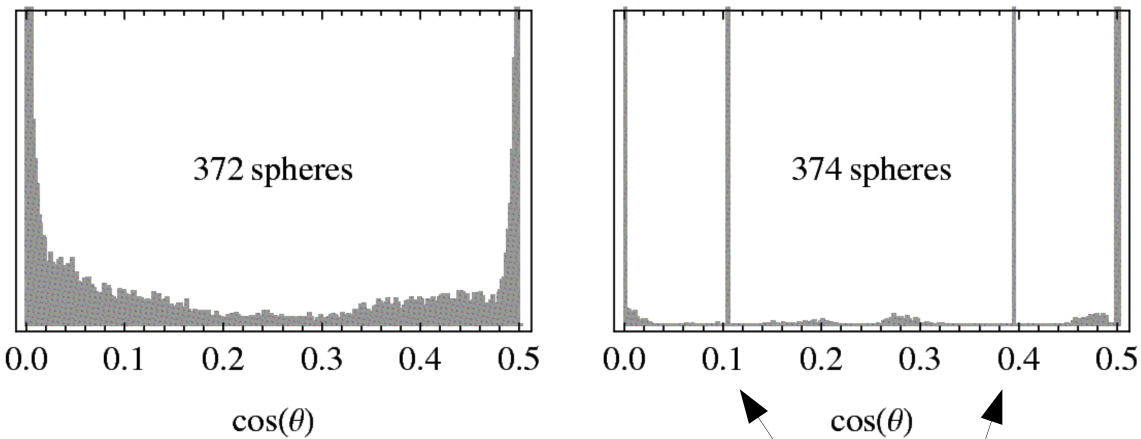


Gravel & Elser, Phys. Rev. E (2008)

