Quasi-Packing Spheres with Ratio Conditions

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Our research is devoted to non-standard packing problems where either non-overlapping, or containment, or both conditions are allowed to be **violated.**

These problems we refer to as **quasi-packing**.

Motivation

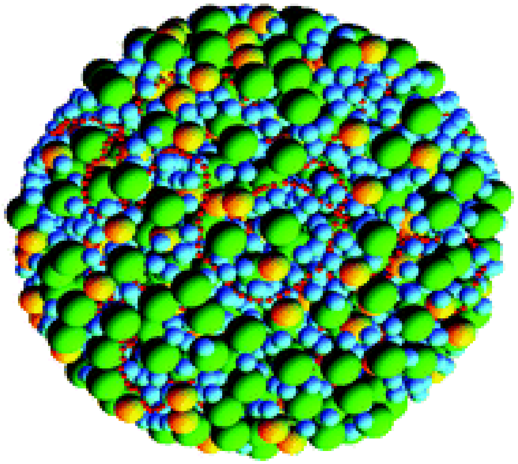
- A relaxation of classical containment arises, e.g., in analyzing experimentally the porous material by extracting a volumetric sample (container) for further investigation, or by mathematical simulation of the material structure in the sample. Only parts of some spheres may remain in the sample.

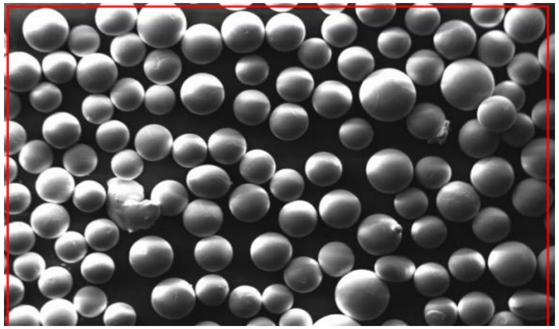
Motivation

- Allowing a controlled overlap is frequently used in natural sciences since soft spheres can be modeled as hard spheres with a limited overlap. This corresponds to partial overlapping of spheres.

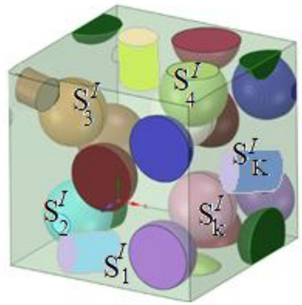
- The ratio conditions are used to maintain a certain structure of a porous media under different particle configurations (fractions).

Study of the properties of biological structures/alloy powder





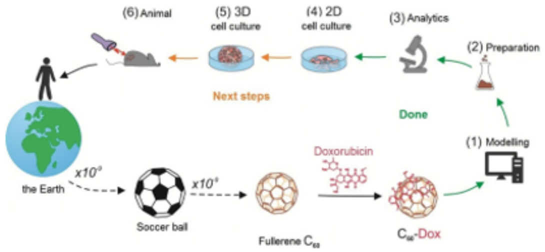
Modeling Nanostructures (study of the mechanical characteristics of 3D nanocomposites for different structural parameters)

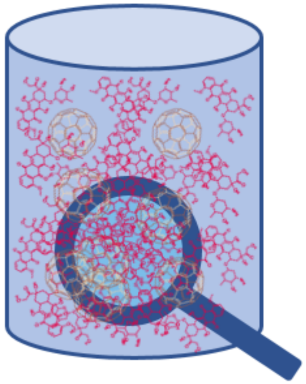


Representative volume element with spherical and non-spherical inclusions

Nano: Doxorubicin-C_{60} Fullerene Nanocomplexation

colloid solution in water





- Molecular Modeling
- Atomic Force Microscopy
- UV/vis Spectroscopy
- Isothermal Titration
- Diffusion-ordered NMR spectroscopy
- HPLC-MS/MS
- Dynamic Light Scattering
- Zeta-potential

Problem Formulation

Let S_0 be a container (for example, spherical container with a given radius R and centered at $(0, 0, 0)$).

In addition, a family $\mathbf{S} = \{S_i(u_i), i = 1, \ldots, n\}$ of spheres $S_i(u_i) = \{u \in \mathbf{R}^3 : \| u - u_i \| \leq r_i\}$ centered at $u_i = (x_i, y_i, z_i)$ is given.

It is assumed that there are K different radii of the spheres and n_k spheres of type k, $(k = 1, 2, \ldots K)$, $n = \sum_{k=1}^{K} n_k$.

Ratio Quasi-Packing Spheres (RQPS). Find the maximum number of spheres $S_i(u_i)$ from the family $\mathbf{S}$ under the following conditions:

- *partial overlapping of* S_i and S_j, $1 \le i < j \le n$
- *quasi-containment of* S_i into S_0, $i = 1, \ldots, n$
- *ratio condition* for spheres of K types, $k = 1, \ldots, K$

- ***Partial overlapping condition***

The partial overlapping condition $\|u_i - u_j\| \geq (r_i + r_j - \delta_{ij})$ means that the minimal distance between centers u_i and u_j of two spheres $S_i(u_i)$ and $S_j(u_j)$ having radii r_i and r_j is at least $r_i + r_j - \delta_{ij}$.

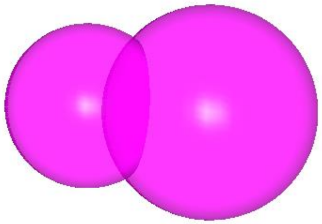


Figure 1. Partial overlapping $\|u_i - u_j\| = r_i + r_j - \delta_{ij}$.

$\delta_{ij} = (r_i + r_j)^* \delta_0$, $\delta_0 \geq 0$ is a given positive parameter of allowable pairwise overlapping of spheres.

