Jamming in Hard-Sphere Packings

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Sphere Packings

Consider packing of N spheres with *configuration* $\mathbf{R} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$:

$$P(\mathbf{R}) = \left\{ \mathbf{r}_i \in \Re^d \; : \; \|\mathbf{r}_i - \mathbf{r}_j\| \geq D \; \forall j \neq i \right\}$$

An **unjamming motion** $\Delta\mathbf{R}(t)$, $t \in [0, 1]$, is a *continuous displacement* of the spheres along the path $\mathbf{R} + \Delta\mathbf{R}(t)$, $\Delta\mathbf{R}(0) = 0$, such that all *relevant constraints are observed* $\forall t$ and some of the particle *contacts are lost* for $t > 0$.

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Easy to test for! Each sphere has to have at least $d+1$ contacts with neighboring spheres, not all in the same d-dimensional hemisphere.

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Not trivial to test for!

Example: `Graphics/Honeycomb.2.1.collective.unjamming.wrl`

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What about **uniformly stable** in Connelly?

- Deformable spheres
- Distance to infeasibility vs. subpacking size
- ε as function of wavelength for periodic systems

Example: `Graphics/Honeycomb.1.1.strict.unjamming.wrl`

Rigidity Theory

A *periodic* packing $\widehat{P}(\mathbf{R})$ is generated by replicating a finite *generating packing* $P(\widehat{\mathbf{R}})$ on a lattice $\boldsymbol{\Lambda} = \{\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d\}$:

$$\mathbf{r}_{\widehat{i}(\mathbf{n}_c)} = \widehat{\mathbf{r}}_i + \boldsymbol{\Lambda}\mathbf{n}_c \,, \; \mathbf{n}_c \in Z^d$$

$$\Delta\mathbf{r}_{\widehat{i}(\mathbf{n}_c)} = \Delta\widehat{\mathbf{r}}_i + (\Delta\boldsymbol{\Lambda})\mathbf{n}_c$$

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Ideal (gapless) packings: *A packing is rigid if and only if it is infinitesimally rigid*, for packings in a concave hard-wall container or for periodic BCs (Connelly).

ASD

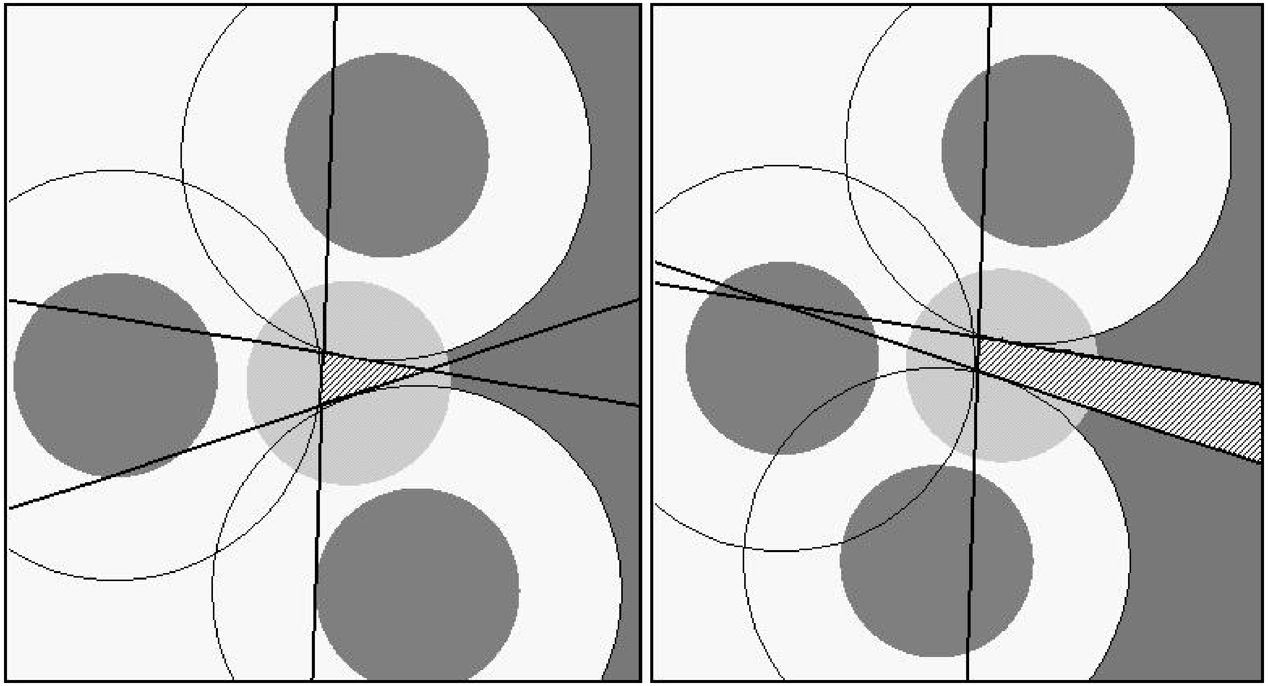
Approximation of small displacements for a *feasible displacement* $\Delta \mathrm{R}$:

$$\|\widetilde{\mathbf{r}}_i - \widetilde{\mathbf{r}}_j\| = \|(\mathbf{r}_i - \mathbf{r}_j) + (\Delta\mathbf{r}_i - \Delta\mathbf{r}_j)\| \geq D$$

$$(\Delta\mathbf{r}_i - \Delta\mathbf{r}_j)^T \mathbf{u}_{i,j} \leq \Delta l_{i,j} \text{ for all } \{i,j\}$$

- $\{i,j\}$ represents a *potential contact*
- $\Delta l_{i,j} = \|\mathbf{r}_i - \mathbf{r}_j\| - D$ is the *interparticle gap*, and
- $\mathbf{u}_{ij} = \frac{\mathbf{r}_j - \mathbf{r}_i}{\|\mathbf{r}_i - \mathbf{r}_j\|}$ is the unit contact vector

Validity of ASD



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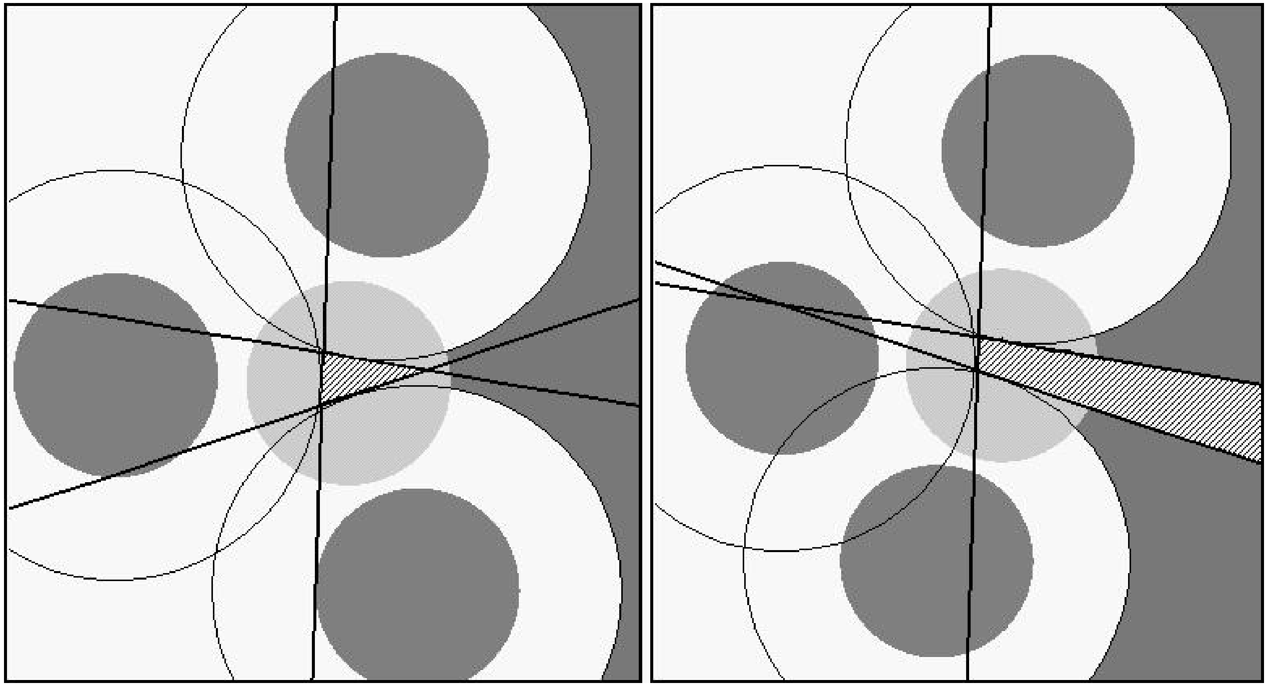

Q1: How to deal with finite gaps?

