UNIVERSITY OF LIVERPOOL

LEVERHULME TRUST

The Leverhulme Research Centre for Functional Materials Design

Periodic packings in the light of crystal structure prediction.

First Year Progress Report

Miloslav Torda

Supervisors:
Prof Yannis Goulermas
Dr Vitaliy Kurlin
Prof Graeme M. Day
Dr Linjiang Chen

Advisors:
Prof Leszek A. Gasieniec
Prof Rahul Savani

diamond
Hartree Centre
Science & Technology Facilities Council
Imperial College London
ICNS
King Abdullah University of Science and Technology
University of Southampton

Table of Contents

MOTIVATION

Motivation

Mathematical crystal

- A structure built of one or a few different kinds of discrete units, arranged in more or less modular fashion
- In our case the module is a space filling polyhedron.
- A model of a real crystal.

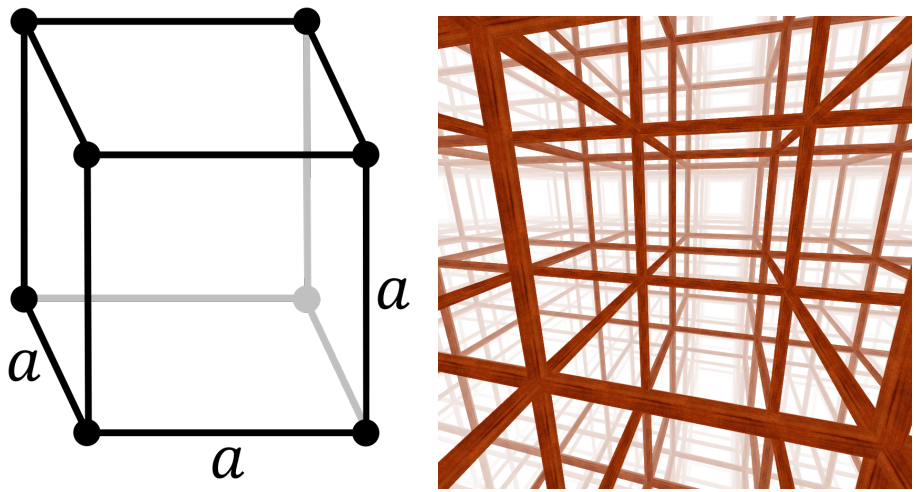


Figure: Left: Cubic module. Right: Cubic crystal

Motivation

Crystal structure prediction

- The calculation of crystal structures of solids from first principles (QED).
- Calculations are based on
  - Force field methods.
  - Density functional theory.
- In principle an optimization problem of finding structures with minimal energy.

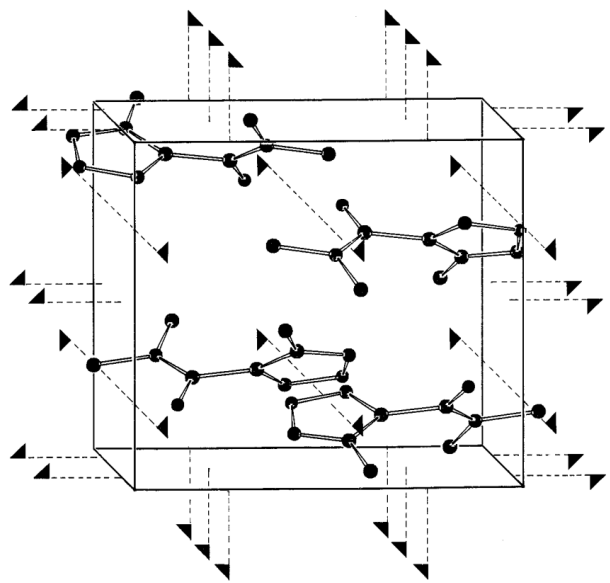


Figure: Example of a molecular crystal module

Motivation

Lennard-Jones potential

$$U_{LJ} = 4\epsilon \left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^{6}}{r^{6}} \right)$$

- ϵ - Lennard-Jones potential well depth.
- σ - The finite distance at which the inter-particle potential is zero.
- r - The distance between two particles.

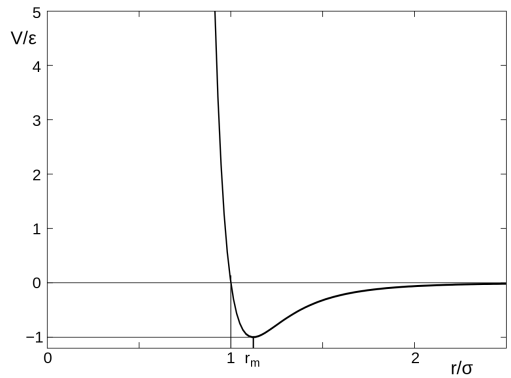


Figure: U_{LJ} graph

Motivation

Lennard-Jones potential stationary points

Potential for atoms:

$$U_{LJ} = \sum_{i<j} 4\epsilon_{ij} \left(\frac{\sigma_{ij}^{12}}{r_{ij}^{12}} - \frac{\sigma_{ij}^{6}}{r_{ij}^{6}} \right)$$

Potential for molecules:

$$U_{LJ} = \sum_{a \in A} \sum_{b \in B} 4\epsilon_{ab} \left(\frac{\sigma_{ab}^{12}}{r_{ab}^{12}} - \frac{\sigma_{ab}^{6}}{r_{ab}^{6}} \right)$$

	Stationary point index															
N	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
4	1	1	2	1	1	0	0									
5	1	2	4	6	6	2	1	0								
6	2	3	13	24	30	26	16	5	1	0						
7	4	12	44	98	168	190	168	101	45	11	1	0				
8	8	42	179	494	1000	1458	1619	1334	852	388	125	26	1	0		
9	21	165	867	2820	6729	12 093	16 292	16 578	13 226	8286	4053	1444	376	56	1	0
10	64	635	4074	16 407	46 277	*97 183*										
11	170	2424	17 109	*47 068*												
12	515	8607	*27 957*													
13	1509	28 756	*88 079*													

Figure: Stationary points of U_{LJ} for atoms.