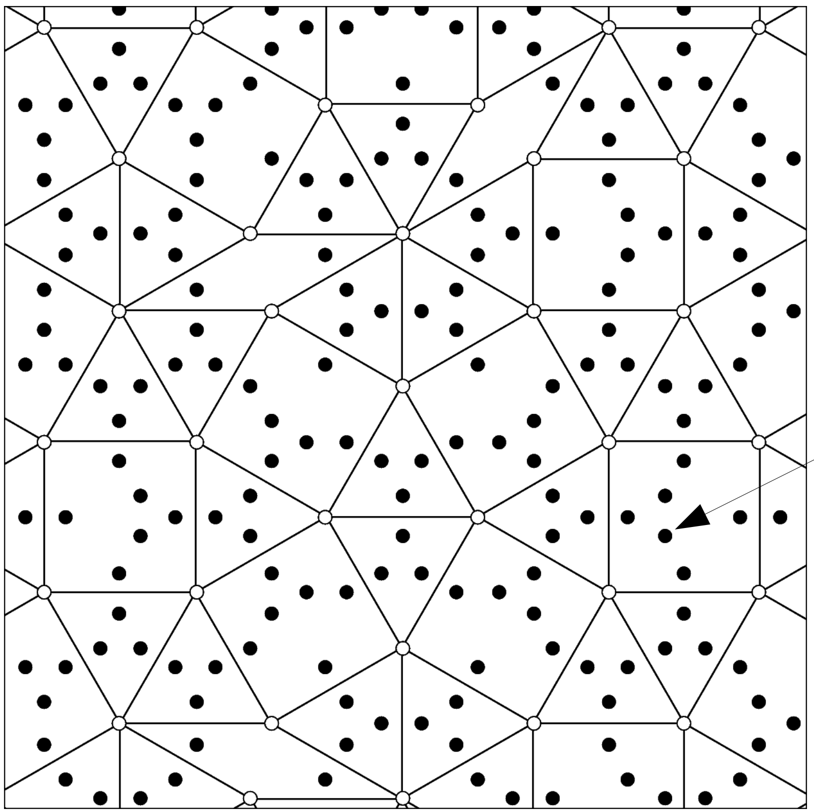
Finite packing problems



The kissing number problem in 10D



$$(3 \pm \sqrt{3})/12$$

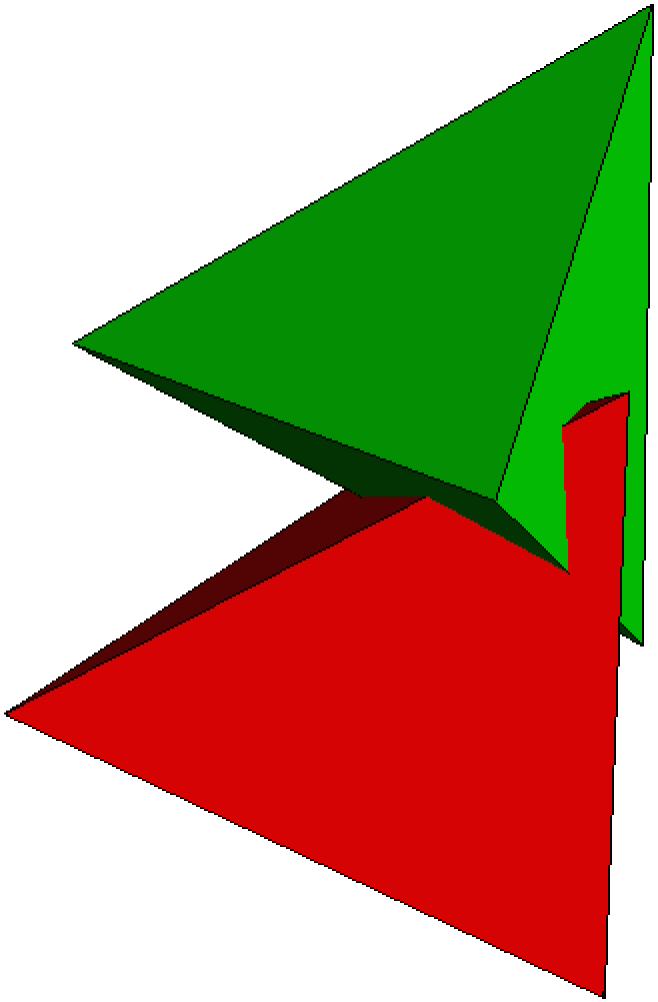


$$A_2 \oplus A_2 \oplus D_4$$

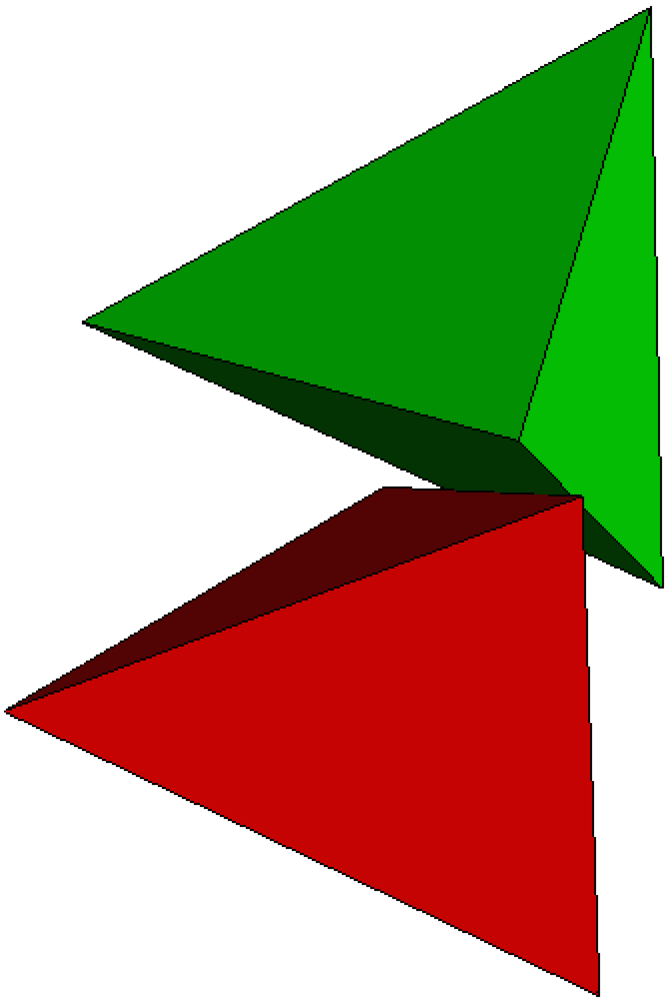
Special dimensions matter!

Elser & Gravel, Disc. Compu. Geom. (2008)

Generalization to non-spherical Particles



Generalization to non-spherical Particles



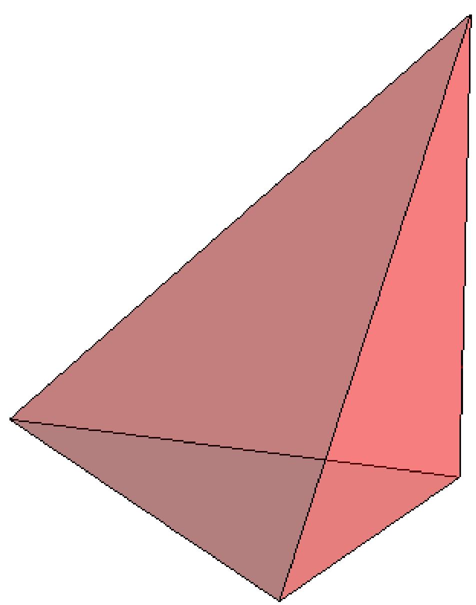
Generalization to non-spherical Particles

A

"divided" packing constraints (rigidity relaxed)

