UNIVERSITY OF LIVERPOOL

LEVERHULME TRUST

The Leverhulme Research Centre for Functional Materials Design

Aspects of Uncertainty Quantification in Materials Discovery

Miloslav Torda

Knowledge bite

diamond

Hartree Centre
Science & Technology Facilities Council

Imperial College London

ICNS

King Abdullah University of Science and Technology

University of Southampton

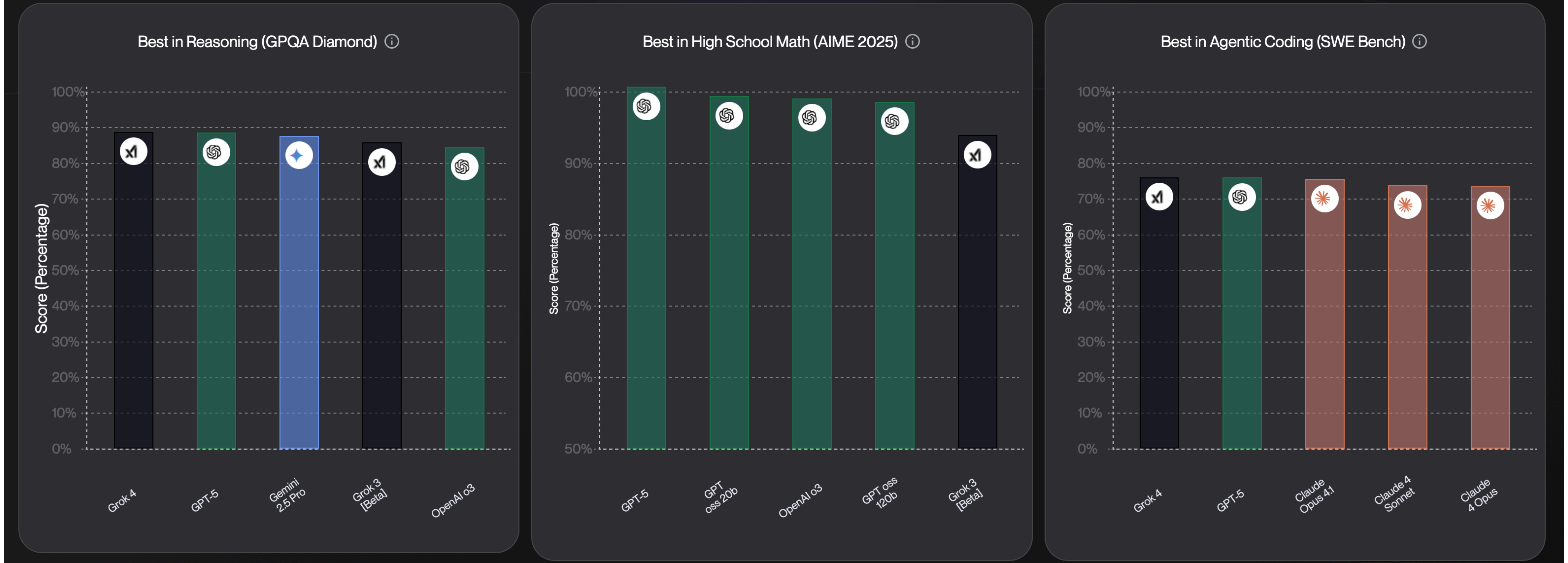
Are You Confident?

UPDATED 11 Sept 2025

LLM Leaderboard

This LLM leaderboard displays the latest public benchmark performance for SOTA model versions released after April 2024. The data comes from model providers as well as independently run evaluations by Vellum or the open-source community. We feature results from non-saturated benchmarks, excluding outdated benchmarks (e.g. MMLU). If you want to evaluate these models on your use-cases, try Vellum Evals.

Top models per tasks



Are You Confident?

write me a script visualizing an icosahedron in matlab

Thought for 39s >

Here's a compact, modern MATLAB script that builds an icosahedron from first principles (golden-ratio coordinates), then renders it nicely with lighting, vertex markers, and a wire overlay. It uses `patch` with Faces/Vertices as documented by MathWorks. MathWorks

matlab   Copy

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% Visualize a regular icosahedron with shading, edges, and vertex markers.
% Cleve-style: short, clear, and vectorized.

% Geometry (golden rectangles)
phi = (1+sqrt(5))/2;
V = [
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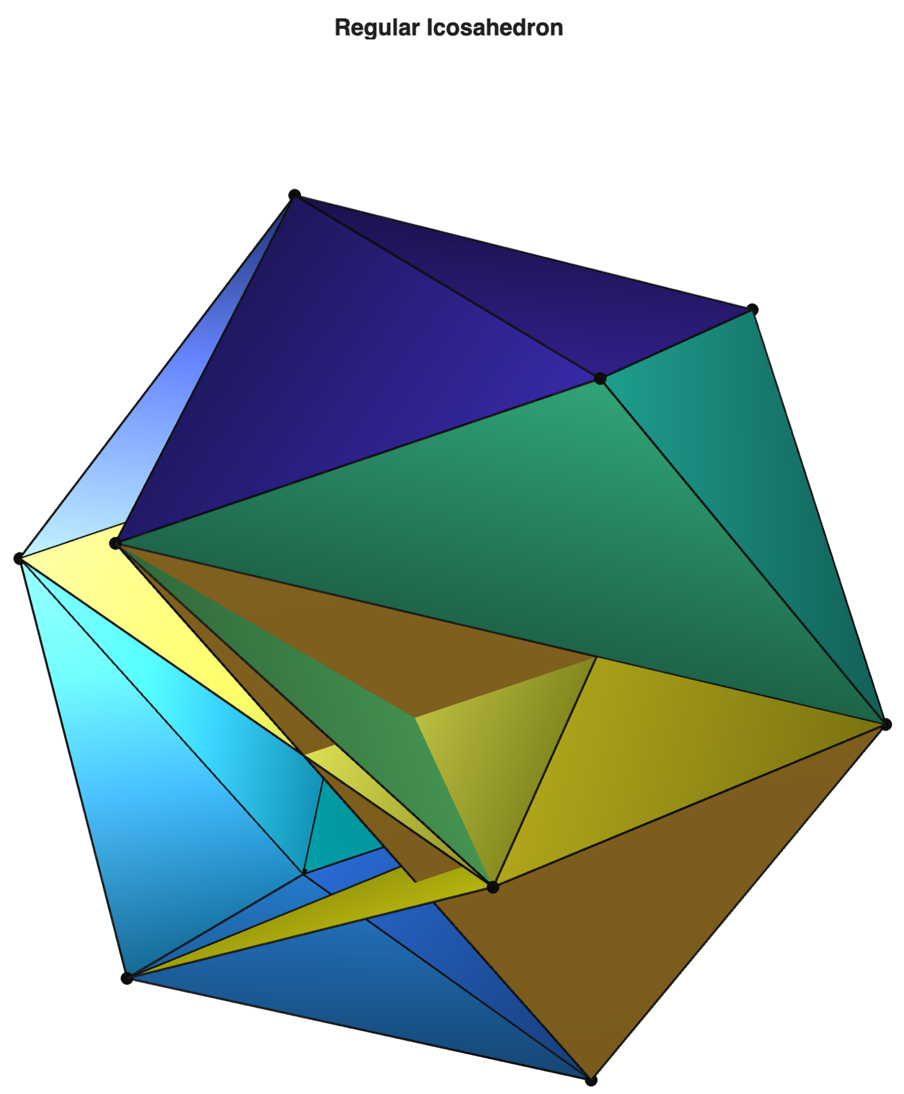

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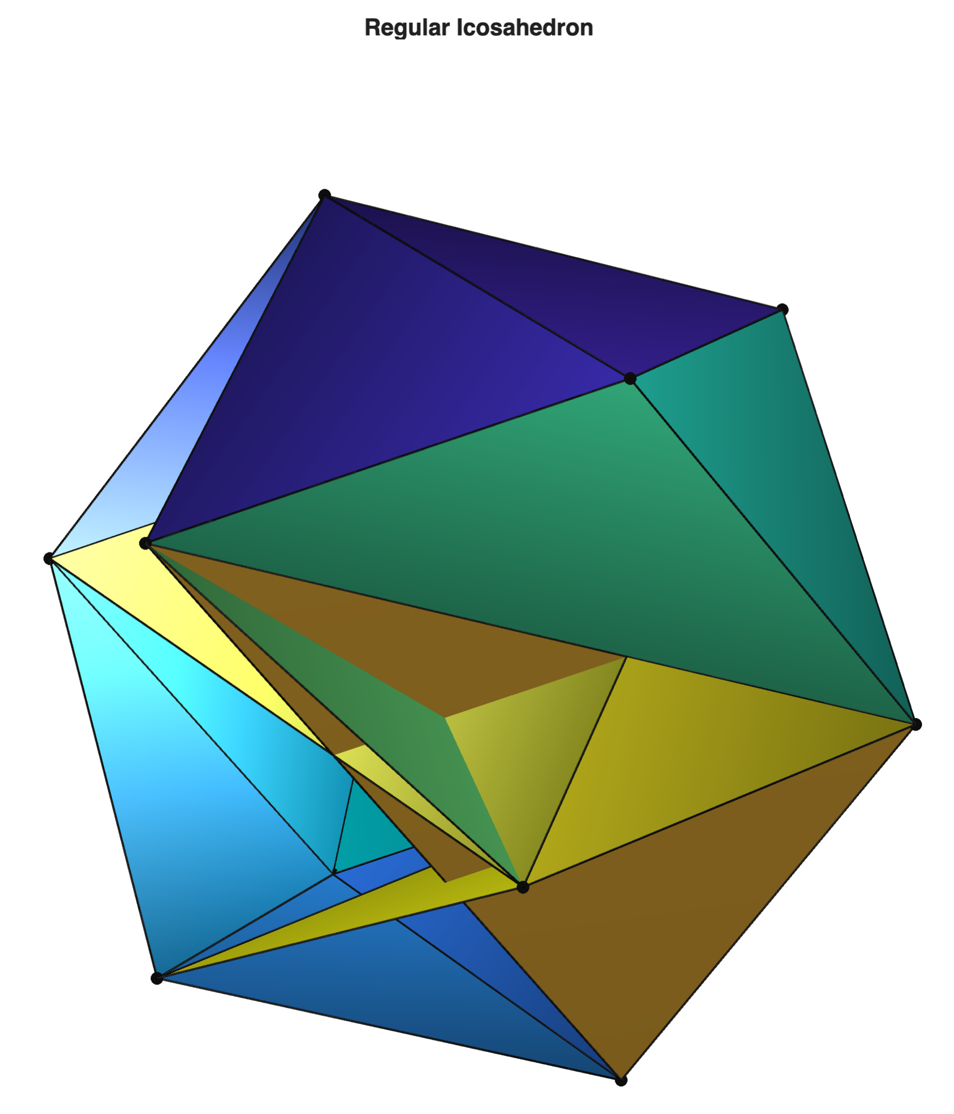

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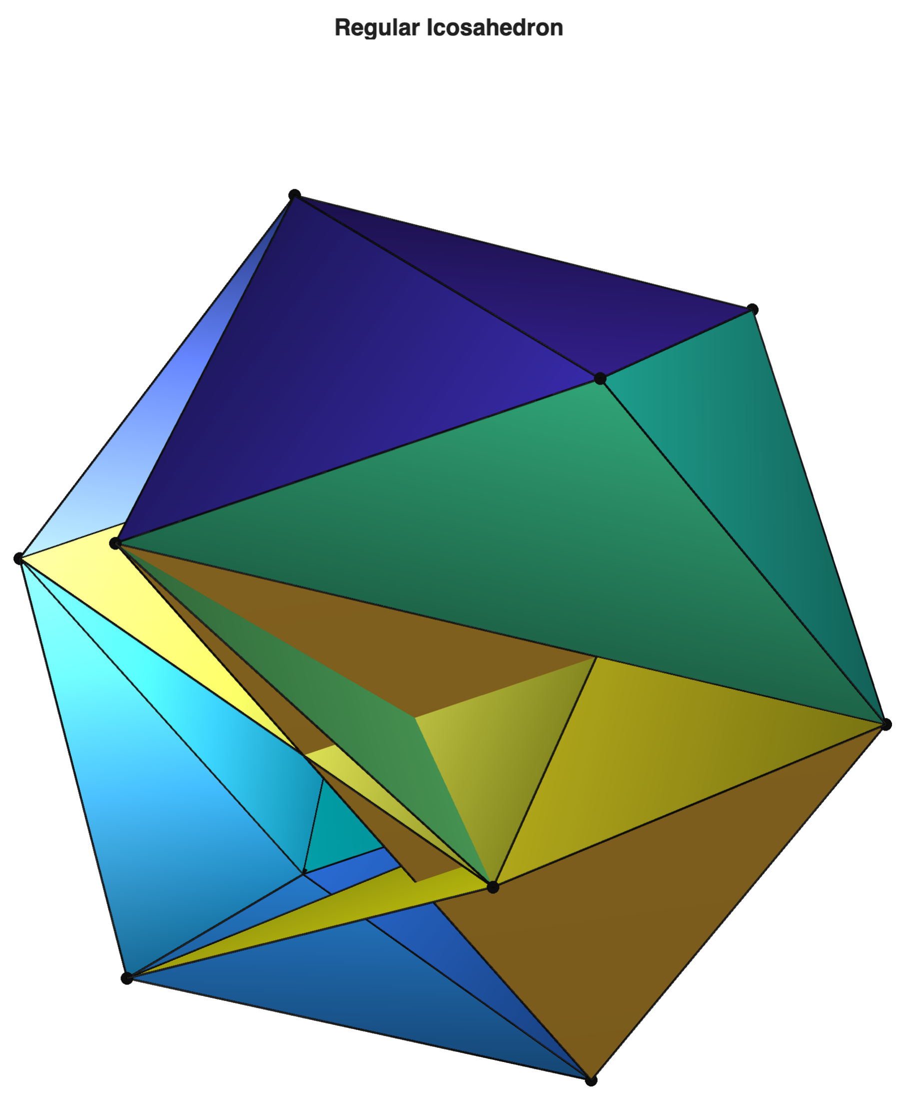

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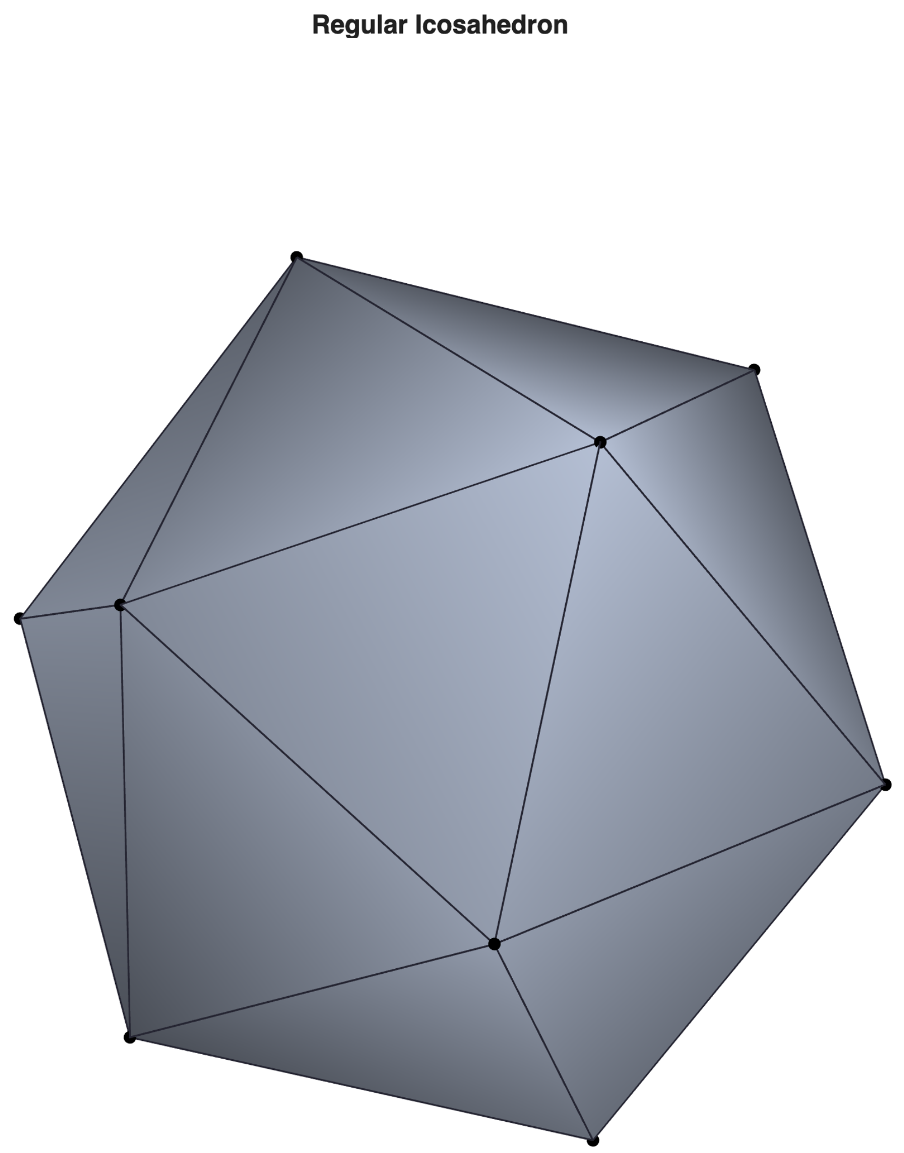

Epistemic or Systematic Uncertainties

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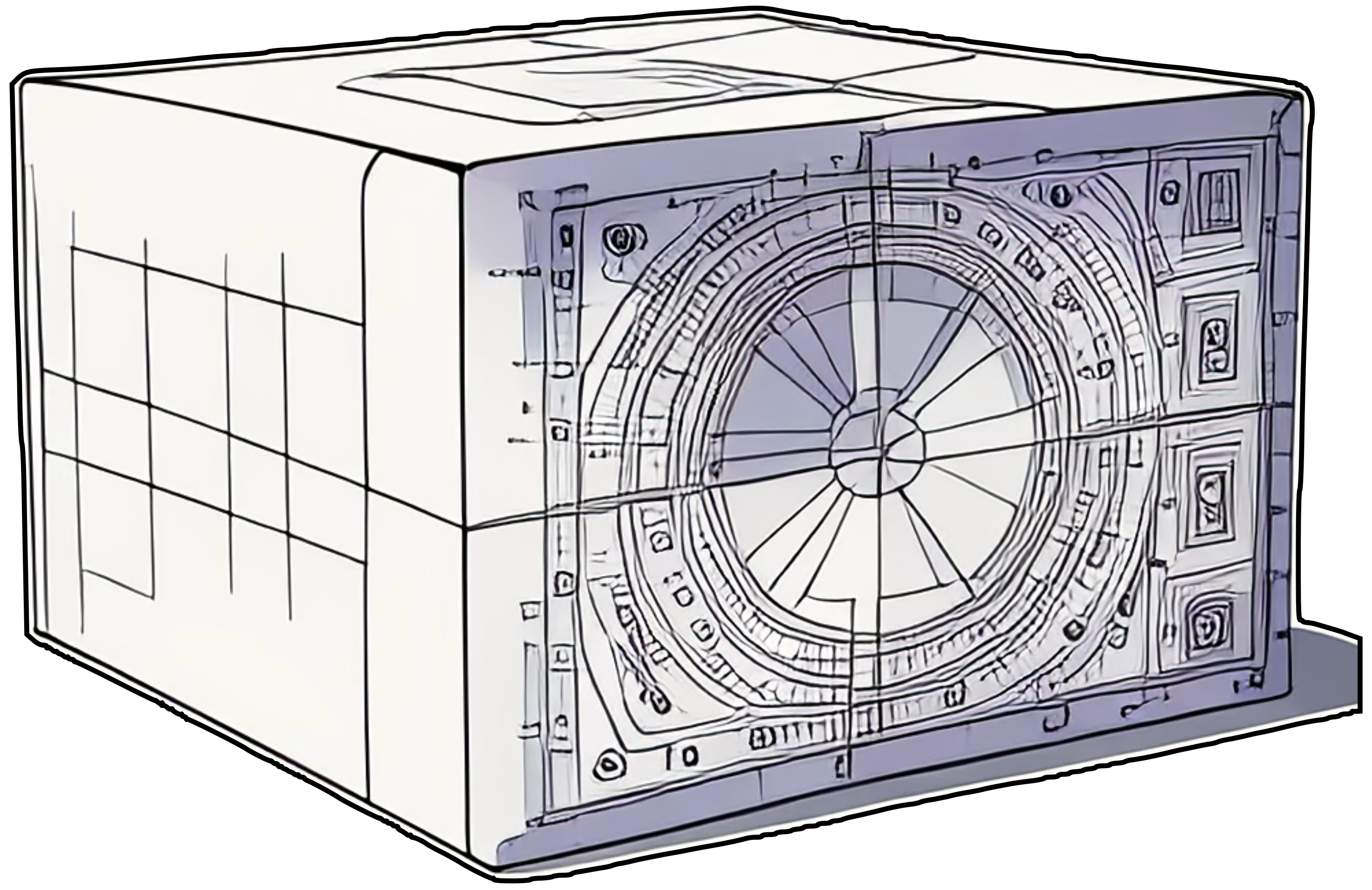

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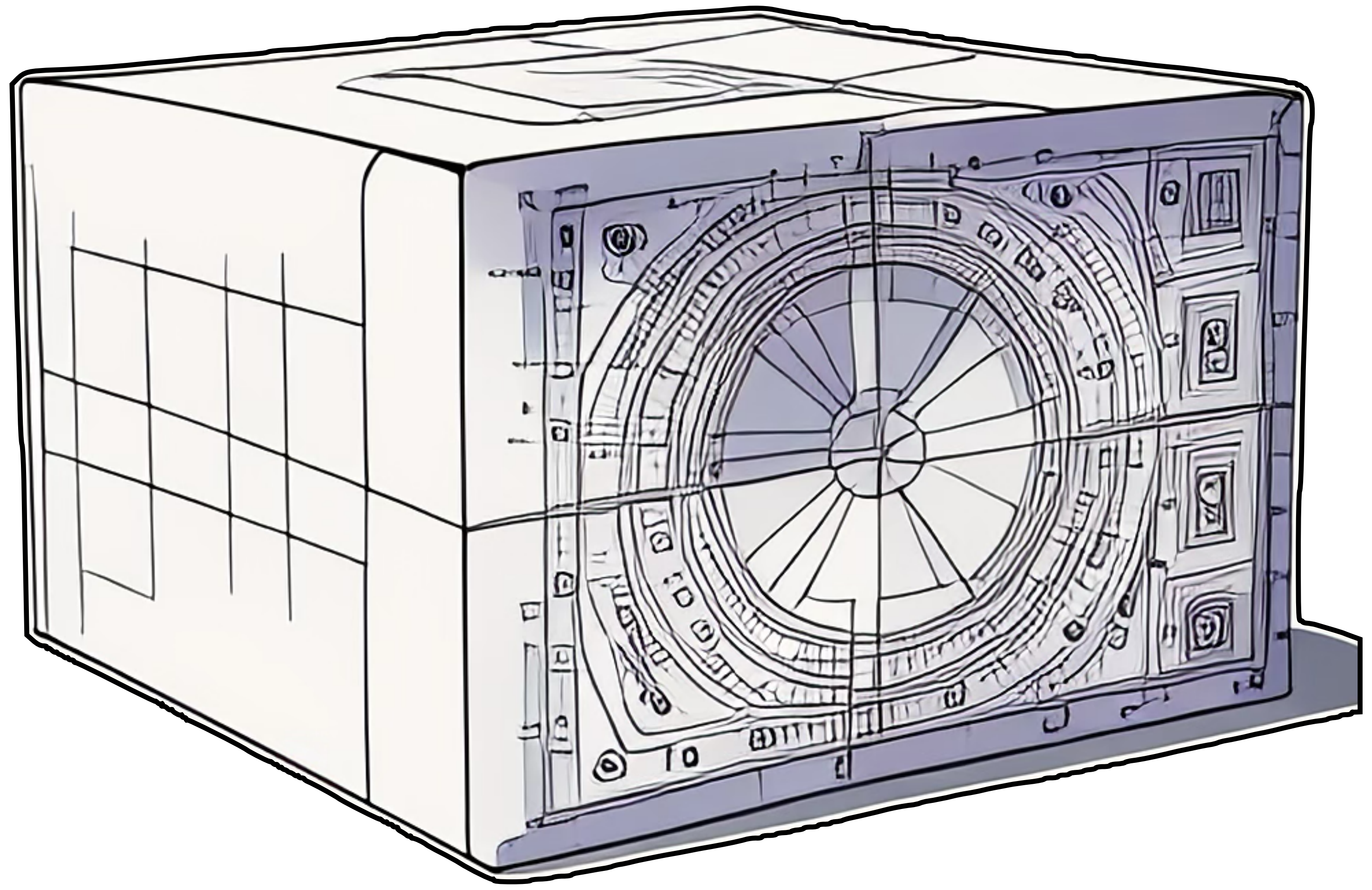

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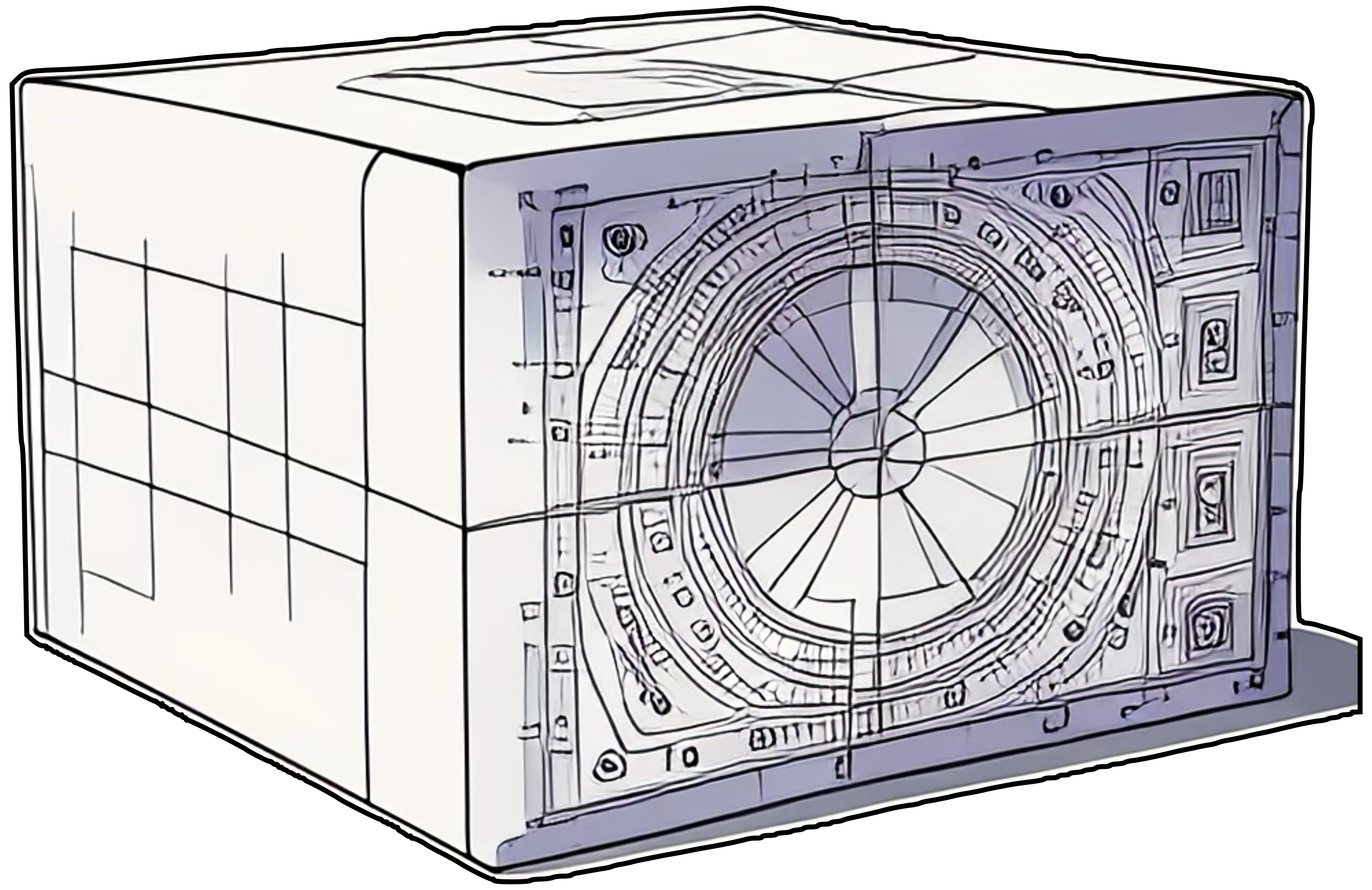

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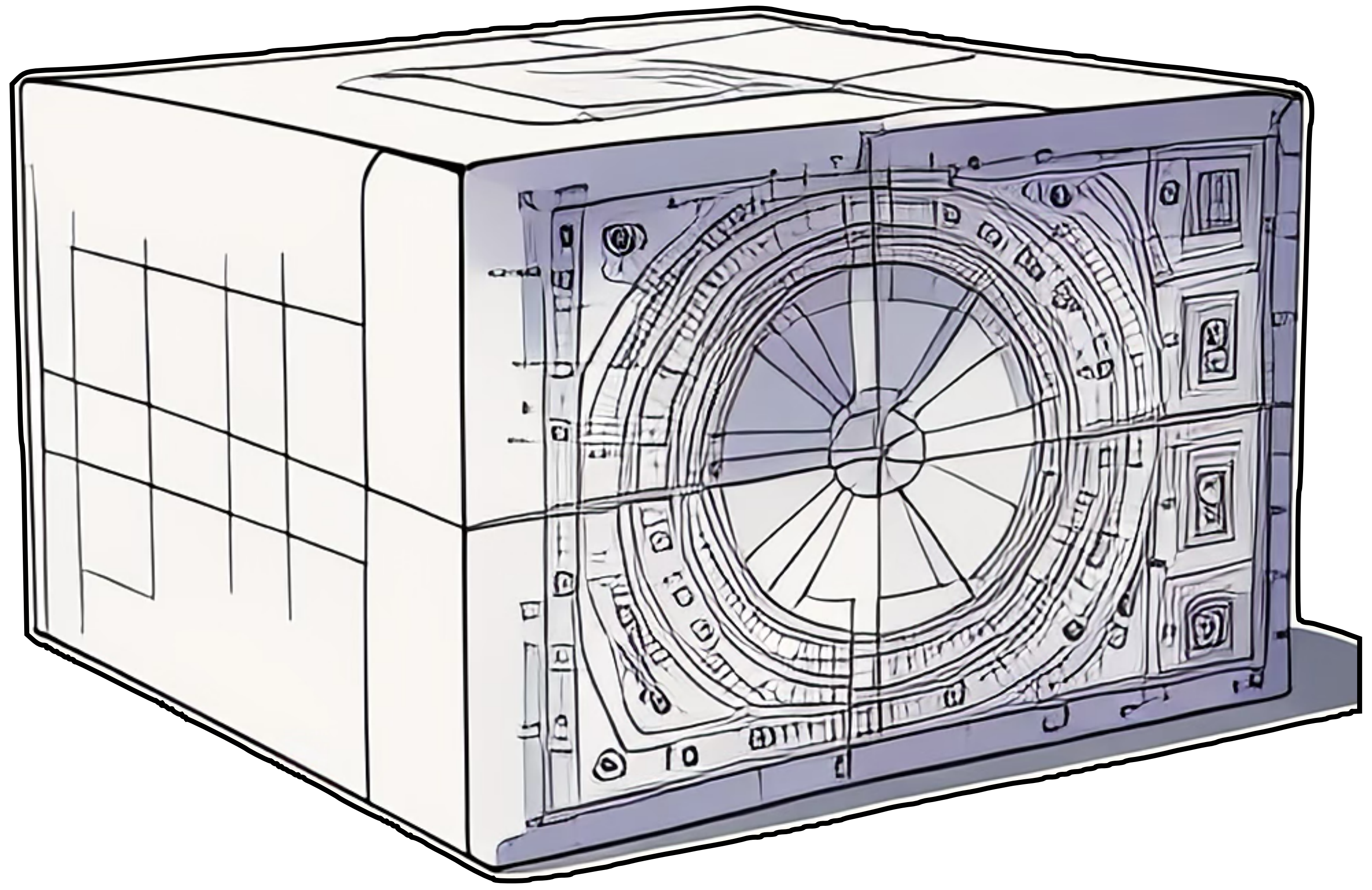

