Jamming in Hard-Sphere Packings

Aleksandar Donev

Collaborators: *Salvatore Torquato, Frank Stillinger, Robert Connelly*

Program in Applied and Computational Mathematics

and *Princeton Materials Institute*

`http://atom.princeton.edu/donev`

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

Local Jamming

No unjamming motions $\Rightarrow$ **jammed packing**. From Torquato & Stillinger:

Locally jammed Each particle in the system is locally trapped by its neighbors, i.e., it cannot be translated while fixing the positions of all other particles. Compare to **1-stable** in Connelly.

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.

Collective Jamming

Collectively jammed Any locally jammed configuration in which no subset of particles can simultaneously be displaced so that its members move out of contact with one another and with the remainder set. Compare to **finitely stable** in Connelly, or **rigid** for finite packings.

Not trivial to test for!

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

Strict Jamming

Strictly jammed Any collectively jammed configuration that disallows all globally uniform volume-nonincreasing deformations of the system boundary (*container* for hard-wall and *unit cell* for periodic BCs). Compare to **periodically stable** in Connelly.

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 $\mathbf{\Lambda} = \{\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_d\}$:

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

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

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

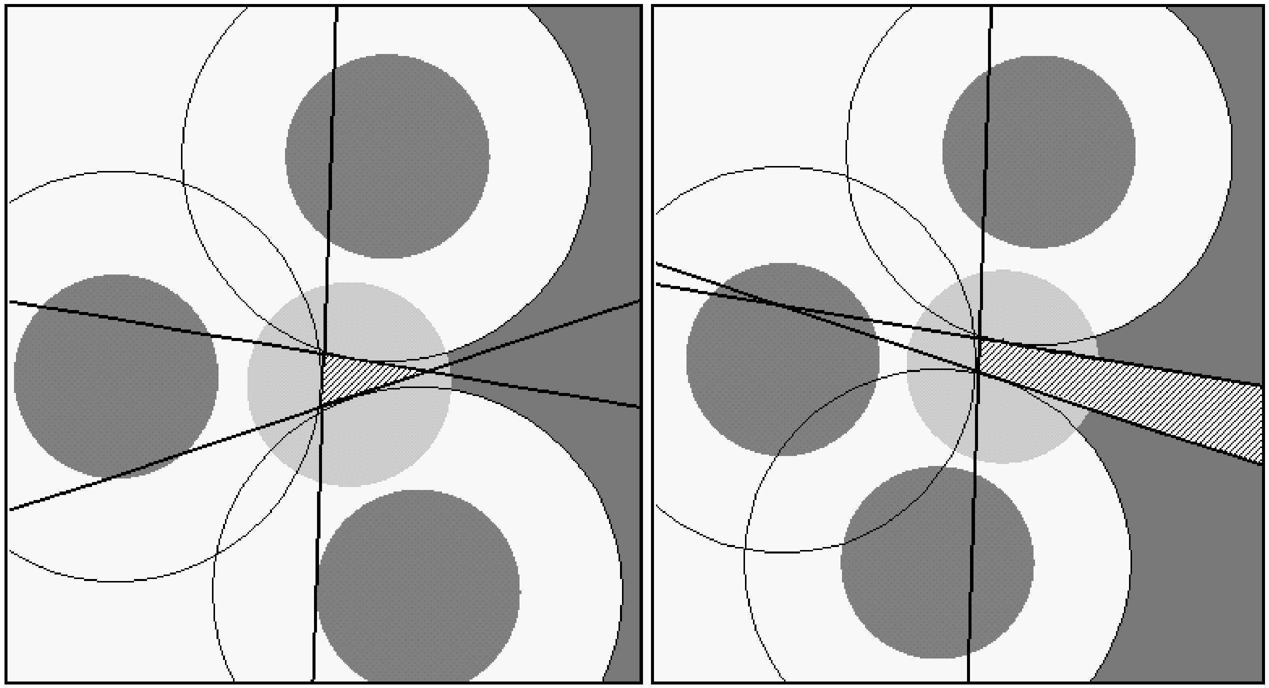
Approximation of small displacements for a *feasible displacement* $\Delta\mathrm{R}$:

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

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

- $\{i,j\}$ 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



Q1: How to deal with finite gaps?

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

Rigidity Matrix

Rigidity Matrix:

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

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).

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):

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

such that $$\mathbf{A}^T \Delta\mathbf{R} \leq 0$$

and also look at contact network as a bar framework.

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:

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

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

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

Strict Jamming with PBC

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

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

$$\text{Strain}\ \boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}^{T}=(\Delta\mathbf{\Lambda})\mathbf{\Lambda}^{-1}$$

Lattice deformation models *macroscopic non-expansive strain*.