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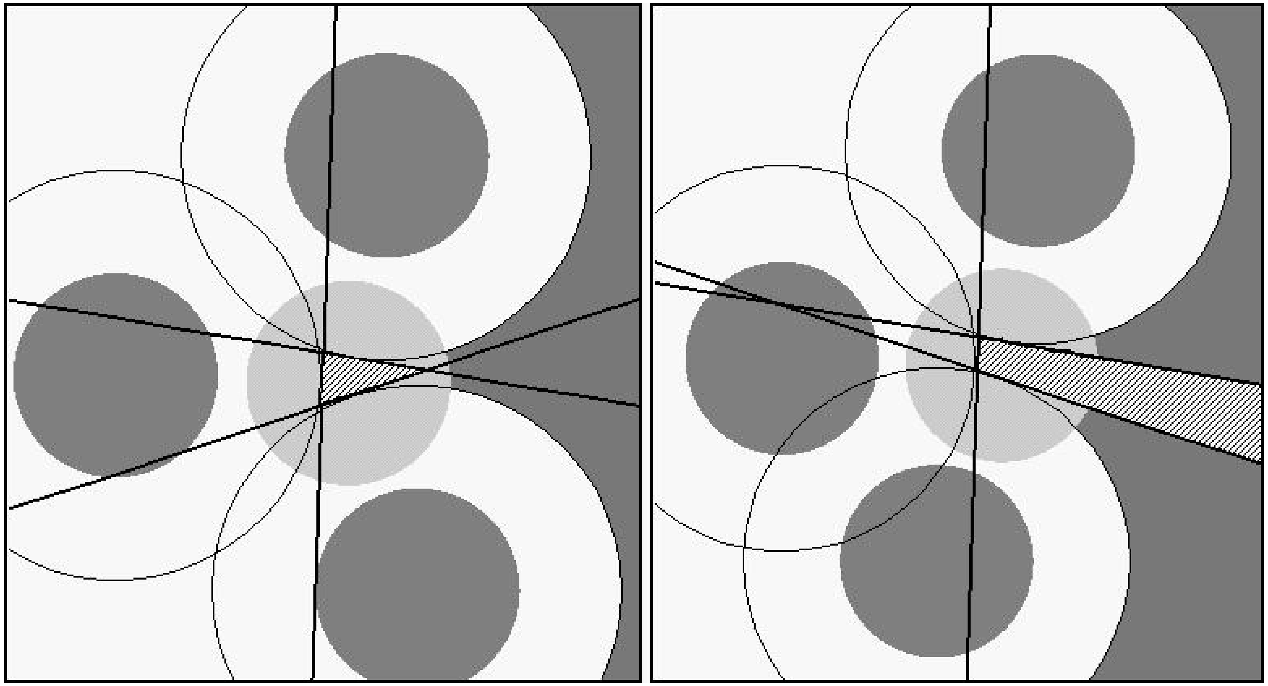

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Compare our geometrical definitions to dynamical concepts like **rearrangement** and **caging**?

Rigidity Matrix

Rigidity Matrix:

$$\mathbf{A} = \begin{array}{r c} & \{i,j\} \\ & \downarrow \\ \begin{array}{r} \\ i \rightarrow \\ \\ j \rightarrow \\ \\ \end{array} & \begin{bmatrix} \vdots \\ \mathbf{u}_{ij} \\ \vdots \\ -\mathbf{u}_{ij} \\ \vdots \end{bmatrix} \end{array}$$

Also known as the **equilibrium** matrix or the transpose of the **compatibility** matrix.

Contact Network

System of linear inequality impenetrability constraints:

$$\mathbf{A}^T \Delta \mathbf{R} \leq \Delta \mathbf{l}$$

Contact network of the packing is a *tensegrity framework*, namely a *strut framework* (Connelly).

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Examples:

1. `Graphics/LS.10.2D.contact.wrl`
2. `Graphics/LS.100.2D.contact.wrl`
3. `Graphics/LS.500.2D.contact.wrl`

Jamming as Feasibility Problem

Gapless packings (excluding trivial motions):

$$\min_{\Delta \mathbf{R}} \sum_{\{i,j\}} (\mathbf{A}^T \Delta \mathbf{R})_{i,j} = \min \left(\mathbf{A}\mathbf{e}\right)^T \Delta \mathbf{R}$$

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Packings with gaps:

$$\mathbf{A}^T \Delta\mathbf{R} \leq \Delta\mathbf{l}$$

$$\exists\, \{i,j\} : \quad \left|\left(\mathbf{A}^T \Delta\mathbf{R}\right)_{\{i,j\}}\right| \geq \Delta l_{\text{large}} \gg \overline{\Delta l}$$

Randomized LP Test

Displacement formulation:

$$\begin{array}{rll} & \max_{\Delta\mathbf{R}} \mathbf{b}^T \Delta\mathbf{R} & \text{for virtual work} \\ \text{such that} & \mathbf{A}^T\Delta\mathbf{R} \le \Delta\mathbf{l} & \text{for impenetrability} \\ & |\Delta\mathbf{R}| \le \Delta R_{\text{max}} & \text{for boundedness} \end{array}$$

for *random loads* $\mathbf{b}$.