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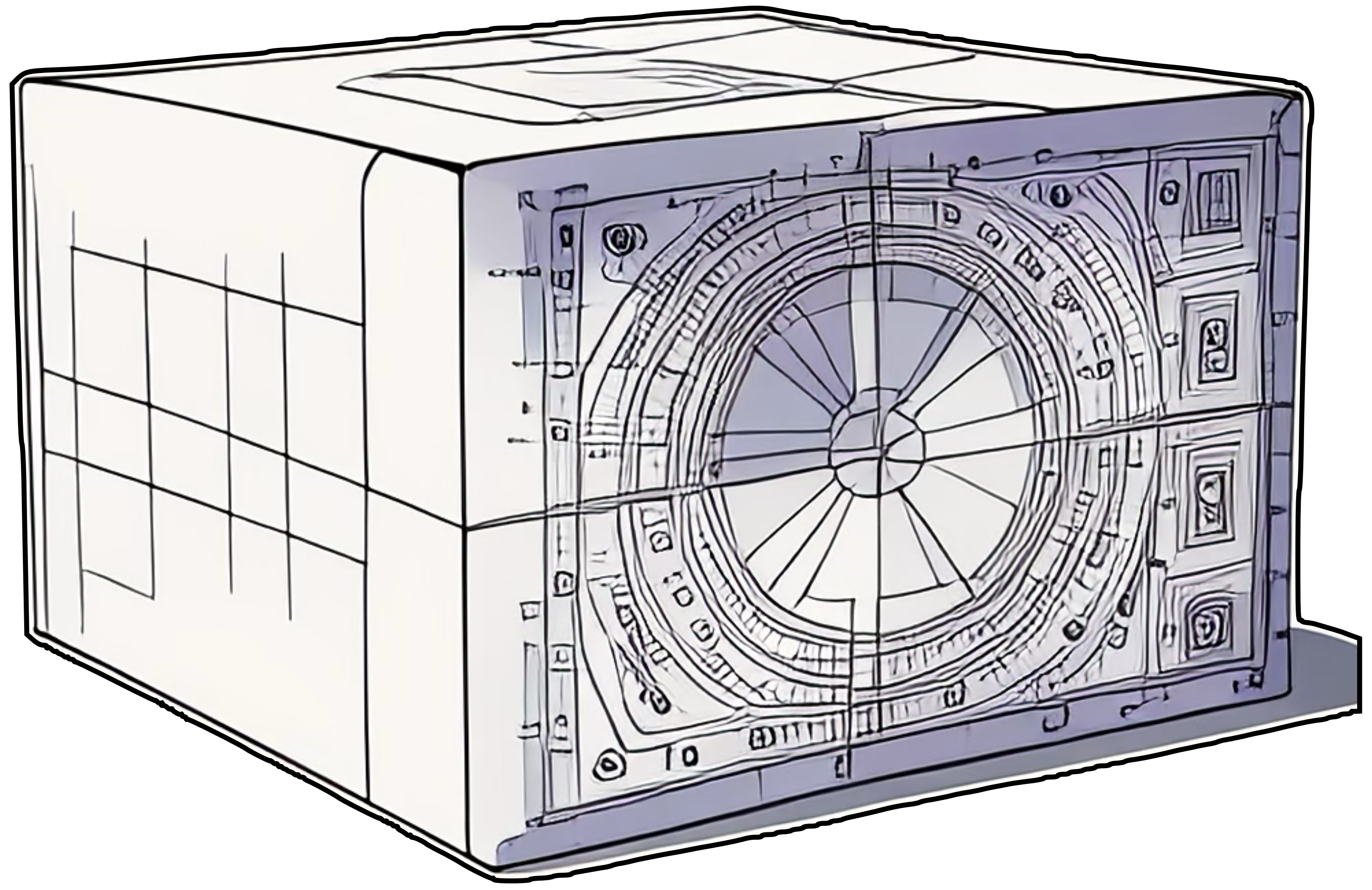

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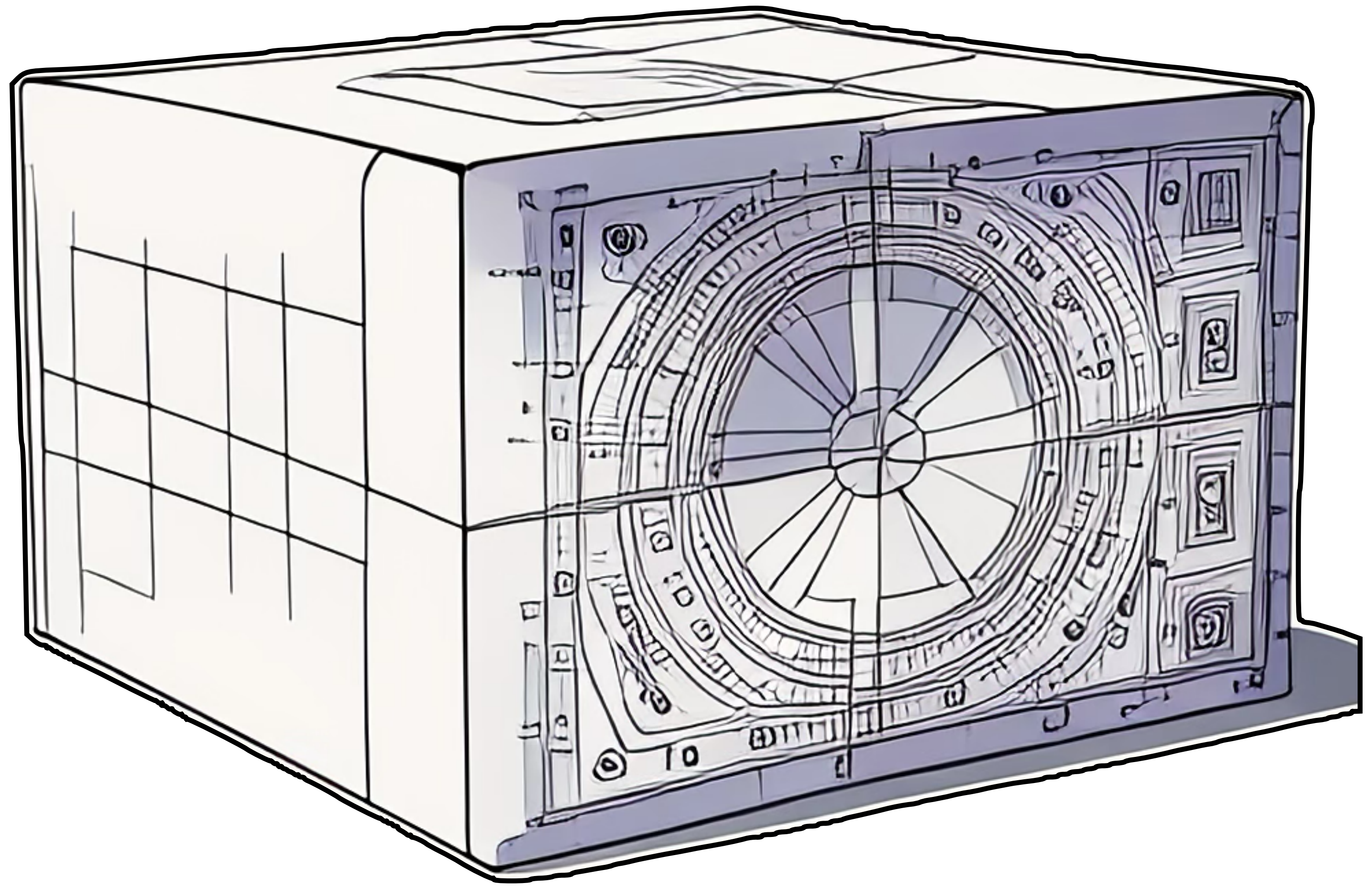

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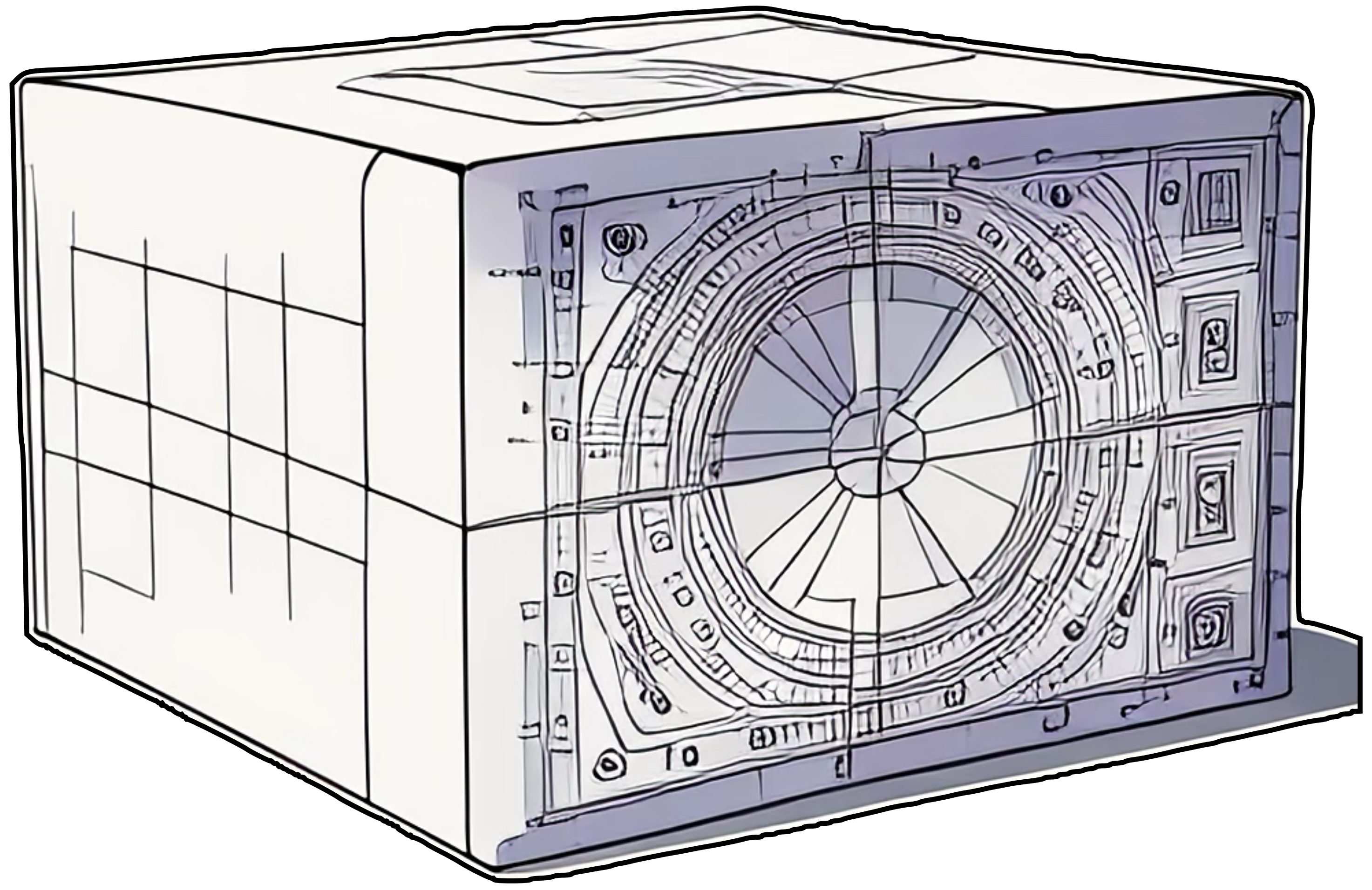

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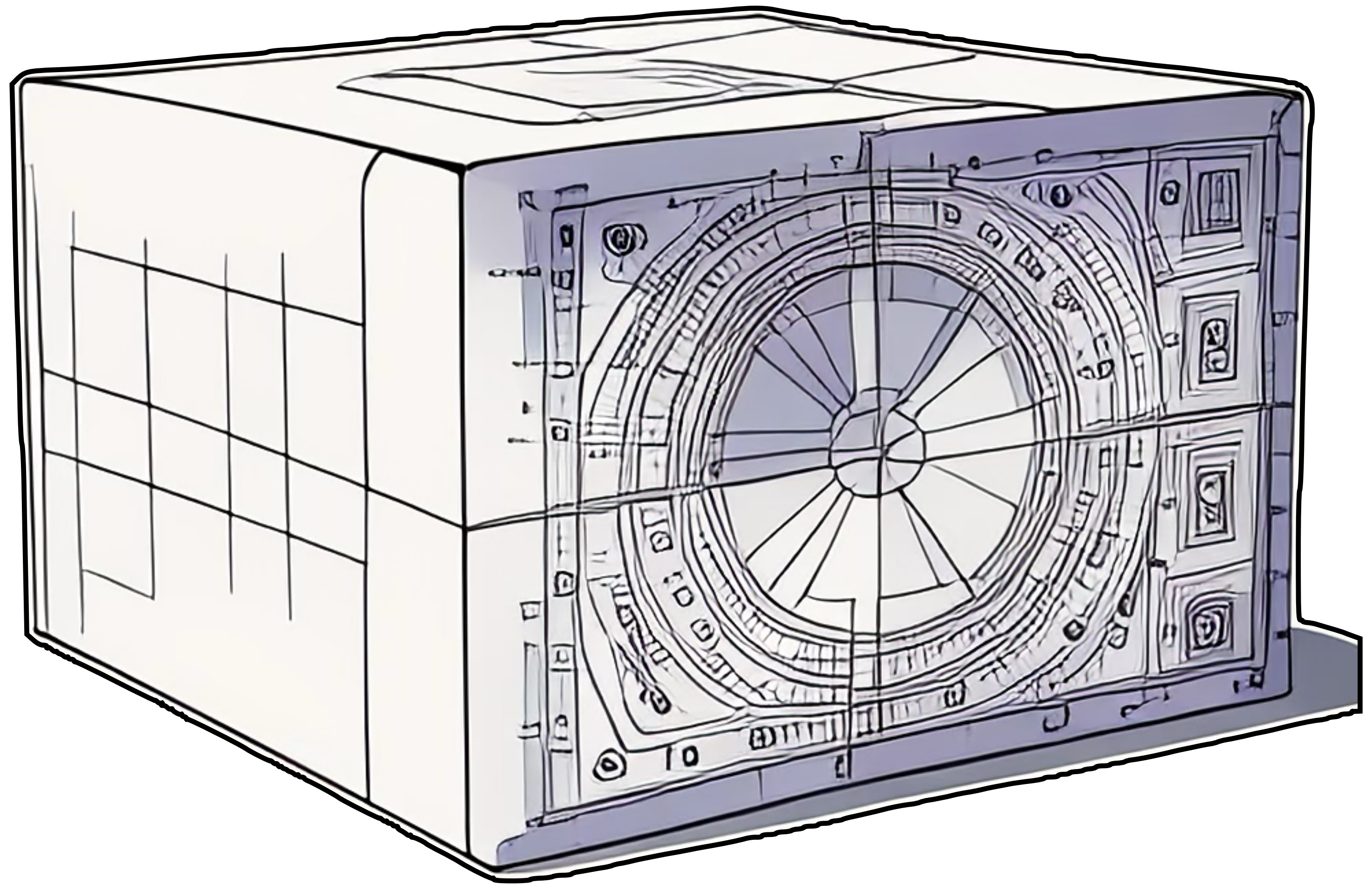

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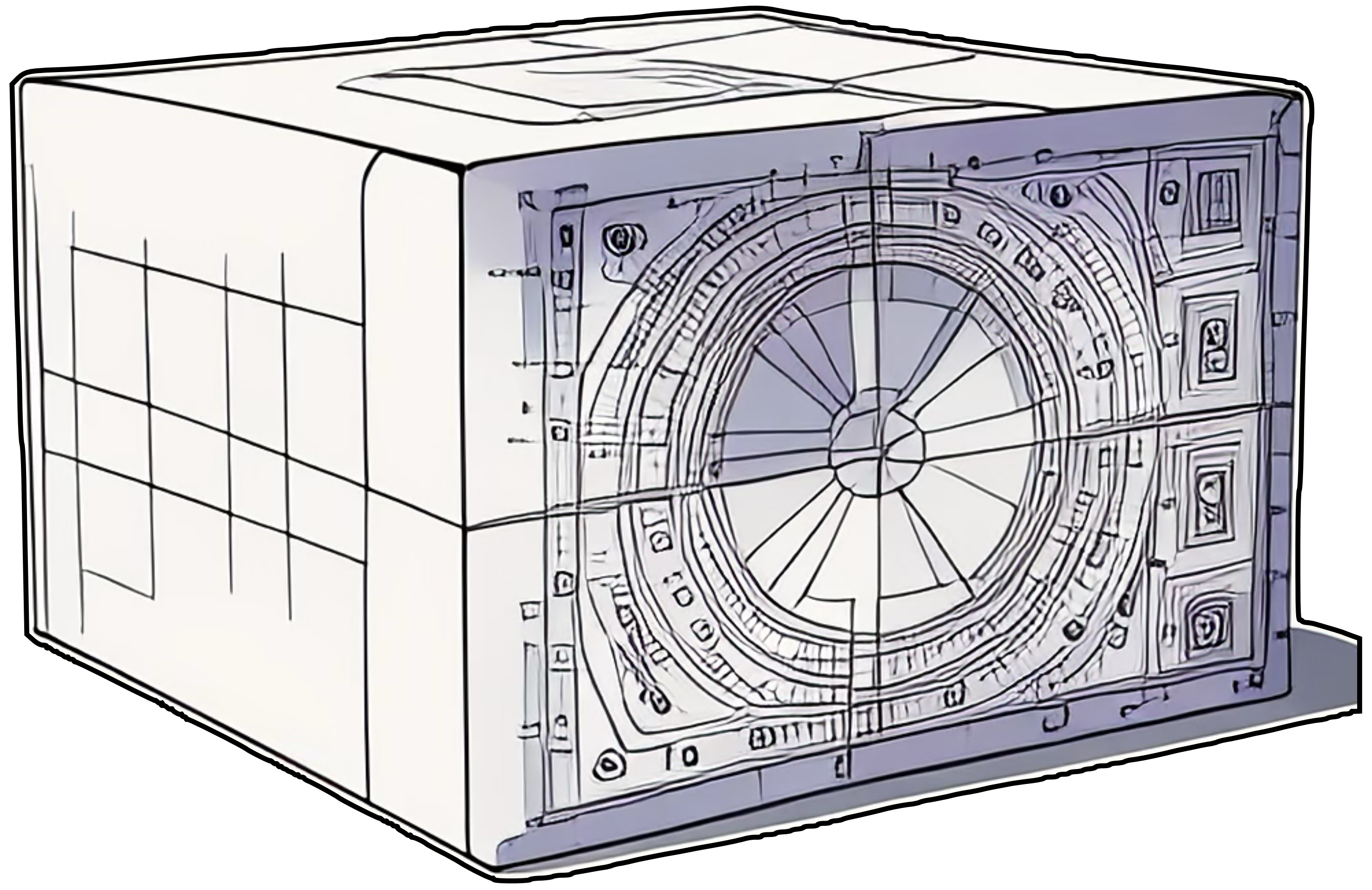
  - **Propagate systematic uncertainties through models to construct interval estimates**



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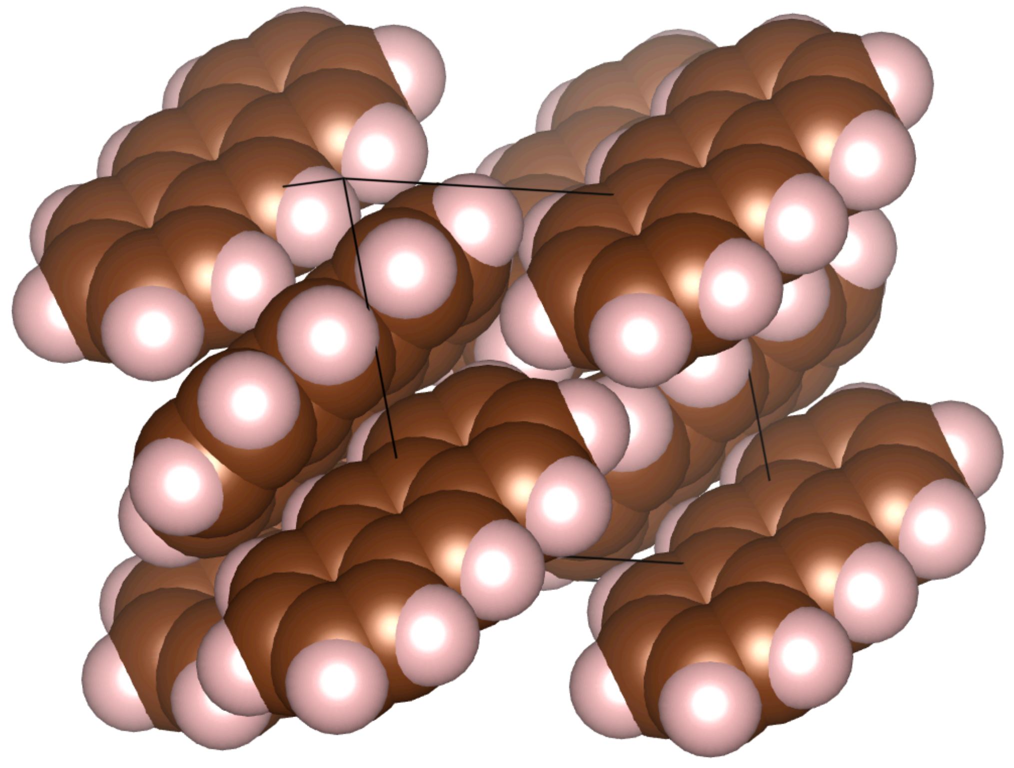
Example: Computing the Packing Coefficient

- Packing coefficient for periodic configurations: $\rho = \dfrac{\text{vol}(O)}{\text{vol}(U)}$



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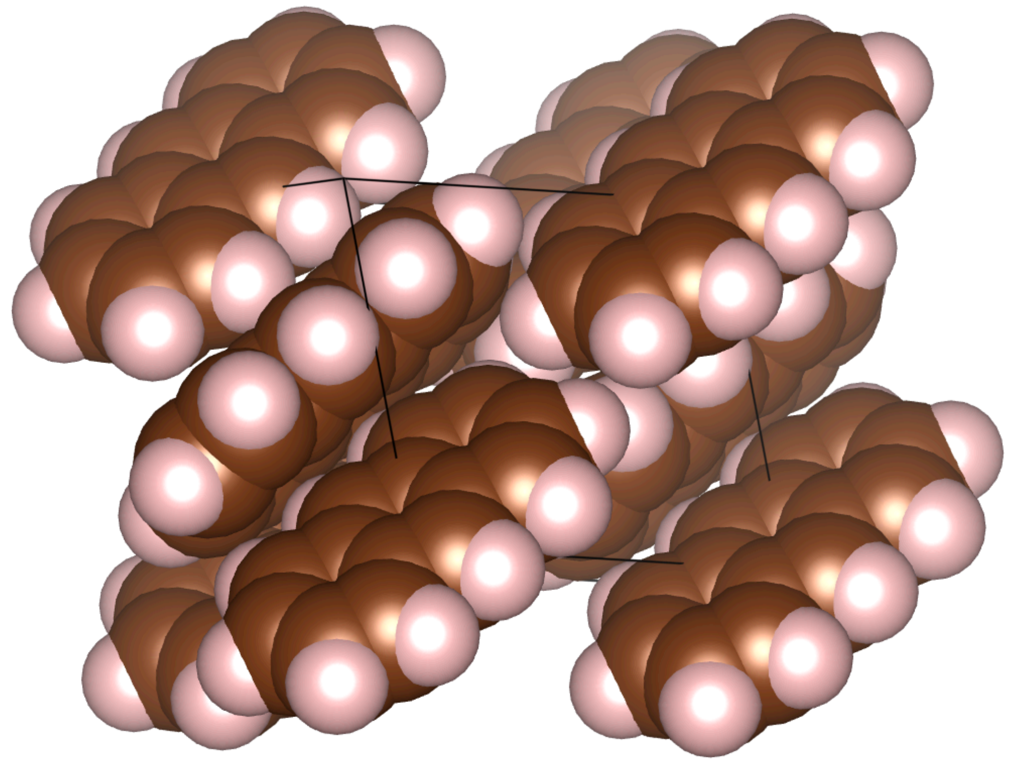

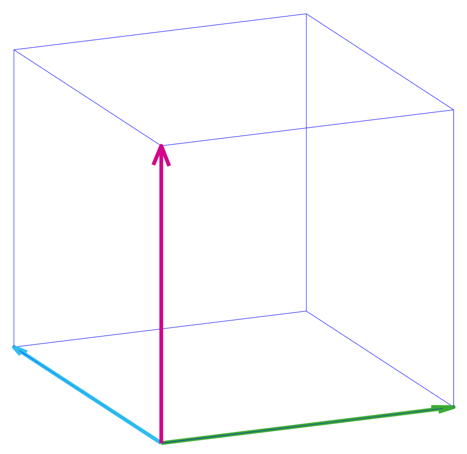

- $\text{vol}(U) = \det(U)$

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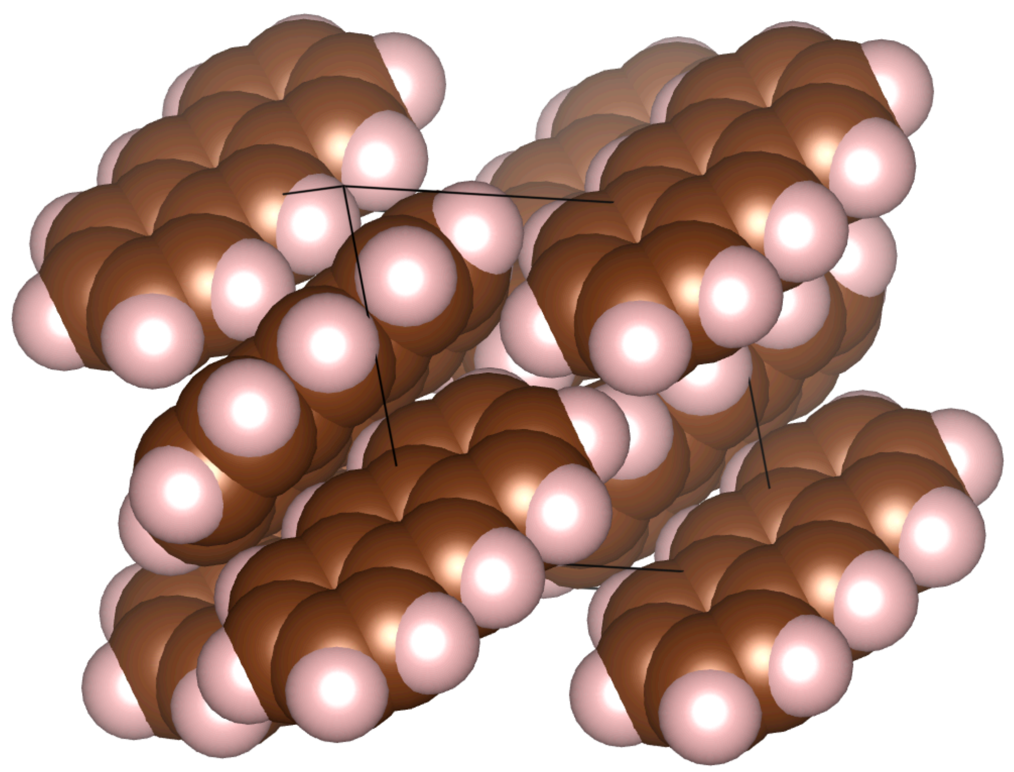

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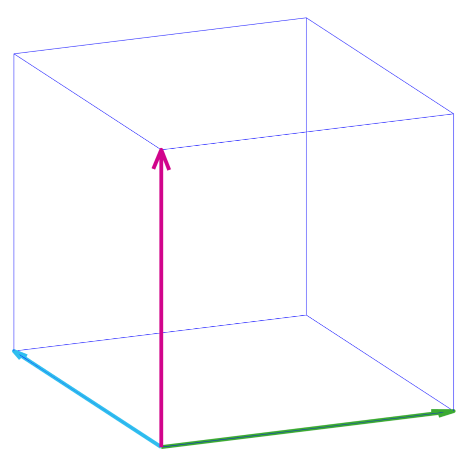

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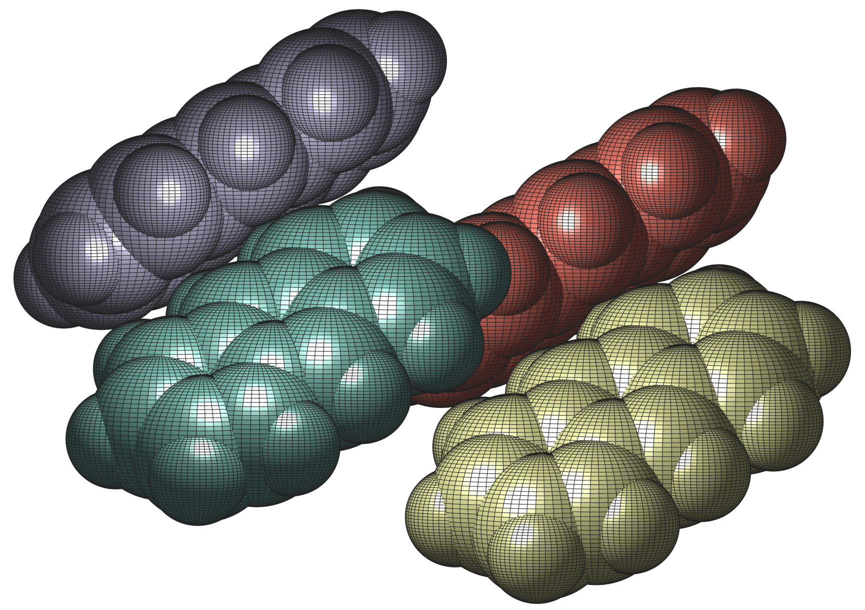

- $\mathrm{vol}(O) = \displaystyle\int_O dV$
  - **O - subset of occupied by the van der Waals spheres**
  - **dV - natural volume form on $\mathbf{R}^3$**

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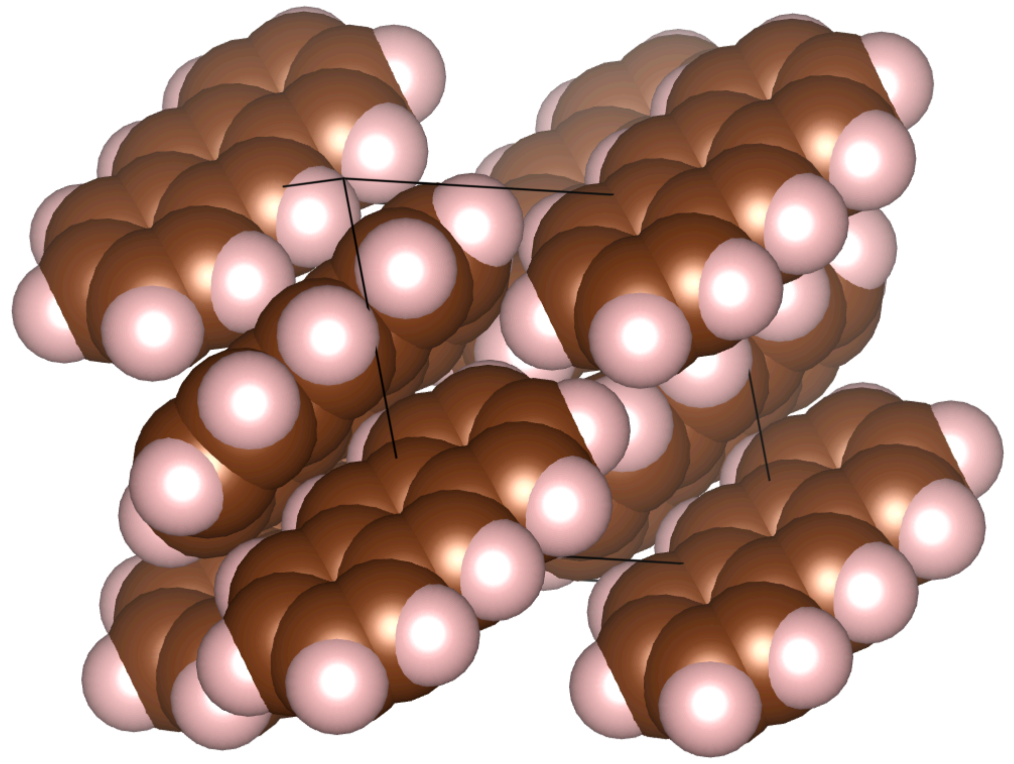