Motivation

Energy vs. density

- Dense packed structures tend to have lower energies

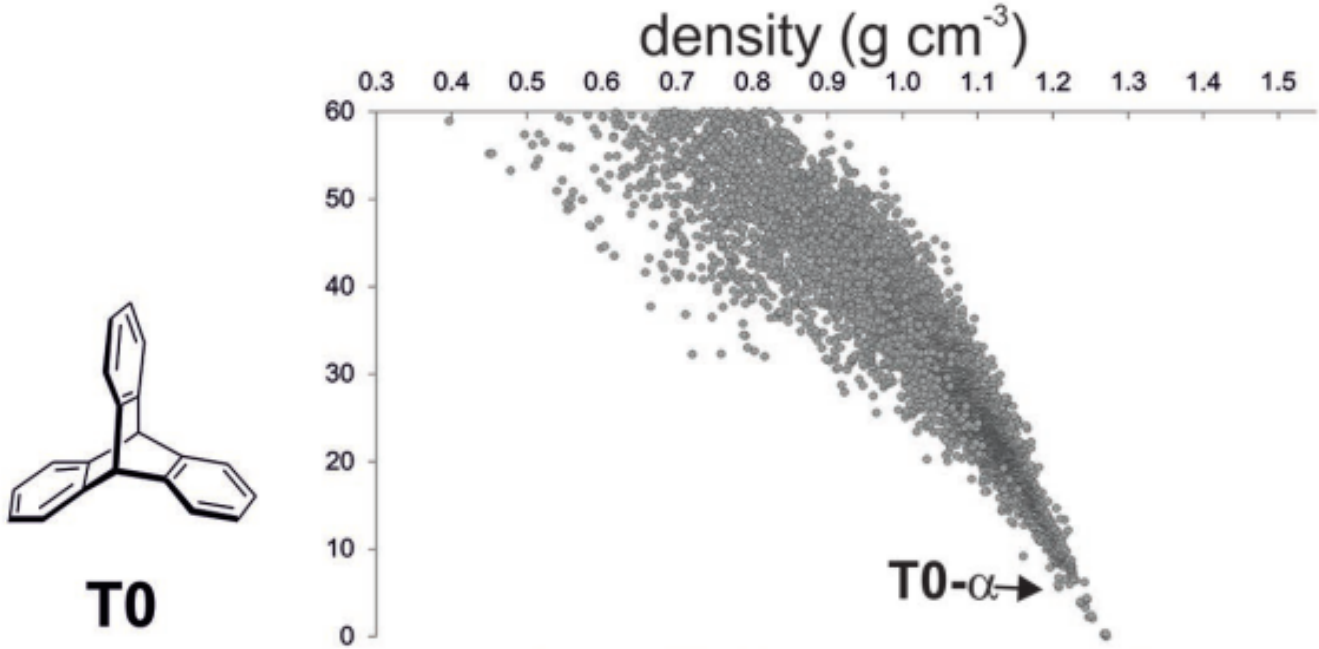
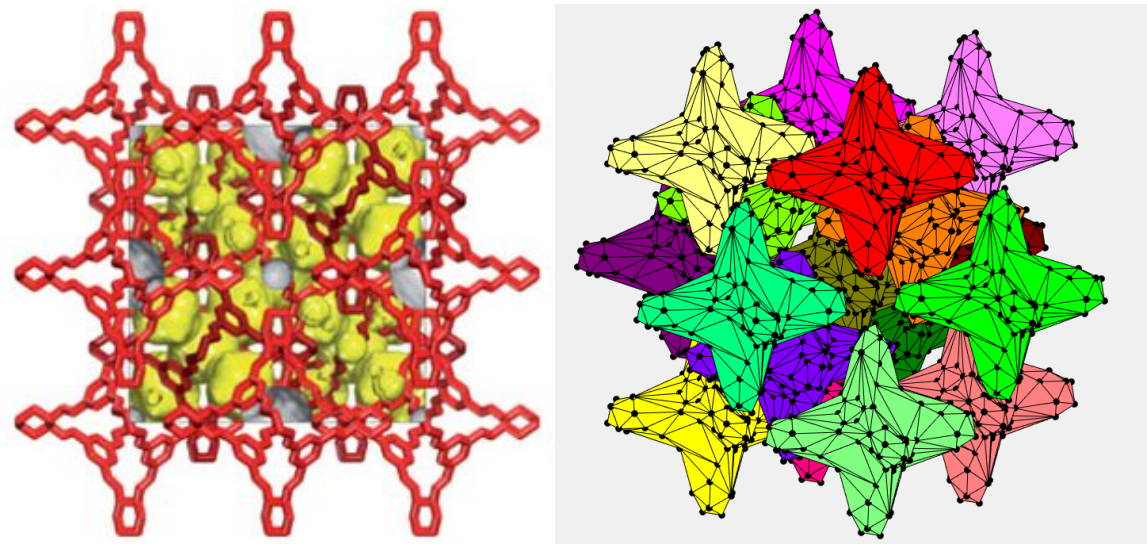


Figure: T0 CSP Lattice energy landscape

Motivation

Molecular packings

- Find dense packings of molecules approximated by polyhedra.
- Optimize packing density instead of energy.
- Use the resulting structures as starting positions in CSP.



(a) (b)

Figure: (a) Organic cage molecule 3 crystal structure. (b) α-shape of organic cage molecule 3.

PACKING

Packing

18th Hilbert problem

"How can one arrange most densely in space an infinite number of equal solids of 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 great as possible?"

D. Hilbert, Mathematical problems, Bull. Amer. Math. Soc., vol. 8, pages 437-479, 1902.

Definition

The system of sets $S_1,\ S_2, \ldots$ is said to form a packing into the set S, if

$$S_i \cap S_j = \emptyset \ (i \neq j)$$
$$\bigcup_i S_i \subset S$$

i.e if no two of the sets $S_1,\ S_2, \ldots$ have any element in common and each element of the sets $S_1,\ S_2, \ldots$ belongs to S.

Packing

Our setting

- $S = \mathbf{E}^3$
- $S_1,\ S_2, \ldots$ is a finite collection or countably infinite of translates of rotations of a single compact set K.
- Translate of K is a set of all points $k + a$, where $k \in K$, and a is a fixed point or vector.
- Rotation is a set of all points Rk for $k \in K$ and $R \in SO(3) = \{A \in \mathbb{R}^{3\times 3} : A^T A = I,\ \det A = 1\}$.

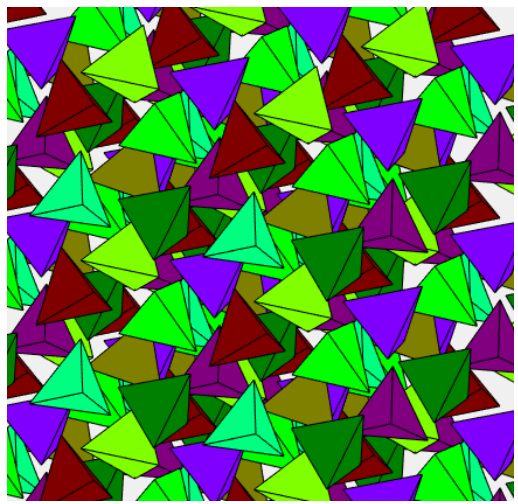


Figure: A packing with tetrahedra

Definition

The density $\rho(\mathcal{K})$ of the packing $\mathcal{K}$ is

$$\rho(\mathcal{K}) = \limsup_{c \to \infty} \rho(\mathcal{K}, C)$$

where

$$\rho(\mathcal{K}, C) = \frac{1}{\mathtt{vol}(C)} \sum_{(R_j K + a_i) \cap C \neq \emptyset} \mathtt{vol}(R_j K + a_i).$$

- $\{a_i\}$ be a sequence of points.
- $\{R_j : R_j \in SO(3)\}$ a collection of rotations.
- K a set with finite volume $\mathtt{vol}(K)$.
- C a cube with the edge length c.
- $\mathcal{K} = \{R_j K + a_i\}$ a system of sets that forms a packing.
- If $\rho(\mathcal{K})$ is a packing then $0 \leq \rho(\mathcal{K}) \leq 1$.