- *Quasi-containment condition*

Quasi-containment condition $\|u_i\| \leq R + \varepsilon_i$ assures that the maximal distance between the centers of S_i and a spherical container S_0 is at most $R + \varepsilon_i$, $\varepsilon_i \in [-r_i, r_i]$ is a given parameter

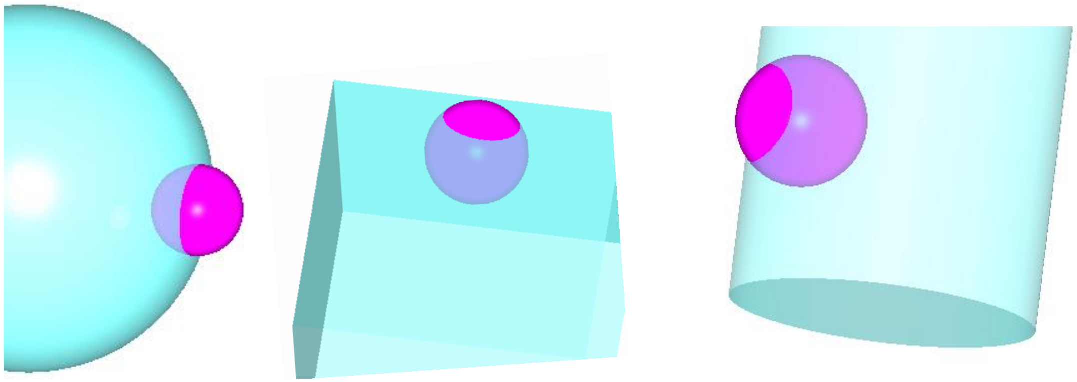


Figure 2. Examples of quasi-containment: spherical container, cuboidal container, cylindrical container

- ***Ratio condition***

Ratio condition $\tau_k^- \le \tau_k \le \tau_k^+$ $(0 \le \tau_k^- \le \tau_k^+ \le 1)$ for $k = 1, \ldots, K$ defines a certain correspondence (proportion) between the number of packed spheres of different radii.

τ_k = (number of packed spheres of *k-th* type)/(total number of packed spheres)

We distinguish between **strict** $(\tau_k^- = \tau_k^+)$ or **non-strict** $(\tau_k^- < \tau_k^+)$ ratio conditions.

- ***Mixed-Integer NonLinear Programming Model for RQPS***

$$\max \sum_{i=1}^{n} \pi_i \tag{1}$$

subject to

$$\pi_i \psi_i(u_i) \geq 0, \quad i = 1, \ldots, n, \tag{2}$$

$$\pi_i \pi_j \varphi_{ij}(u_i, u_j) \geq 0, 1 \leq i < j \leq n, \tag{3}$$

$$\tau_k^- \sum_{i=1}^{n} \pi_i \leq \sum_{i \in I_k} \pi_i \leq \tau_k^+ \sum_{i=1}^{n} \pi_i, \quad k = 1, \ldots, K, \tag{4}$$

$$\pi_i \in \{0, 1\}, \quad u_i \in \mathbf{R}^3, \quad i = 1, \ldots, n, \tag{5}$$

$$I_1 = \{1, \ldots, n_1\}, \ldots, \quad I_K = \{n - n_K + 1, \ldots, n\}, \quad I = I_1 \cup \ldots \cup I_K, \quad \sum_{k=1}^{K} n_k = n,$$

$$\psi_i(u_i) = R + \varepsilon_i - \|u_i\|, \quad \varphi_{ij}(u_i, u_j) = \|u_i - u_j\| - (r_i + r_j - \delta_{ij}).$$

Packing spheres are known to be NP-hard [1].

Global solvers can find provably optimal solutions to model (1)–(5) for small problem instances.

A heuristic approach is proposed to find reasonable feasible solutions for larger instances.

Heuristic Approach

The main idea of the proposed heuristic algorithm is reducing the original problem (1)-(5) to a sequence of quasi-packing problems of a given number of scaled spheres in a given container.

The objective is to maximize the scaling parameter (and, with this, to grow up the spheres to the original size) subject to the ratio conditions.

Each of quasi-packing problems is stated as a nonlinear programming problem

$$\max \lambda \quad (6)$$

subject to

$$-\|u_i\| + (R + \lambda\varepsilon_i) \geq 0, \quad i = 1, \ldots, l, \quad (7)$$

the quasi-containment of scaled sphere λS_i in $S_0(\lambda\varepsilon_i) = \{u \in \mathbf{R}^3 : \|u\| \leq R + \lambda\varepsilon_i\}$

$$\|u_i - u_j\| - \lambda(r_i + r_j - \delta_{ij}) \geq 0, 1 \leq i < j \leq l, \quad (8)$$

the partial overlapping of scaled spheres λS_i and λS_j

$$0 \leq \lambda \leq 1, \quad u_i \in \mathbf{R}^3, \quad i = 1, \ldots, l \ . \quad (9)$$

Our algorithm involves three main stages:

Stage 1. Generation of a minimal set of spheres (minimal block), $\mathbf{I}_{\min}$, that satisfies ratio conditions.

Stage 2. Multiple sequential placement of the spheres in $\mathbf{I}_{\min}$ meeting the quasi-packing and ratio conditions. Creation of an aggregate set $\mathbf{I}_s$ (accumulation of $\mathbf{I}_{\min}$ blocks).

Stage 3. Placement of additional spheres to the quasi-packing found at Stage 2 meeting the quasi-packing and ratio conditions.

For solving NLP problems we use a decomposition algorithm[1]

[1]Romanova, T.; Stoyan, Y.; Pankratov, A.; Litvinchev, I.; Marmolejo, J.A. Decomposition Algorithm for Irregular Placement Problems. In Advances in Intelligent Systems and Computing; Intelligent Computing and Optimization, 2020; Volume 1072, pp. 214–221.