B

"concurrence" + rigidity constraints



Generalization to non-spherical Particles

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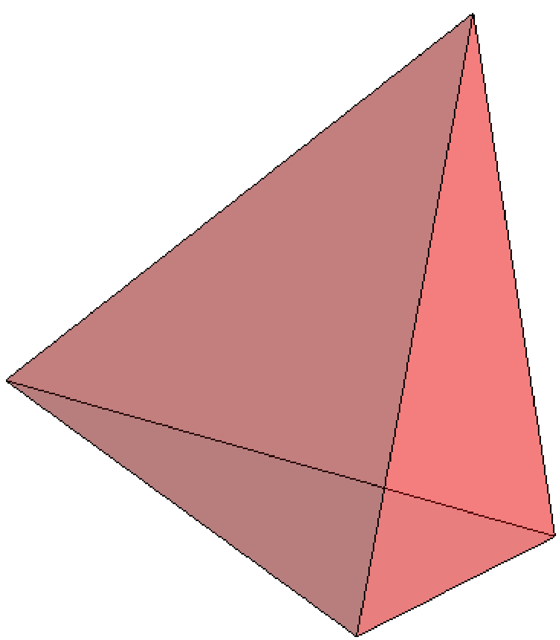
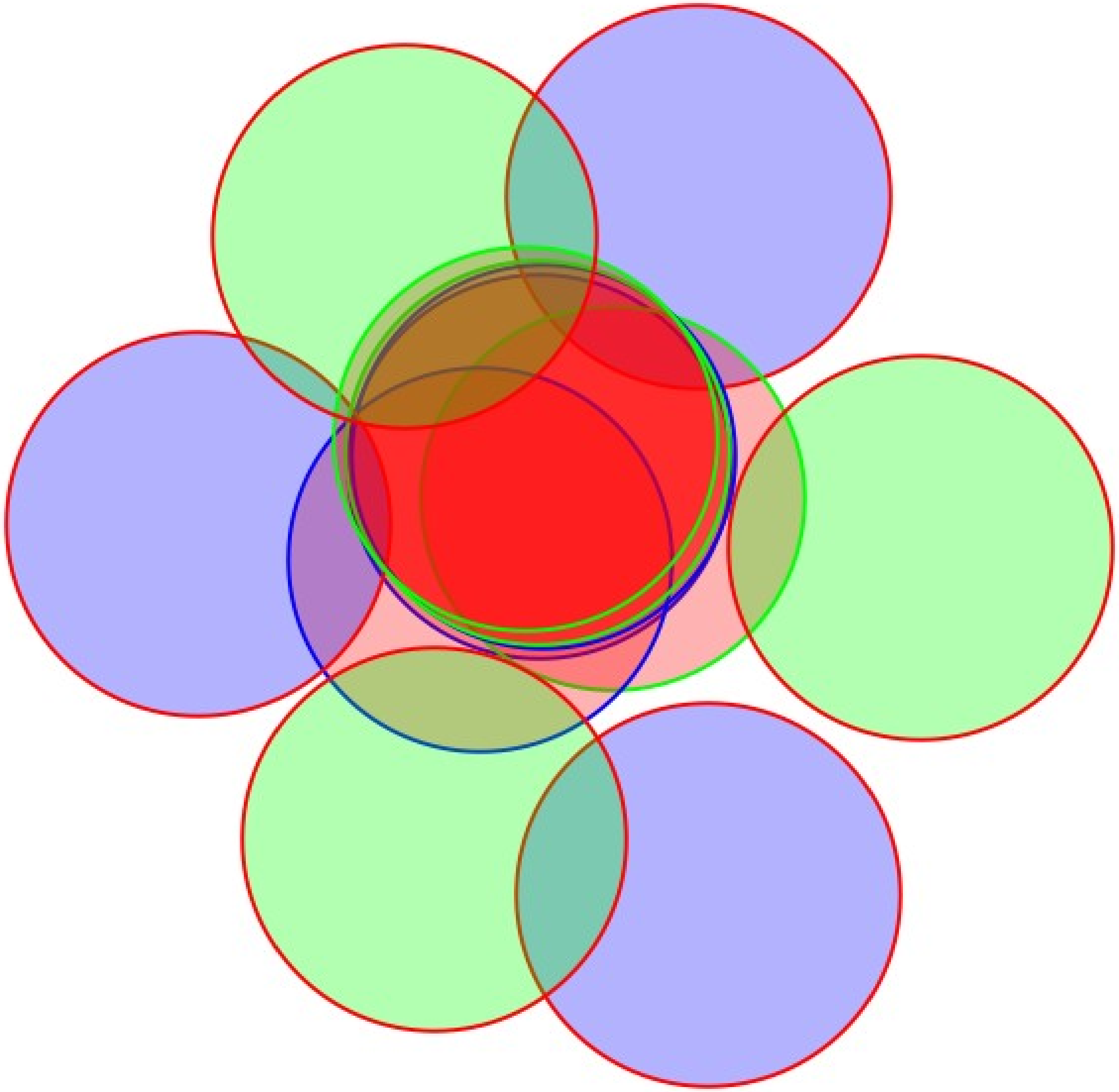