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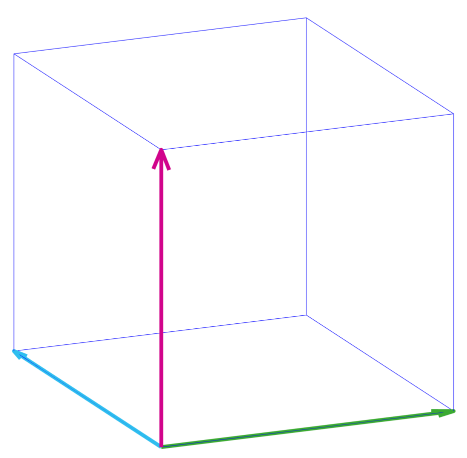

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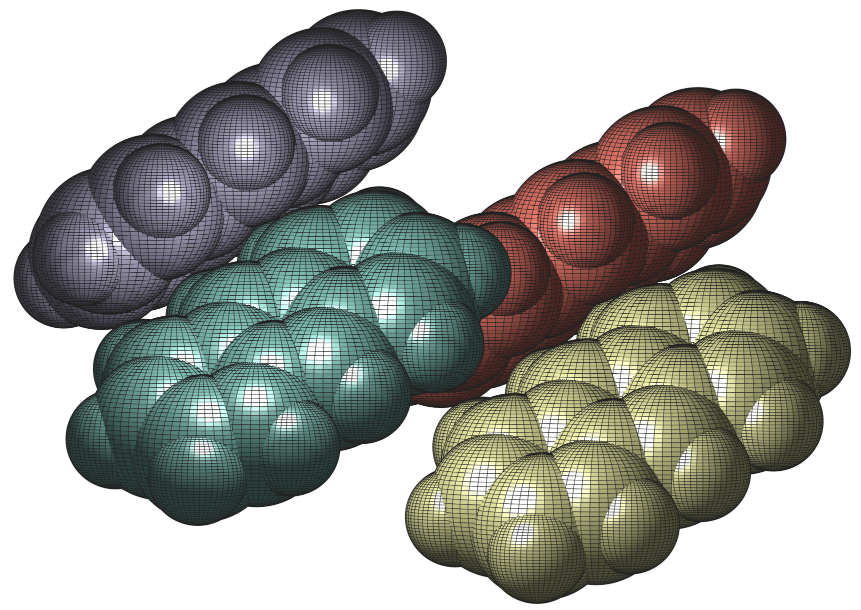

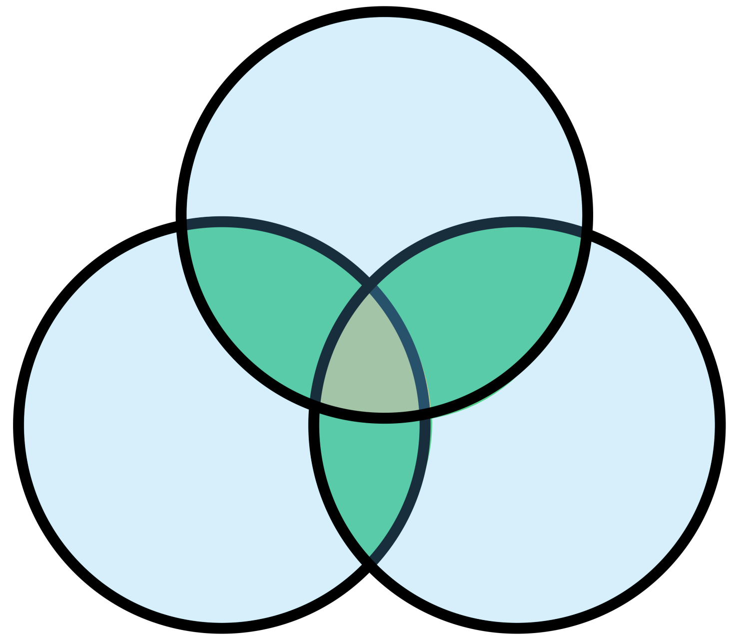

$S_1 + S_2 + S_3 - S_1 \cap S_2 - S_1 \cap S_3 - S_2 \cap S_3 + S_1 \cap S_2 \cap S_3$

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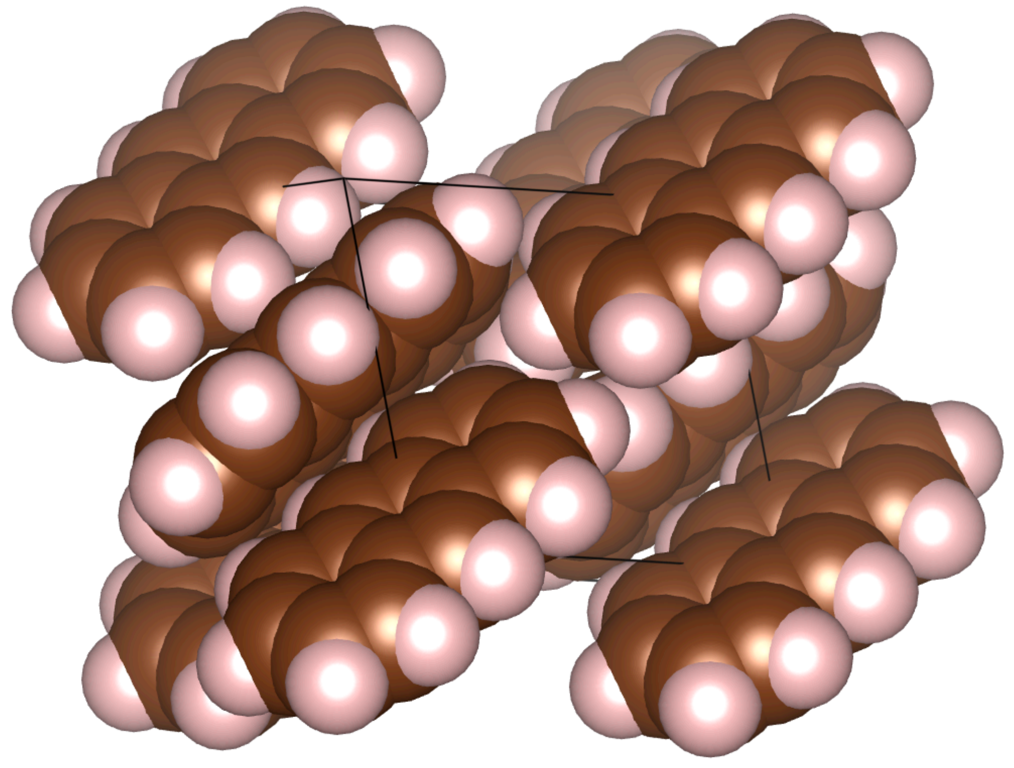
Alternative: Monte-Carlo Estimation

- $\text{vol}(O) = \int \mathbf{1}_O dU$
  - $\mathbf{1}_O$ - indicator function over U



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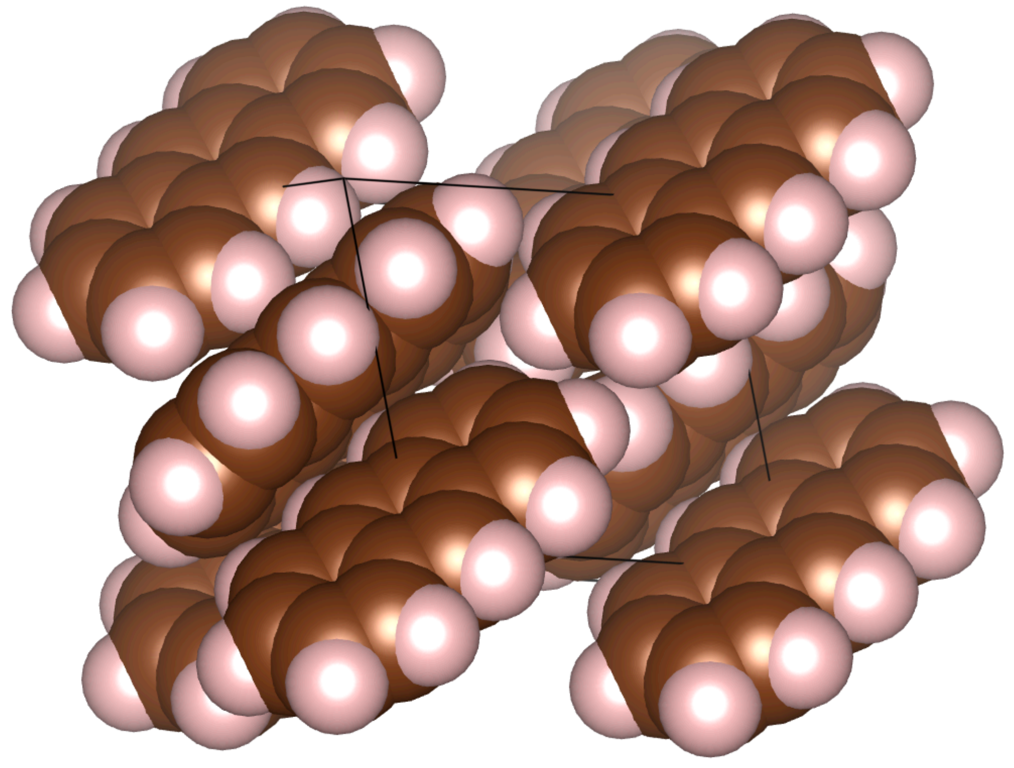

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- Change of coordinates to an integral over the unit cube C

$$\text{vol}(O) = \int \mathbf{1}_{U^{-1}O} \text{det}(U) dC$$

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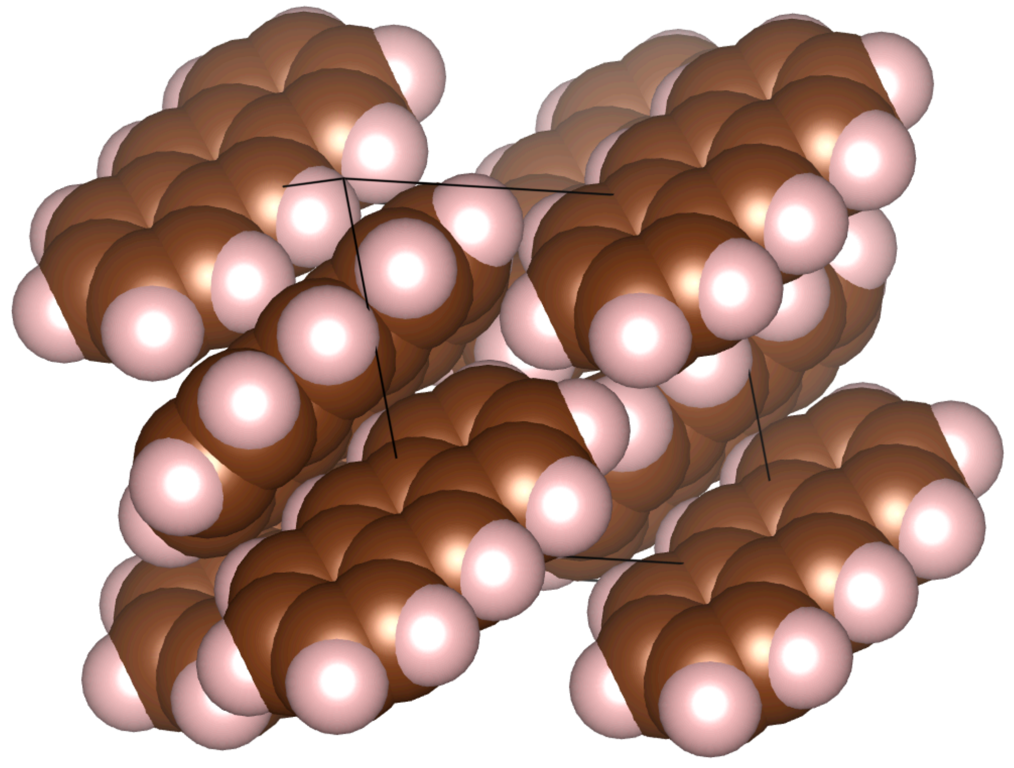

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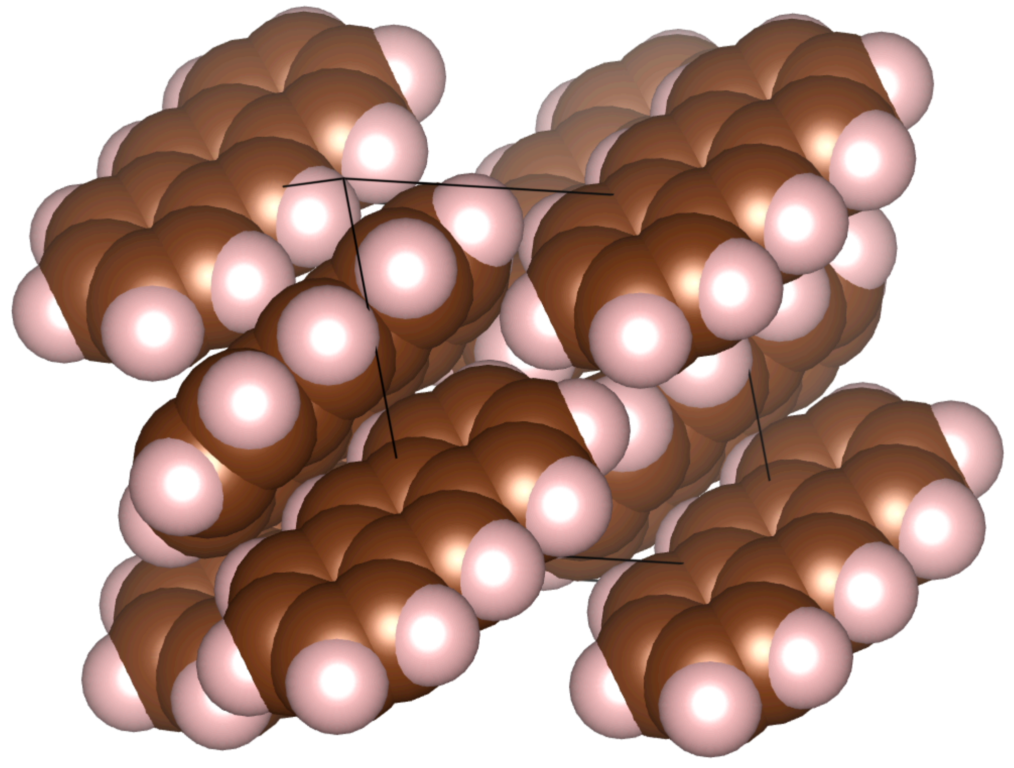

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- Uniform random variable on a unit cube $C \sim \mathbf{X}$

$$\rho = \mathbf{E}\left[1_{U^{-1}O}\right] = \mathrm{P}\left(X \in U^{-1}O\right)$$

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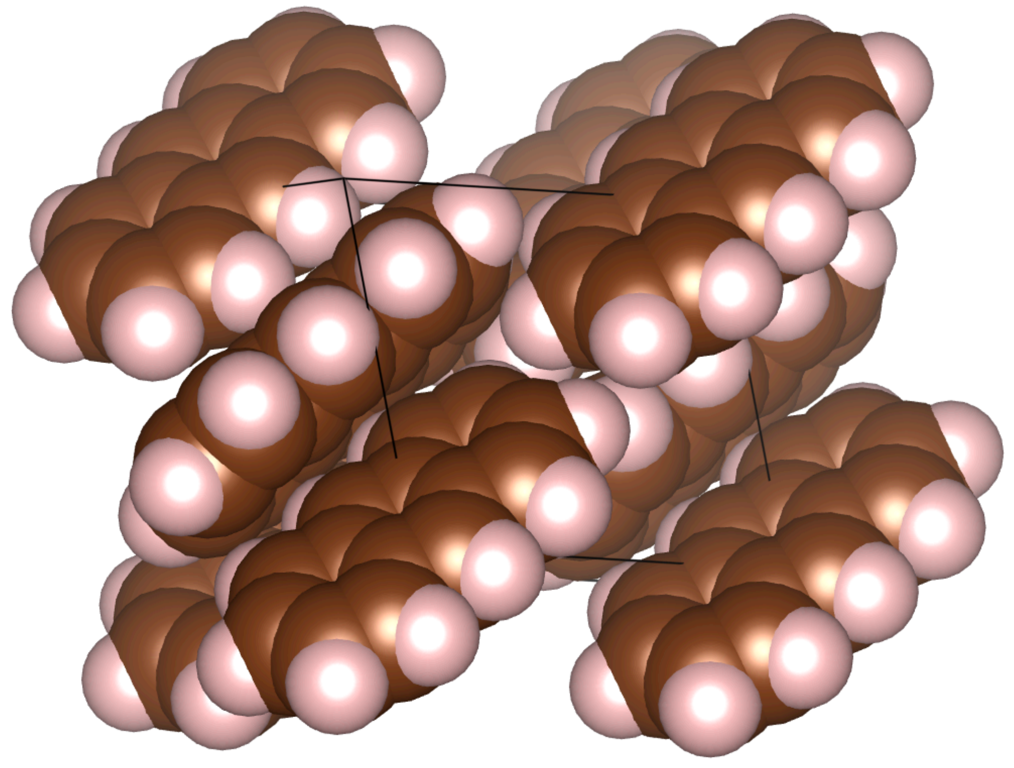

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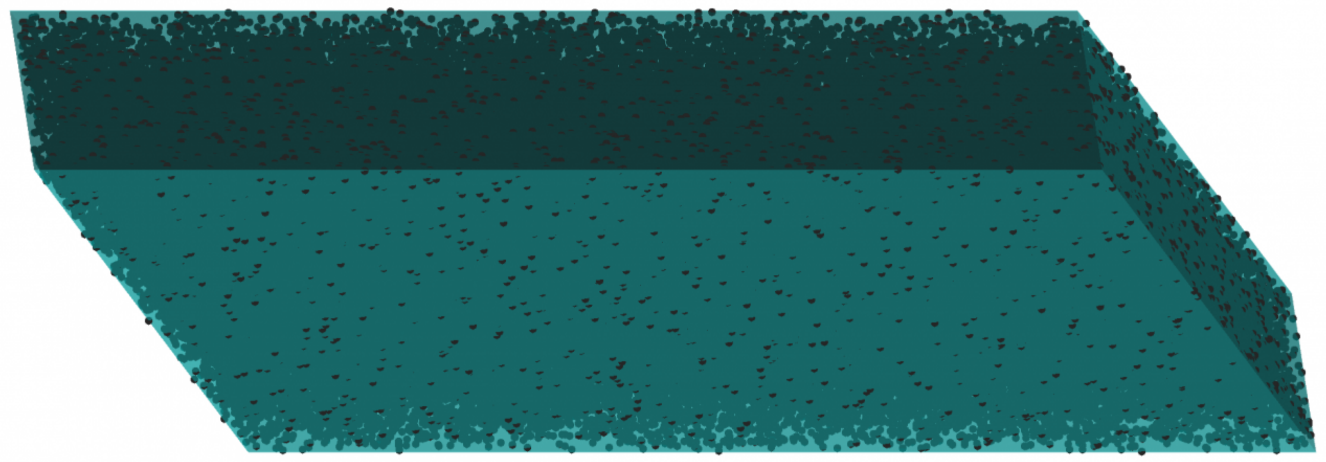

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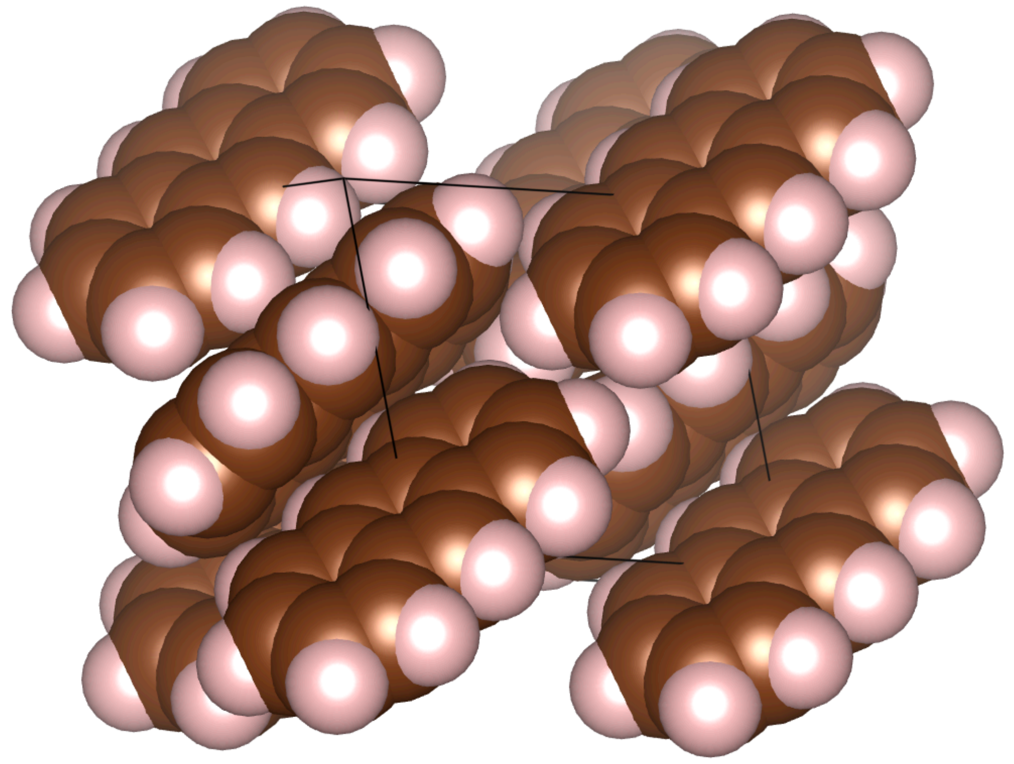

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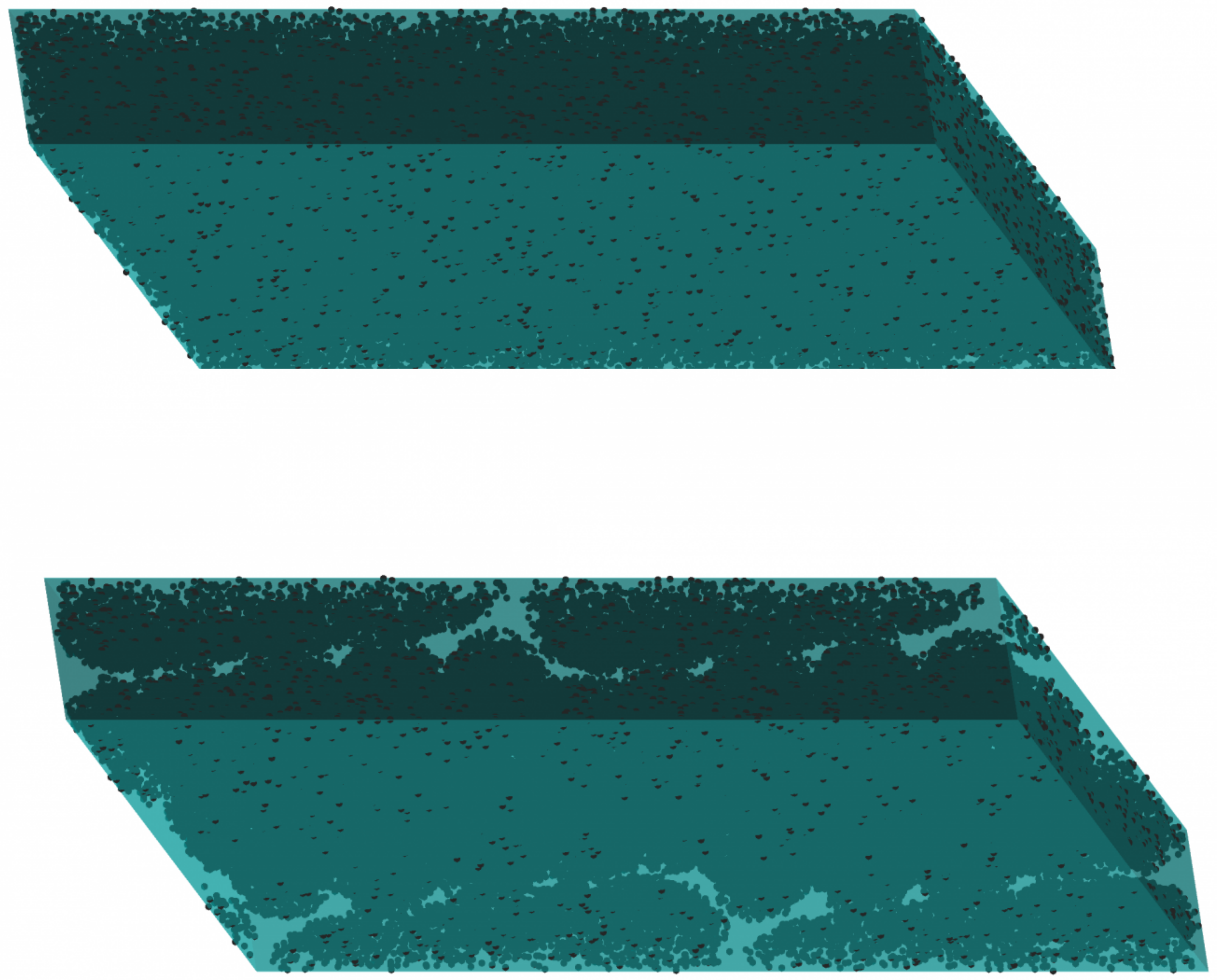

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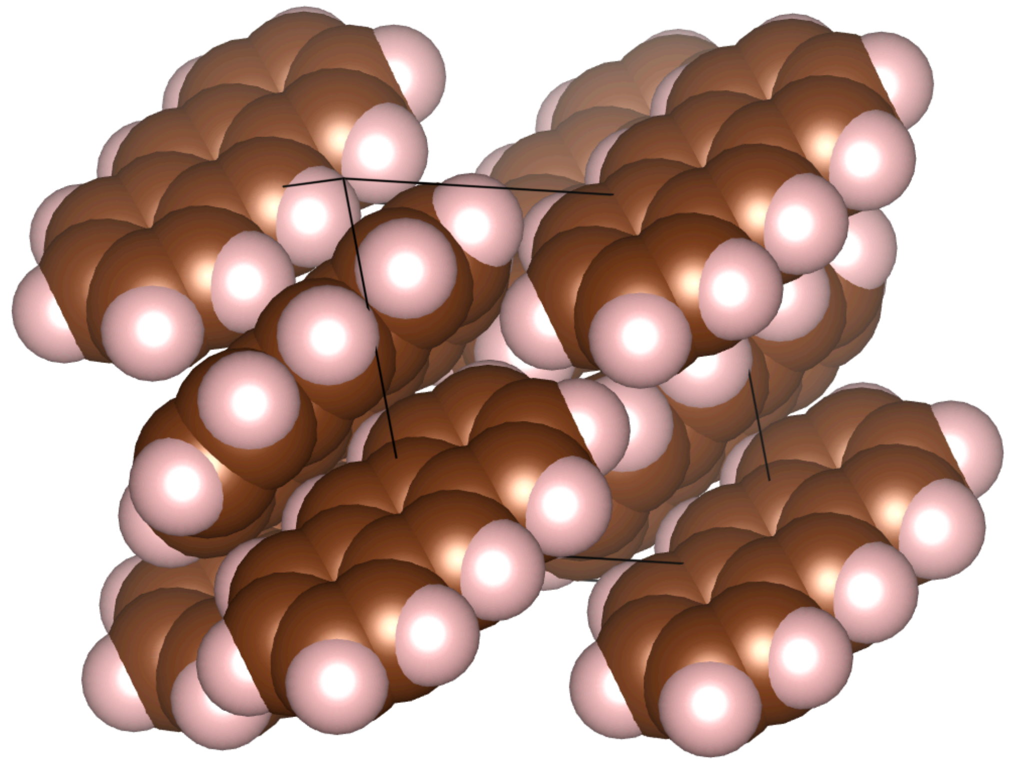
- Draw realisations o a random vector

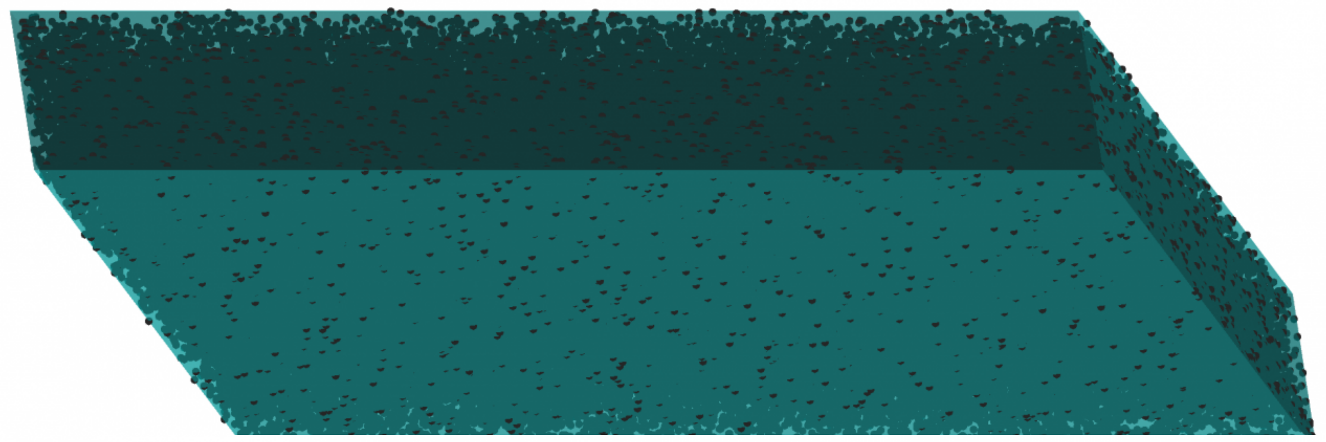
$$X_1, \ldots X_N \sim C$$

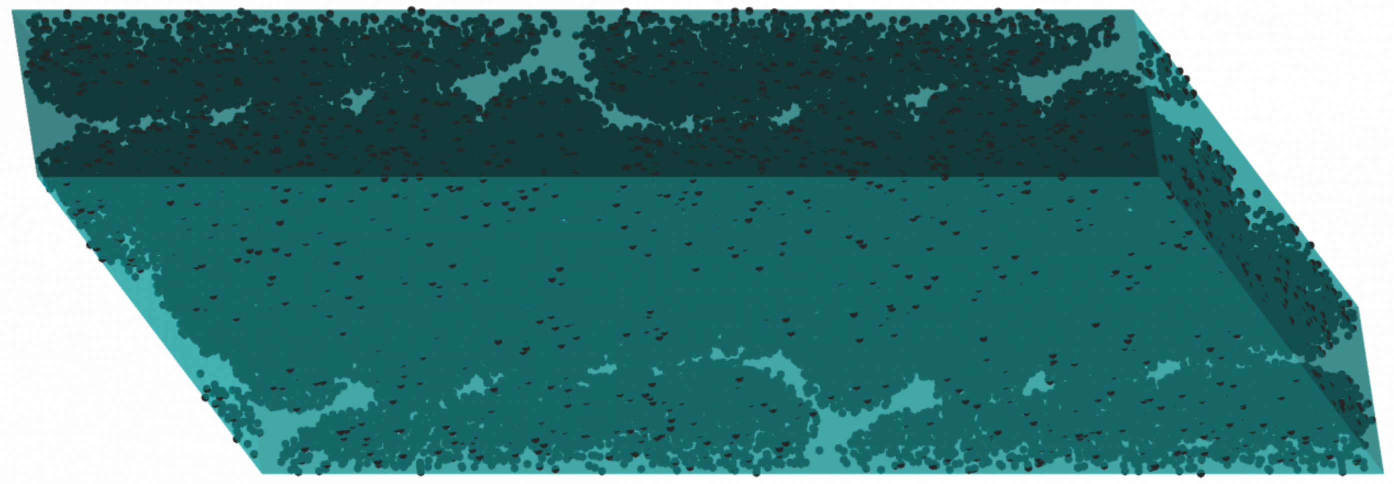
- Estimate the packing coefficient $\hat{\rho} = \dfrac{\#\{X_i \in U^{-1}O\}}{N}$