Algorithm

Let $\tau'_k \in [\tau_k^-, \tau_k^+]$, $\sum_{k=1}^{K} \tau'_k = 1$ for $k \in K$.

Step 1. Set $q := 1$.

Step 2. Repeat $q := q + 1$ until $q\tau'_k - \lfloor q\tau'_k \rfloor = 0$ for $k \in K$.

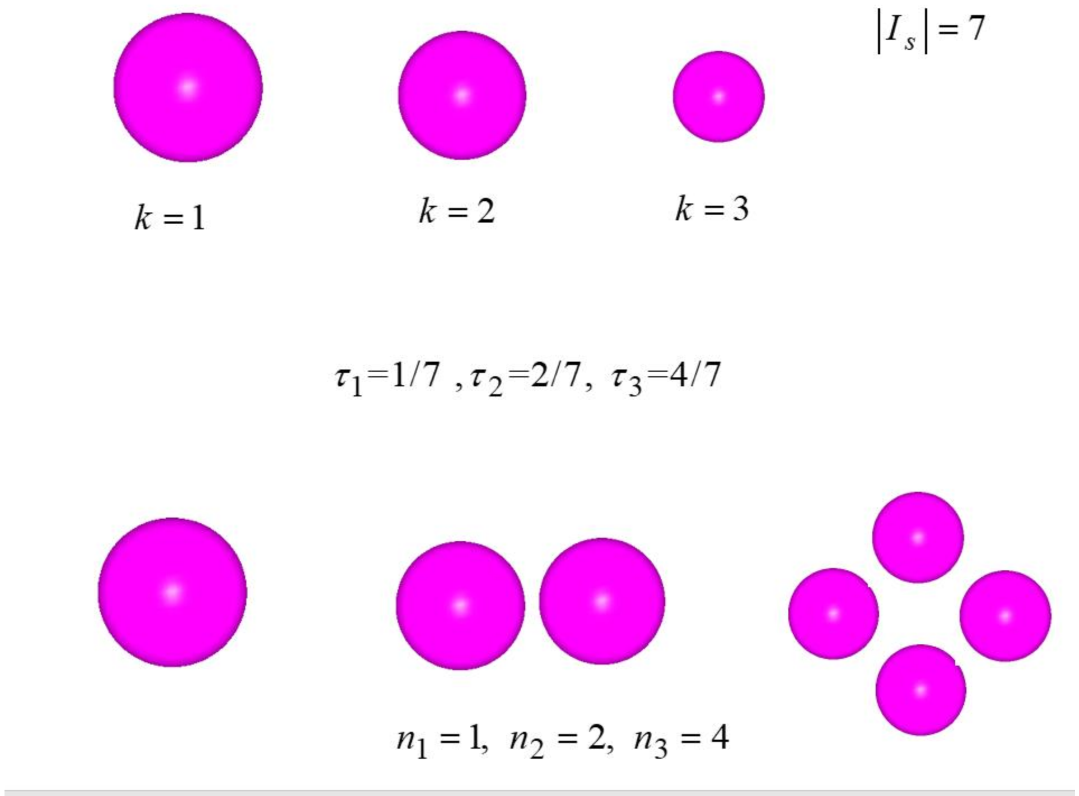
Here $\lfloor \bullet \rfloor$ is the floor function.

Then the minimum index set $\mathbf{I}_{\min}$ is formed (***Steps 3–5***).

Step 3. Set $k := 1$, $\mathbf{I}_{\min} := \varnothing$.

Step 4. If $k = K + 1$, then go to Step 6.

Step 5. Set $\mathbf{I}_{\min} := \mathbf{I}_{\min} \cup \bigcup_{j=1}^{q\tau'_k} \{i_{k_j}\}$, $k := k + 1$ and go to Step 4.


$|I_s| = 7$
$k=1$
$k=2$
$k=3$
$\tau_1=1/7$, $\tau_2=2/7$, $\tau_3=4/7$
$n_1=1$, $n_2=2$, $n_3=4$

Further the aggregate index set $\mathbf{I}_s$ having cardinality l and meeting the quasi-packing and the ratio conditions is constructed (***Steps 6–8***).

Step 6. Set $\mathbf{I}_s := \varnothing$, $l := 0$.

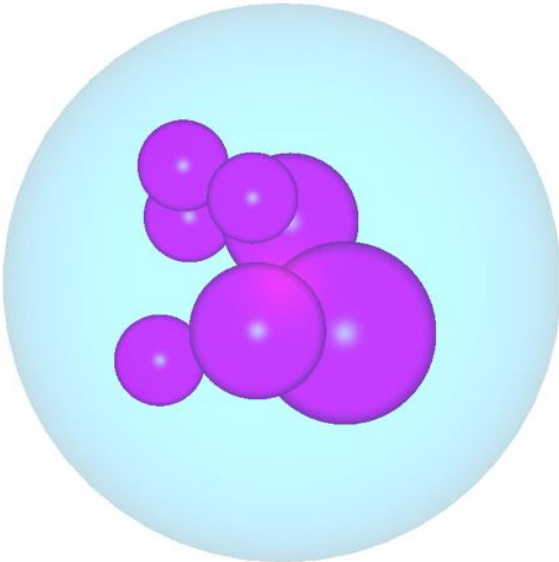
Step 7. Set $\mathbf{I}_s := \mathbf{I}_s \bigcup \mathbf{I}_{\min}$, $l := l + q$.

Step 8. Search for a local maximum of the problem (6)–(9) for the set $\mathbf{I}_s$ using a local optimization solver combined with the decomposition procedure.

At the next step, we verify the quasi-packing conditions and update the set $\mathbf{I}_s := \mathbf{I}_s \setminus \mathbf{I}_{\min}$ (***Step 9***).