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

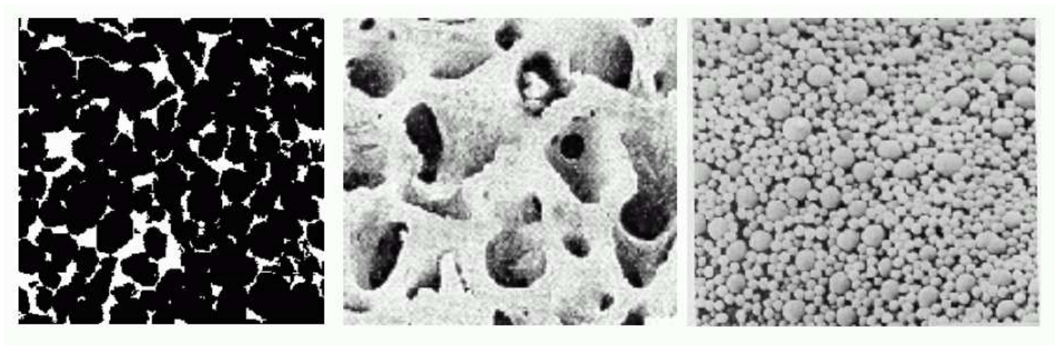
Heuristic Tests

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`
  - Failure: `Graphics/Kagome.unjamming.LS.wrl`

Not rigorous and reliable; But it is very fast!

Order Metrics

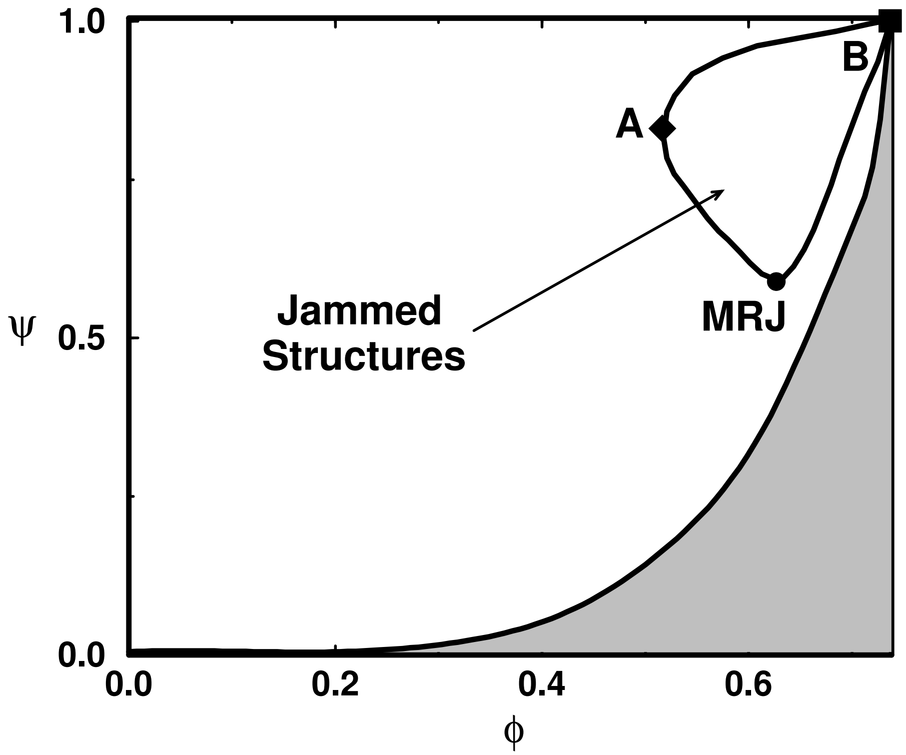


A scalar **order metric** $0 \le \psi \le 1$ is needed to replace correlation functions.

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.

All of the 3D random packings we tested were strictly jammed.

Random packings in 2D near MRJ *typically* have $\varphi \approx 83\%$, but they *can* be densified further to $\varphi \approx 91\%$.

None of the 2D packings were strictly jammed, though some were collectively jammed.

Why?

Packing Algorithms

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

Modified definition: *A packing is jammed iff there is a jammed subpacking*.

How to find jammed subpackings (sensitivity analysis, recursive LP)?

Are exceptions of measure zero for MRJ?

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

Jammed Backbones

Special jammed subpackings:

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

- (Minimal) Irreducible Infeasible Subsystem (minimally jammed subpacking)
- (Maximum) Feasible Subsystem (NP hard) (critical clusters)

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

Low-Density Jamming

There are locally jammed packings of vanishing density (covering fraction) (K. Baroczky)

What is the lowest density **saturated packing**?

How about point *A* for collectively and strictly jammed (with PBC)?

- Subpackings of the triangular lattice: *No divacancies!*

  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

Physicists focus on **macroscopic** (averaged) displacements (strains) and forces (stresses).

Typical definition of a glass is “disordered material that can resist shear”.

Kagome lattice can support any global loading, but is not jammed (`Graphics/Kagome.1.1.strict.unjamming.wrl`).

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.

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.

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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- *Rigid Circle And Sphere Packings*, **Robert Connelly** *et al.*, Structural Topology, *Part I: Finite Packings*, 14:43-60, 1988, *Part II: Infinite Packings*, 16:57, 1991

References (physics)

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