Definition

Let $\mathbf{a_1}, \mathbf{a_2}, \ldots, \mathbf{a_n}$ be n linearly independent vectors in $\mathbf{E}^n$. The set $\Lambda = \{u_1\mathbf{a_1} + u_2\mathbf{a_2} + \cdots + u_n\mathbf{a_n} \mid u_i \in \mathbb{Z}\}$ is called a **lattice.**

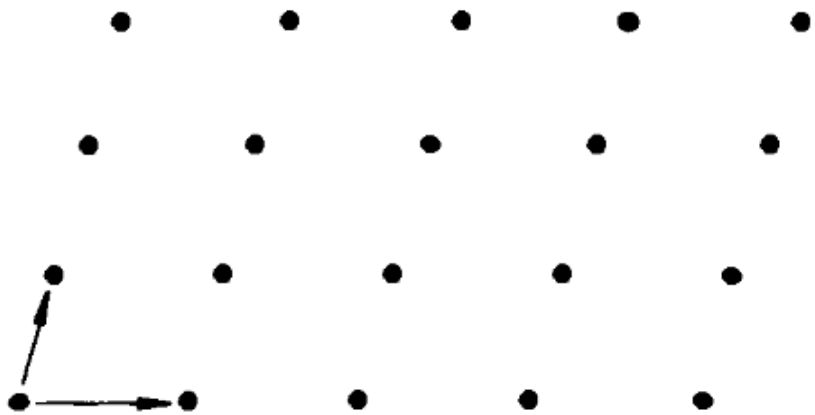


Figure: A plane lattice

Definition

A lattice packing $\mathcal{K}_L$ is a system of translates of a given set K i.e.

$$\mathcal{K}_L = \{K + \mathbf{a} \mid \mathbf{a} \in \Lambda\}$$

if it is a packing into the whole space.

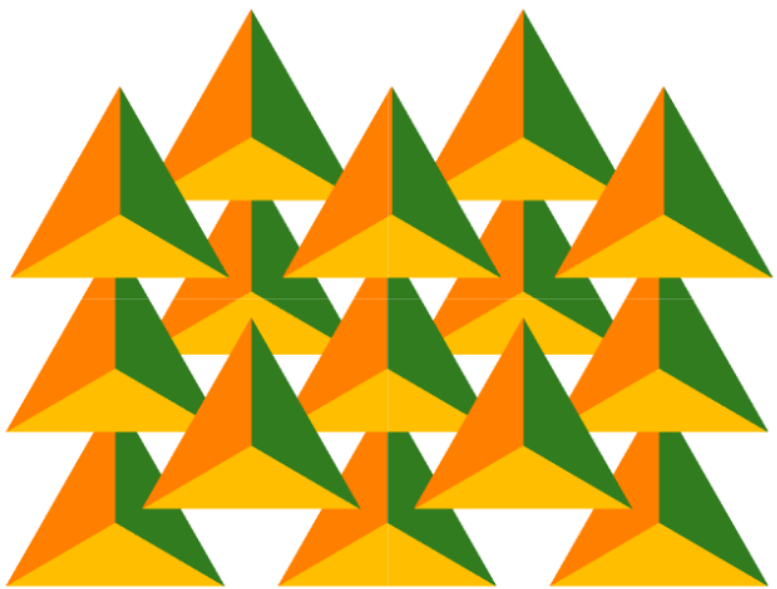


Figure: The densest lattice packing with the tetrahedron.

Definition

A periodic packing $\mathcal{K}_P$ is a system of translates and rotations of a given set K, that is

$$\mathcal{K}_P = \{R_i K + \mathbf{a_i} + \mathbf{b_j} \mid i = 1, 2, \ldots, N;\ j = 1, 2, \ldots\}$$

if it is a packing into the whole space.

- $\mathbf{a_1}, \mathbf{a_2}, \ldots, \mathbf{a_N}$ is a set of points
- $\mathbf{b_1}, \mathbf{b_2}, \ldots \in \Lambda$
- $R_1, R_2, \ldots, R_N \in SO(3)$.

Theorem

Let K be a bounded set with positive measure, let C be a cube (with its edges parallel to the coordinate axes) with edge-length $s(C)$, and let T be a non-singular affine transformation. Let $\mathbf{a_1}, \mathbf{a_2}, \ldots, \mathbf{a_N}$ be a set of points, and let $\mathbf{b_1}, \mathbf{b_2}, \ldots$ be the points of the lattice of all points that have integral multiples of $s(C)$ for co-ordinates. Let $\mathcal{K}_P$ be the periodic system of sets

$$K + \mathbf{a_i} + \mathbf{b_j} \ \ (i = 1, 2, \ldots, N;\ j = 1, 2, \ldots)$$

and let $T\mathcal{K}_P$ denote the system of sets

$$T\left(K + \mathbf{a_i} + \mathbf{b_j}\right) \ \ (i = 1, 2, \ldots, N;\ j = 1, 2, \ldots).$$

Then

$$\rho\left(T\mathcal{K}_P\right) = \rho\left(\mathcal{K}_P\right) = \frac{N\mathtt{vol}(K)}{\mathtt{vol}(C)}.$$

Lattice packing:

$$\rho(\mathcal{K}_L) = \frac{\mathtt{vol}(K)}{|\det(\Lambda)|}$$

Periodic packing:

$$\rho(\mathcal{K}_P) = \frac{N\mathtt{vol}(K)}{|\det(\Lambda)|}$$

Packing

Problem statement

Find a periodic packing $\mathcal{K}_{\max}$ of N congruent copies of a given set K such that

$$\mathcal{K}_{\max} = \operatorname*{argmax}_{\mathcal{K}_P} \rho(\mathcal{K}_P).$$

Packing

Bodies K for which the densest packing is known

BODY	SOURCE
Circular disk in $\mathbb{E}^2$	[Thu10]
Parallel body of a rectangle	[Fej67]
Intersection of two congruent circular disks	[Fej71]
Centrally symmetric n-gon (algorithm in $O(n)$ time)	[MS90]
Ball in $\mathbb{E}^3$	[Hal05]
Ball in $\mathbb{E}^8$	[Via17]
Ball in $\mathbb{E}^{24}$	[CKM17]
Truncated rhombic dodecahedron in $\mathbb{E}^3$	[Bez94]