Alternative: Monte-Carlo Estimation

- N=100000 $\#\left\{X_i \in U^{-1}O\right\} = 76812$







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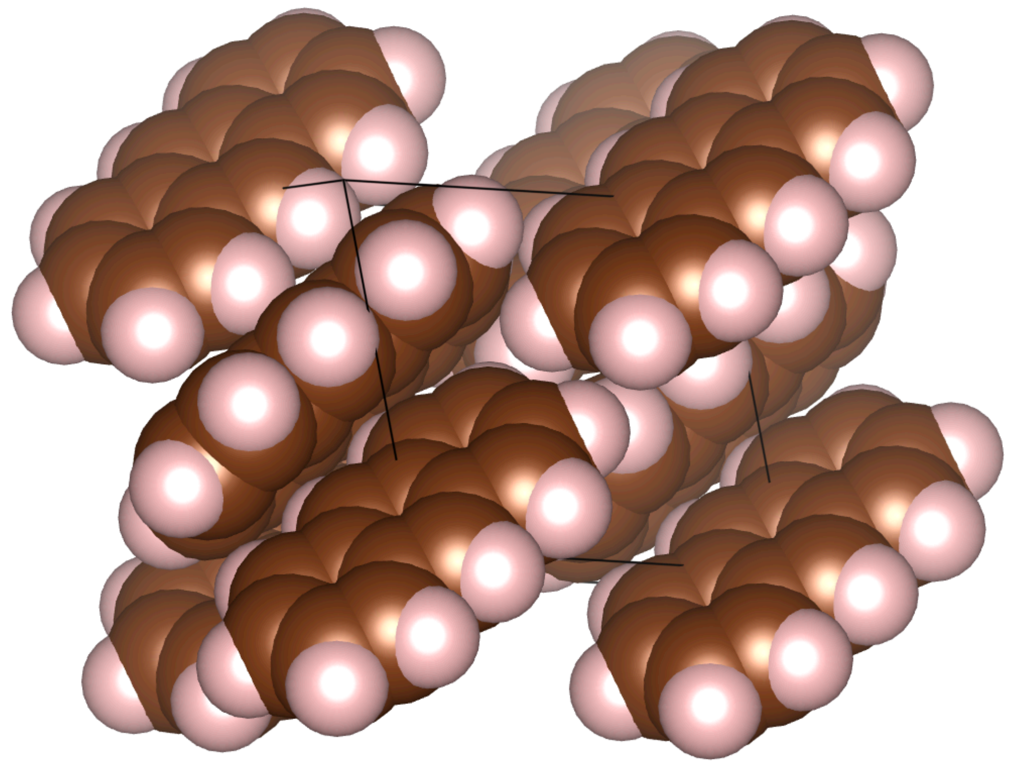

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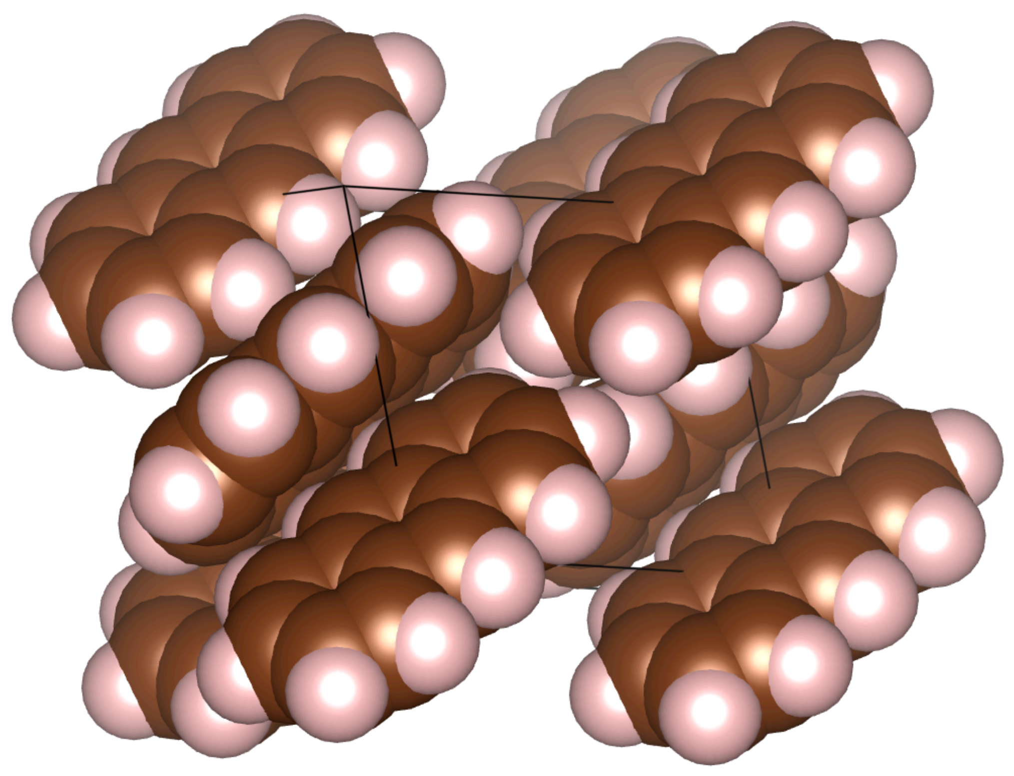
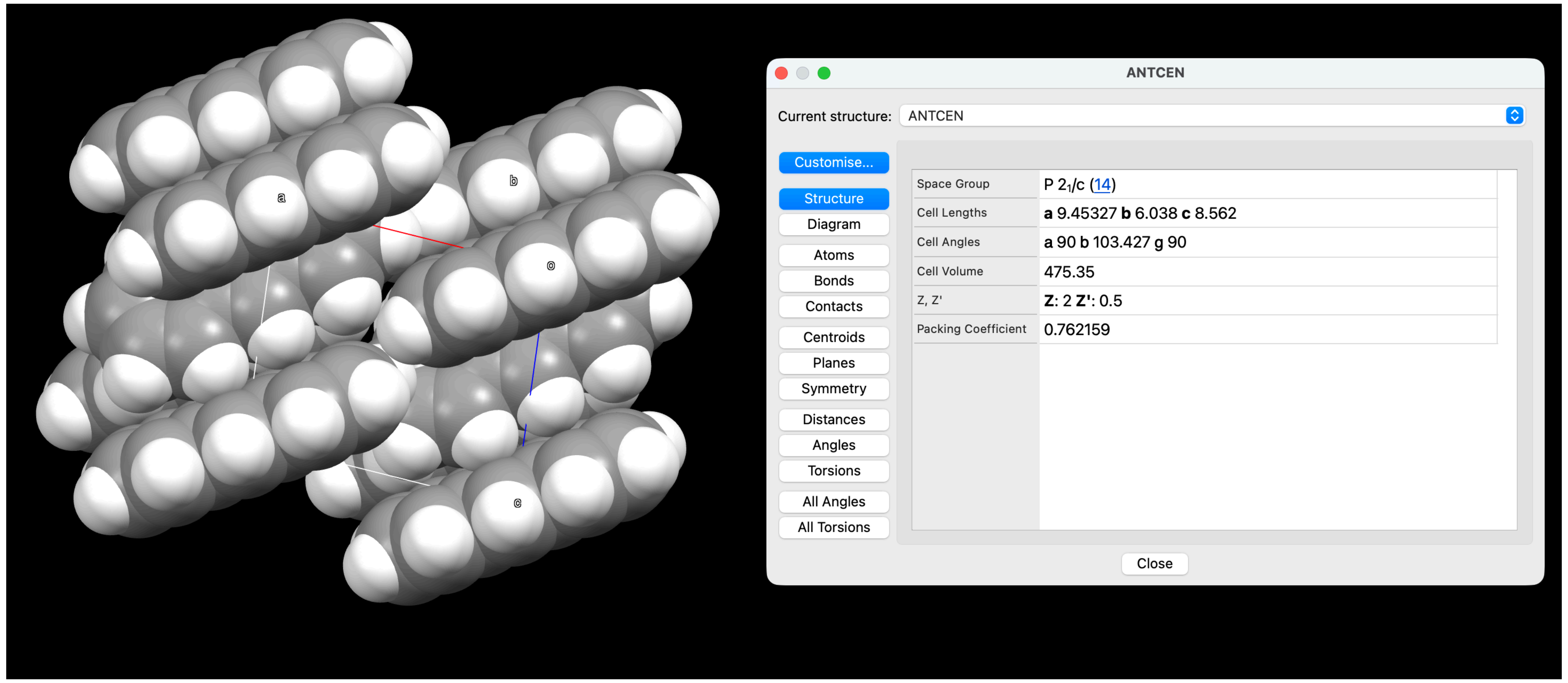
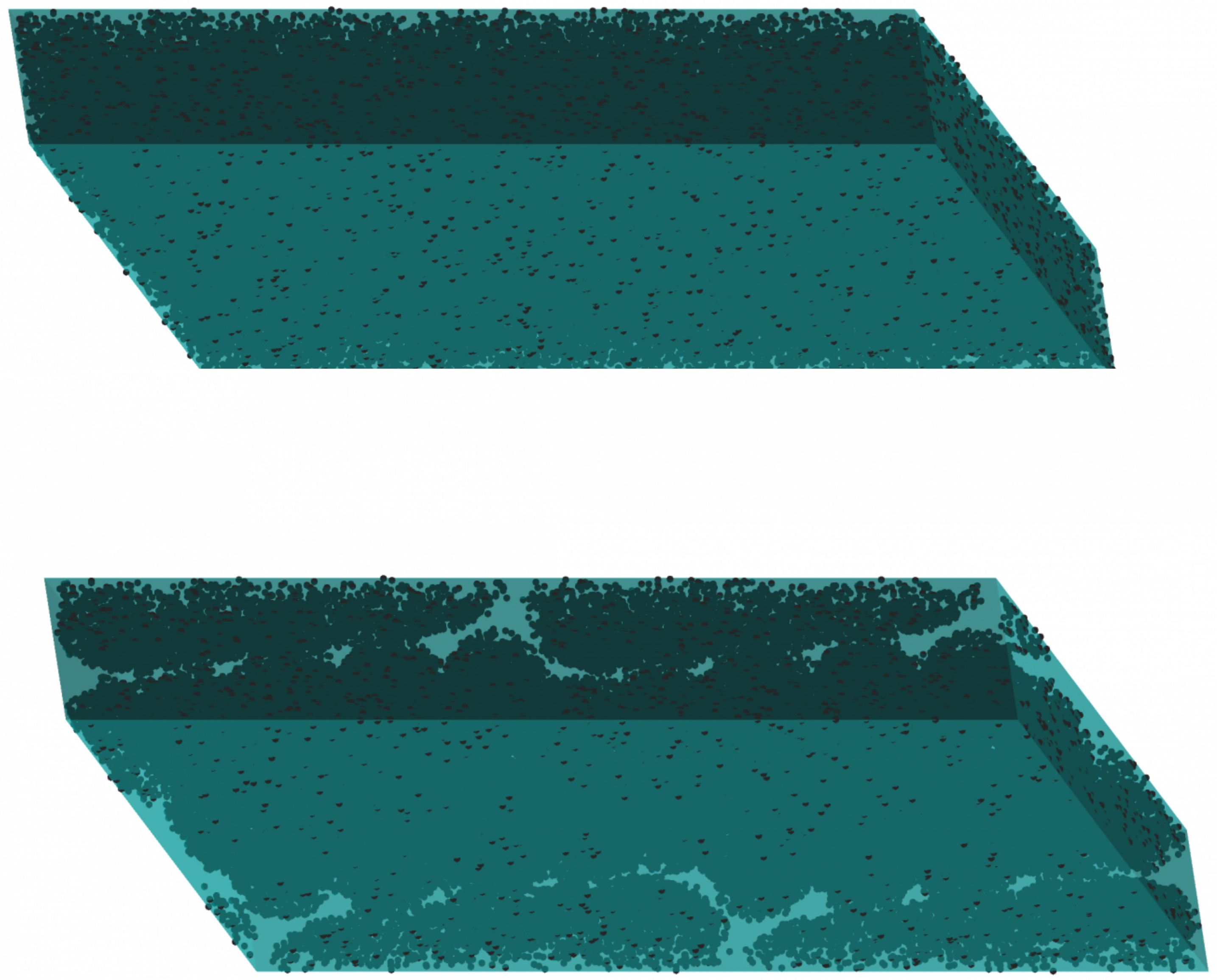
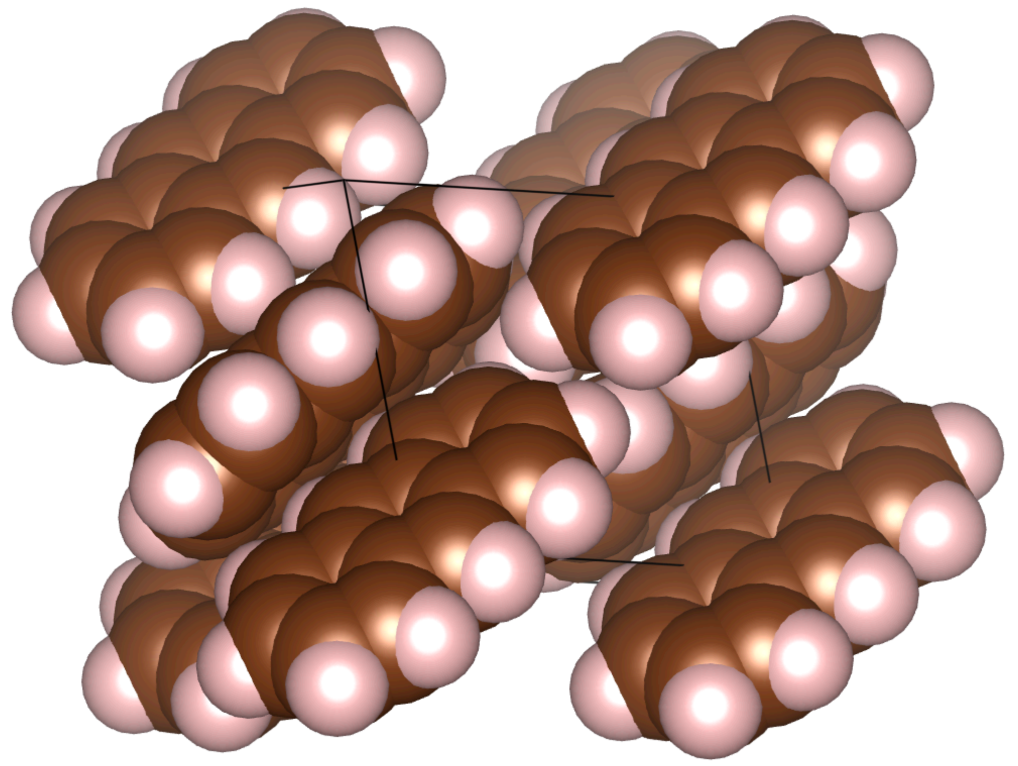


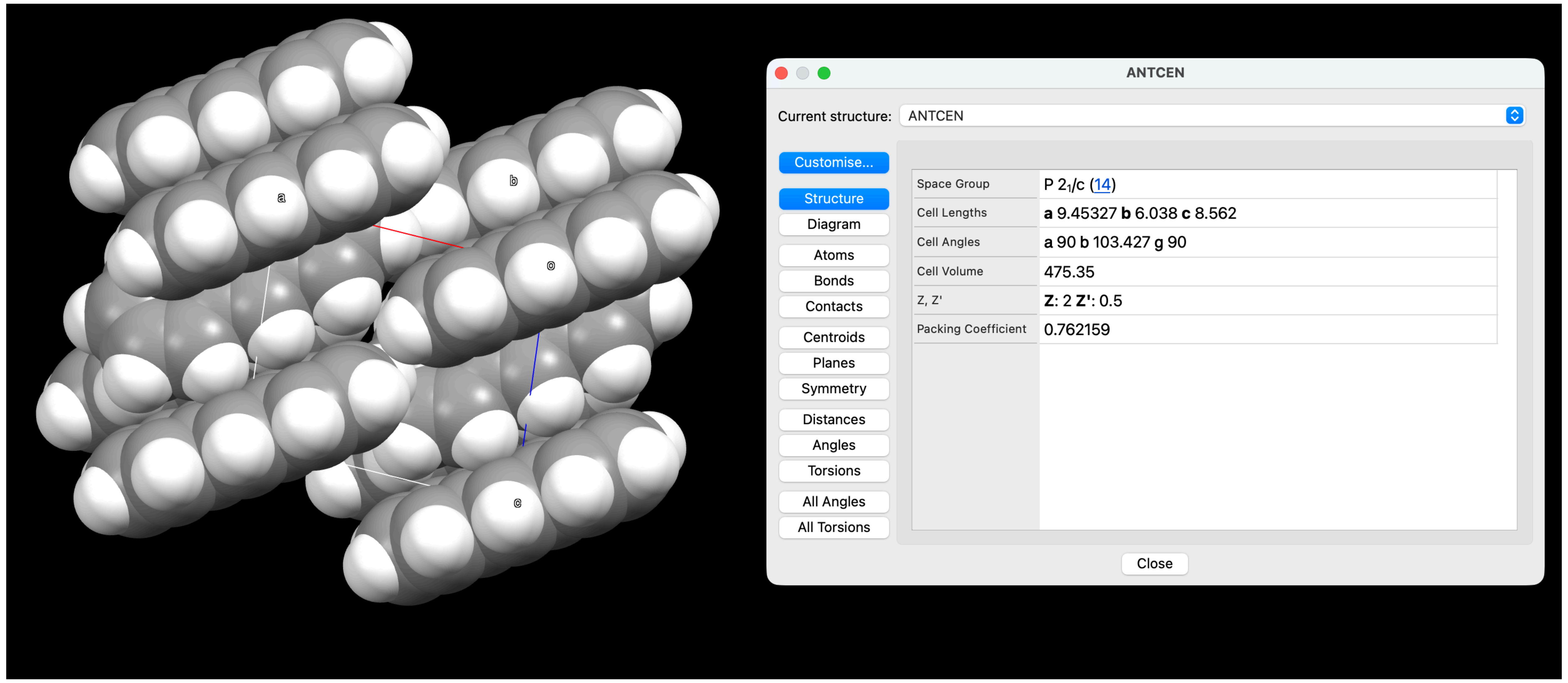


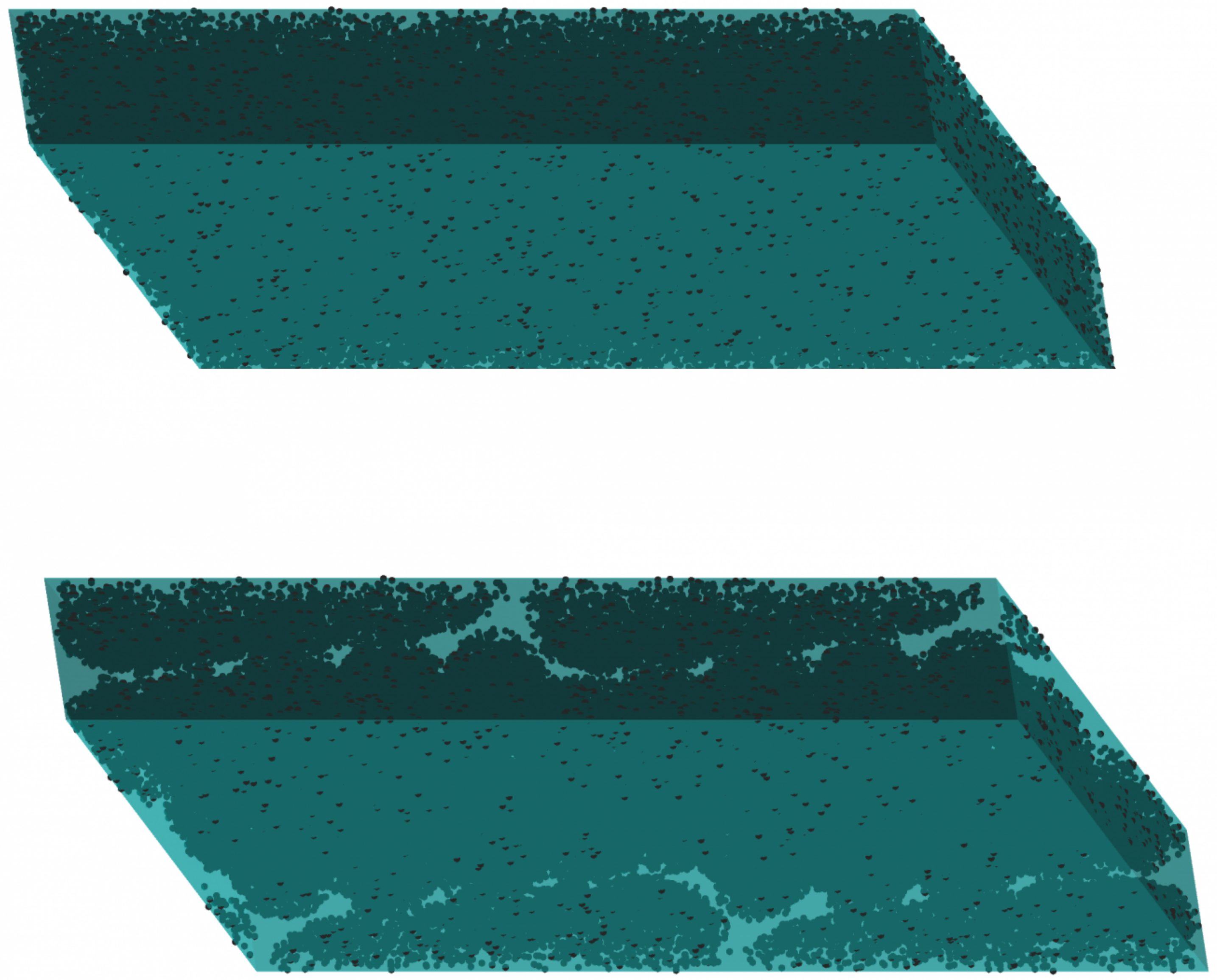


Alternative: Monte-Carlo Estimation

- N=100000 $\#\{X_i \in U^{-1}O\} = 76812$
- $\hat{\rho} = 0.76812$
- CCDC Mercury: 0.762159
- Which point estimate to trust?







Interval Estimate of the Packing Coefficient

- X_i - Bernoulli trial $\quad \mathbf{X} = \sum_{i=1}^{N} X_i \quad$ binomially distributed random variable

Expected value: $N\rho$

Variance: $N\rho\left(1-\rho\right)$

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z **-** $1-\alpha$ **quantile of the standard normal distribution**

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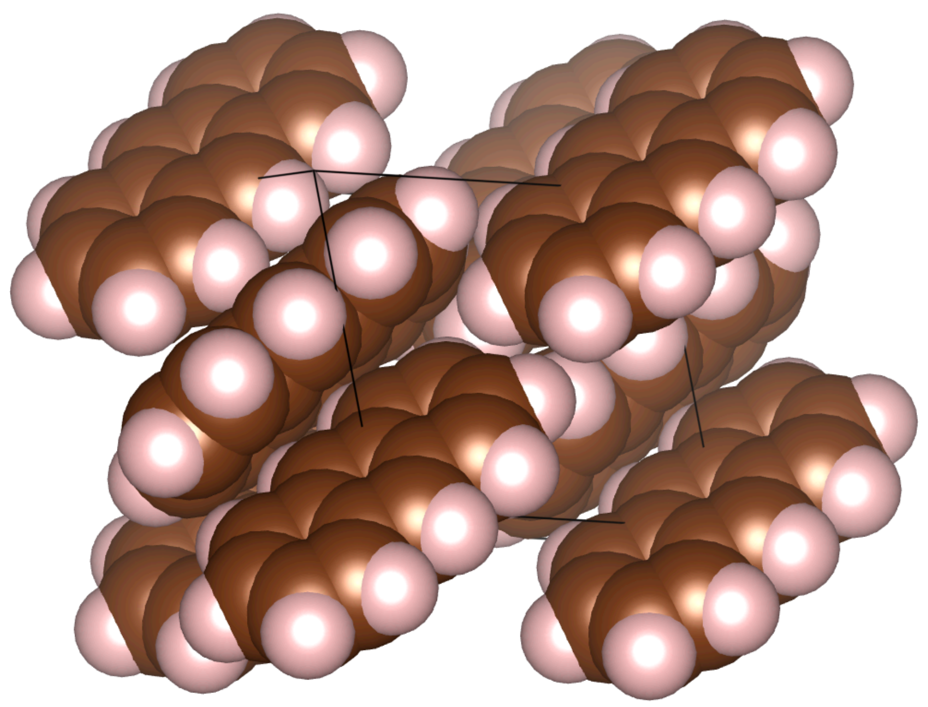

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- N=100,000: 0.76812
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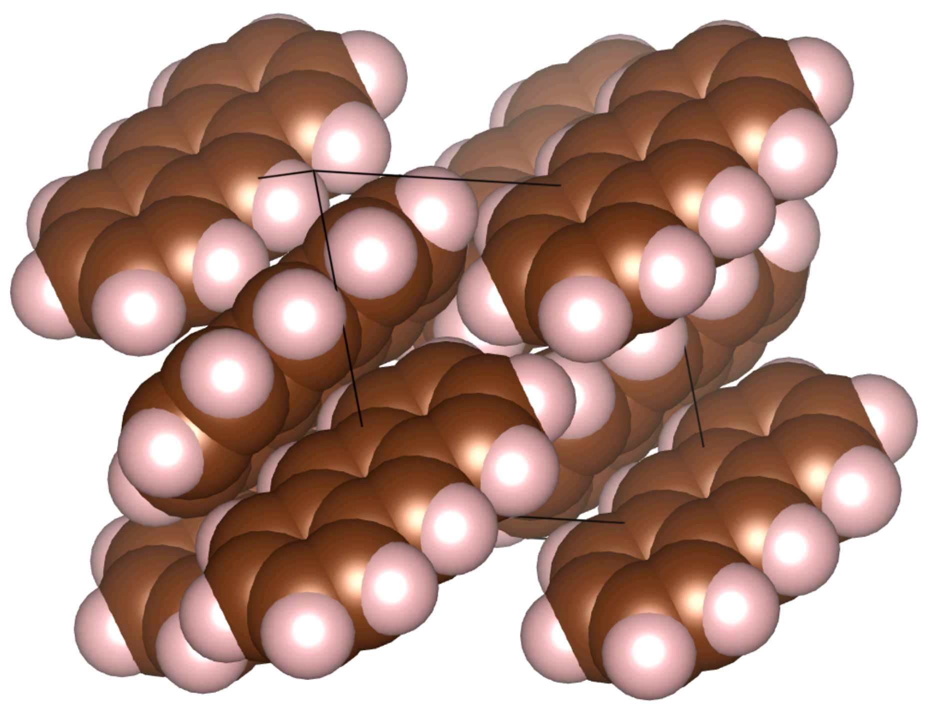
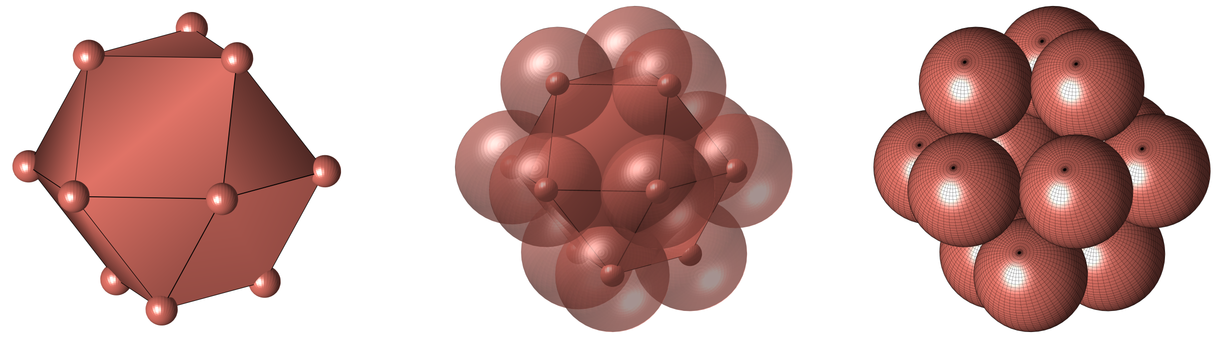


Estimating Packing Coefficient of a Model Molecule

- A collection of equal spheres with centres on the vertices of a cuboctahedron.