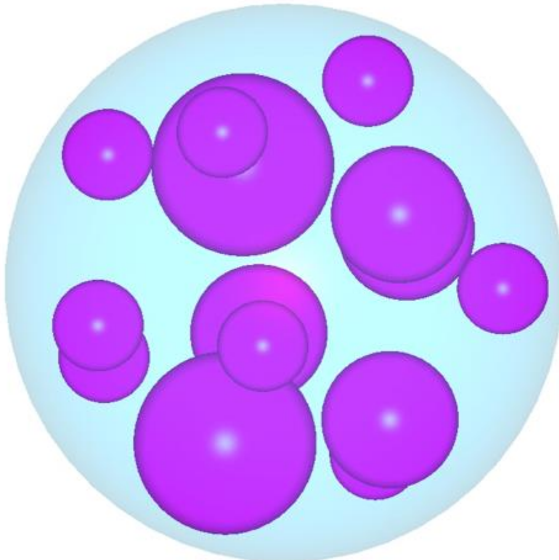
Step 9. If $\lambda = 1$, then go to Step **7**; otherwise ($\lambda < 1$) set $\mathbf{I}_s := \mathbf{I}_s \setminus \mathbf{I}_{\min}$, $l := l - q$ and go to Step 10.

$|I_s| = 7$ $\tau_1 = 1/7, \tau_2 = 2/7, \tau_3 = 4/7$ $l = 1 \cdot |I_s| = 7$

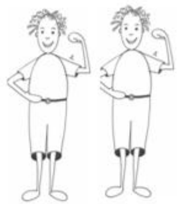


$n_1 = 1, \; n_2 = 2, \; n_3 = 4$

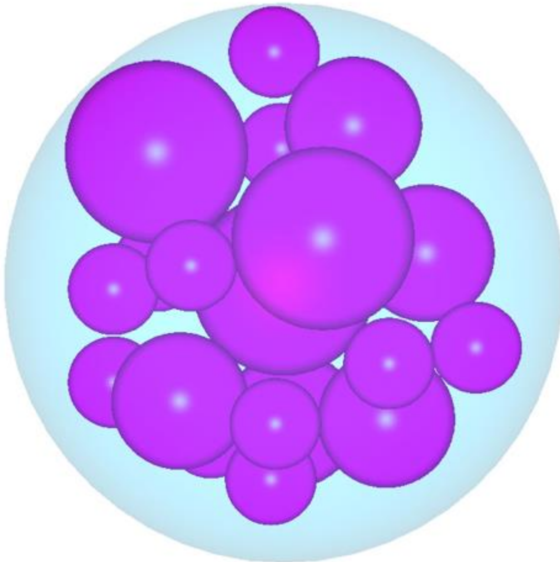
$|I_s| = 7$ $\tau_1 = 1/7$, $\tau_2 = 2/7$, $\tau_3 = 4/7$ $l = 2 \cdot |I_s| = 14$

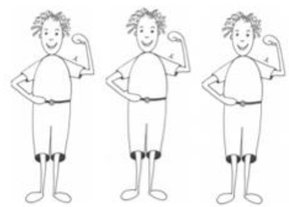


$n_1 = 2,\ n_2 = 4,\ n_3 = 8$



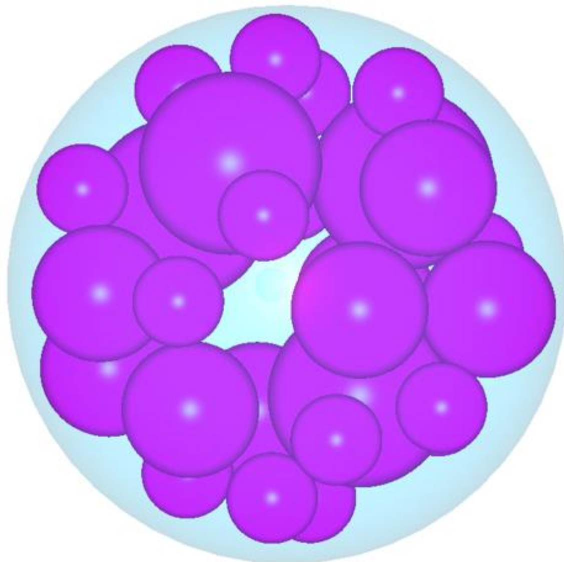
$|I_s| = 7$ $\tau_1 = 1/7$, $\tau_2 = 2/7$, $\tau_3 = 4/7$ $l = 3 \cdot |I_s| = 21$

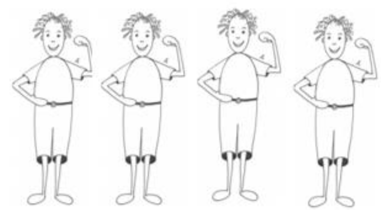




$n_1 = 3$, $n_2 = 6$, $n_3 = 12$

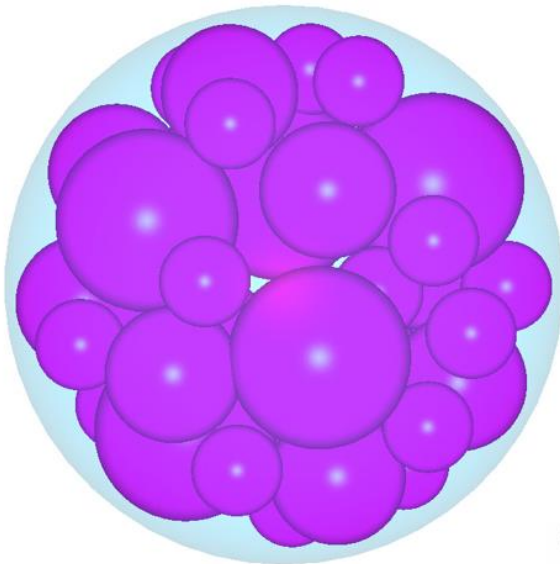
$|I_s| = 7$ $\tau_1 = 1/7$, $\tau_2 = 2/7$, $\tau_3 = 4/7$ $l = 4 \cdot |I_s| = 28$