Packing

Bodies K $\in$ $\mathbf{E}^3$ for which the densest lattice packing is known

BODY	$\delta_L(K)$	SOURCE
$\{x \mid \lvert x\rvert \le 1,\ \lvert x_3\rvert \le \lambda\} \quad (\lambda \le 1)$	$\pi(3-\lambda^2)^{1/2}/6$	[Cha50]
$\{x \mid \lvert x_i\rvert \le 1,\ \lvert x_1+x_2+x_3\rvert \le \lambda\}$	$\frac{9-\lambda^2}{9}$ for $0<\lambda\le\frac{1}{2}$; $\frac{9\lambda(9-\lambda^2)}{4(-\lambda^3-3\lambda^2+24\lambda-1)}$ for $\frac{1}{2}\le\lambda\le 1$; $\frac{9(\lambda^3-9\lambda^2+27\lambda-3)}{8\lambda(\lambda^2-9\lambda+27)}$ for $1\le\lambda\le 3$	[Whi51]
$\{x \mid \sqrt{(x_1)^2+(x_2)^2}+\lvert x_3\rvert \le 1\}$	$\pi\sqrt{6}/9 = 0.8550332\ldots$	[Whi48]
Tetrahedron	$18/49 = 0.3673469\ldots$	[Hoy70]
Octahedron	$18/19 = 0.9473684\ldots$	[Min04]
Dodecahedron	$(5+\sqrt{5})/8 = 0.9045084\ldots$	[BH00]
Icosahedron	$0.8363574\ldots$	[BH00]
Cuboctahedron	$45/49 = 0.9183633\ldots$	[BH00]
Icosidodecahedron	$(45+17\sqrt{5})/96 = 0.8647203\ldots$	[BH00]
Rhombic Cuboctahedron	$(16\sqrt{2}-20)/3 = 0.8758056\ldots$	[BH00]
Rhombic Icosidodecahedron	$(768\sqrt{5}-1290)/531 = 0.8047084\ldots$	[BH00]
Truncated Cube	$9(5-3\sqrt{2})/7 = 0.9737476\ldots$	[BH00]
Truncated Dodecahedron	$(25+37\sqrt{5})/120 = 0.8977876\ldots$	[BH00]
Truncated Icosahedron	$0.78498777\ldots$	[BH00]
Truncated Cuboctahedron	$0.8493732\ldots$	[BH00]
Truncated Icosidodecahedron	$(19+10\sqrt{5})/50 = 0.8272135\ldots$	[BH00]
Truncated Tetrahedron	$207/304 = 0.6809210\ldots$	[BH00]
Snub Cube	$0.787699\ldots$	[BH00]
Snub Dodecahedron	$0.7886401\ldots$	[BH00]

PRELIMINARY RESULTS

Preliminary results

Monte-Carlo molecular dynamics simulations

- First idea: use stochastic optimization.
- Well explored approach.
- For example by Salvatore Torquato and Yang Jiao
  S. Torquato and Y. Jiao, Dense packings of polyhedra: Platonic and Archimedean solids, Phys. Rev. E, vol. 80, 2009.

Preliminary results

Torquato and Jiao packing algorithm

Algorithm:

- For N number of stages do
  - For M number of cycles do
    - For every polyhedron in a unit cell
      - With probability p translate the polyhedron in a random direction within the unit cell or with $1 - p$ rotate the polyhedron around a random axis by a random angle.
      - Repeat until successful rotation/translation or until J number of attempts.
  - With probability p_u contract the unit cell or with the probability $1 - p_u$ expand the unit cell by a random strain tensor. Repeat until success or until L number of attempts.

Restrictions:

- Only the centres of the packed objects have to be contained inside the unit cell.
- No overlaps between the objects in the unit cell and neighbouring unit cells.

Theorem

Two convex polyhedra do not intersect if and only if there exists a separating plane which is either parallel to a face of one polyhedron or which is parallel to at least one edge of each polyhedron.

- A consequence of Minkowsky's *Separating hyperplane theorem*
- A and B do not overlap $\Leftrightarrow$ orthogonal projections of A and B onto the normal of the separating hyperplane (separating axis) do not overlap.
- For two general polyhedrons with the same number of faces (F) and edges (E) there are $2F + E^2$ potential separating axes.
- Limits the overlap check only to convex sets.

We implemented the Torquato-Jiao packing algorithm in Julia programming language with a modification in the unit cell adaptation acceptance rate:

$$P(\mathcal{K}_t \leftarrow \mathcal{K}_{new}) = \begin{cases} 1 & \text{if } \Delta\rho > 0 \\ e^{\frac{-\Delta\rho}{T_t}} & \text{if } \Delta\rho \leq 0 \end{cases}$$

where $\Delta\rho = \rho(\mathcal{K}_{new}) - \rho(\mathcal{K}_t)$.

Preliminary results

Tetrahedra packing

Left:Initial density 0.06415, **Right**: Output density 0.67045.

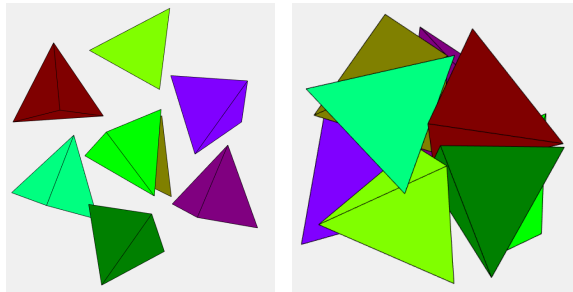


Figure: Single unit cell

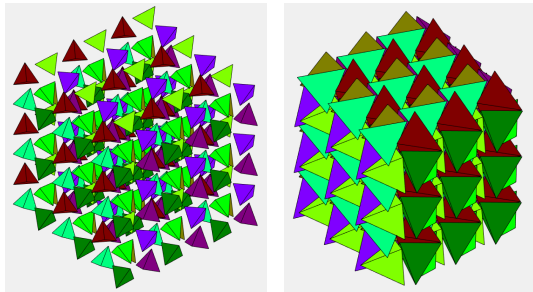


Figure: 27 unit cells

Currently the best achieved density is 0.856347

Preliminary results

Octahedra packing

Left:Initial density 0.1667, **Right**: Output density 0.9178.

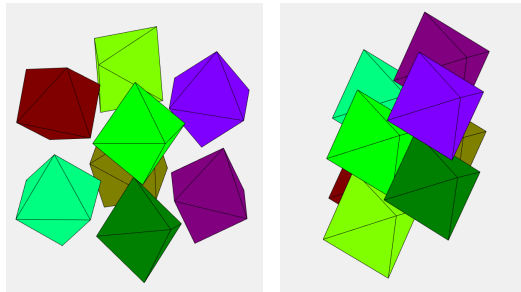


Figure: Single unit cell

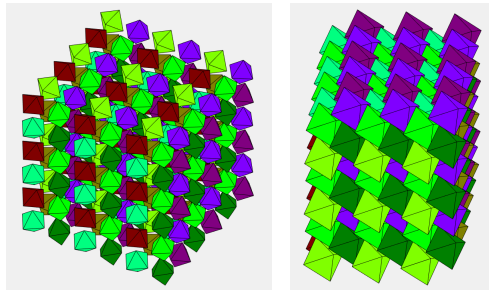


Figure: 27 unit cells

Optimal lattice packing density 0.9474.

Preliminary results

Pentacene modelling

- From a CSP dataset containing 586 pentacene structures we computed minimum euclidean distance between pentacene molecules within every crystal structure. $\min \texttt{dist} = 0.5573$
- Around every pentacene atom we put 14 points uniformly placed on a sphere with the radius $0.5573/2$.
- Computed the convex hull of the resulting point cloud.
- Resulting polyhedron defined by a triangulation with 58 vertices, 112 edges, 168 faces.