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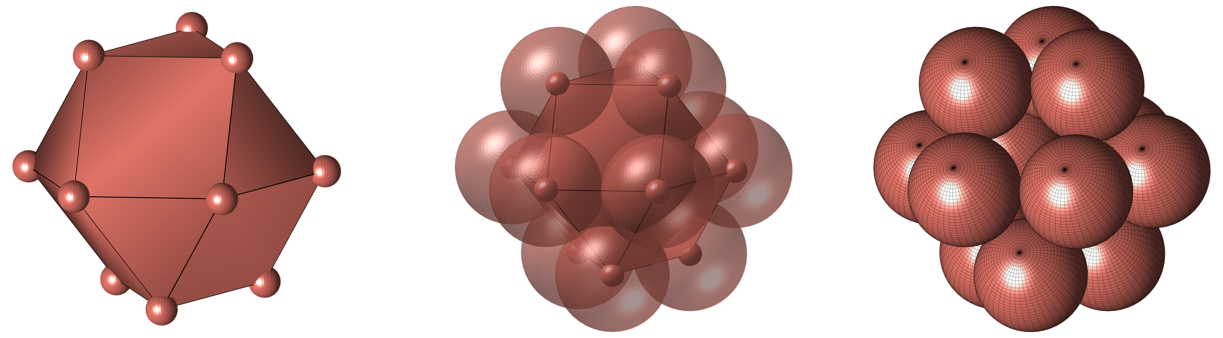
- A collection of equal spheres with centres on the vertices of a cuboctahedron.
    - **Number of vertices: 12**



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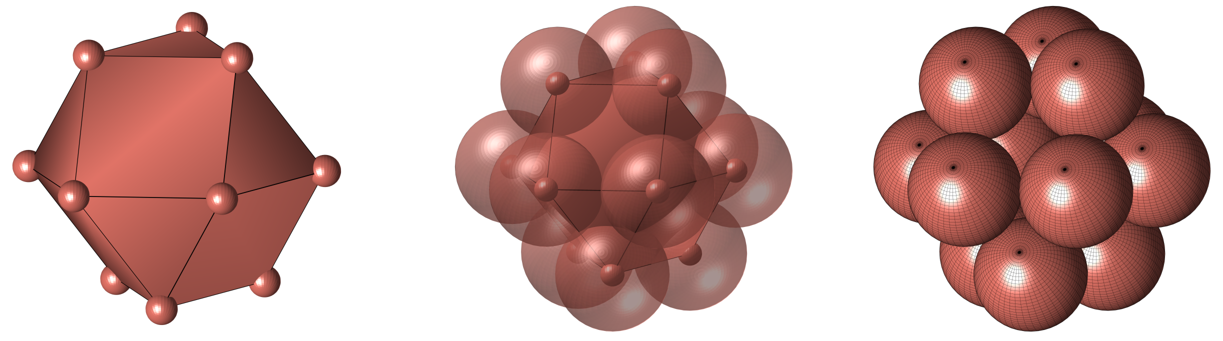
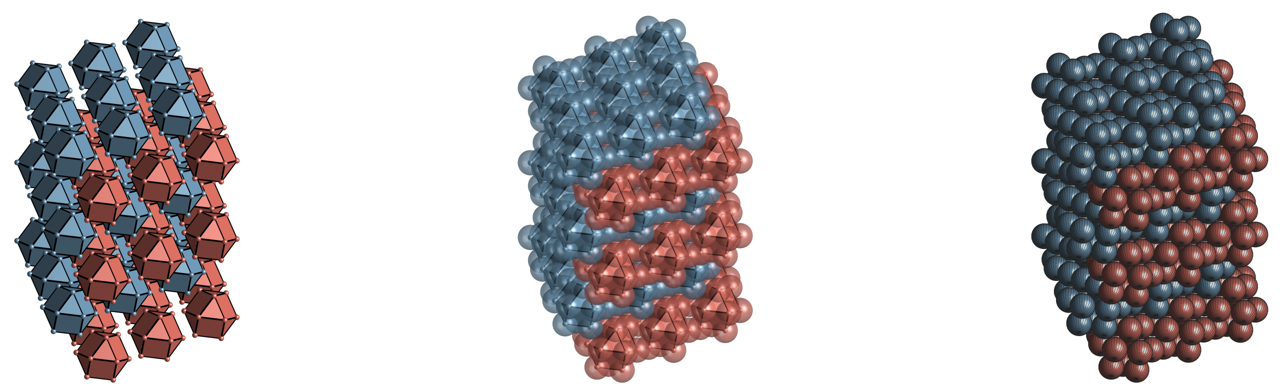


- Densest packing of cuboctahedral molecules

$$\rho = \frac{12}{13}\frac{\pi}{\sqrt{18}} \approx 0.68352...$$



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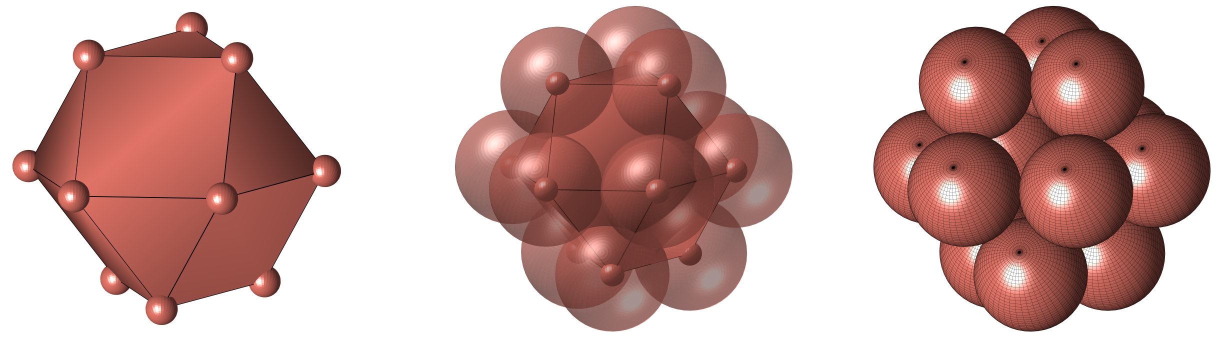
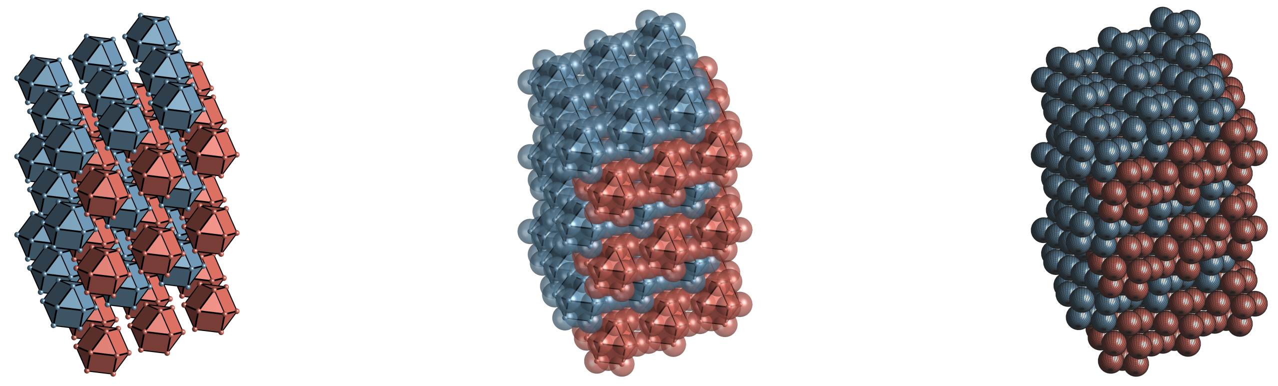
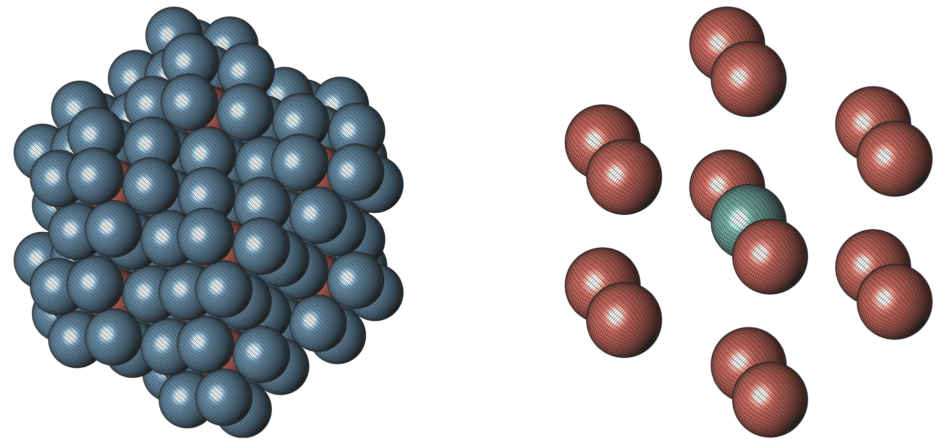




Packing of 15 cuboctahedral molecules

Complementary packing



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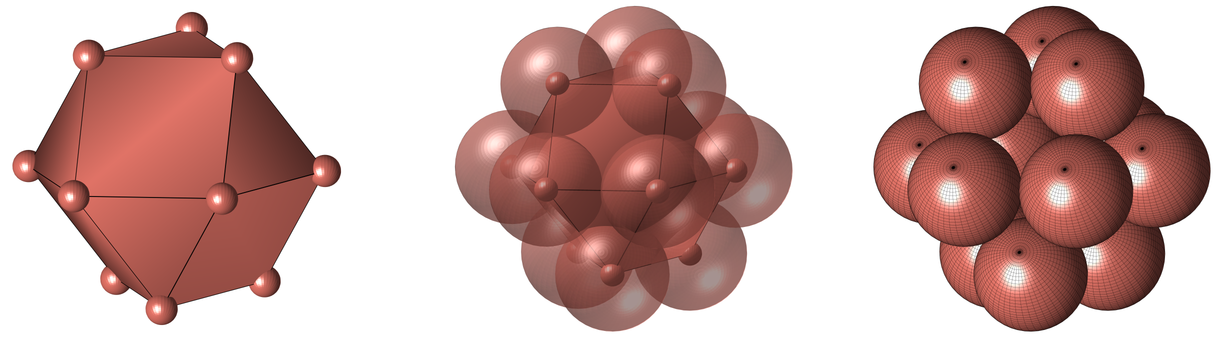

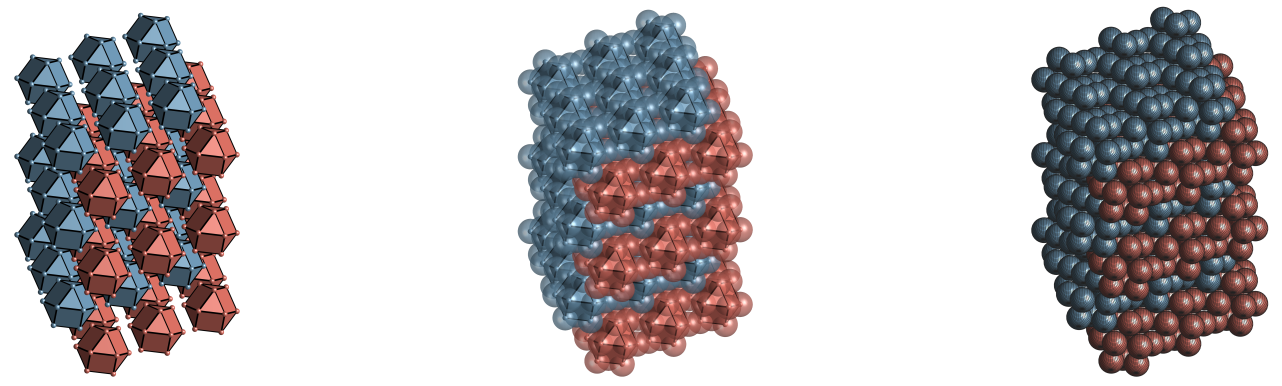

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Complementary packing

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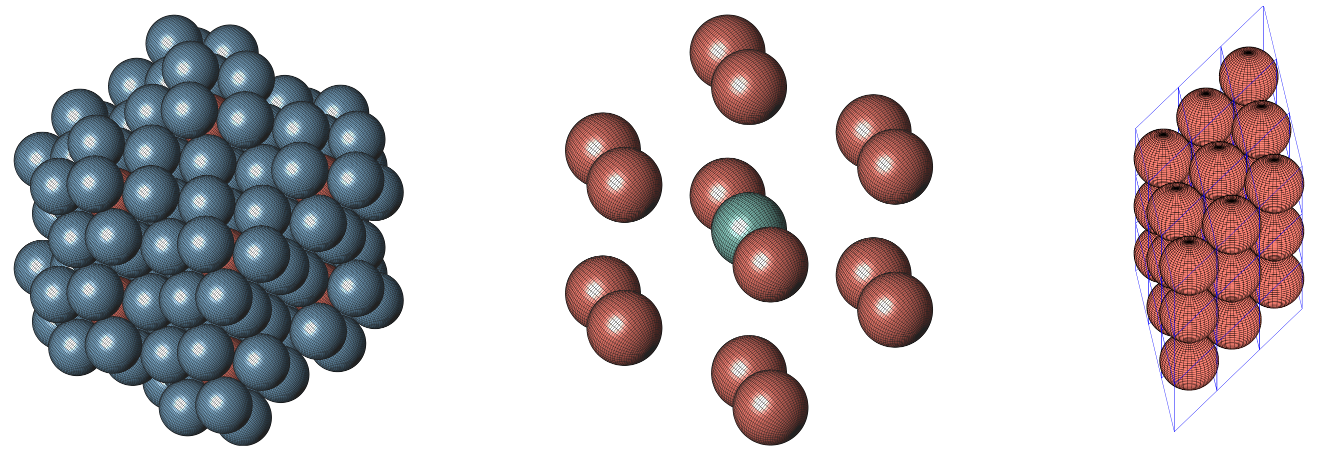

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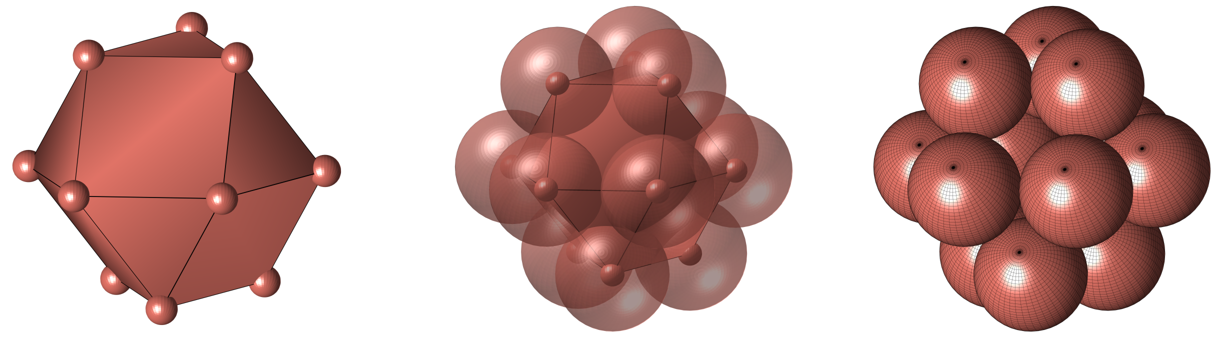

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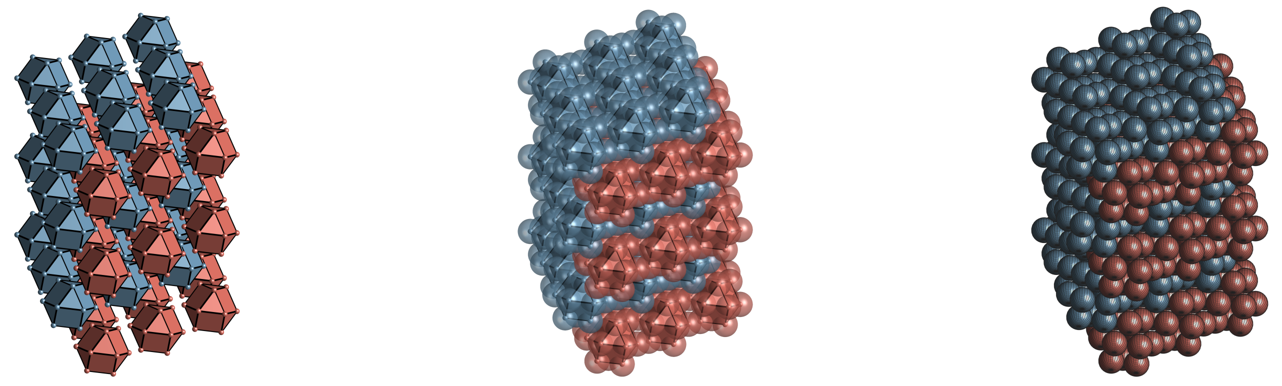

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Packing of 15 cuboctahedral molecules | Complementary packing | FCC close-packing of equal spheres

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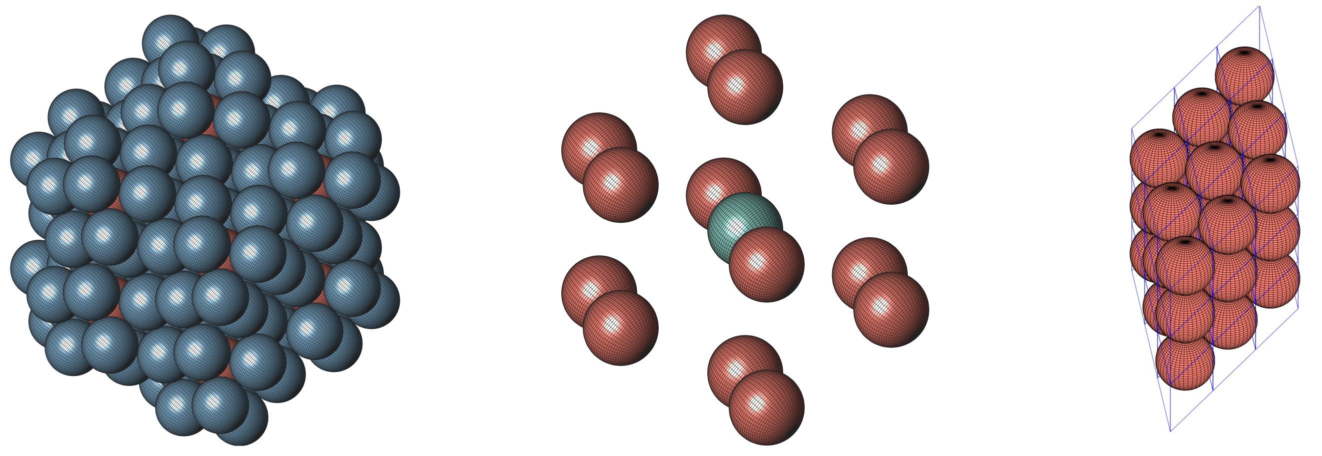

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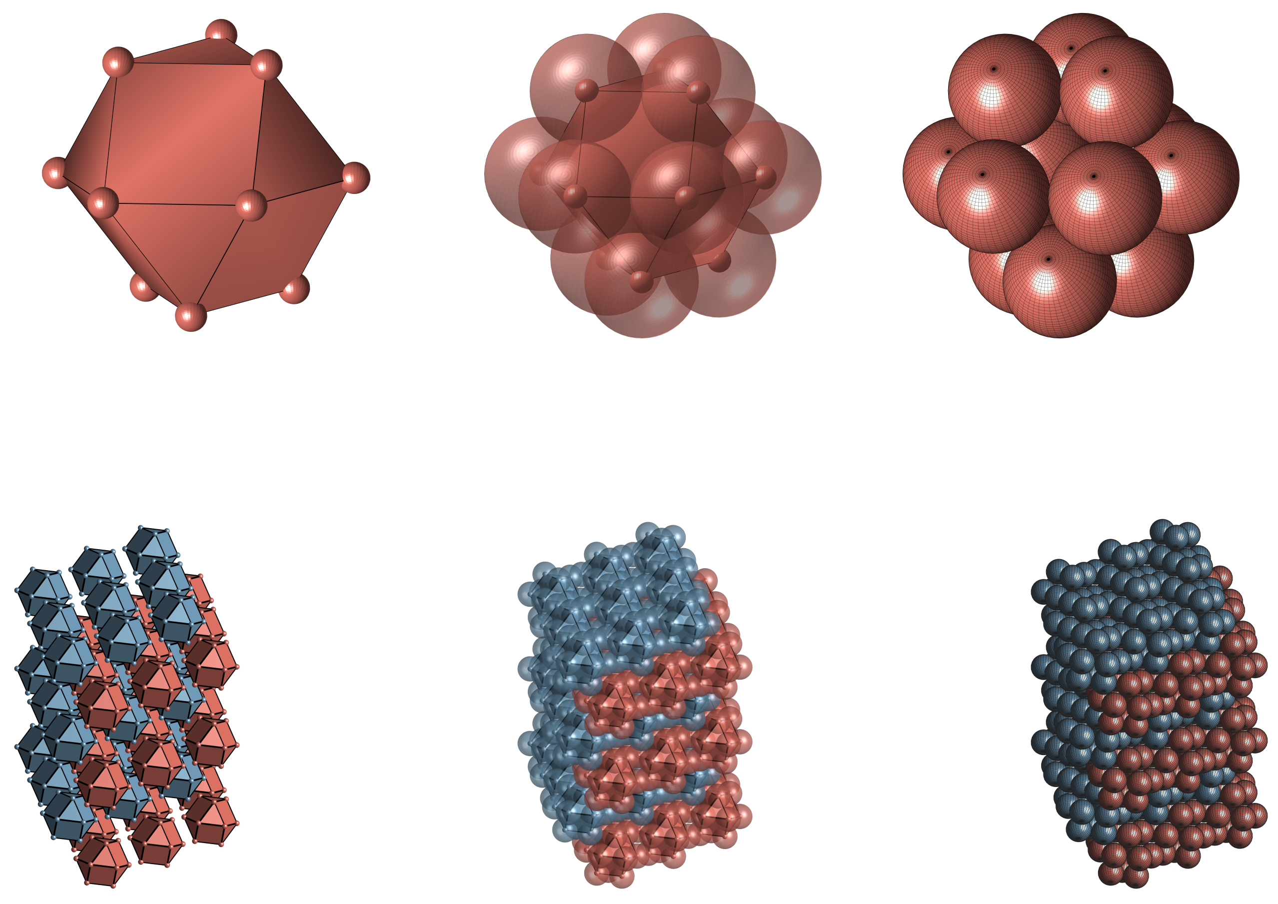

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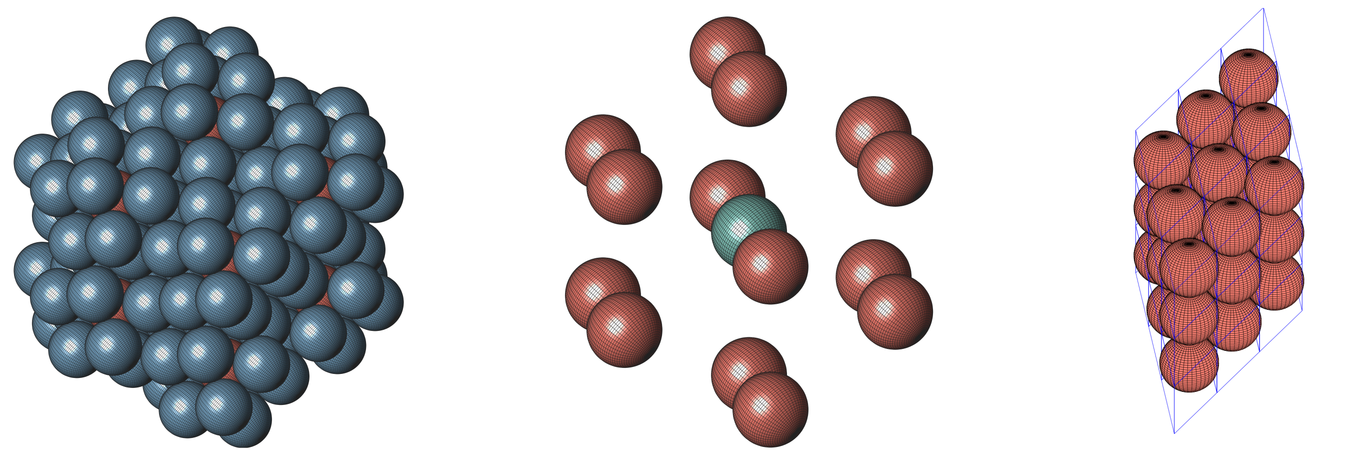

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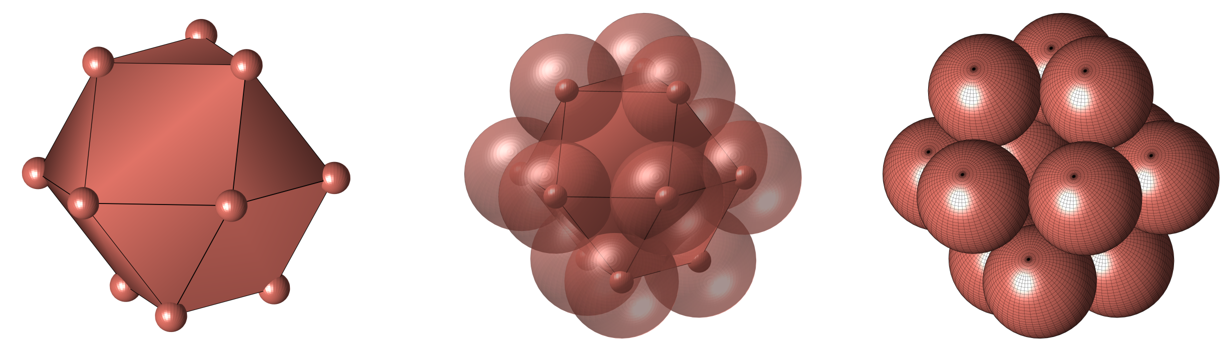

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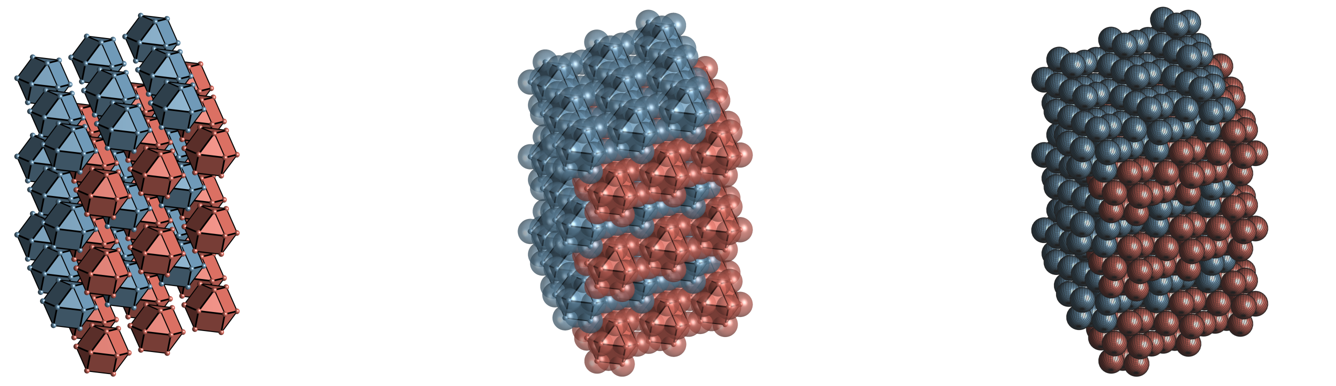

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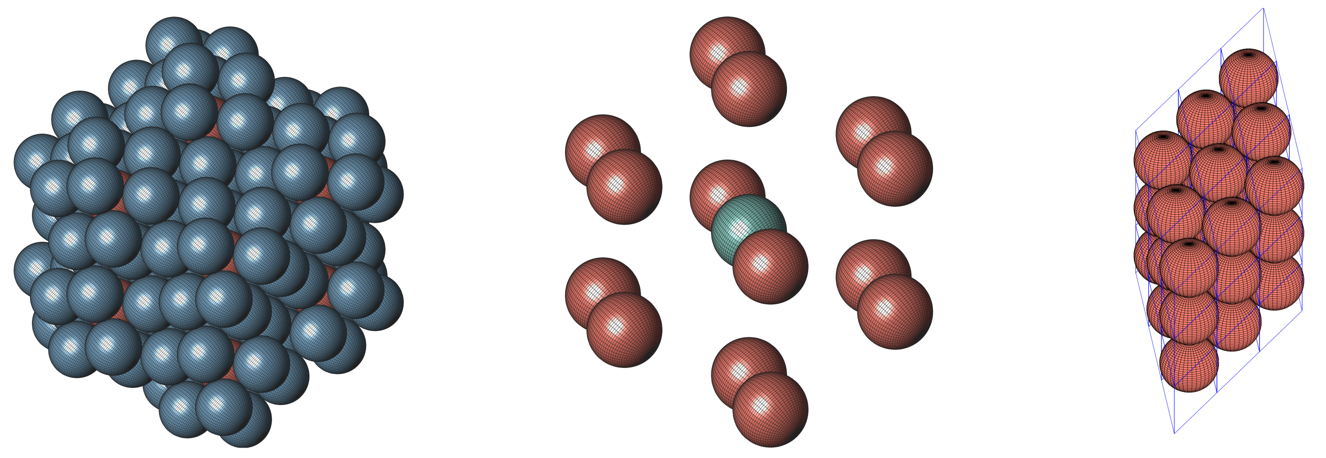

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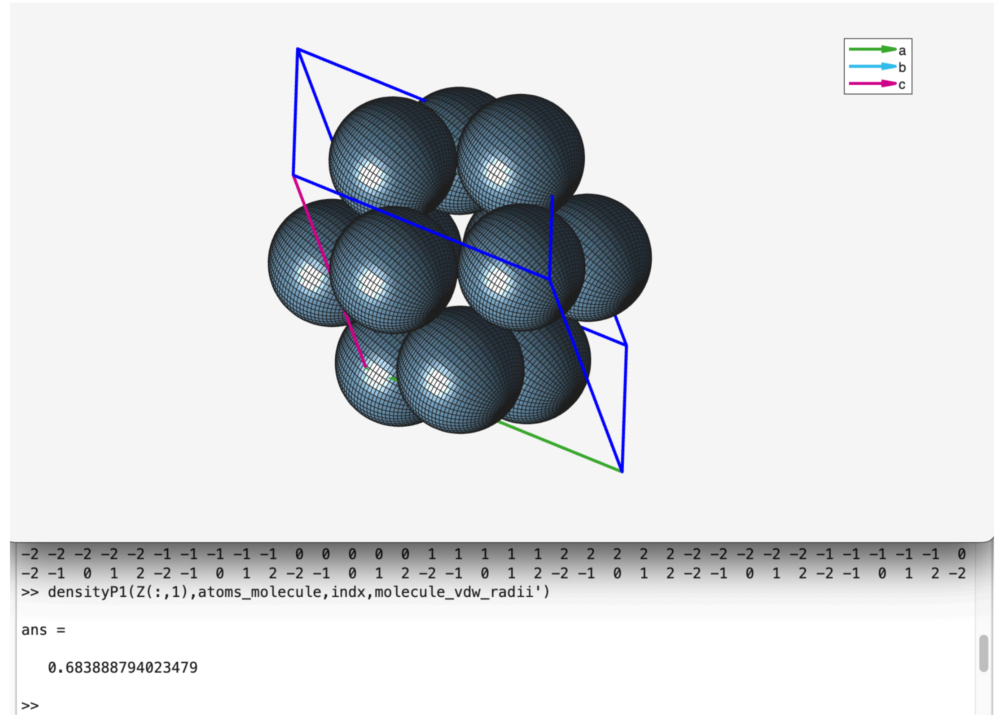

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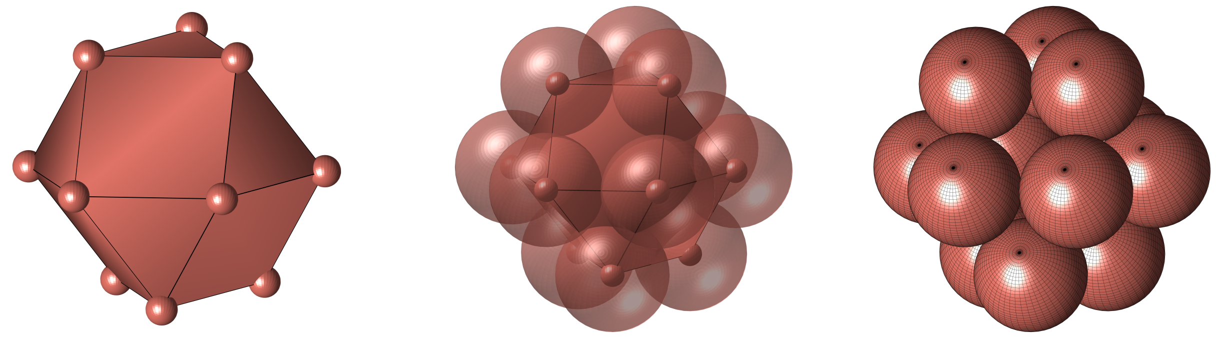

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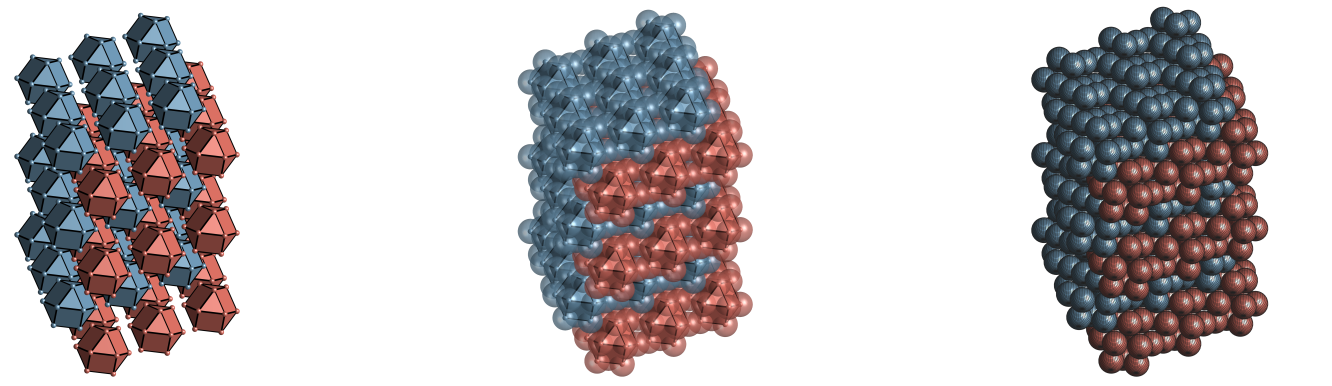

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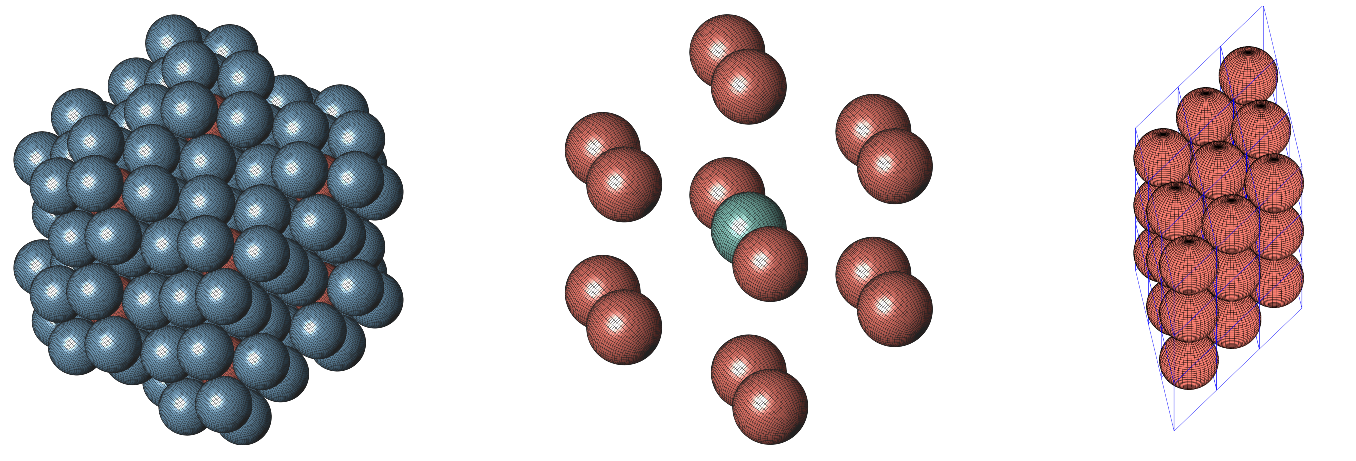