Example: `Graphics/LS.1000.2D.dilute.collective.unjamming.wrl`

Strict Jamming with PBC

$$\det\left[\widetilde{\mathbf{\Lambda}} = \mathbf{\Lambda} + \Delta\mathbf{\Lambda}(t)\right] \leq \det \mathbf{\Lambda} \textit{ for } t > 0$$

$$\mathit{Tr}[(\Delta\mathbf{\Lambda})\mathbf{\Lambda}^{-1}] \leq 0$$

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Lattice deformation models *macroscopic non-expansive strain*.

Example: `Graphics/LS.1000.2D.dense.strict.unjamming.wrl`

Heuristic Tests

Shrink-and-Bump heuristic (modified LS):

- **Pinned Honeycomb**:
  - LP-based unjamming: `Graphics/Honeycomb.unjamming.LP.LS.wrl`
  - Heuristic unjamming: `Graphics/Honeycomb.unjamming.LS.wrl`
- **Pinned Kagome**:
  - Success of heuristic: `Graphics/Kagome.non-unjamming.LS.wrl`
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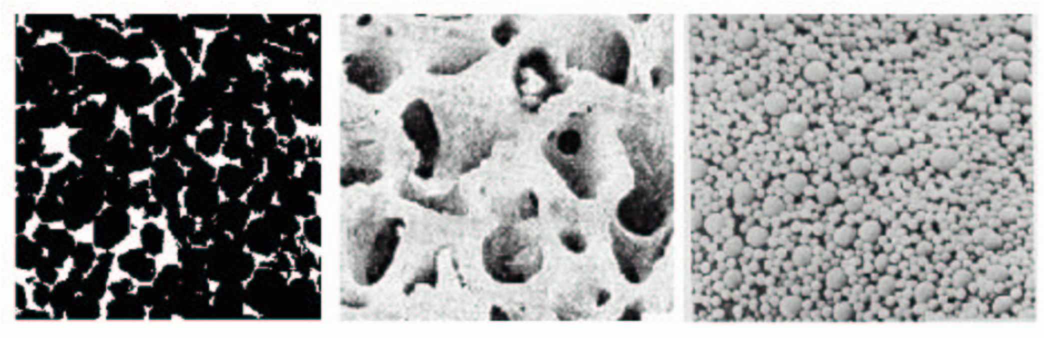
Not rigorous and reliable; But it is very fast!

Order Metrics



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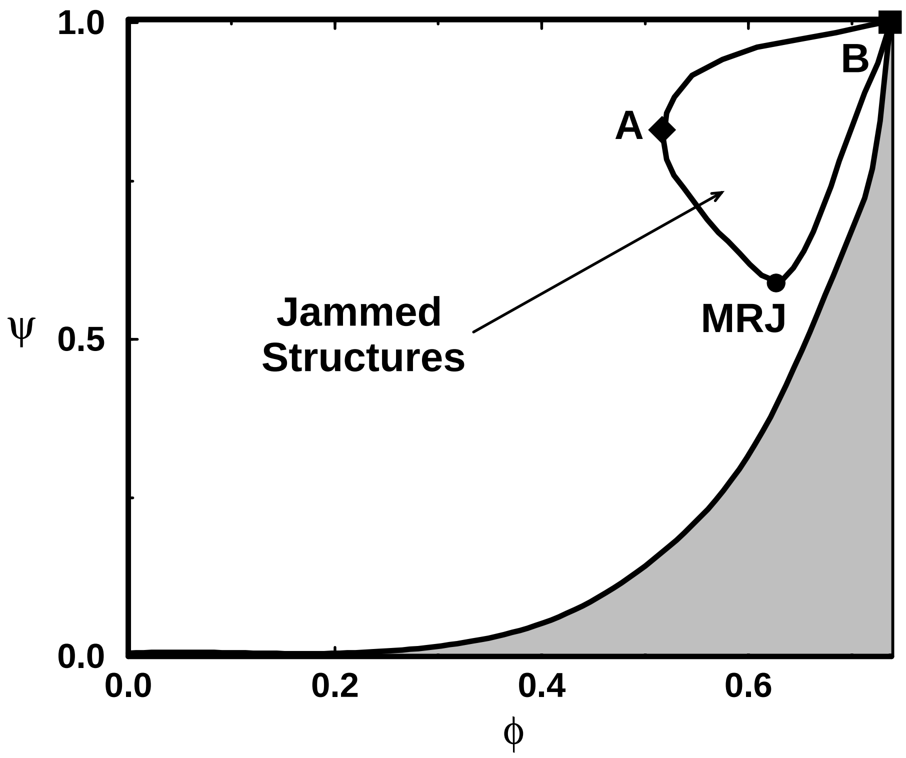
Examples:

- *Bond-orientation* order $\psi \equiv Q_6 = \frac{1}{m} \sum \left| e^{6i\theta} \right|$
- Information (entropy) contents of configuration?

The MRJ State



(*Torquato, Truskett & Debenedetti*) The jammed subspace in the order (ψ)-density (ϕ) plane

Random Packings

Random packings in 3D near MRJ *typically* have $\varphi \approx 64\%$ (`Graphics/LS.500.3D.packing.wrl`), and *cannot* be further densified from this with a variety of algorithms.

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Why?

Packing Algorithms

- Hard particles
  - Dynamical (Lubachevsky-Stillinger `Graphics/LS.100.3D.compression.wrl`)
  - Contact-network building (Zinchenko `Graphics/Zinchenko.3D.500.packing.wrl`)

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- Soft particles
  - Molecular dynamics (annealing)
  - Monte Carlo with stiff potentials
  - Hardening elastic springs

Challenging Packing Algorithms

- **Including the (periodic) cell in the algorithm**
  - Lattice velocity in LS (computational challenge) Compare to Parinello-Rahman MD. All collisions implicitly involve the lattice.
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  - Lattice velocity in LS (computational challenge) Compare to Parinello-Rahman MD. All collisions implicitly involve the lattice.
  - Lattice spring constants
- **Polydisperse packings**
  - Standard LS has problems with large polydispersity Shrink some, grow other particles and shrink the container?
  - Adaptive molecular dynamics?

continued...

- **Packings of ellipsoids (`Graphics/Ellipses_MMs.jpg`)**
  - Rotation is new degree of freedom (counting)
  - LS for ellipses (collision time calculation)
  - Ellipsoidal interaction potentials (e.g., based on overlap volume)

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- **Generating jammed packings**
  - Local jamming is the usual (easy criterion)
  - Need for generating *nearby* jammed states for Monte Carlo (e.g., search for the MRJ)

Jammed Subpackings

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Randomly diluting jammed packings:
How to efficiently test whether a sphere can be removed or not (sensitivity analysis)?

Jammed Backbones

Special jammed subpackings:

$$\text{Infeasible}: \quad \begin{aligned} (\mathbf{Ae})^T \Delta\mathbf{R} &\leq -\varepsilon < 0 \\ \mathbf{A}^T \Delta\mathbf{R} &\leq 0 \end{aligned}$$

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Compare to **backbones** in framework rigidity: What is the analog?

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  Braced Kagome lattice: `Graphics/Kagome.reinforced.contact.wrl`

- Subpackings of the FCC lattice: *No trivancies!*

  FCC random dilution $\phi = 0.52$: `Graphics/Fcc.348_500.packing.wrl`

Stress-Strain Relations

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Do rearrangements (dynamics) play a critical role?

continued...

Static view: For perfect packings, we have a **cone of feasible strains** and a **cone of unsupported loads** (but note non-uniqueness). Describing these in full is NP complete.

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Settle for reduced information? Approximate polyhedral with ellipsoidal cones:

Will give us a “stiffness” matrix for networks of stiff springs (uniqueness).

The End...and Beginning

Jamming is important and interesting, particularly in random packings.

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Future directions (to do):

- Improve LS packing algorithm: deforming cell, polydisperse packings, ellipses, etc.
- Design packing algorithms based on networks of stiff elastic springs.
- Design algorithms to find jammed subpackings, backbones and critical clusters.

continued...

- Explore **statistical geometry** of random packings such as *Voronoi cells*, particularly for the MRJ state.
- Make amorphous strictly jammed 2D packing.

Future directions (to think about):

- How to make dilute jammed packings.
- Unambiguous identification of the MRJ.
- Jamming, caging, rearrangement, and reality.
- Macroscopic stress-strain relations in jammed packings.

References (math)

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