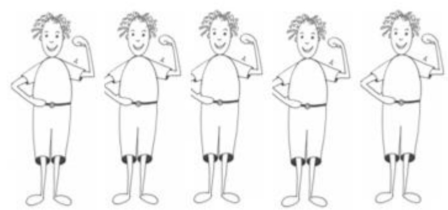




$n_1 = 4$, $n_2 = 8$, $n_3 = 16$

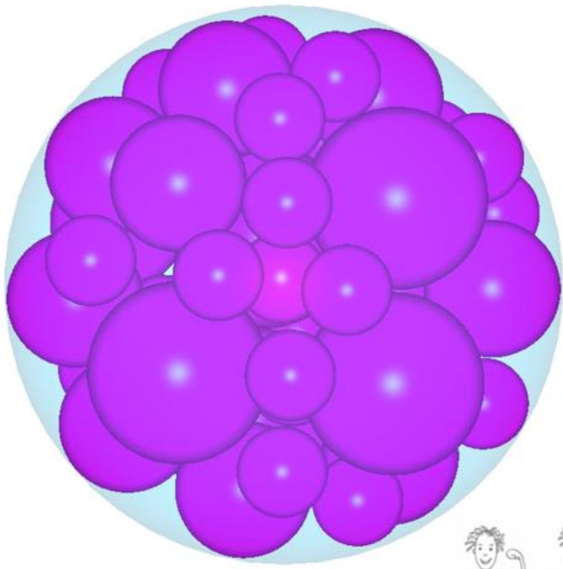
$|I_s| = 7$ $\tau_1 = 1/7$, $\tau_2 = 2/7$, $\tau_3 = 4/7$ $l = 5 \cdot |I_s| = 35$



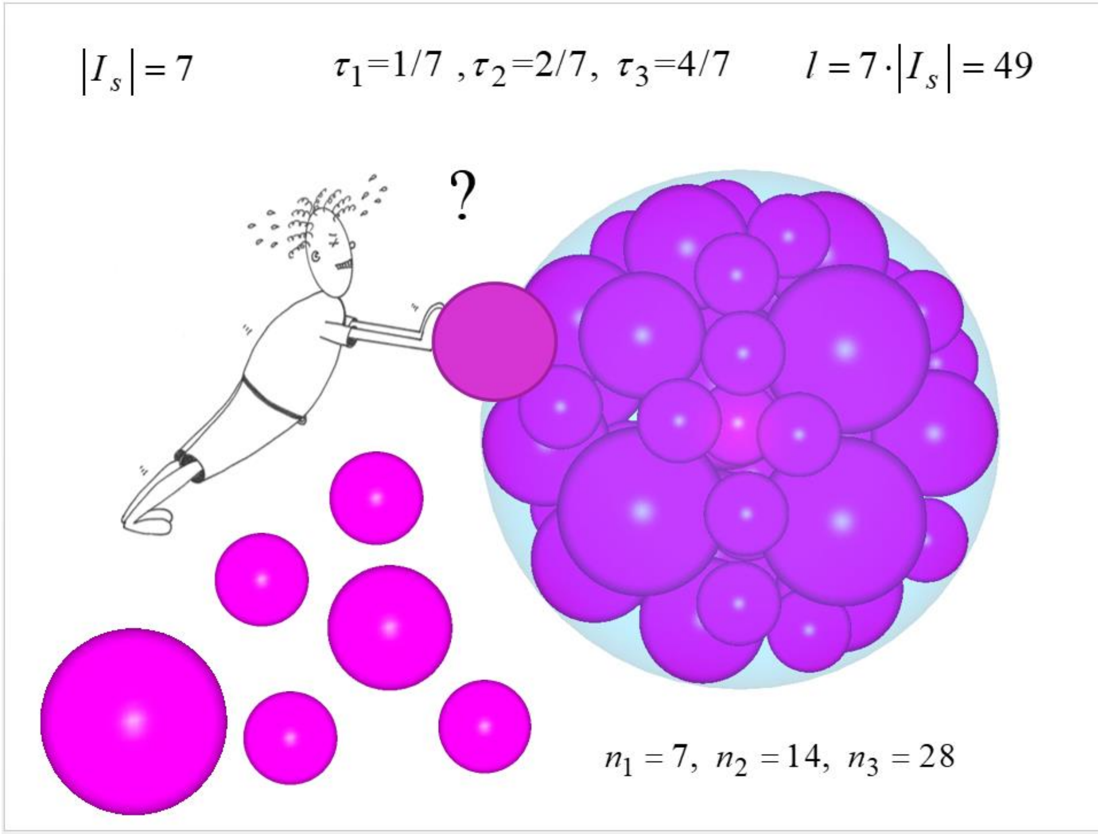


$n_1 = 5$, $n_2 = 10$, $n_3 = 20$

$|I_s| = 7$ $\tau_1 = 1/7$, $\tau_2 = 2/7$, $\tau_3 = 4/7$ $l = 6 \cdot |I_s| = 42$



$n_1 = 6$, $n_2 = 12$, $n_3 = 24$


$|I_s| = 7$
$\tau_1=1/7$, $\tau_2=2/7$, $\tau_3=4/7$
$l = 7 \cdot |I_s| = 49$
?
$n_1 = 7$, $n_2 = 14$, $n_3 = 28$

For the case of the strict ratio conditions we provide a stopping criterion of our algorithm at ***Step* 10.**

Step 10. If $\tau_k^- = \tau_k^+$, $k = 1, \ldots, K$, then stop the algorithm with $n^* := l$; otherwise go to Step 11.