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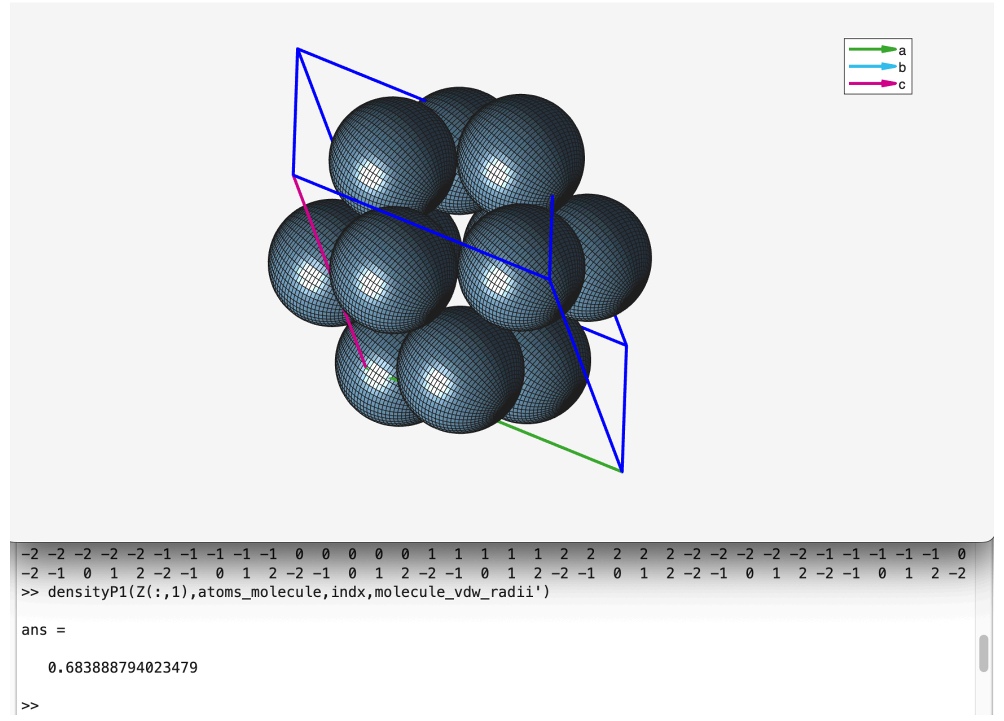

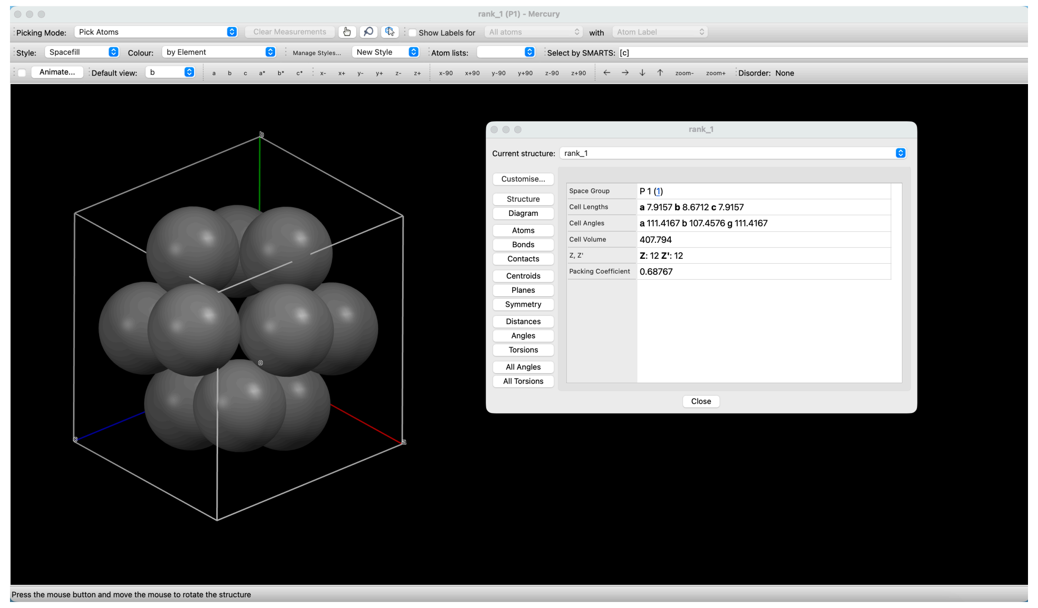

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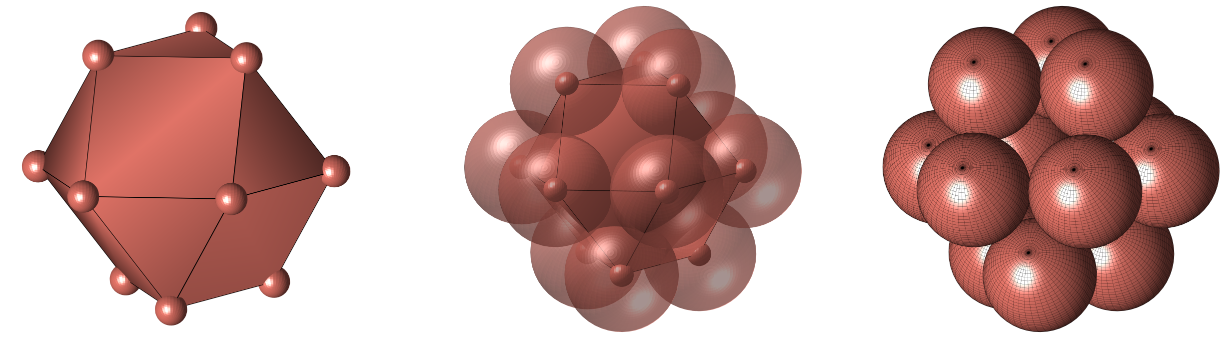

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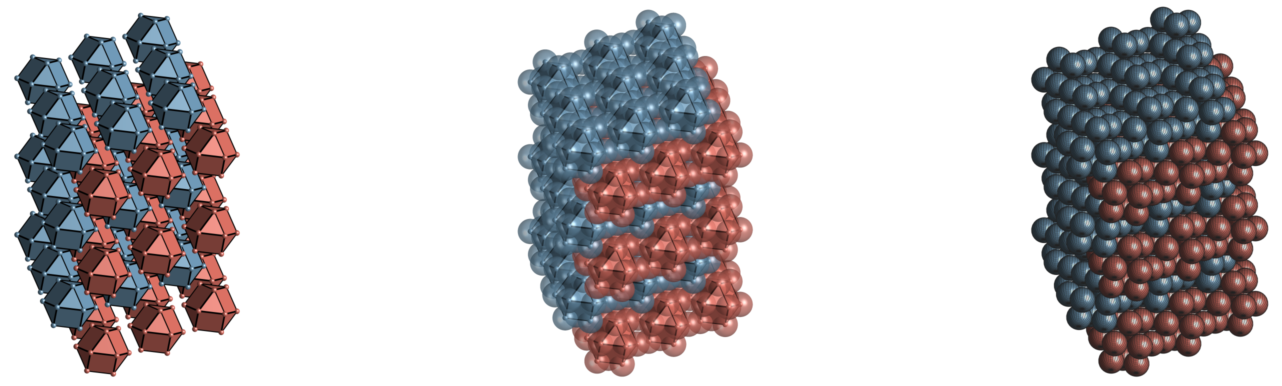
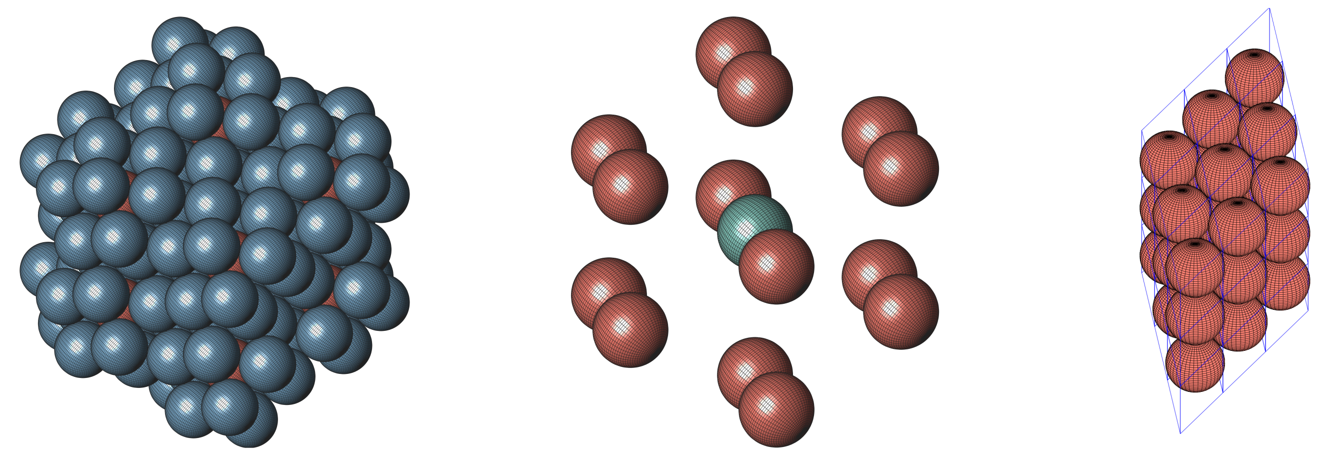


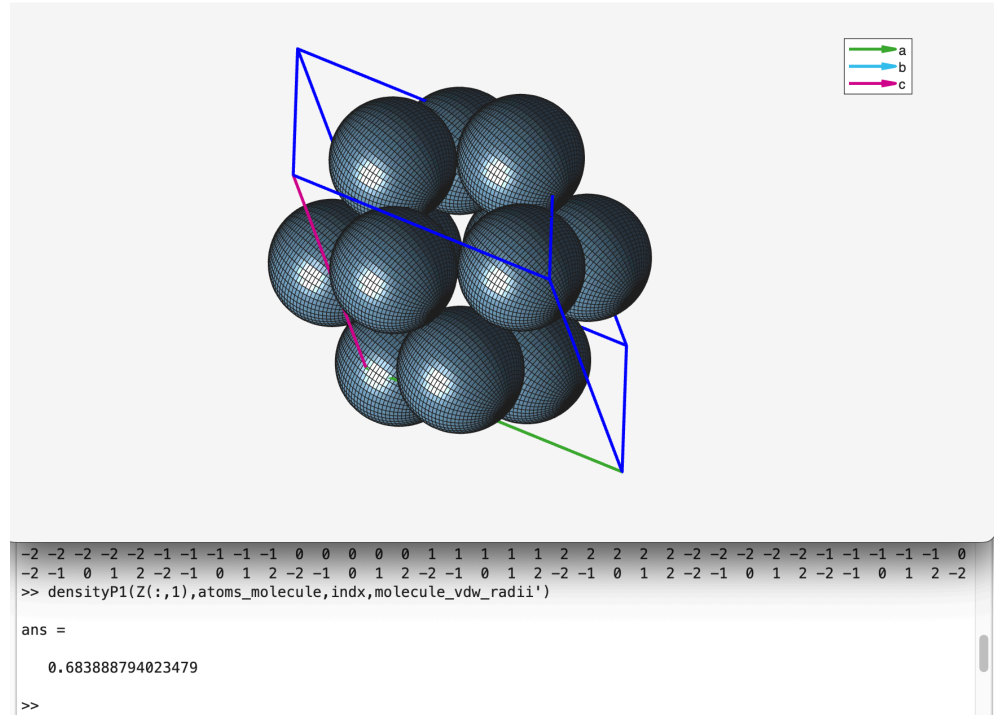
Packing of 15 cuboctahedral molecules

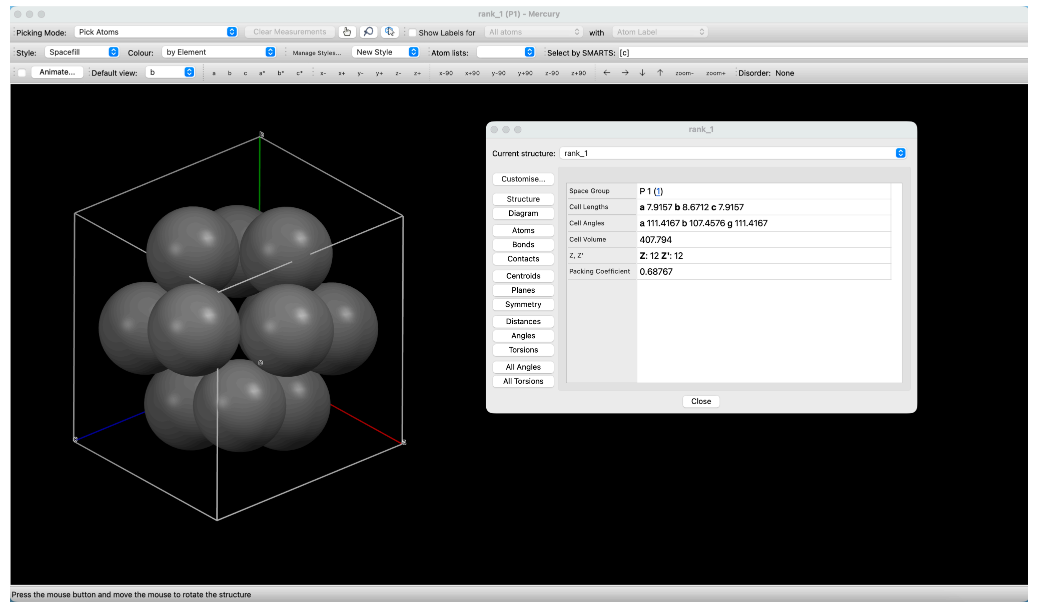
Complementary packing

FCC close-packing of equal spheres



- $\hat{\rho} \approx 0.683888$ $\epsilon = 0.00036$ $N = 9{,}370{,}000$
- CCDC Mercury: 0.68767 $\epsilon = 0.00415$





Hales, T. C. (2005). A proof of the Kepler conjecture. *Annals of mathematics*, 1065-1185.

Optimisation Under Uncertainty

- Stochastic optimisation problems

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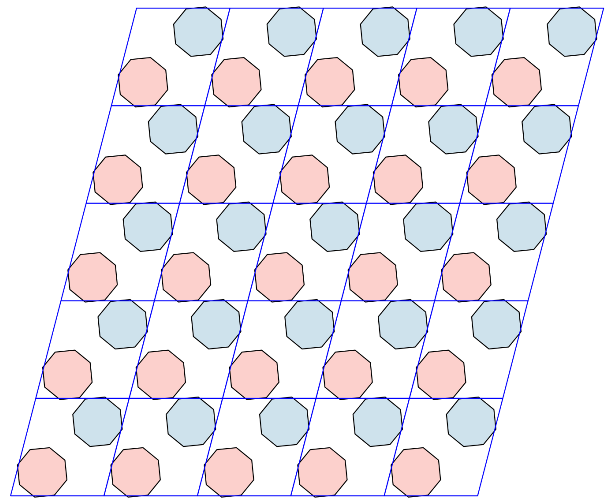

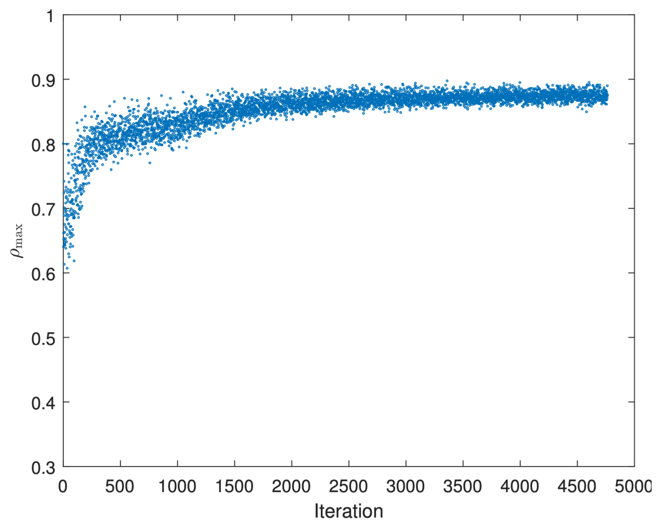

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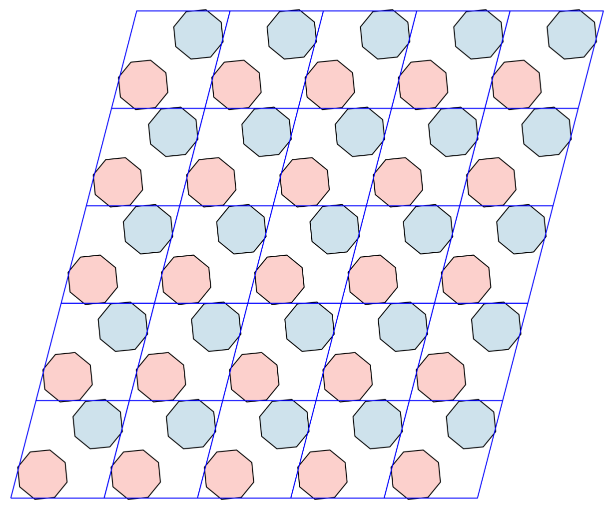

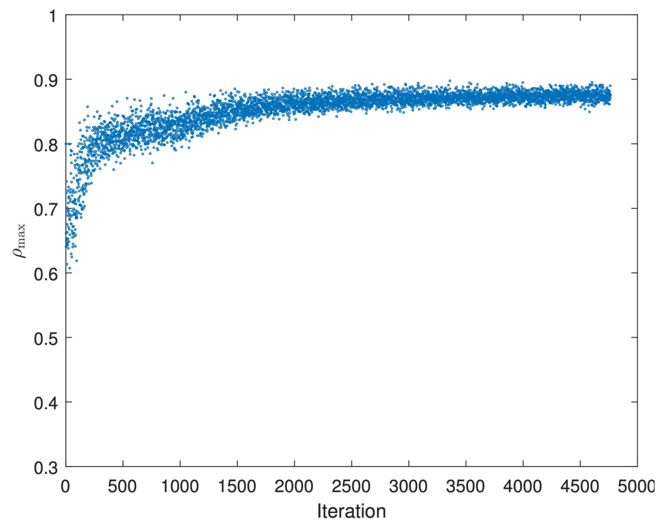

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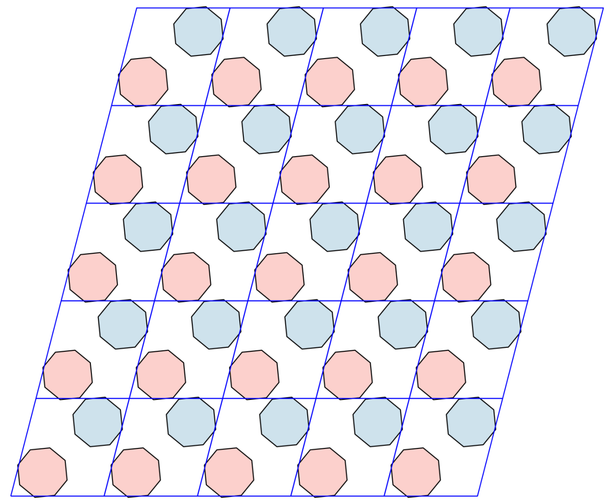

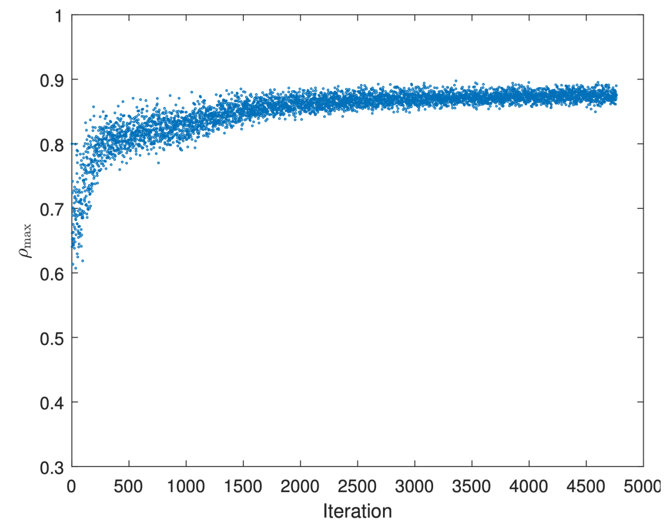

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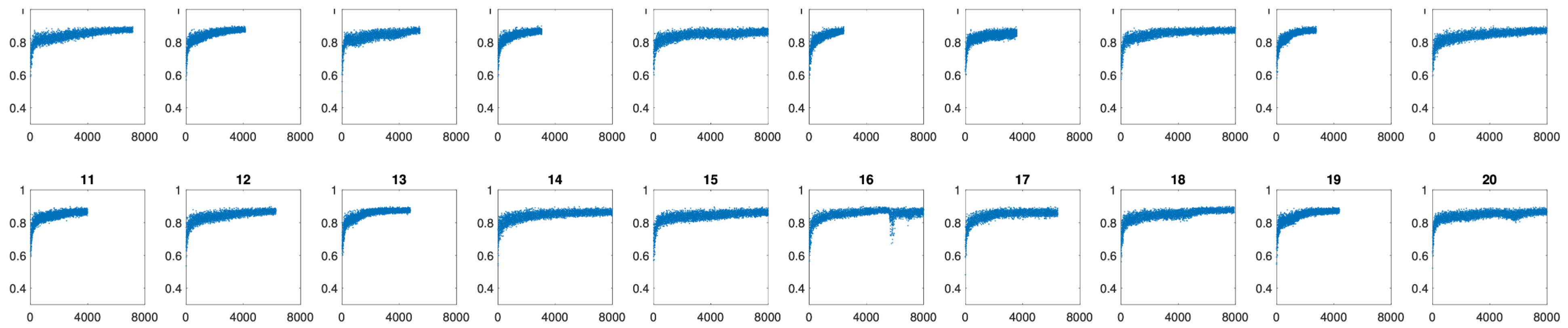

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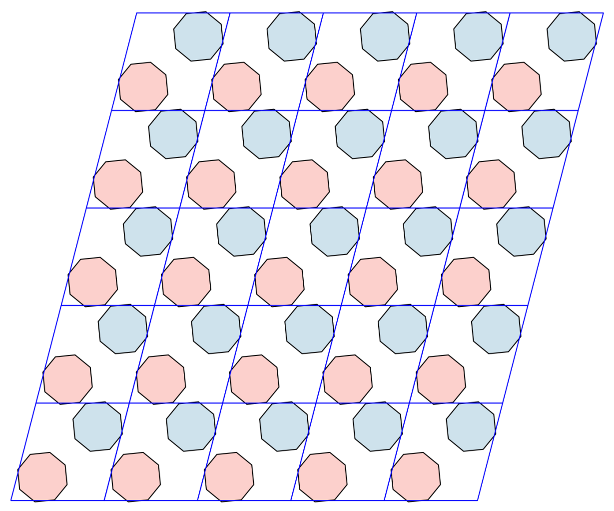

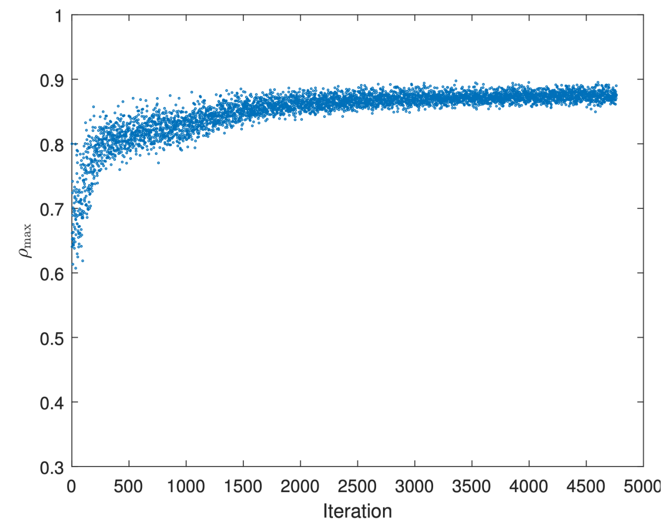

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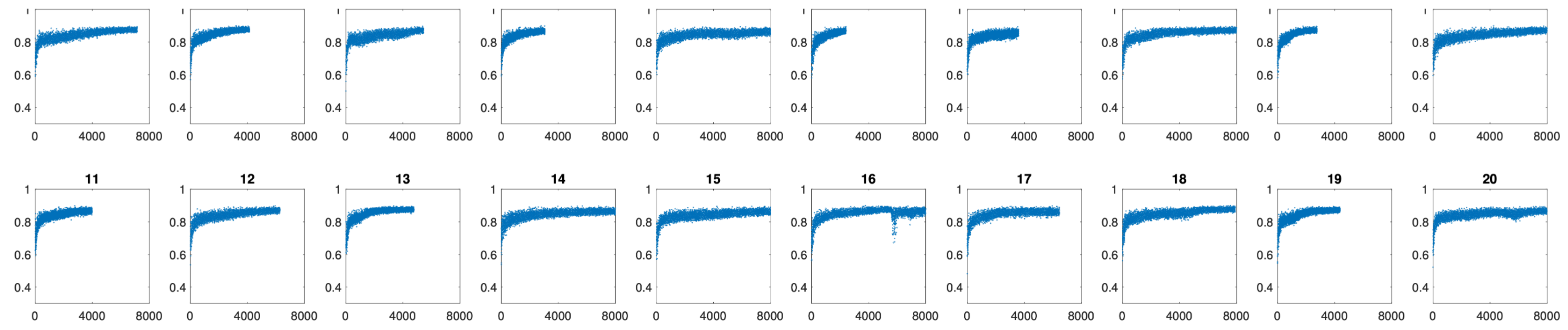

- How to express confidence in the best solution found?
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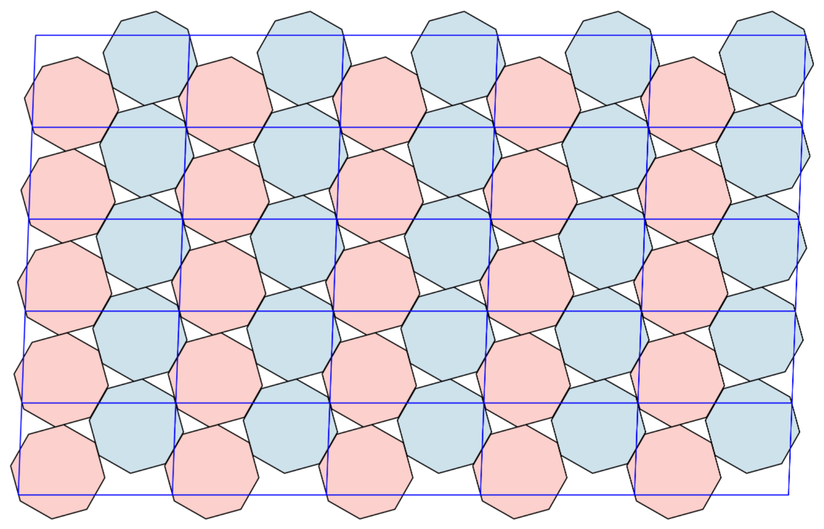
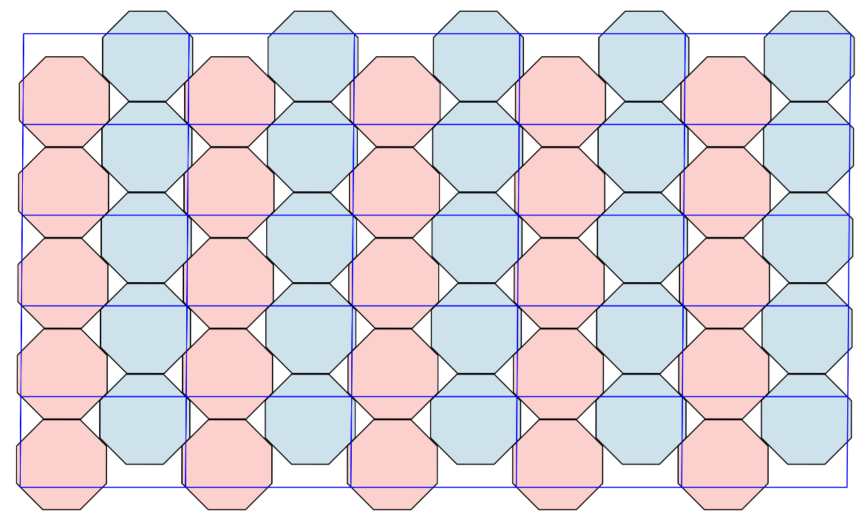
- Hodges-Lehmann estimator of the pseudomedian of 20 runs

$$\hat{m} = 0.8970032$$



Highest maximal packing solution

$\rho = 0.89984$



Lowest maximal packing solution

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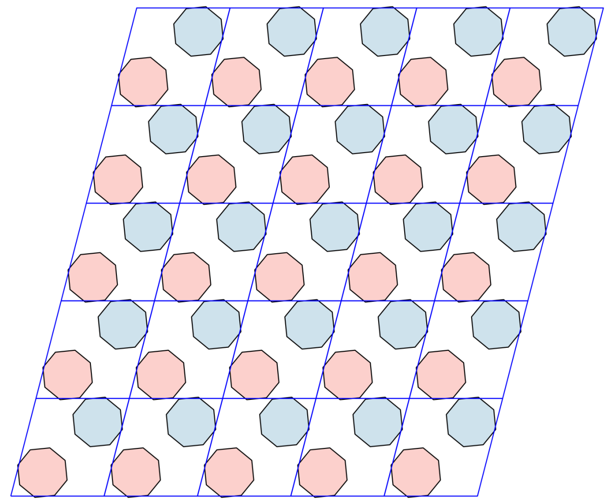

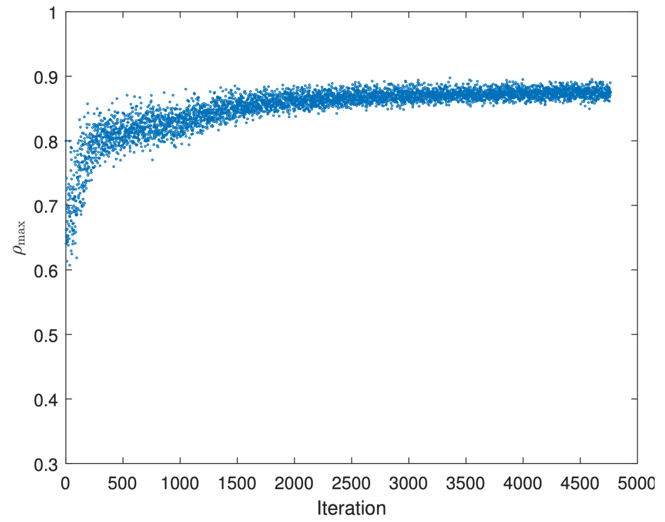

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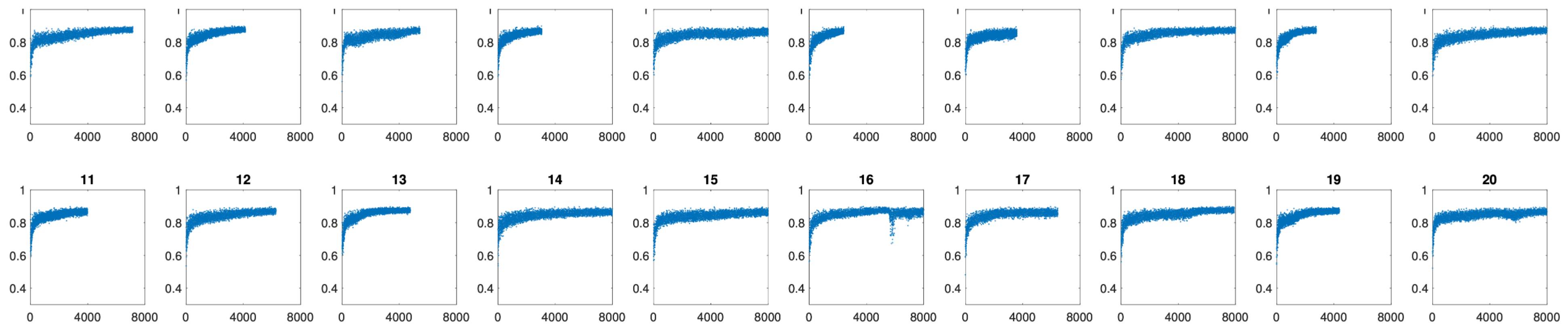