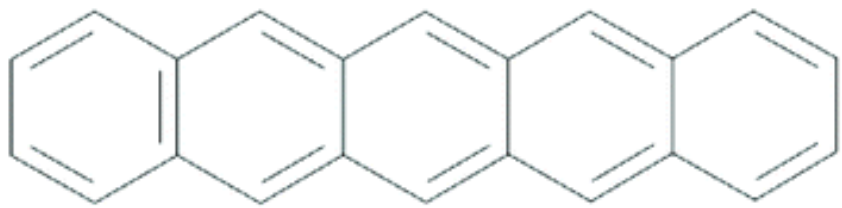
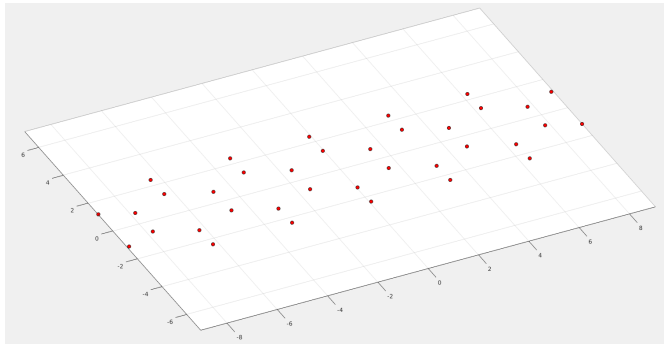


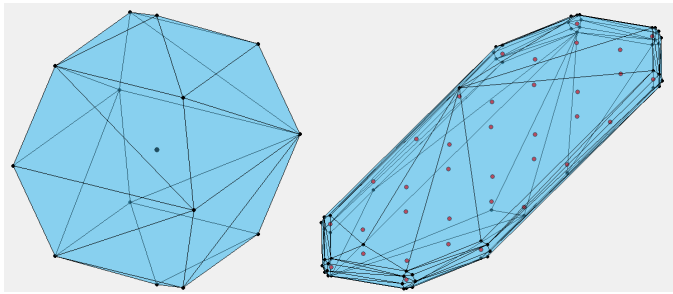
Figure: Pentacene

Preliminary results

Pentacene modelling



(a)

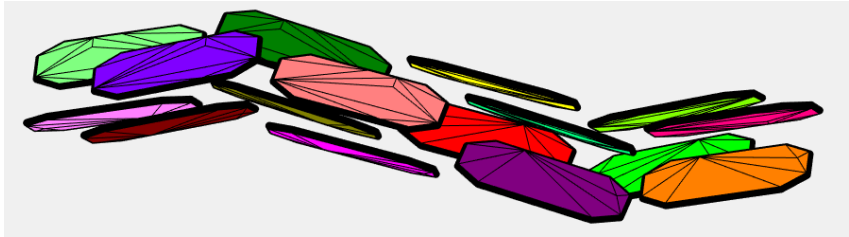


(b) (c)

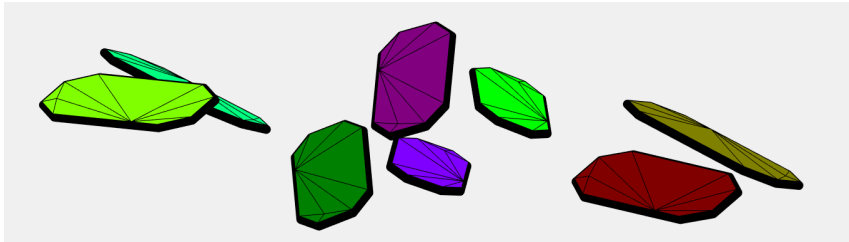
Figure: (a) Centers of atoms of pentacene. (b) 14 points placed on a sphere with radius 0.5573/2. (c) Convex hull of the resulting point cloud with centres of pentacene atoms inside (red).

Preliminary results

Pentacene modelling



(a)

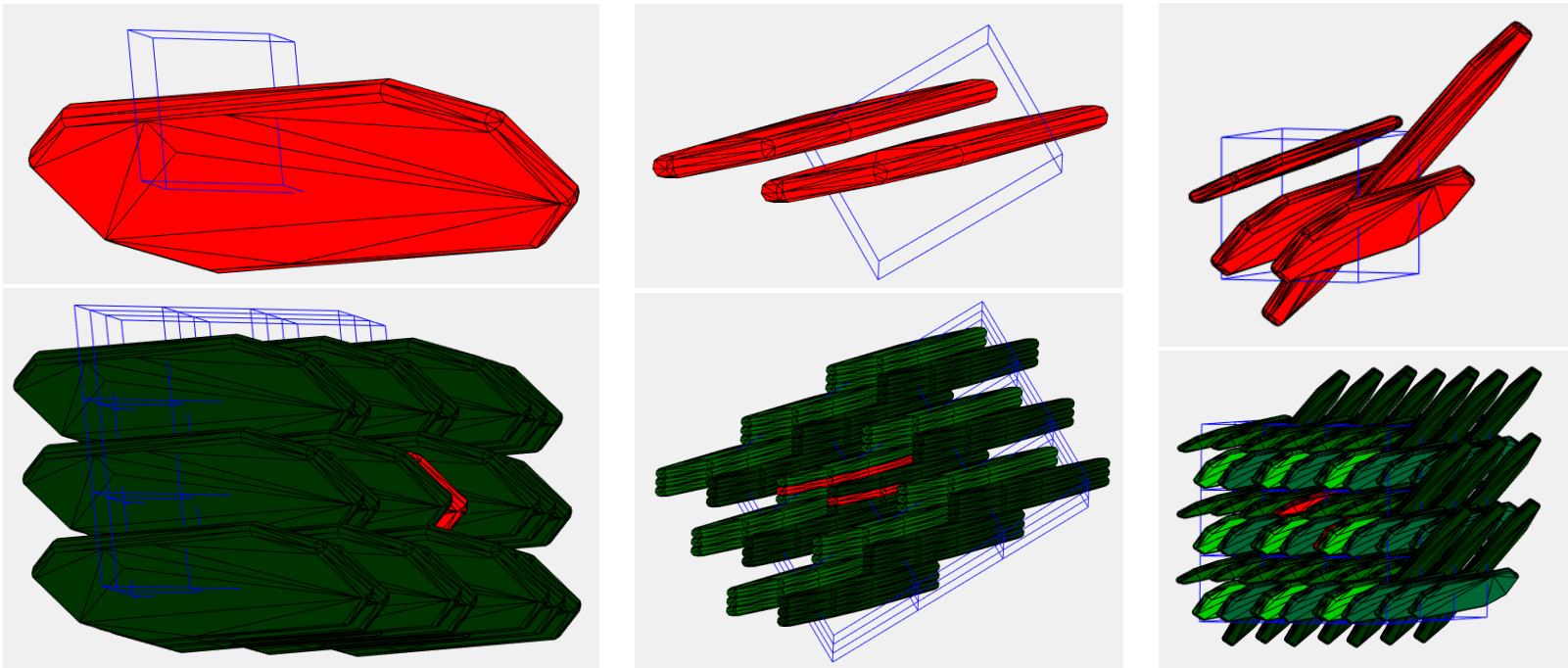


(b)

Figure: (a) A model of the pentacene crystal structure from the CSP dataset. (b) The crystal structure where the minimum distance between two pentacene molecules is attained.