An addition of single spheres to the set $\mathbf{I}_s$ meeting the ratio and quasi-packing conditions are produced at ***Steps 11–14.***

Step 11. Set $k := K$.

Step 12. If $k \geq 1$, then set $\mathbf{I}_s := \mathbf{I}_s \bigcup \{i_k\}$, $l := l + 1$ and go to Step 16; otherwise stop the algorithm with $n^* := l$.

Step 13. If $\mathbf{I}_s$ meets (4), then go to Step 14**;** otherwise set $\mathbf{I}_s := \mathbf{I}_s \setminus \{i_k\}$, $l := l - 1$, $k := k - 1$ and go to Step 12.

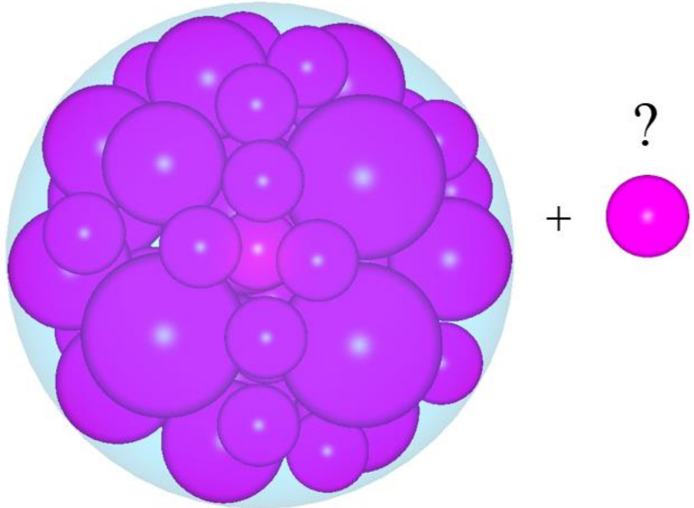
$|I_s| = 7$

$\tau_1^- = 1/7 - 0.1, \tau_1^+ = 1/7 + 0.1$

$\tau_2^- = 2/7 - 0.1, \tau_2^+ = 2/7 + 0.1$

$\tau_3^- = 4/7 - 0.1, \tau_3^+ = 4/7 + 0.1$

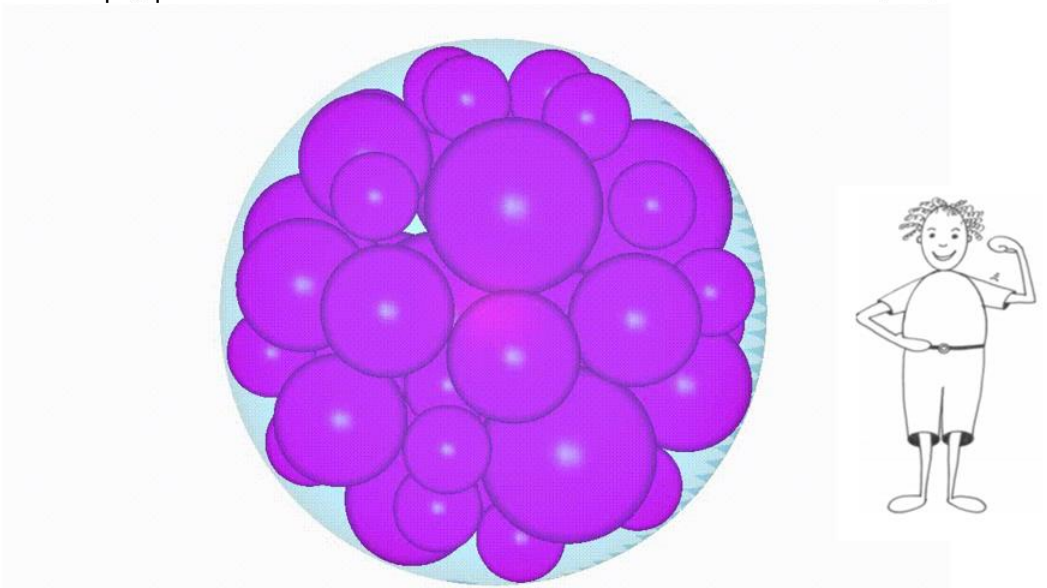
$l = 6 \cdot |I_s| = 42$



$n_1 = 6, \; n_2 = 12, \; n_3 = 24 + 1$?

Step 14. Search for a local maximum of the problem (6)–(9) for the sphere set $\mathbf{I}_s$. If $\lambda = 1$, then go to Step 11; otherwise set $\mathbf{I}_s := \mathbf{I}_s \setminus \{i_k\}$ and stop the algorithm with $n^* := l - 1$.

$|I_s| = 7 \qquad n_1 = 6,\ n_2 = 12,\ n_3 = 25 \qquad l = 6 \cdot |I_s| + 1 = 43$



$\tau_1^- = 1/7 - 0.1, \tau_1^+ = 1/7 + 0.1; \tau_2^- = 2/7 - 0.1, \tau_2^+ = 2/7 + 0.1; \tau_3^- = 4/7 - 0.1, \tau_3^+ = 4/7 + 0.1$

$\tau_1 \approx 0.1395, \tau_2 \approx 0.2791, \tau_3 \approx 0.5814$

Computational Results

To verify the model (1)-(5) the global optimization solver BARON[1] was used to solve small problem instances.

BARON was executed at NEOS server (State-of-the-Art Solvers for Numerical Optimization. https://neos-server.org/neos/) with AMPL (A Modeling Language for Mathematical Programming)[2] applied for modeling optimization problem (1)-(5).