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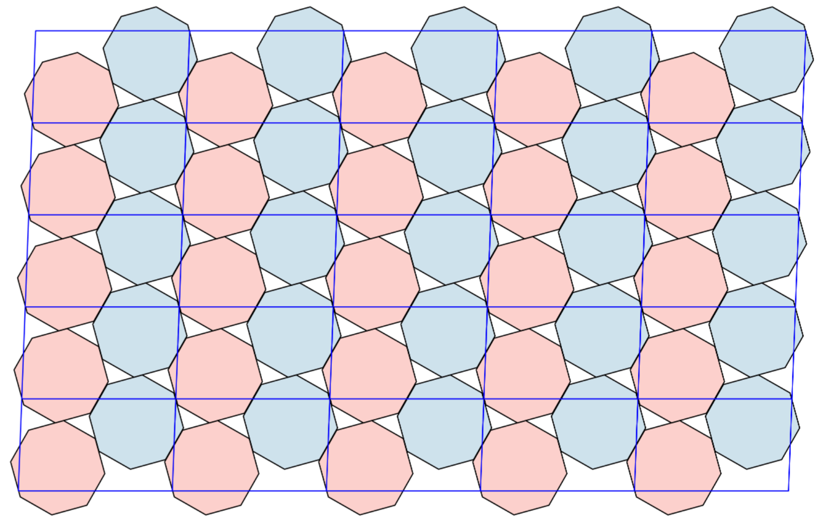
- 95% confidence interval based on Wilcoxon's signed rank test

$$(0.8959246, 0.8980686)$$



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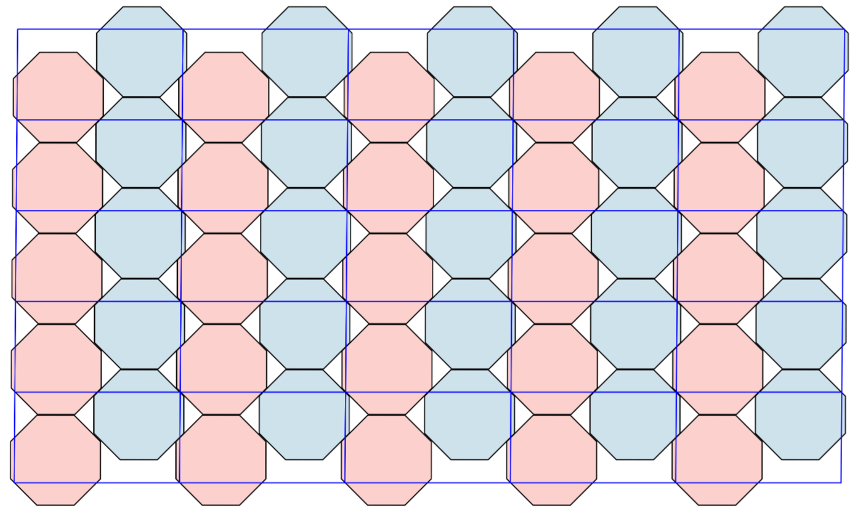

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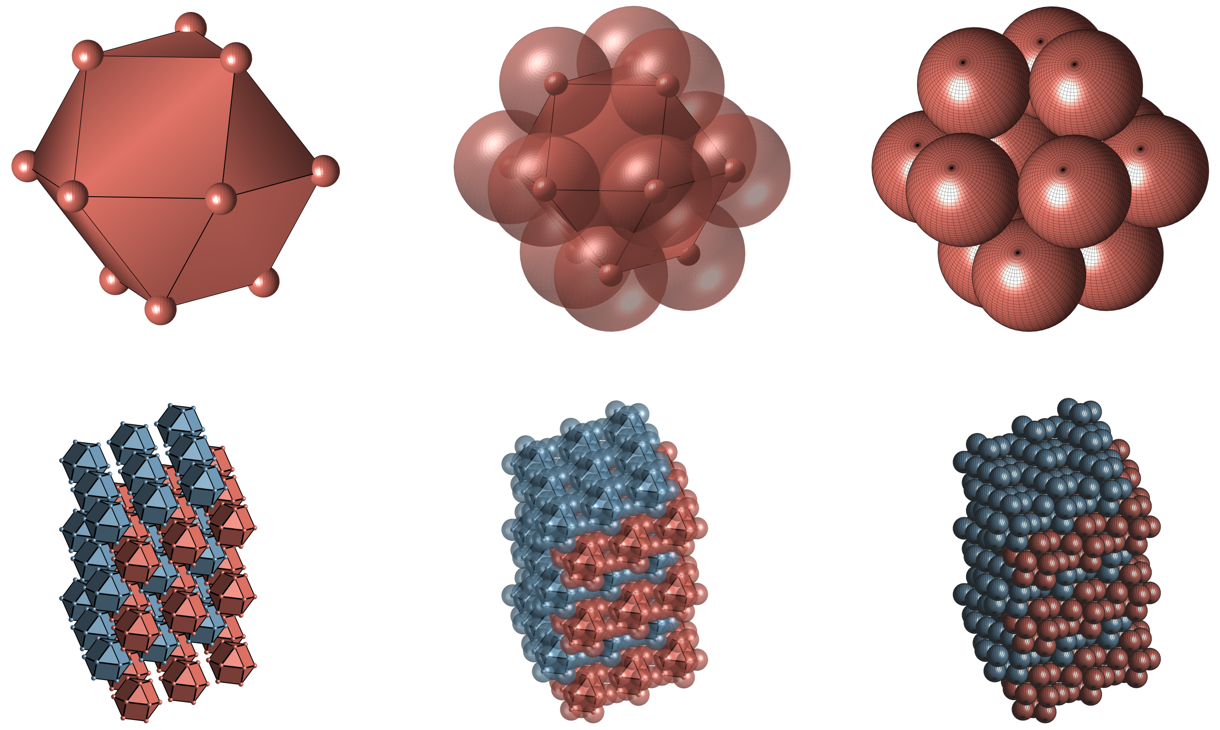

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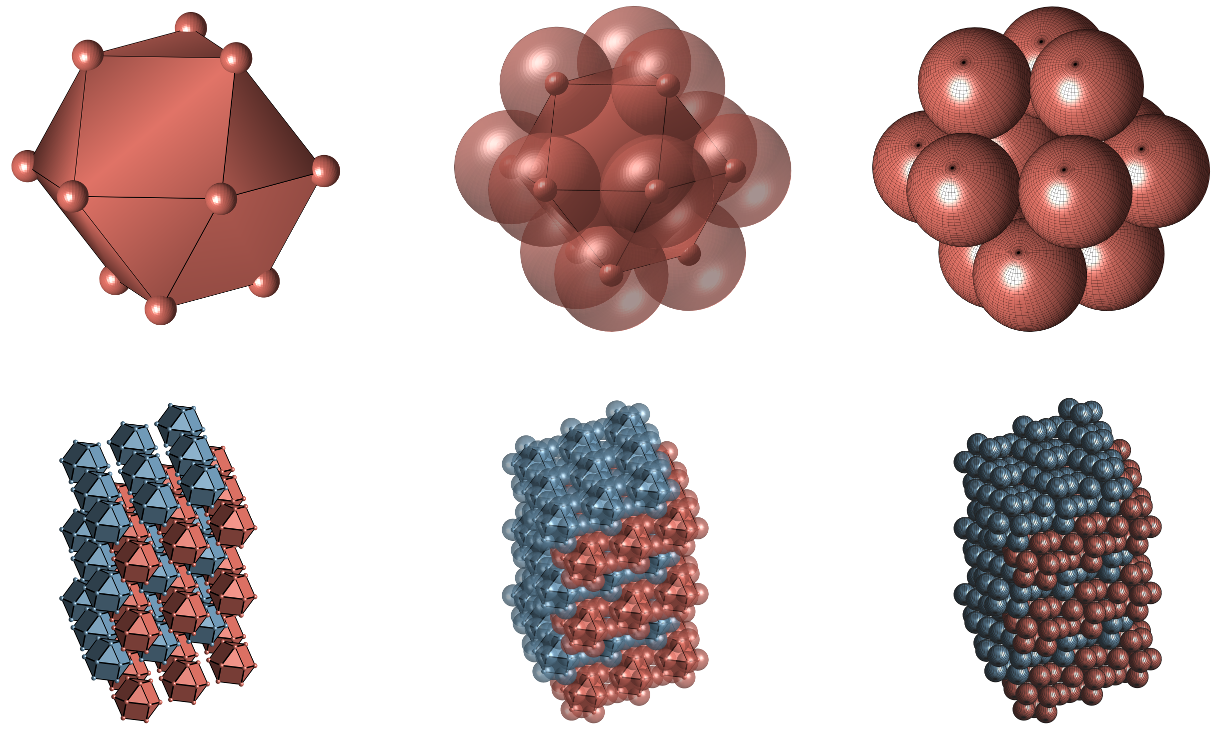

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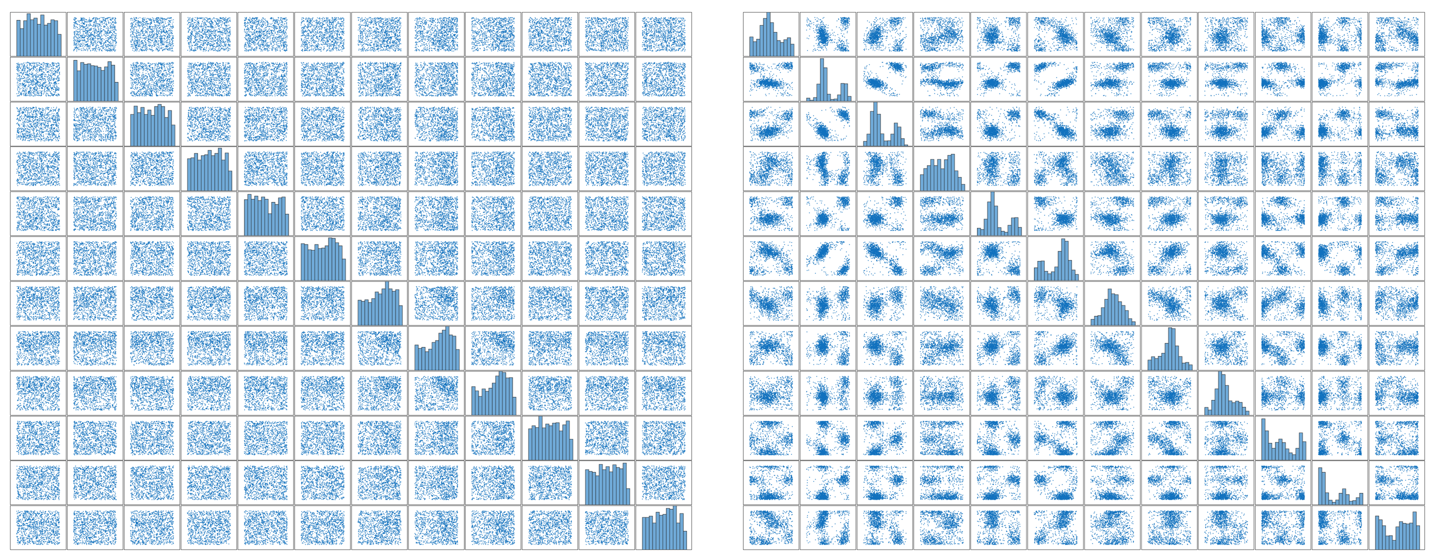

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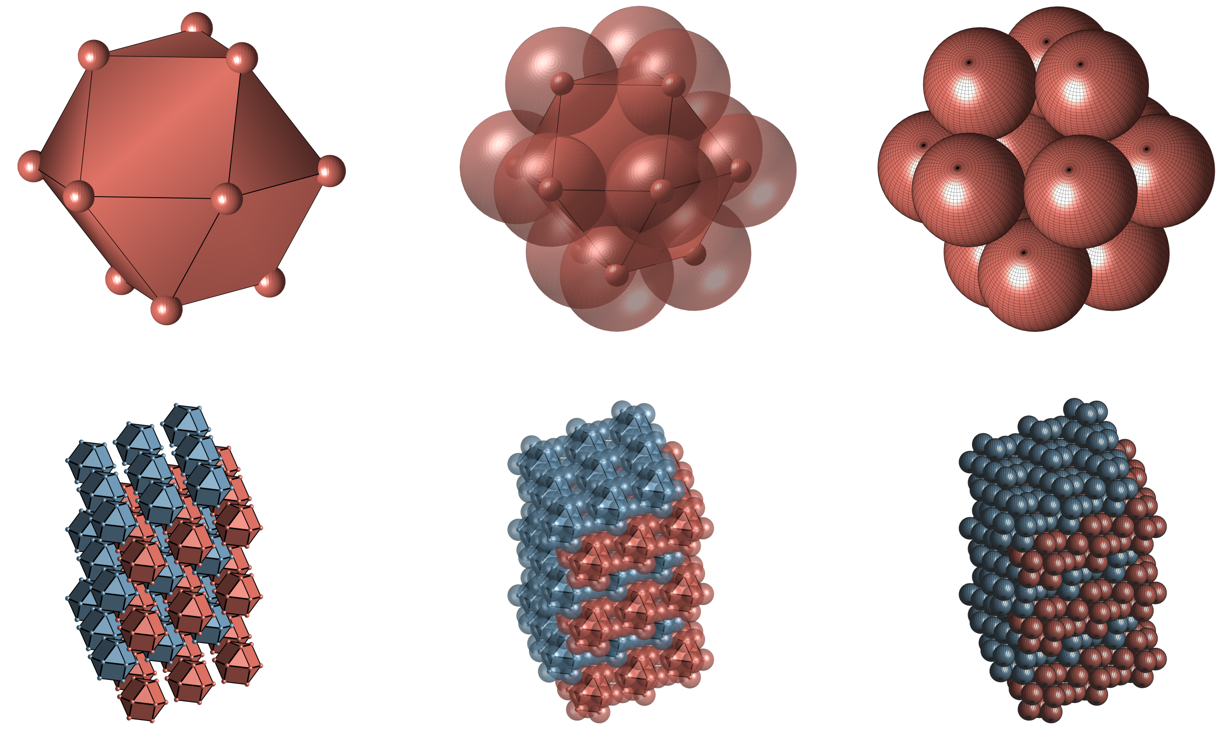

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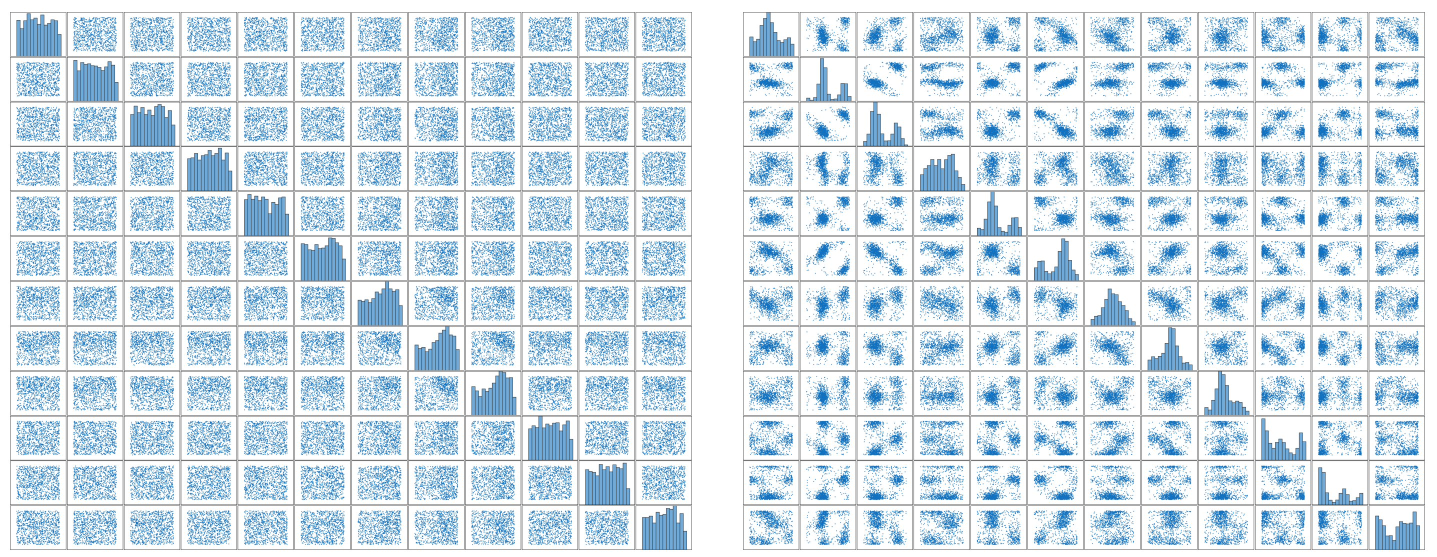

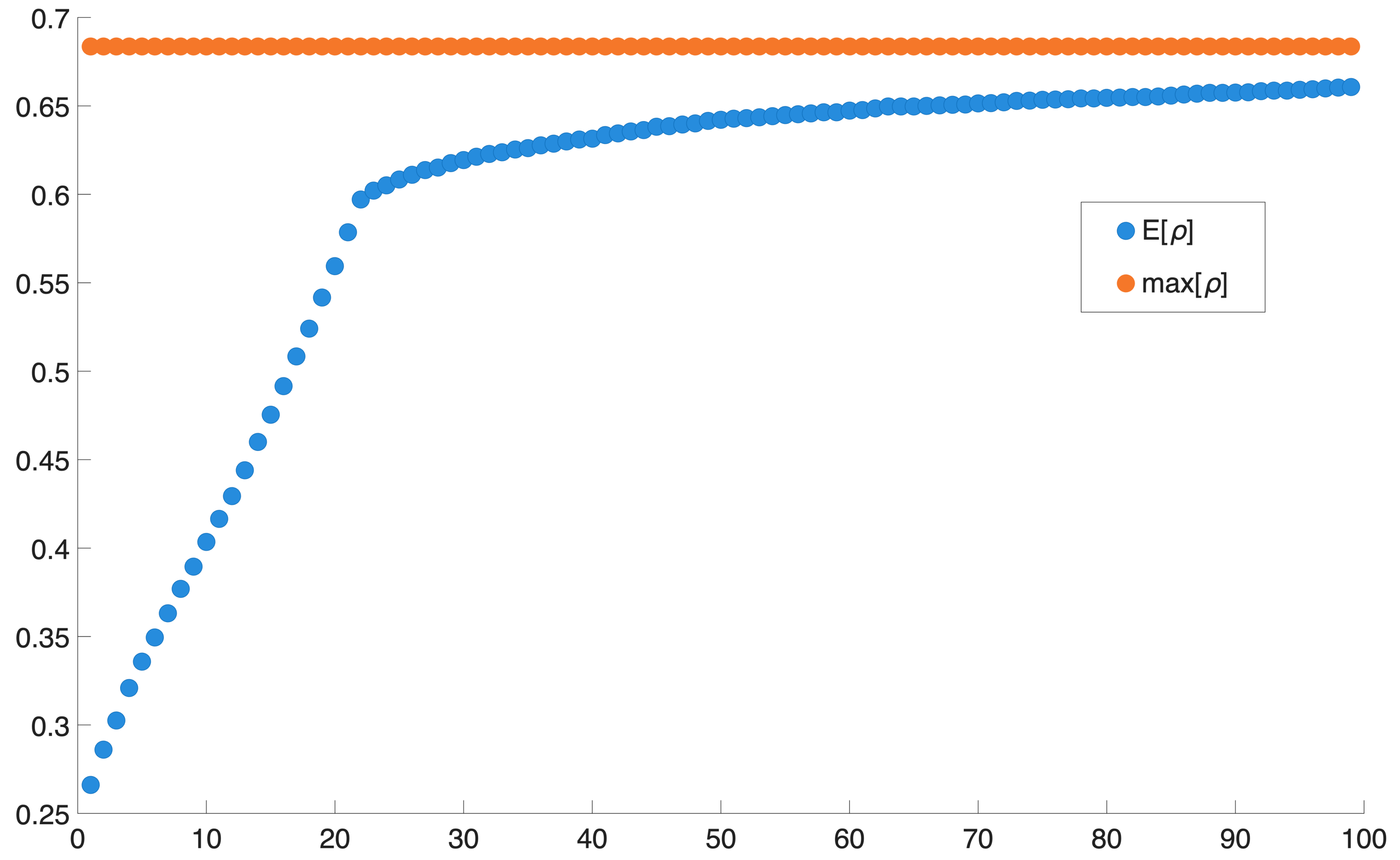

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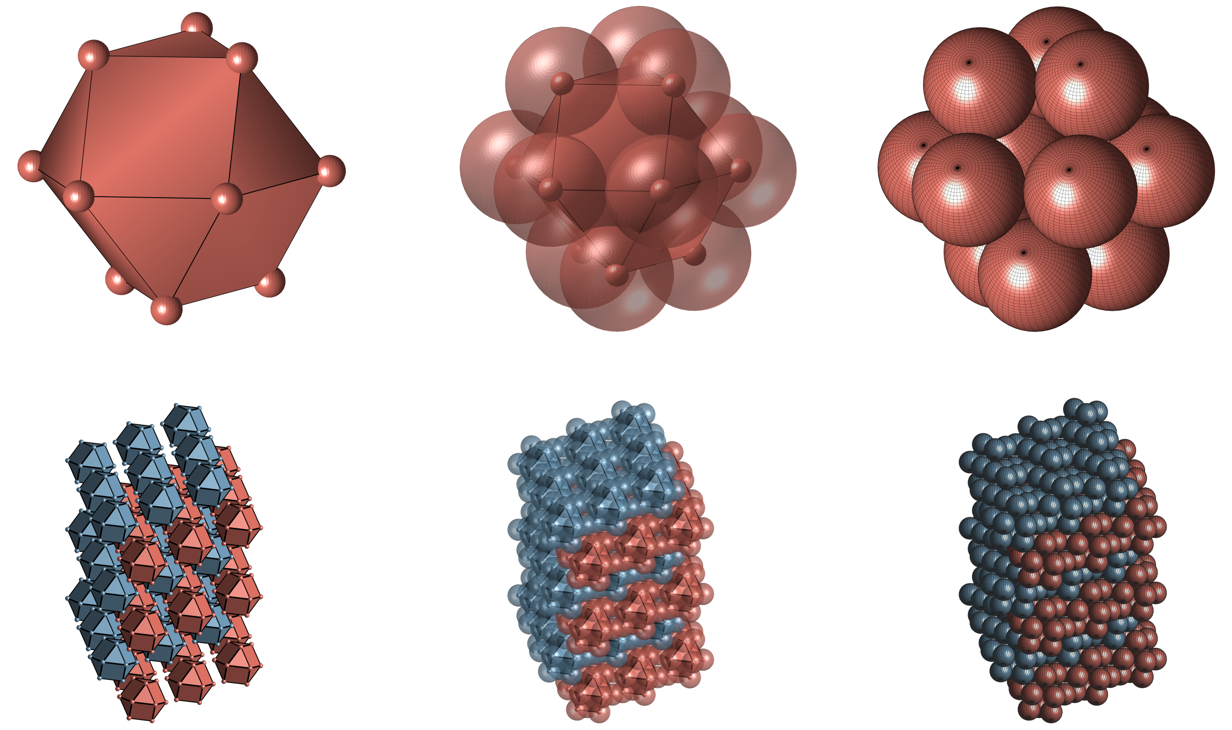

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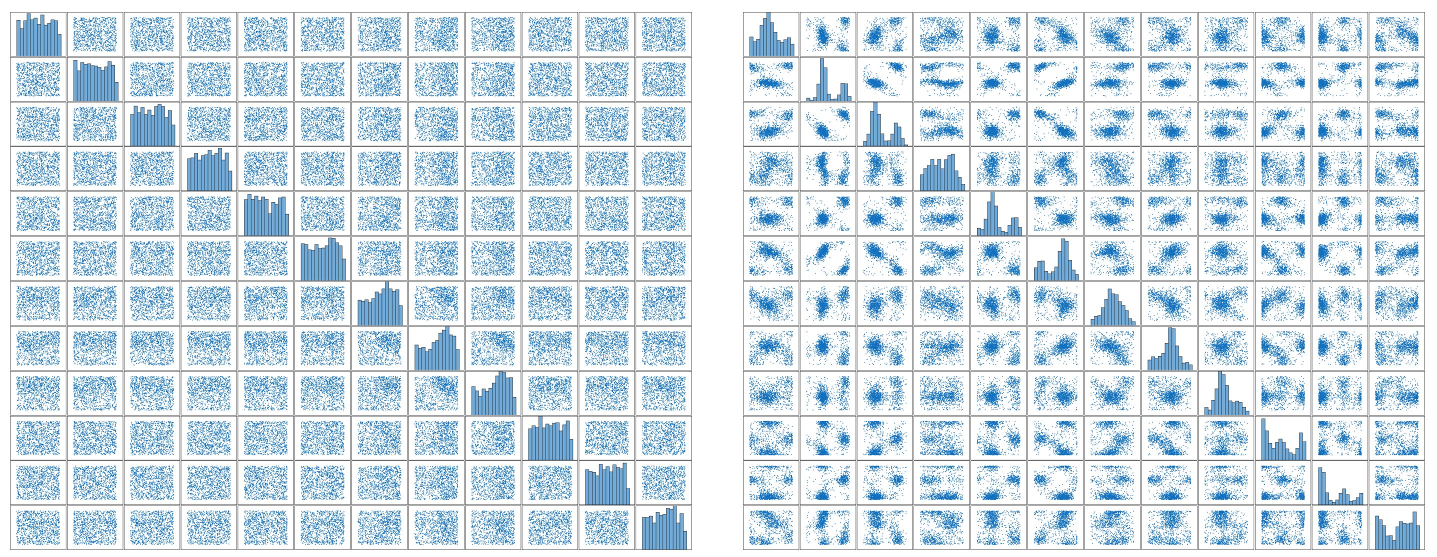

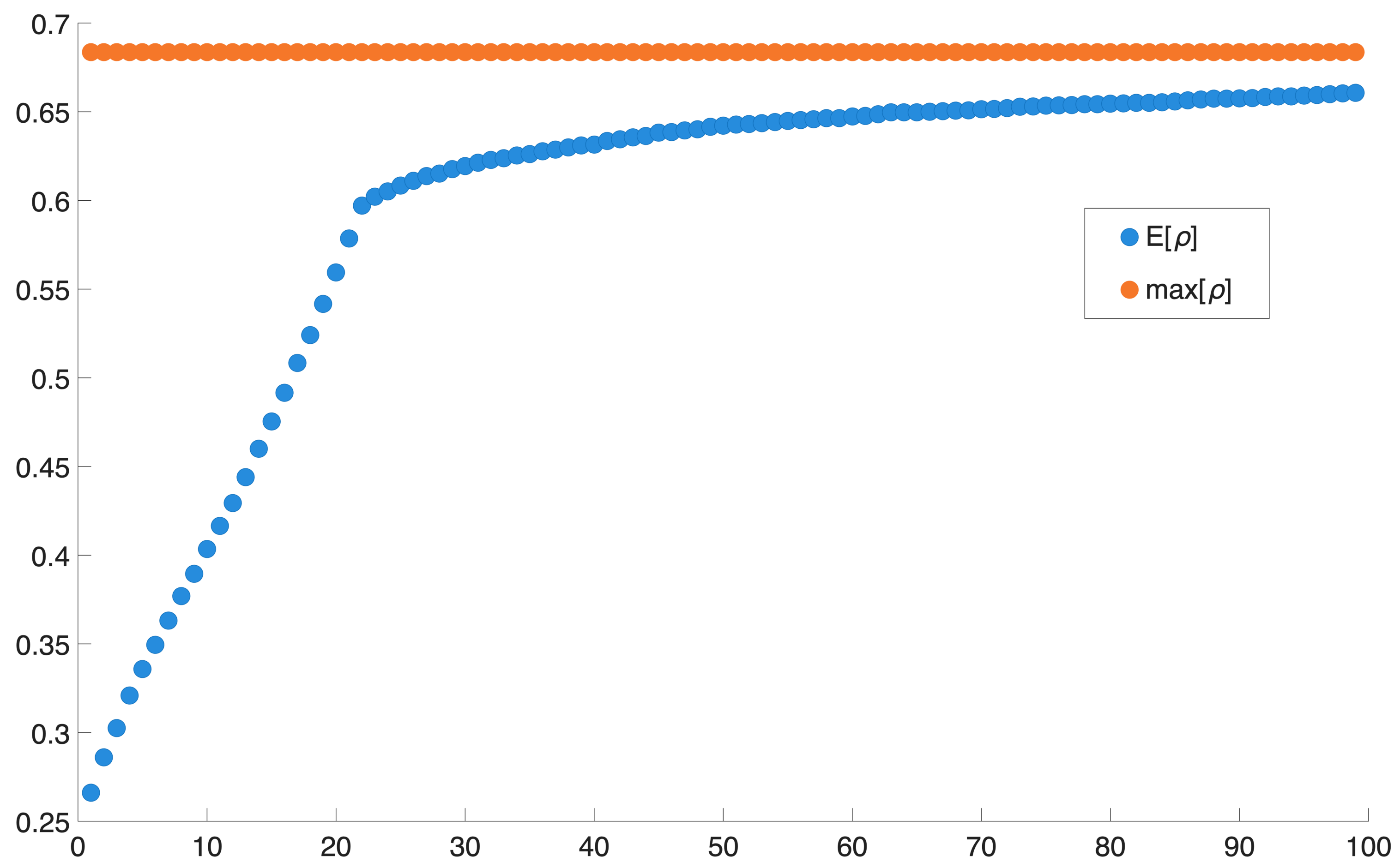

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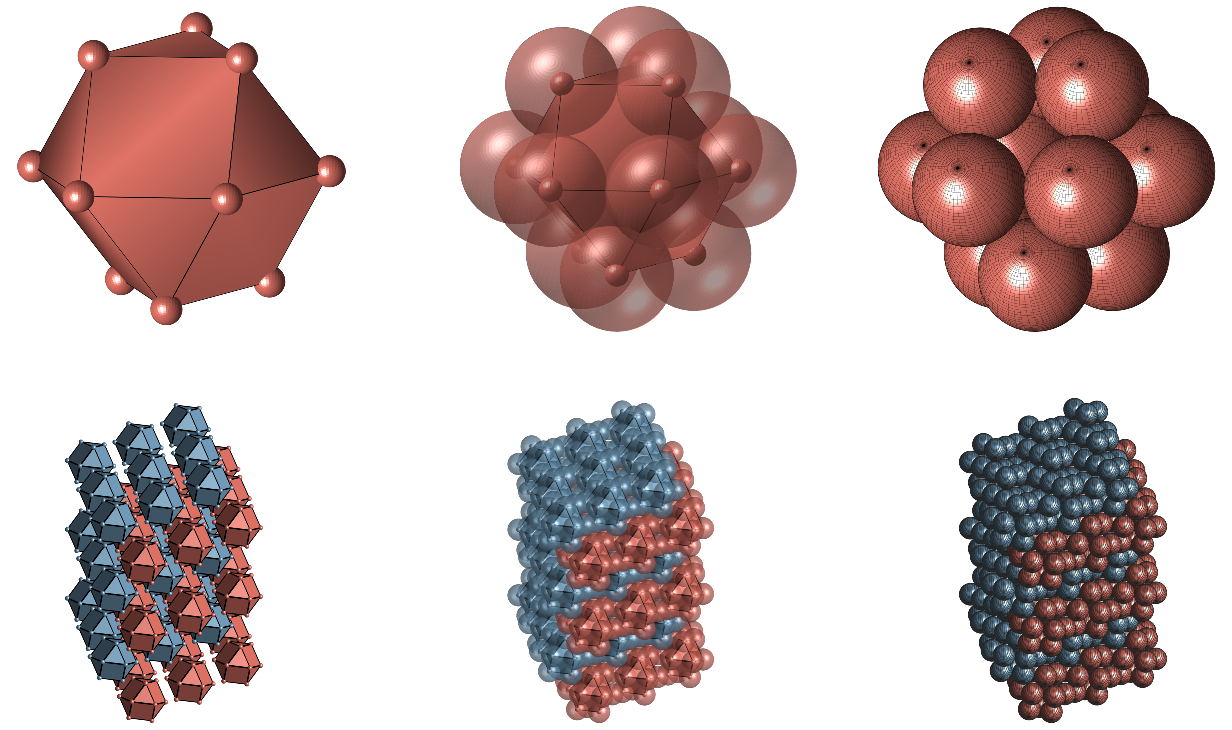
- **Stopping Criterion**: stop when the optimality gap falls below 0.1%