Generalization to periodic packings

replicas → replicas + periodic images



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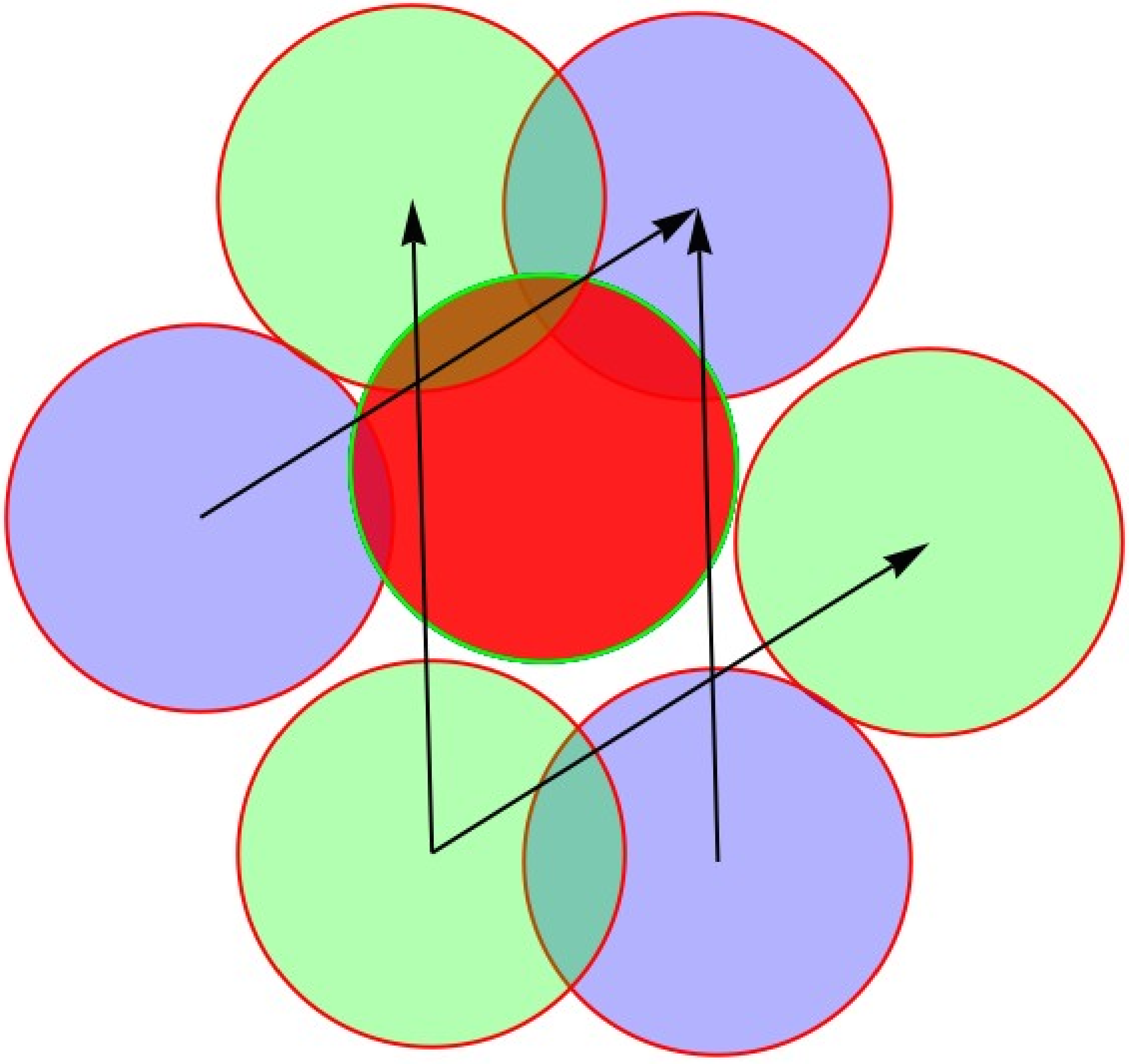
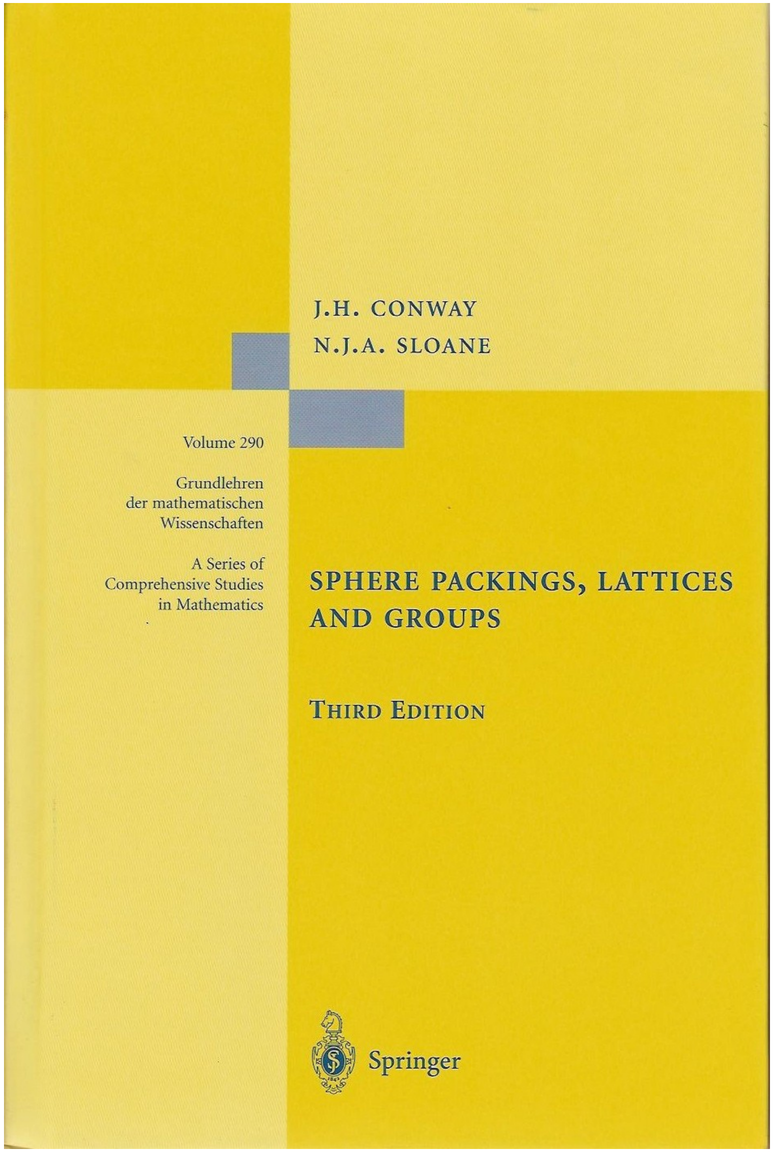


