Packing tetrahedra and other figures using *Divide and Concur*

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General packing problem

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

2D periodic examples:

$\varphi = 0.817$
$N = 1$

$\varphi = 0.854$
$N = 2$

$\varphi = 0.921$
$N = 2$

$\varphi_{\text{max}}(K)$ for $d > 2$ known only for spheres, space-filling solids.
From Hilbert's 18\textsuperscript{th} problem:

“How can one arrange most densely in space an infinite number of equal solids of a given form, e.g., \textit{spheres} with given radii or \textit{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?”
Some upper and lower bounds

- 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)

- 1 – $2.6 \times 10^{-25}$ Gravel et al. (2010)
Rogers bound

$\varphi(B) \leq 0.7796$

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

$\varphi(B) \leq 0.7796$

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

The tetrahedron can easily fill its Voronoi region
Regular tetrahedra do not fill space

Missing angle: 7.4°

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 $\varepsilon$
Optimization challenge:
1. Prove $\varphi \leq 1 - \varepsilon$, where $\varepsilon > 0$
2. Maximize $\varepsilon$
2'. Minimize length of proof

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

11 By applying this argument iteratively: $\varphi(T) \leq 1 - (2.6...) \times 10^{-25}$
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Lower bounds (densest known packings)


Icosahedral packing: $\phi = 0.7166$
N=20

“Welsh” packing: $\phi = 0.7175$
N=34

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

PNAS (2006)
Densest known packings

2. Chen (2008)

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

$N=18$

$\varphi_{\text{max}}(T) > \varphi_{\text{max}}(B)$
Densest known packings


Challenge for numerical search: highly frustrated optimization problem

Search often got stuck at local optima
Densest known packings

4. Kallus et al. (2009)

Method: “divide and concur”

φ = 0.8547
N = 4 (!)
All tetrahedra equivalent
(tetrahedron-transitive packing)


5. Chen et al. (2010)

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

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 $> \varphi$

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:

\[ A = \text{permutations of "acgiknp"} \]

\[ B = \text{7-letter English words} \]
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 $\Omega$

simple constraints:
easy, efficient \textit{projections} to A, B

\[
P_A(x) = y \in A \quad \text{s.t.} \quad ||x-y|| \text{ is minimized}
\]
Brief (incomplete) history of

\[ x_{i+1} = x_i + P_B(2P_A(x_i) - x_i) - P_A(x_i) \]


splitting scheme for numerical PDE solutions


rediscovery, control theory motivation, phase retrieval


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
Dividing the Constraints
Dividing the Constraints
Projection to concurrence constraint
Projection to concurrence constraint
A

No overlaps between designated replicas

“divided” packing constraints

B

All replicas of a particular figure concur

“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

Finite packing problems

The kissing number problem in 10D

372 spheres

374 spheres

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

\[ A_2 \oplus A_2 \oplus D_4 \]

Special dimensions matter!

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

A
“divided” packing constraints (rigidity relaxed)

B
“concurrence” + rigidity constraints
Generalization to periodic packings

replicas \rightarrow \text{replicas + periodic images}
Generalization to periodic packings

replicas → replicas + periodic images
Sphere packing and kissing in higher dimensions

Densest known lattice packing in $d$ dimensions:

<table>
<thead>
<tr>
<th>$d$</th>
<th>$\Lambda_{densest}$</th>
<th>$\phi_{densest}^{(L)}$</th>
<th>$\langle N_{iter} \rangle$</th>
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<tr>
<td>2</td>
<td>$A_2$</td>
<td>0.90690</td>
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<td>3</td>
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Lattice with highest known kissing number in $d$ dimensions:

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<th>$\tau_{highest}^{(L)}$</th>
<th>$\langle N_{iter} \rangle$</th>
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“physical” tetrahedra