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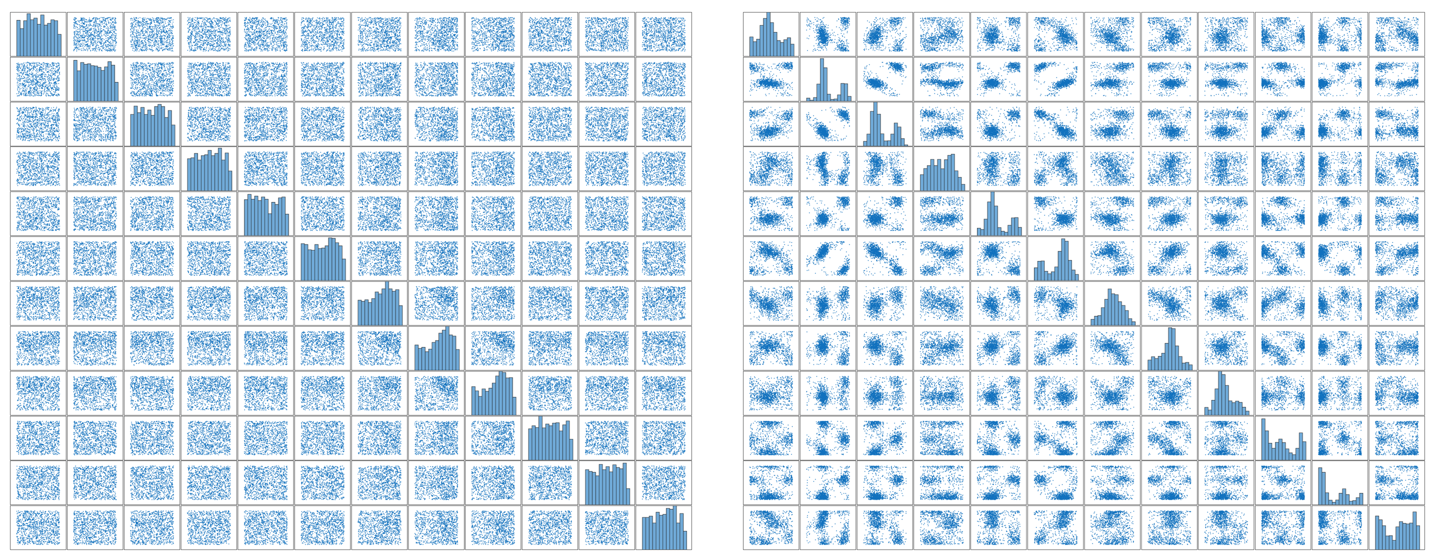

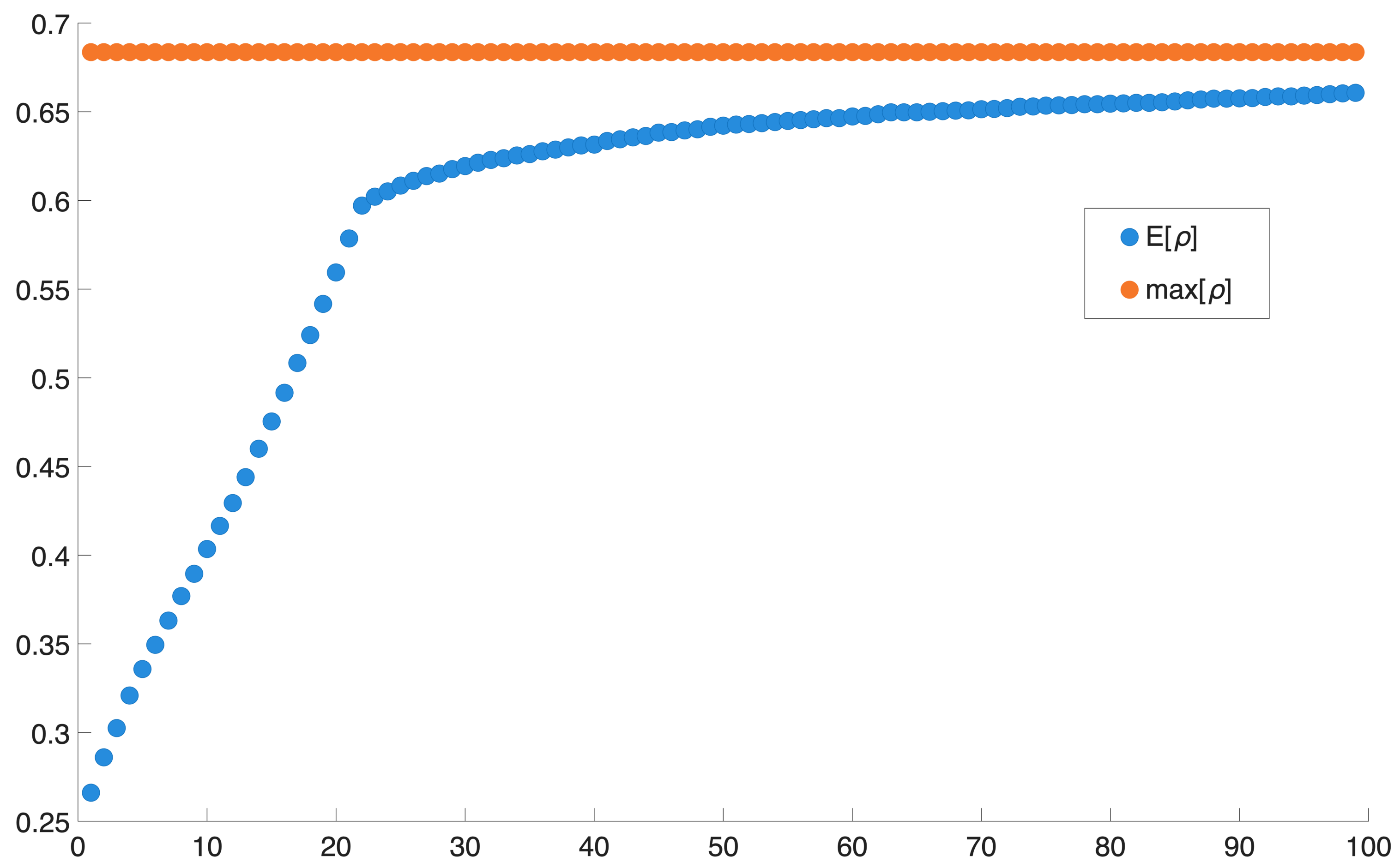

Uncertainties in Predictive Estimation

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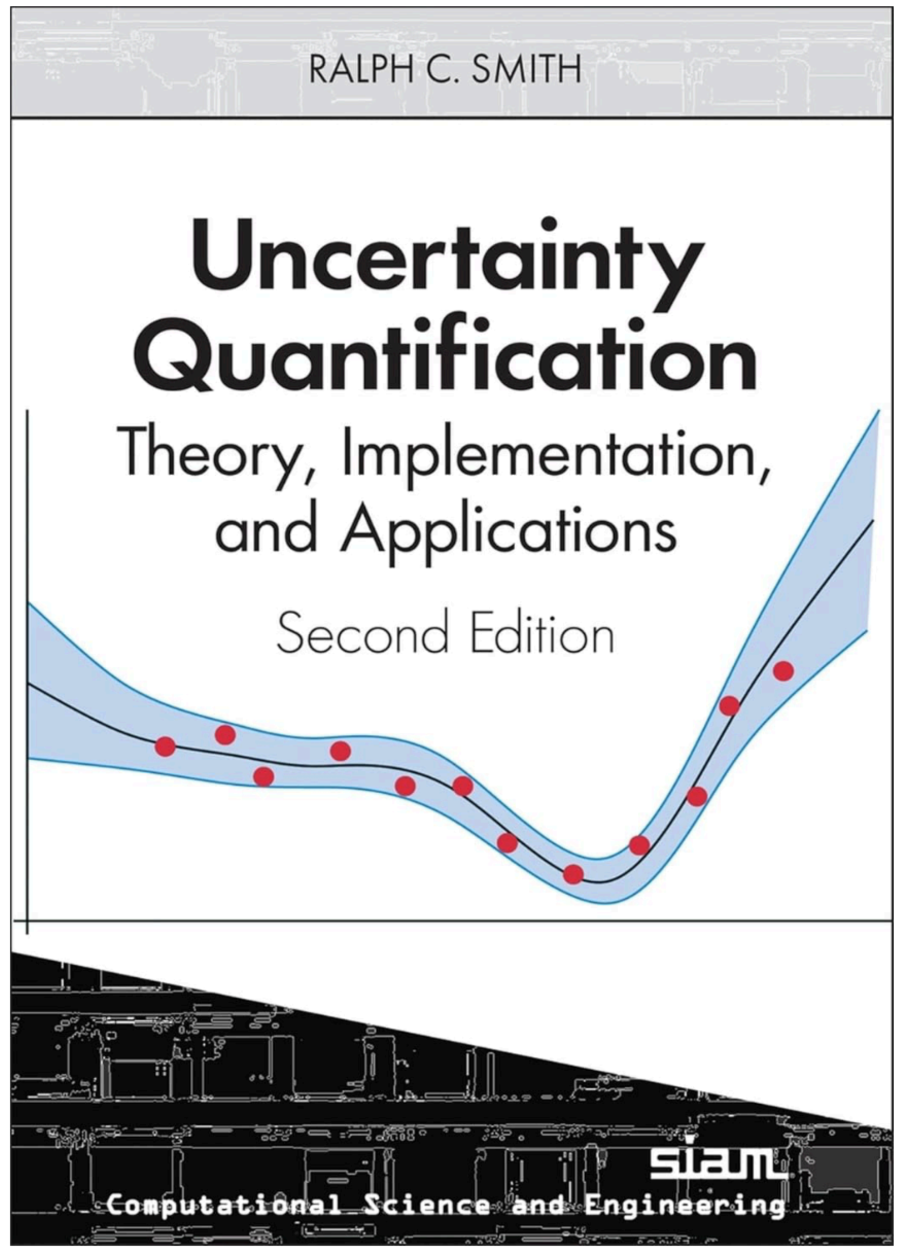

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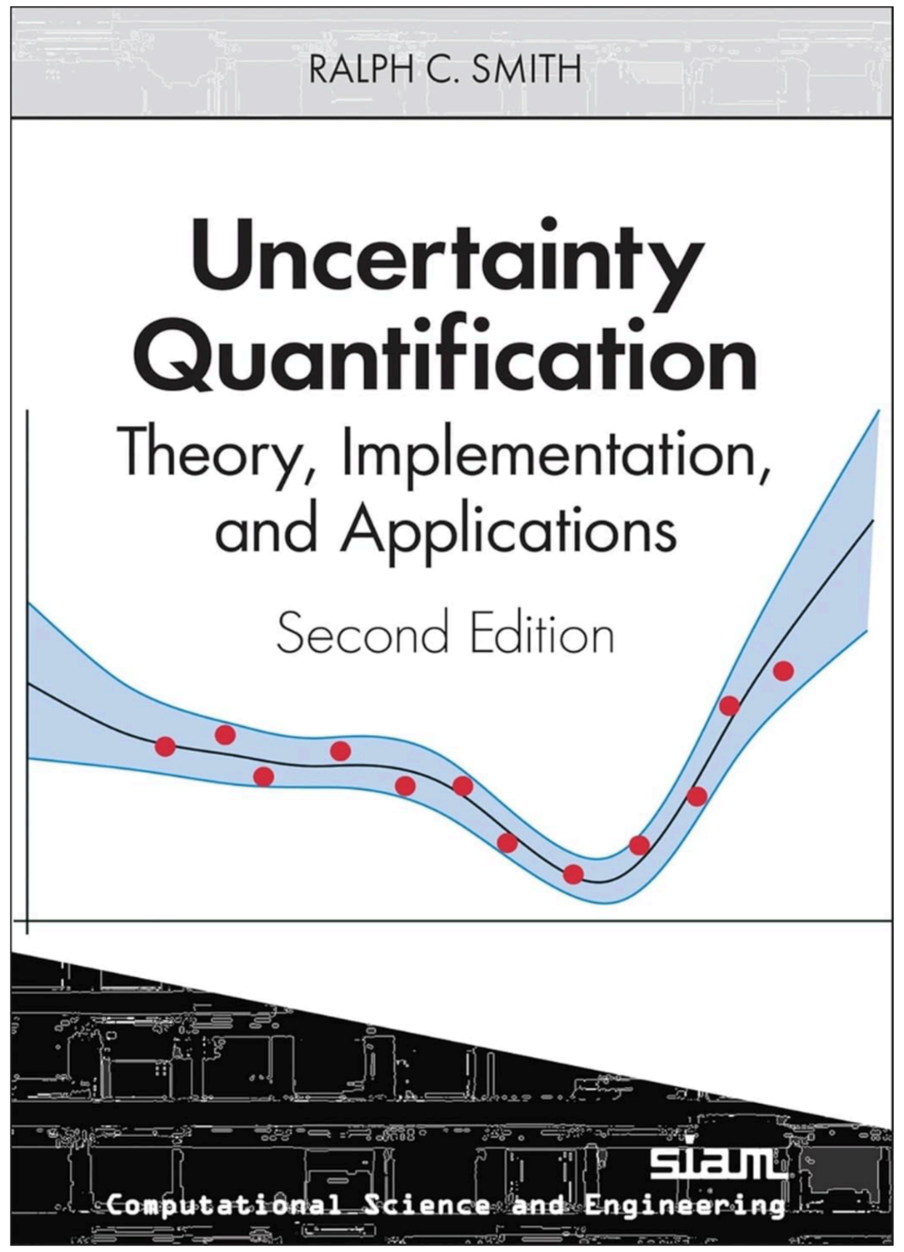

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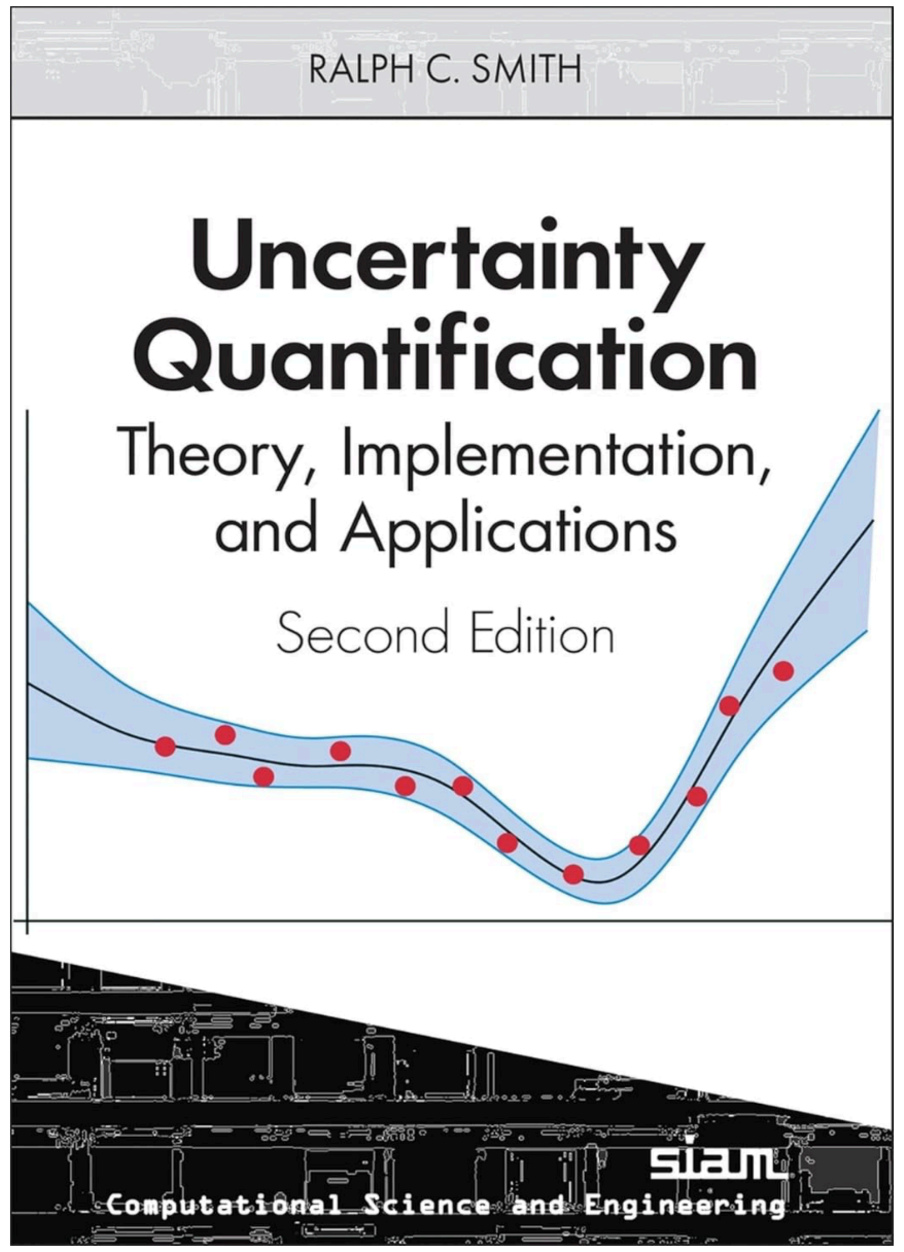

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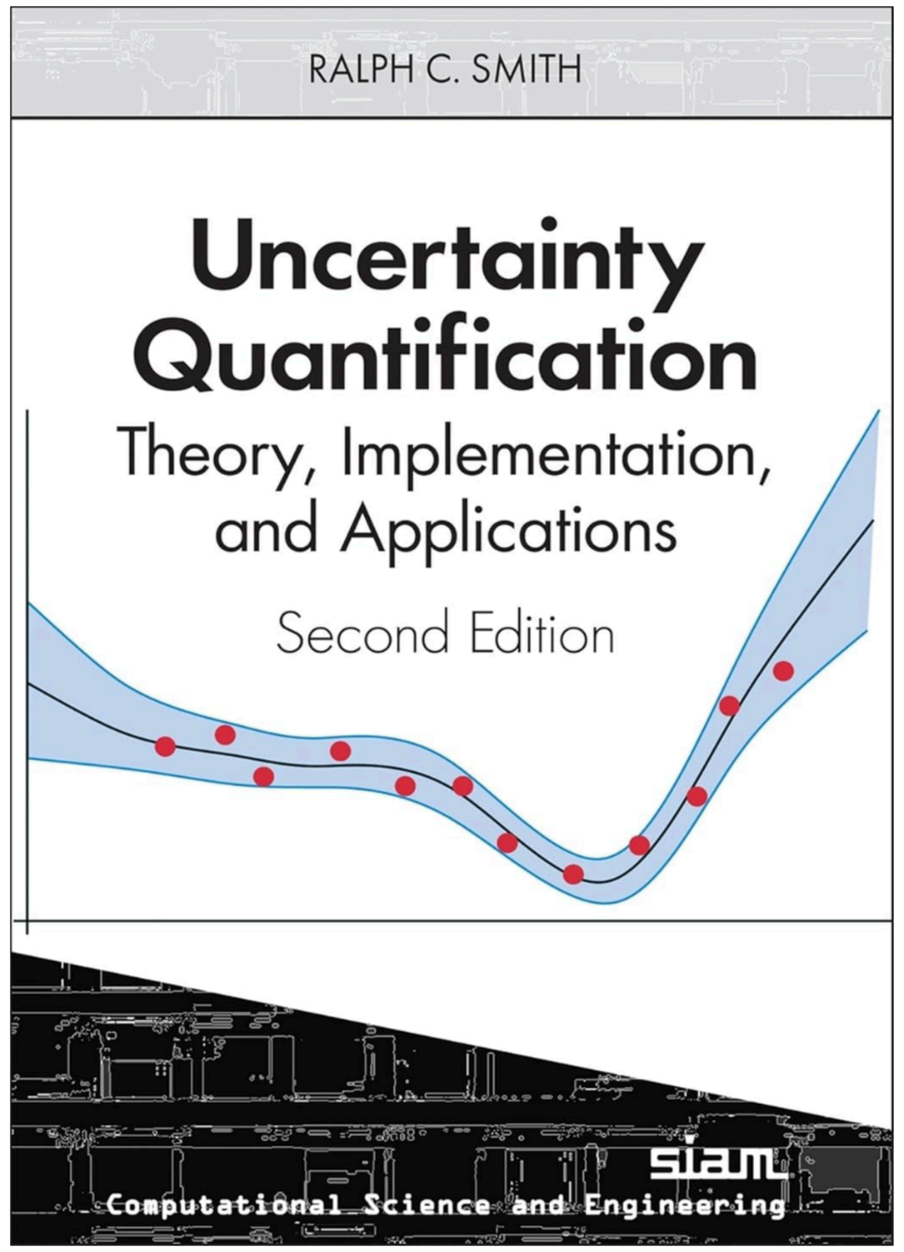

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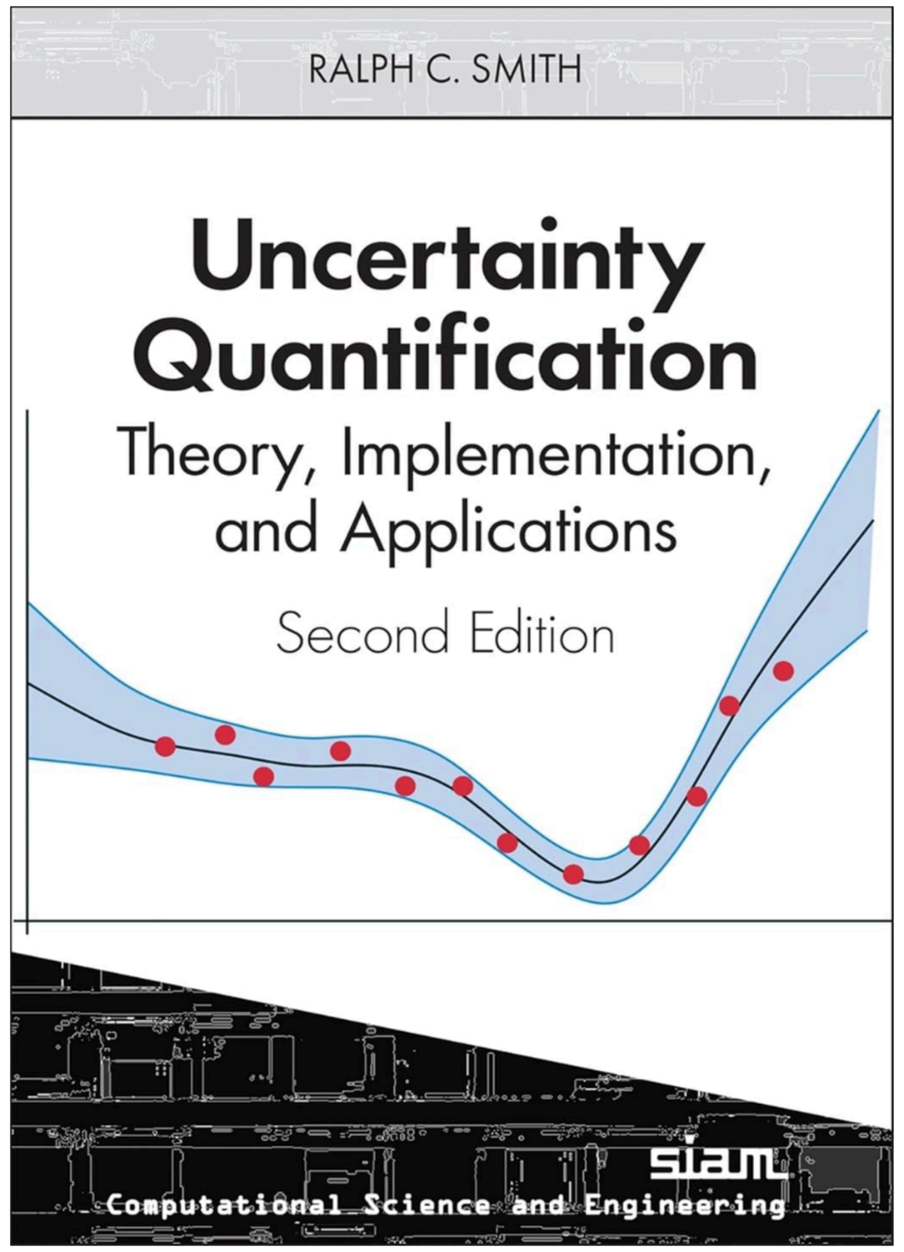

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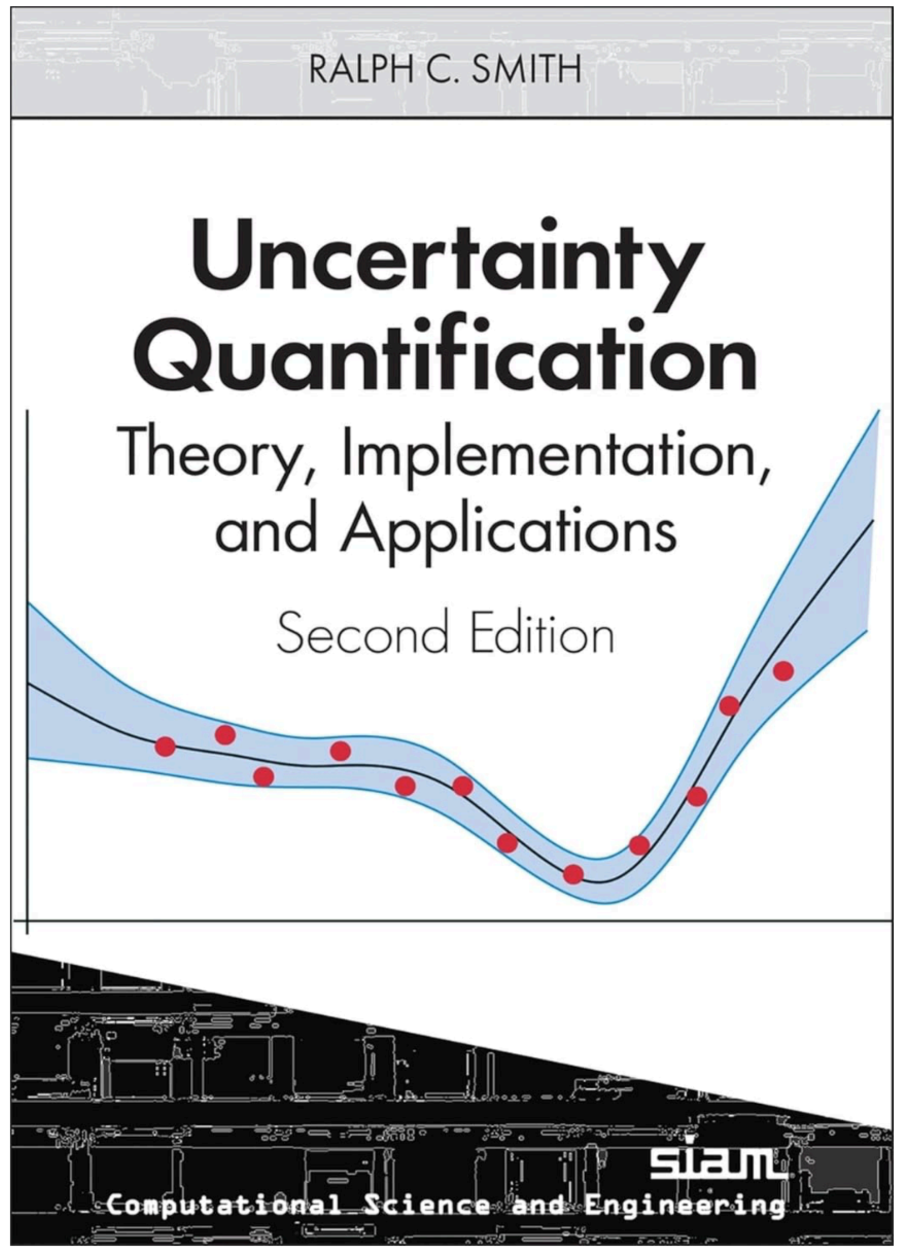

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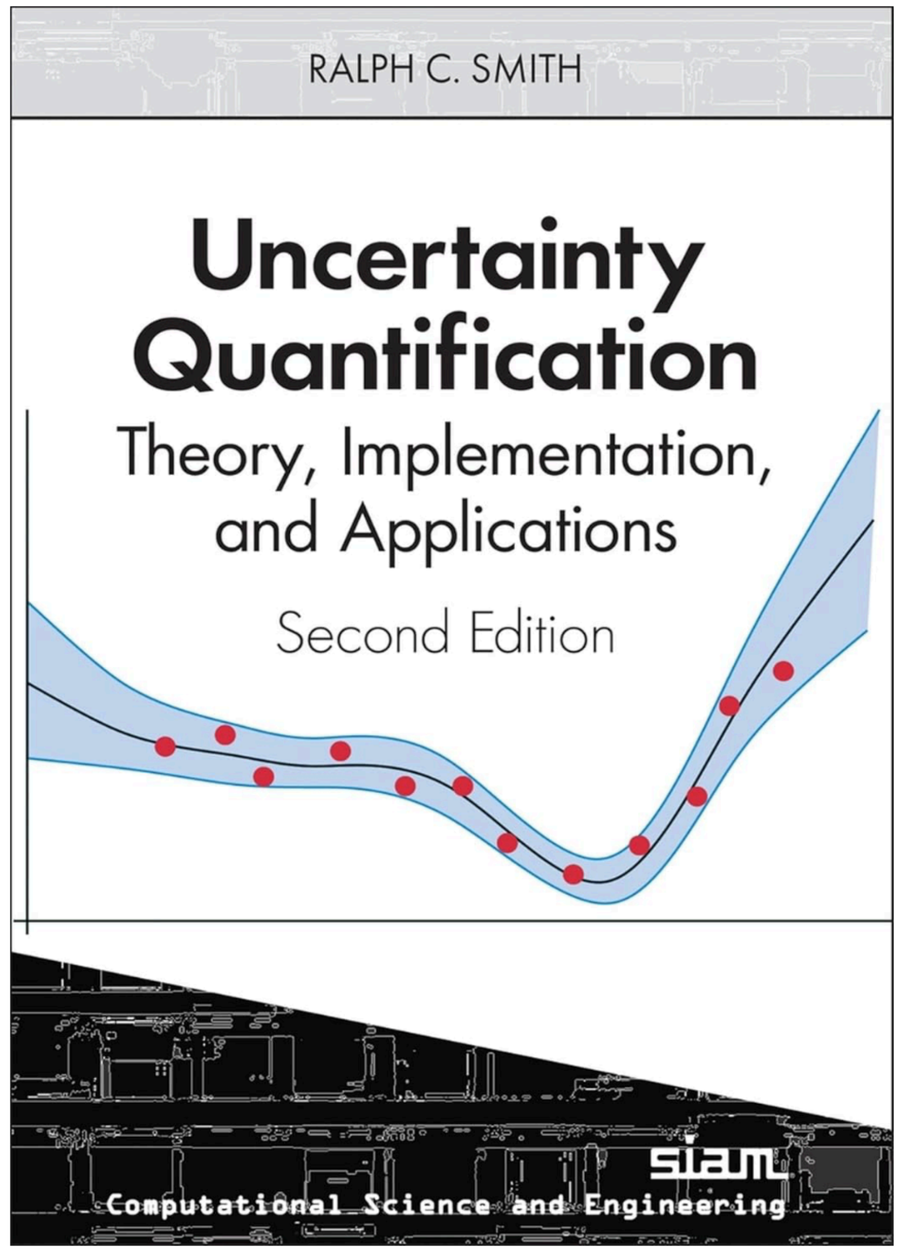

- When **extrapolating** to contexts outside those for which we have observations of the physical system, it is essential to impose **strict prior information** on the permissible function space used to construct $\delta(x_i)$.

THANK YOU

The authors thank the Leverhulme Trust for funding this research via the Leverhulme Research Centre for Functional Materials Design