[1]Sahinidis N.: BARON user manual v. 2022.11.3 (2022). http://www.minlp.com/downloads/docs/baronmanual.pdf
Tawarmalani M., Sahinidis N.V. A polyhedral branch-and-cut approach to global optimization. Math. Program. 103(2), 225-249 (2005)
[2]Fourer, R., Gay, D.M., Kernighan, B.W.: AMPL: A Modeling Language for Mathematical Programming. 2nd ed., Duxbury Press/Brooks/Cole Publishing Company (2002)

The nonlinear optimization problems (6)-(9) arising in the heuristic algorithm were solved by the local optimization solver IPOPT (https://coin-or.github.io/Ipopt/) combined with the decomposition procedure.

Computational Results

Three types of instances were used in the computational experiments.

In the first case classical packing problems without violation of non-overlapping and containment conditions ($\varepsilon_i = -r_i$, $\delta_{ij} = 0$) were generated.

The second group is composed of packing problems with non-overlapping ($\varepsilon_i = -r_i$) and quasi-containment ($\varepsilon_i \in [-r_i, r_i]$) conditions.

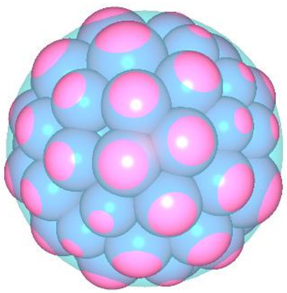
In the last group partial overlapping ($0 \le \delta_{ij} \le (r_i + r_j) * \delta_0$) and quasi-containment ($\varepsilon_i \in [-r_i, r_i]$) were permitted.

Strict ($\tau_k^- = \tau_k^+$) and non-strict ($\tau_k^- < \tau_k^+$) ratio conditions (4) were considered.

Computational Results Obtained by BARON

Input and output data for Instance 1

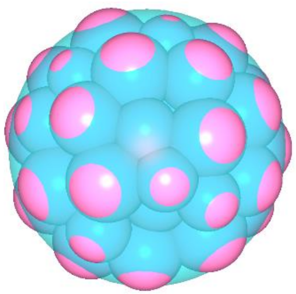
Instance	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#1	1	11	1.1	-1	0.2	0.2	50	10	0.2	222.149	0.1850096
$R=5$	2	10	1.2	-1	0.2	0.2		10	0.2		
$K=5$	3	10	1.3	-1	0.2	0.2		10	0.2		
$\delta_0=0.2$	4	12	1.4	-1.1	0.2	0.2		10	0.2		
	5	14	1.5	-1.2	0.2	0.2		10	0.2		



The global solution for Instance 1

Input and output data for Instance 2

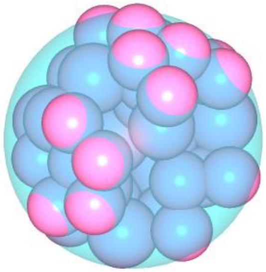
Instance	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#2	1	10	1.1	-1	0.1	0.3	53	10	0.188679	72.3216	0.1410674
$R=5$	2	9	1.2	-1	0.1	0.3		9	0.169811		
$K=5$	3	9	1.3	-1	0.1	0.3		9	0.169811		
$\delta_0=0.2$	4	13	1.4	-1.1	0.1	0.3		13	0.245283		
	5	12	1.5	-1.2	0.1	0.3		12	0.226415		



The global solution for Instance 2

Input and output data for Instance 3

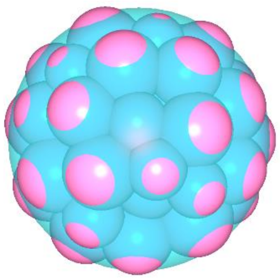
Instance	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#3 $R=5$ $K=3$ $\delta_0=0.2$	1	24	1.2	-0.7	0.6	0.6	40	24	0.6	98.4785	0.4056054
	2	15	1.3	-1	0.2	0.2		8	0.2		
	3	10	1.4	-1.1	0.2	0.2		8	0.2		



The global solution for Instance 3

Input and output data for Instance 4

Instance	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#4 $R=5$ $K=3$ $\delta_0=0.2$	1	24	1.2	-0.7	0.5	0.7	48	24	0.5	79.458	0.2499254
	2	15	1.3	-1	0.1	0.3		14	0.291667		
	3	10	1.4	-1.1	0.1	0.3		10	0.208333		

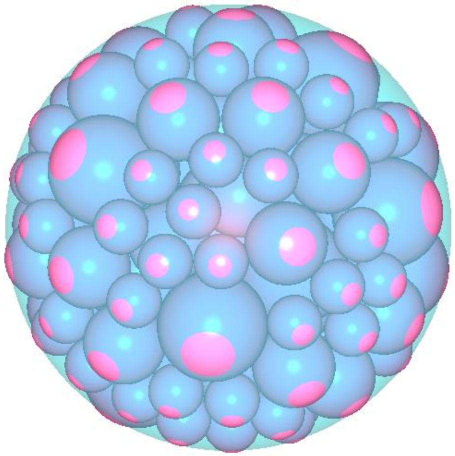


The global solution for Instance 4

Computational Results Obtained by the Heuristic

Input and output data for Instance 5

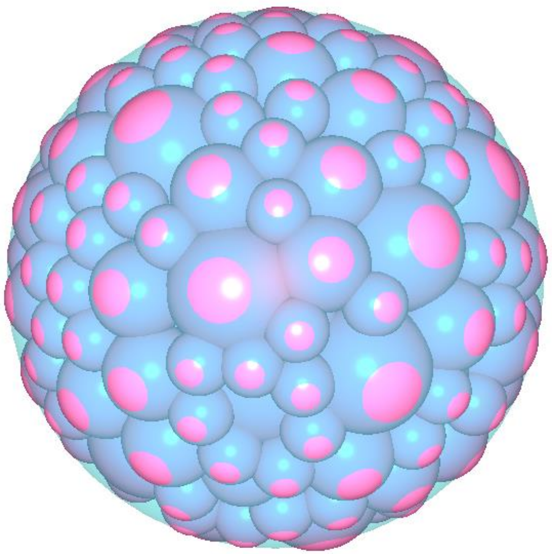
Instance #	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#5 $R=8$, $K=3$, $\delta_0=0$	1	50	2	-1.8	1/7	1/7	112	16	1/7	50	0.414063
	2	100	1.5	-1.35	2/7	2/7		32	2/7		
	3	200	1	-0.9	4/7	4/7		64	4/7		