Sphere packing and kissing in higher dimensions



Densest known lattice packing in *d* dimensions:

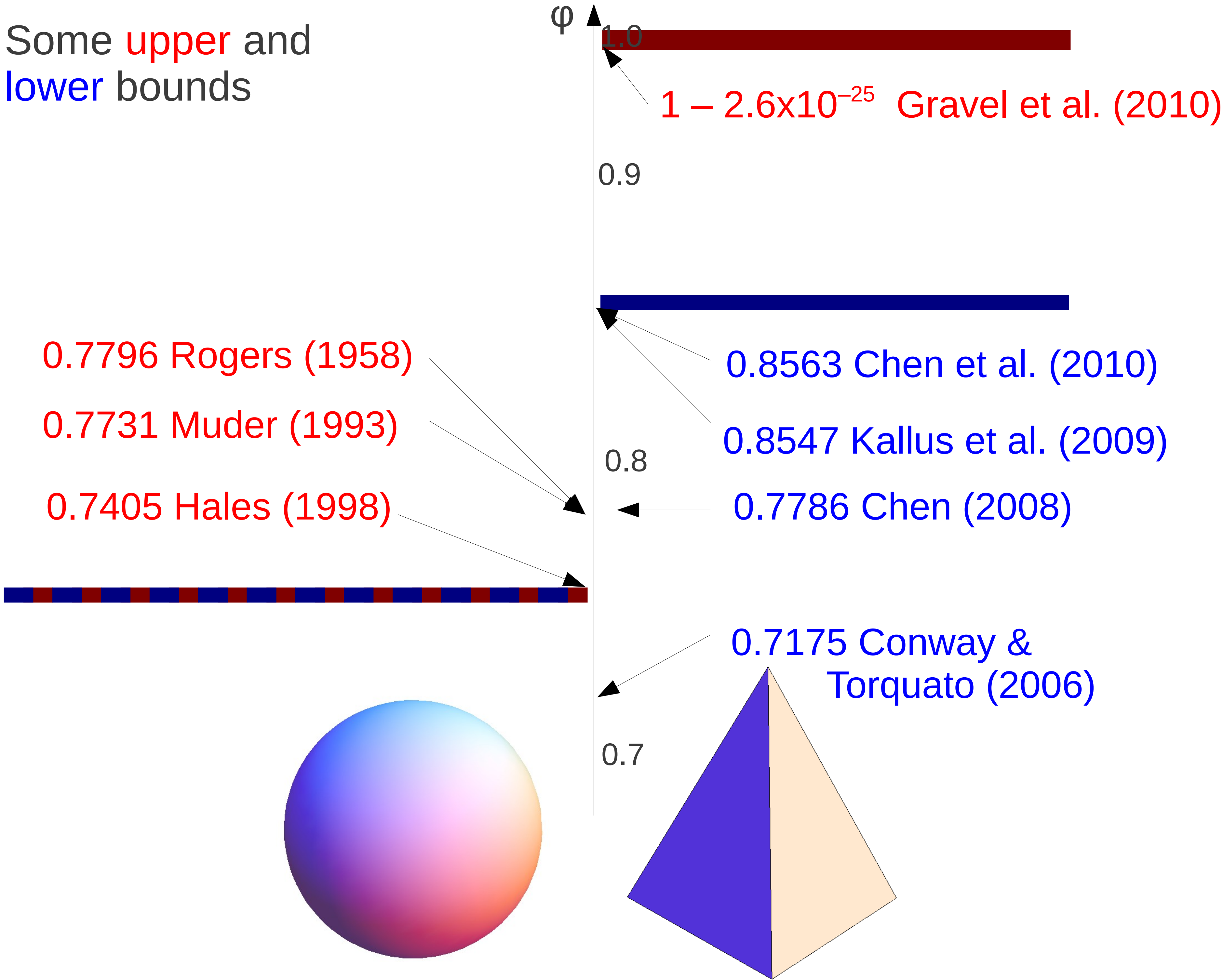
d	Λ_{densest}	$\phi^{(L)}_{\text{densest}}$	$\langle N_{\text{iter}} \rangle$
2	A_2	0.90690	42
3	D_3	0.74047	230
4	D_4	0.61685	191
5	D_5	0.46526	308
6	E_6	0.37295	173
7	E_7	0.29530	217
8	E_8	0.25367	99
9	Λ_9	0.14577	161
10	Λ_{10}	0.092021	394
11	K_{11}	0.060432	421
12	K_{12}	0.049454	397
13	K_{13}	0.029208	577
14	Λ_{14}	0.021624	1652