Preliminary results

Pentacene packing

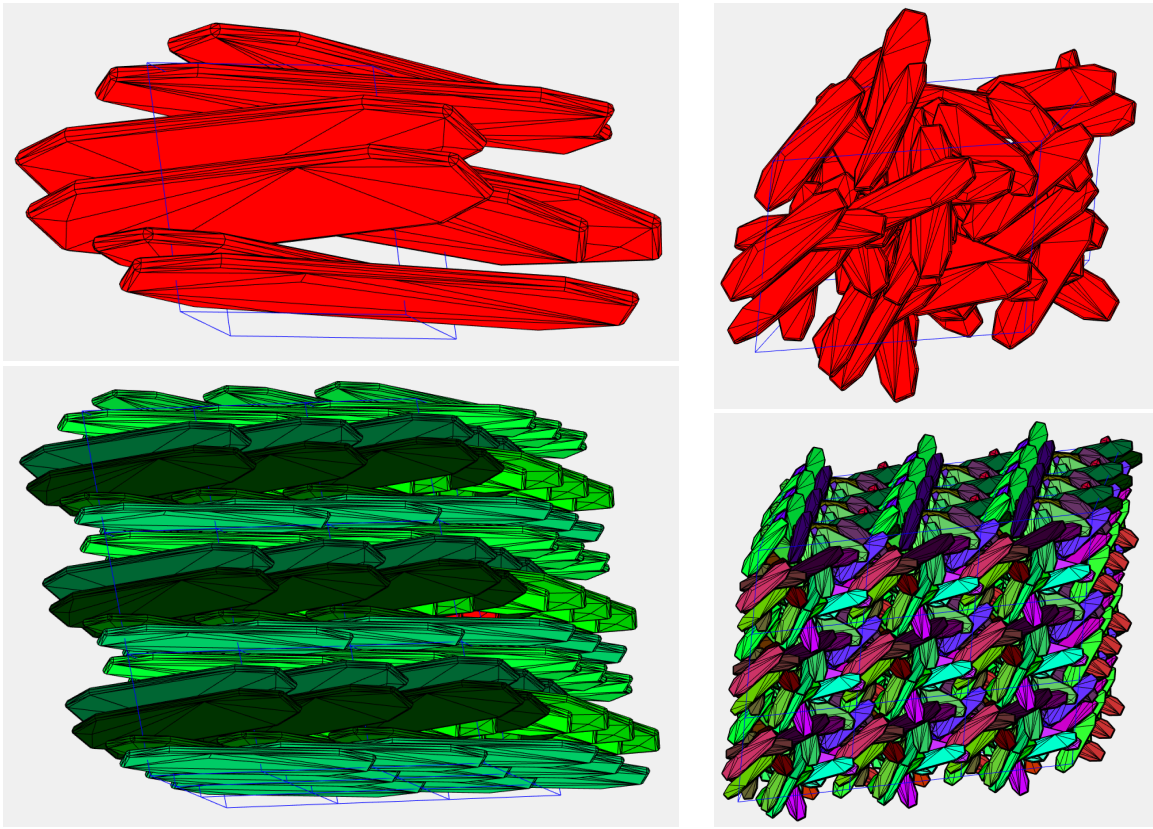


(a) (b) (c)

Figure: Densities of packings of (a) 1 $\rho \approx 1$, (b) 2 $\rho \approx 1$, (c) 4 $\rho = 0.8093$ pentacene models.

Preliminary results

Pentacene packing



(a) (b)

Figure: Densities of packings of (a) 8 $\rho = 0.6940$ and (b) 54 $\rho = 0.1521$ pentacene models.

The model:

- $\Lambda = \left\{ p_1 u_1 + p_2 u_2 \mid p_1, p_2 \in [0,1]; u_1, u_2 \in \mathbb{R}^2 \right\}$ a unit cell defined by the set of generators $\overline{\Lambda} = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}$
- $T_0 = \left\{ \phi_1 \binom{1}{0} + \phi_2 \binom{0}{1} - \binom{\frac{1}{3}}{\frac{1}{3}} \mid 0 \leq \phi_1 + \phi_2 \leq 1 \right\}$ a 2-simplex centred at the origin.

The model (continued):

- N copies of T_0 translated by $c_k \in \mathbb{R}^2$ and rotated by $R_k \in SO(2)$:

$$T_k = \left\{ \overline{\Lambda} c_k + R_k p_0 \mid p_0 \in T_0 \right\}$$

where $c_k = \begin{pmatrix} x^k \\ y^k \end{pmatrix} \in [0,1] \times [0,1]$ and $R_k = \begin{pmatrix} \cos\theta_k & -\sin\theta_k \\ \sin\theta_k & \cos\theta_k \end{pmatrix}$ for $k = 1, 2, \ldots, N$ and $\theta_k \in [0, 2\pi]$.

- Translates $T_k^{i,j}$ of T_k in the neighbouring unit cells

$$T_k^{i,j} = \left\{ \overline{\Lambda} \begin{pmatrix} i \\ j \end{pmatrix} + p_k \mid p_k \in T_k \right\}$$

for $i, j \in \{-2, -1, 0, 1, 2\}$.

Problem statement:

$$\min \mathtt{obj} = \min \mathtt{vol}(\Lambda) = \min \det(\overline{\Lambda}) = \min u_{11}u_{22} - u_{12}u_{21}$$

as a function of $4 + 3N$ variables i.e
$\mathtt{obj}(u_{11}, u_{12}, u_{21}, u_{22}, c_1, \ldots, c_N, \theta_1, \ldots, \theta_N)$, subject to

$$c_i \in [0,1] \times [0,1];\ \ i = 1, 2, \ldots, N$$
$$\mathtt{Int}(T_k) \cap \mathtt{Int}(T_l^{i,j}) = \emptyset$$

where $\mathtt{Int}(\cdot)$ is the interior of a set, $k, l = 1, 2, \ldots, N$,
$i, j = -2, -1, 0, 1, 2$, excluding the case when $l = k, i = 0, j = 0$.

Observation:

- For intersection check of two simplexes it's enough to check if the vertices of one simplex do not lie inside the other simplex.
- All simplexes are rotations and translations of T_0

- Define separating hyperplanes by

$$\alpha_h x + \beta_h y + \gamma_h = 0$$

for $h = 1, 2, 3$ where $\alpha_h, \beta_h, \gamma_h$ are given by the edges of T_0.

- Vertices of T_0:

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \in \texttt{Vert}(T_0)$$

.

- Vertices of T_k:

$$\begin{pmatrix} x_k^{0,0} \\ y_k^{0,0} \end{pmatrix} = \overline{\Lambda} c_k + R_k \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \in \texttt{Vert}(T_k)$$

- Vertices of $T_l^{i,j}$:

$$\begin{pmatrix} x_l^{i,j} \\ y_l^{i,j} \end{pmatrix} = \overline{\Lambda} \left(c_l + \begin{pmatrix} i \\ j \end{pmatrix} \right) + R_l \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \in \texttt{Vert}(T_l^{i,j})$$

- Vertices of T_k in the coordinate system of $T_l^{i,j}$:

$$\begin{pmatrix} \tilde{x}_k^{0,0} \\ \tilde{y}_k^{0,0} \end{pmatrix} = R_l^{-1} \left[\begin{pmatrix} x_k^{0,0} \\ y_k^{0,0} \end{pmatrix} - \overline{\Lambda} \left(c_l + \begin{pmatrix} i \\ j \end{pmatrix} \right) \right]$$