A feasible solution for Instance 5

Input and output data for Instance 6

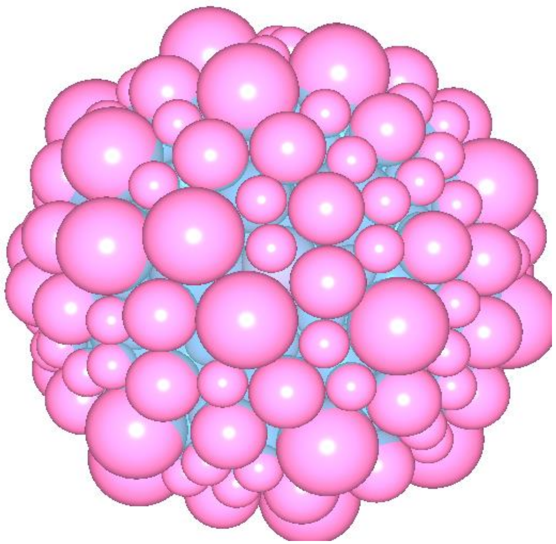
Instance #	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#6 $R=8$, $K=3$, $\delta_0=0.2$	1	50	2	-1.8	1/7	1/7	210	30	1/7	47	0.129044
	2	100	1.5	-1.35	2/7	2/7		60	2/7		
	3	200	1	-0.9	4/7	4/7		120	4/7		



A feasible solution for Instance 6

Input and output data for Instance 7

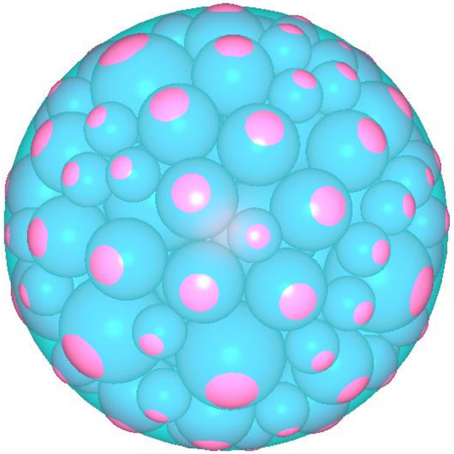
Instance #	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#7 $R=9$, $K=3$, $\delta_0=0$	1	50	2	0.2	1/7-0.01	1/7+0.01	246	35	0.1423	471	0.211930
	2	100	1.5	0.15	2/7-0.01	2/7+0.01		70	0.2846		
	3	200	1	0.1	4/7-0.01	4/7+0.01		141	0.5732		



A feasible solution for Instance 7

Input and output data for Instance 8

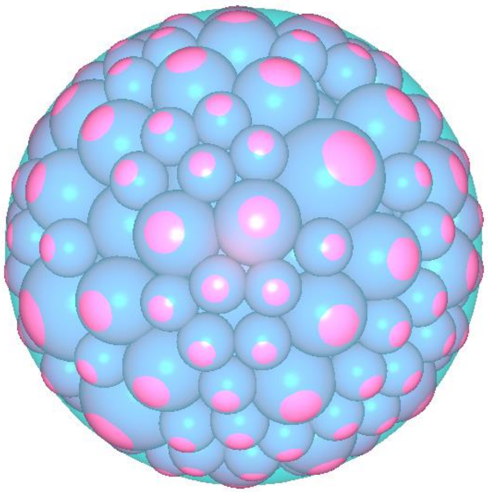
Instance #	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#8 $R=8$, $K=3$, $\delta_0=0$	1	50	2	-1.8	1/7-0.01	1/7+0.01	118	16	0.1356	18	0.393993
	2	100	1.5	-1.35	2/7-0.01	2/7+0.01		34	0.2881		
	3	200	1	-0.9	4/7-0.01	4/7+0.01		68	0.5763		



A feasible solution for Instance 8

Input and output data for Instance 9

Instance #	Input data						Output data				
	k	n_k	radius of $\{i_k\}$	ε_k	τ_k^-	τ_k^+	n^*	n_k^*	τ^*	Time (sec)	Porosity
#9 $R=8$, $K=3$, $\delta_0=0.1$	1	50	2	-1.8	1/7-0.01	1/7+0.01	152	21	0.1382	147	0.24759
	2	100	1.5	-1.35	2/7-0.01	2/7+0.01		43	0.2829		
	3	200	1	-0.9	4/7-0.01	4/7+0.01		88	0.5789		



A feasible solution for Instance 9

Conclusions

A sphere quasi-packing model that allows controlled violation of non-overlapping and containment conditions was developed. Ratio constraints were introduced to establish correspondence between the number of packed spheres of different radii.

Corresponding MINLP formulation, as well as the heuristic strategy for obtaining good feasible solutions were proposed. Proven optimal global solutions for the MINLP formulation were obtained for small instances by the global solver BARON at the NEOS server.

For larger instances with hundreds of spheres the proposed heuristic was successfully implemented providing reasonable feasible solutions.

Future research

To made analyses of granular structures non-spherical shapes can be used, e.g., ellipsoids, cylinders, convex polyhedra and their mixtures. Some results on quasi-packing non-spherical objects are on the way.

Acknowledgements

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