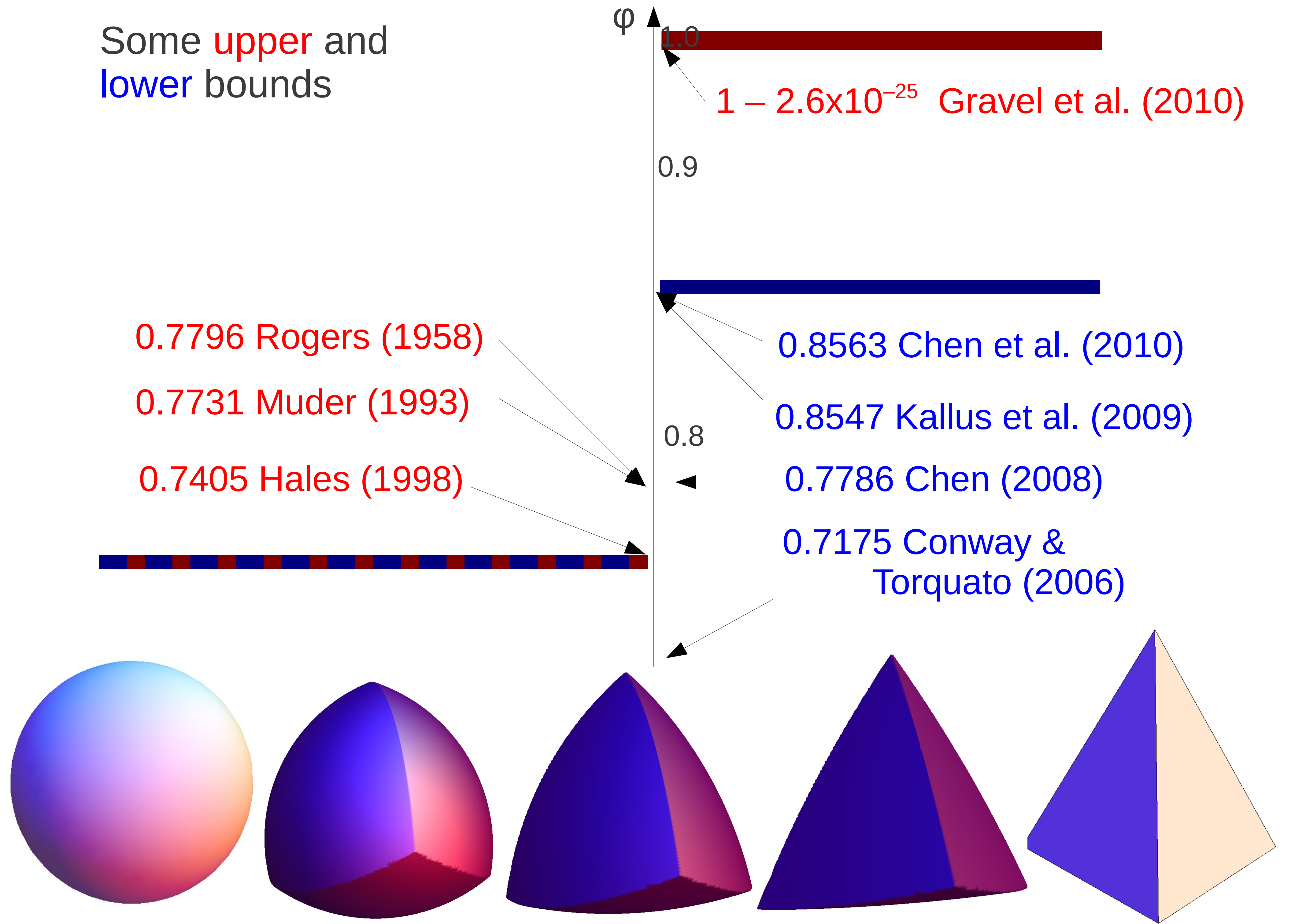
lattice with highest known kissing number in *d* dimensions:

d	Λ_{highest}	$\tau^{(L)}_{\text{highest}}$	$\langle N_{\text{iter}} \rangle$
2	A_2	6	27
3	D_3	12	54
4	D_4	24	132
5	D_5	40	163
6	E_6	72	225
7	E_7	126	597
8	E_8	240	511
9	Λ_9	272	350
10	Λ_{10}	336	438
11	Λ_{11}	438	549

Kallus, Elser, & Gravel, Phys. Rev. E (2010)

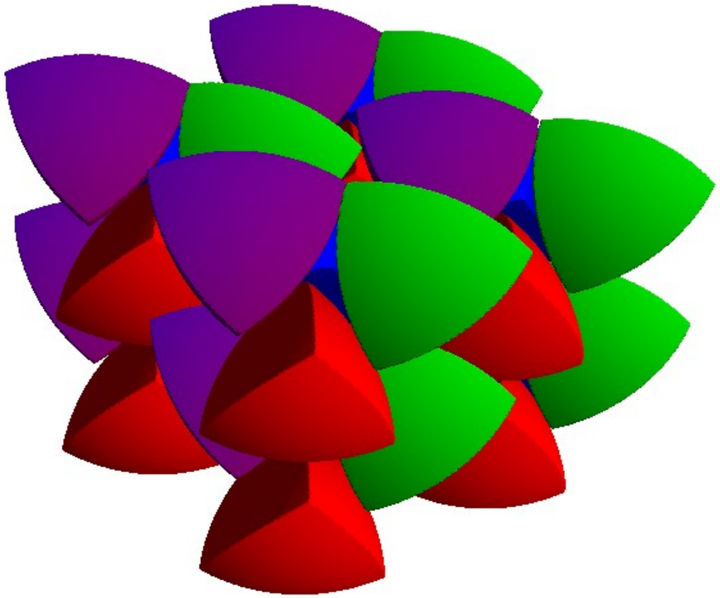
Some upper and lower bounds

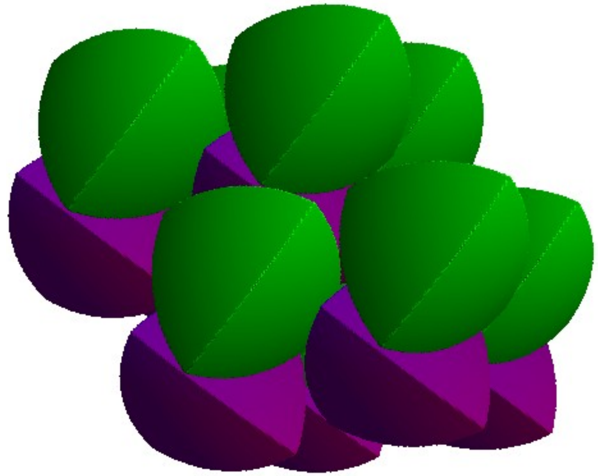


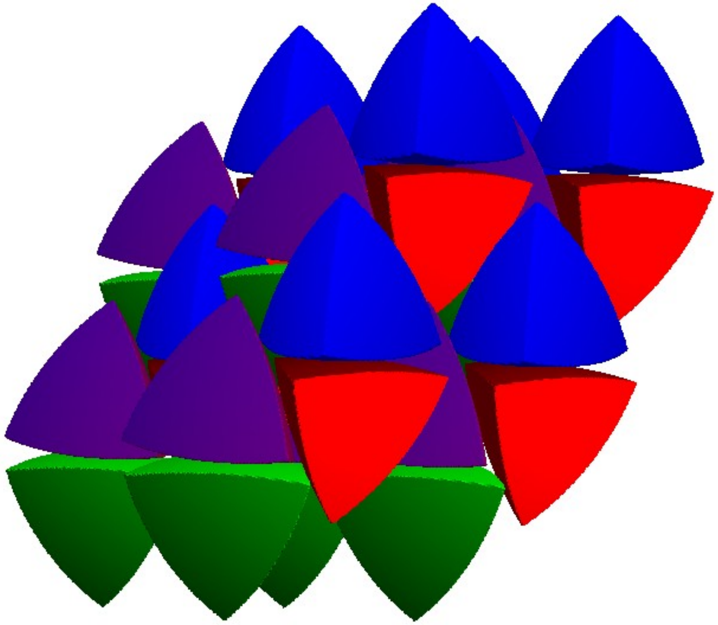