- Vertices of $T_l^{i,j}$ in the coordinate system of T_k:

$$\begin{pmatrix} \tilde{x}_l^{i,j} \\ \tilde{y}_l^{i,j} \end{pmatrix} = R_k^{-1} \left[\begin{pmatrix} x_l^{i,j} \\ y_l^{i,j} \end{pmatrix} - \overline{\Lambda} c_k \right].$$

$$\texttt{Int}(T_k) \cap \texttt{Int}(T_l^{i,j}) = \emptyset$$
$$\Leftrightarrow \min_{i,j,k,l} \max\{ \max_{1\leq h\leq 3} \min_{\binom{x_0}{y_0}\in \texttt{Vert}(T_0)} v_{h,k}^{0,0}, \max_{1\leq h\leq 3} \min_{\binom{x_0}{y_0}\in \texttt{Vert}(T_0)} v_{h,l}^{i,j}\} \geq 0$$

where

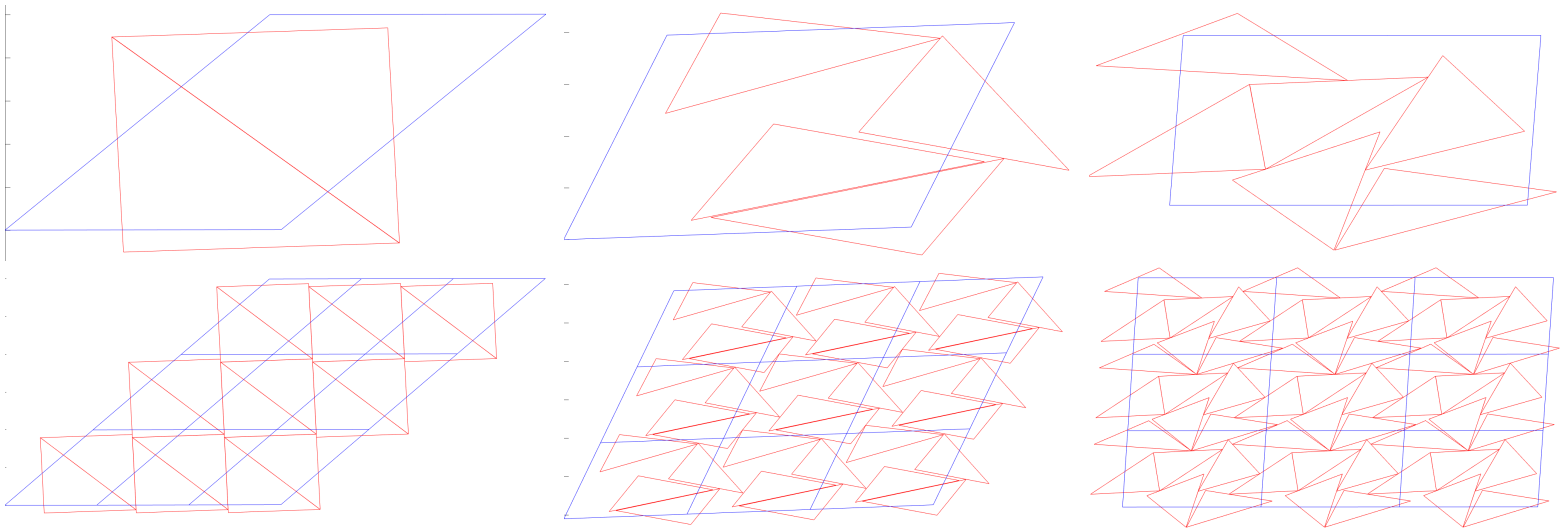
$$v_{h,k}^{0,0} = \alpha_h \tilde{x}_k^{0,0} + \beta_h \tilde{y}_k^{0,0} + \gamma_h$$
$$v_{h,l}^{i,j} = \alpha_h \tilde{x}_l^{i,j} + \beta_h \tilde{y}_l^{i,j} + \gamma_h$$

,$\alpha_h, \beta_h, \gamma_h$ are the coefficients of the separating hyperplanes of T_0 defined in previously and $k, l = 1, 2, \ldots, N$, $i, j = -2, -1, 0, 1, 2$, excluding the case when $l = k, i = 0, j = 0$.

Preliminary results

Experiments: Genetic algorithm

- Tested using Matlab's Global optimization toolbox genetic algorithm.



(a) (b) (c)

Figure: Output configurations of genetic algorithm for the packing of (a) 2 $\rho = 1$, (b) 4 $\rho = 0.6715$, (c) 6 simplexes $\rho = 0.7534$ in a unit cell.

Preliminary results

Experiments: Nonlinear constrained optimization

- Used Matlab's optimization toolbox nonlinear constrained solver
- Implements interior-point method
  - Objective function: a homogeneous polynomial of degree 2 ✓

$$\bigtriangledown \texttt{obj} = (u_{22}, -u_{21}, -u_{12}, u_{11}, 0, \ldots, 0)$$

  - Overlap constrains: continuous but only piecewise differentiable function ×
    - BFGS Hessian approximation

Preliminary results

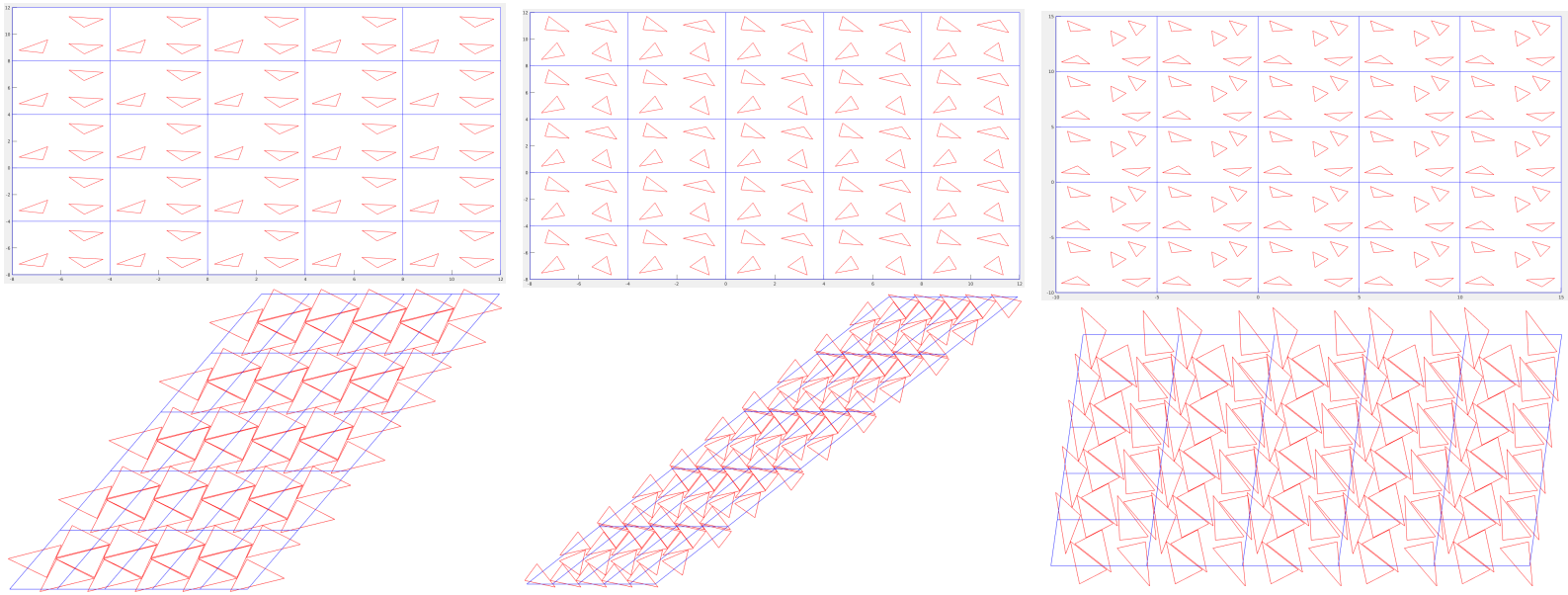
Experiments: Nonlinear constrained optimization

- Packing 2, 3, 4, 5 simplexes in a unit cell.
- 100 runs with random initial configurations (rotations) for each setting.
- Results:
  Setting with 2 simplexes generated optimal solutions but with degenerate unit cells i.e $\det(\bar{\Lambda}) \approx 0$.

Setting	Feasible solutions found	$\bar{\rho}$	$\mathtt{Var}(\rho)$	$\max \rho$
3	39	0.5827	0.0197	0.8118
4	20	0.5850	0.0127	0.7959
5	9	0.5637	0.0111	0.7246

Preliminary results

Experiments: Nonlinear constrained optimization



(a) (b) (c)

Figure: Best solutions found using nonlinear constrained optimization for (a) 3, (b) 4, (c) 5 simplexes in a unit cell. For each case initial (upper image) and output (lower image) configurations are displayed.

FUTURE WORK

1. Geometric model

- Pentacene has 4 main packing types.
- Monte-Carlo packing algorithm $\rightarrow \beta$

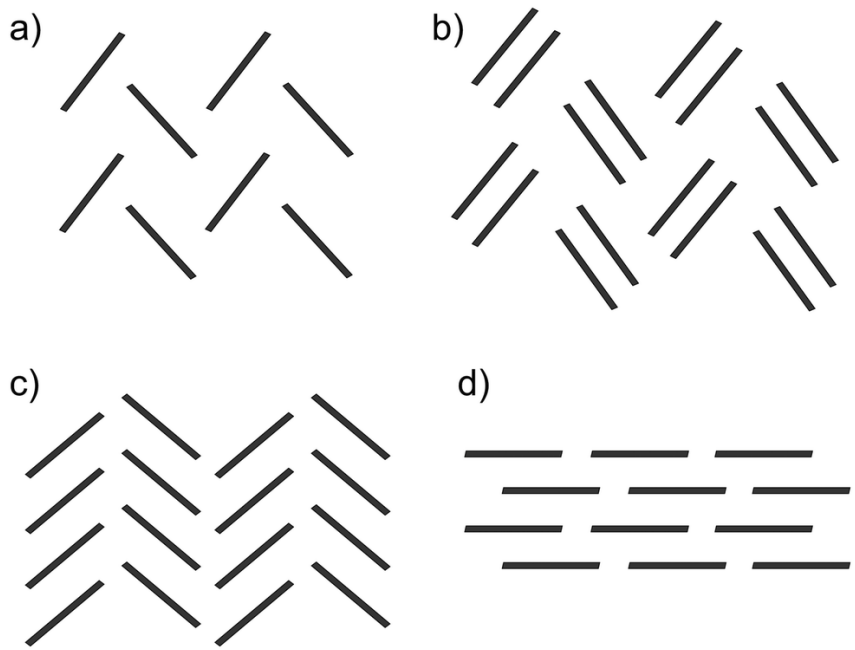


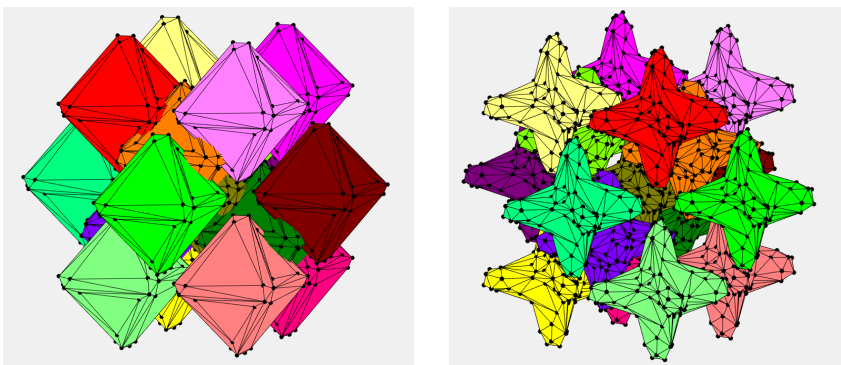
Figure: (a) herringbone; (b) sandwich herringbone; (c) γ and (d) sheet (β).

2. Optimization methods

- Decreasing packing density with increasing number of objects in the unit cell.
- Solutions depend on initial configurations.
- Complicated configuration space $\rightarrow$ Complicated objective function landscape (many hills and valleys) $\rightarrow$ Hill climbing is necessary.

3. Concavity

- Convex hulls of the organic cage molecule crystal structure overlap.
- Spectrum of α-shapes $\rightarrow$ There exists α for which the shapes do not overlap but $\alpha + \epsilon$ there is an overlap for some small ϵ.
- Overlap checks for concave sets are necessary.



(a) (b)

Figure: (a) convex hull and (b) α-shape of an organic cage molecule crystal structure.

1. Geometric model

- Make use of space-groups
- Adjust only one object in the unit cell and the unit cell itself. The rest is given by space-group symmetries (230).

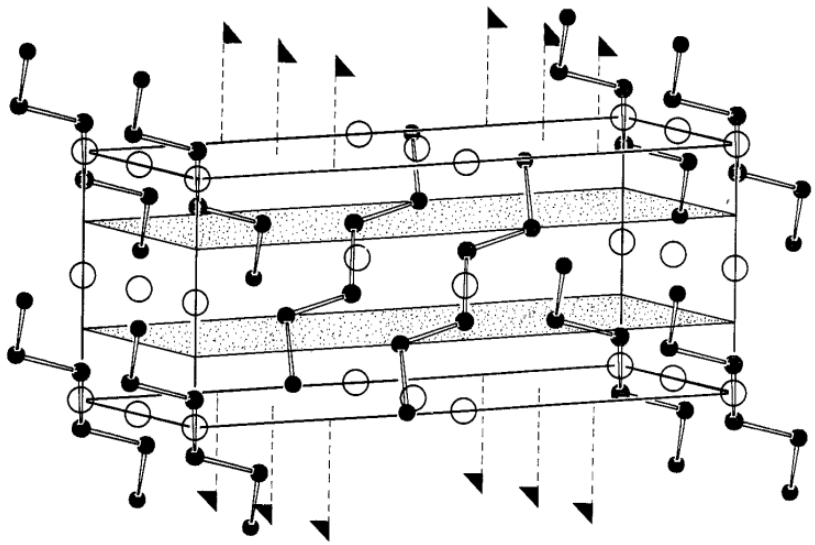


Figure: A $P2_1/c$ crystal structure and its symmetry elements with. Glide planes are emphasized by the shading.

2. **Optimisation methods**
   - Explore black box optimisation methods and replace the Simulated annealing schedule
     - Evolution strategies
       - Covariance matrix adaptation evolution strategy
       - Natural evolution strategy
3. **Concavity**
   - Implement overlap checks for concave polyhedra.
     - Convex decomposition

THANK YOU