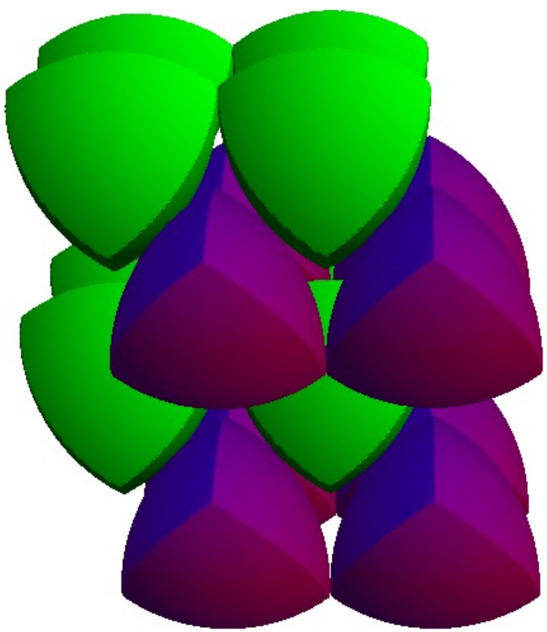
Some upper and
lower bounds
φ
1.0
1 – 2.6x10^{-25} Gravel et al. (2010)
0.9
0.8
0.7796 Rogers (1958)
0.7731 Muder (1993)
0.7405 Hales (1998)
0.8563 Chen et al. (2010)
0.8547 Kallus et al. (2009)
0.7786 Chen (2008)
0.7175 Conway & Torquato (2006)

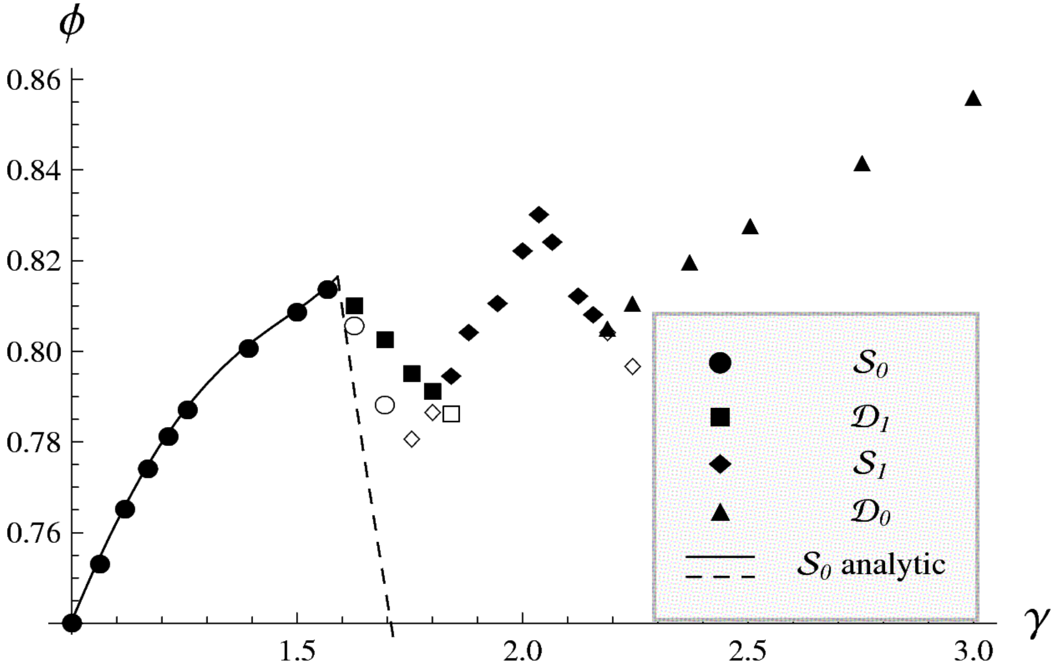
“physical” tetrahedra











Kallus & Elser, preprint (2010)