Globally Optimized Finite Packings of Arbitrary Size Spheres in $\mathbb{R}^d$

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Abstract

This work discusses the following general packing problem-class: given a finite collection of d-dimensional spheres with arbitrarily chosen radii, find the smallest sphere in $\mathbb{R}^d$ that contains the entire collection of these spheres in a non-overlapping arrangement. Generally speaking, analytical solution approaches cannot be expected to apply to this general problem-type, except for very small or certain specially structured sphere configurations. In order to find high-quality numerical (approximate) solutions, we propose a suitable combination of heuristic strategies with constrained global and local nonlinear optimization. We present numerical results for non-trivial model instance-classes of optimized sphere configurations with up to $n = 50$ spheres in dimensions $d = 2,3,4$. Our numerical results for an intensively studied model-class in $\mathbb{R}^2$ are on average within 1% of the entire set of best known results, with new optimized (conjectured) packings for previously unexplored generalizations of the same model-class in $\mathbb{R}^d$ with $d = 3,4$. The results obtained also support the estimation of the optimized container sphere radii and of the packing fraction as functions of the model instance parameters n and $\frac{1}{n}$, respectively.

Key words: General Finite Sphere Packings in $\mathbb{R}^d$ · LGO Solver Suite for Global-Local Constrained Optimization · Hybrid Optimization Approach · Numerical Results and Their Analysis.

1 Introduction and Review

A generic packing problem in the d-dimensional Euclidean space $\mathbb{R}^d$ can be formally described as a non-overlapping arrangement of a given (finite or infinite) collection of objects in that space, optimized according to some well-defined criterion. A frequently used criterion is the packing fraction: typically, this is defined as the fraction of space $\mathbb{R}^d$ covered by an infinite set of identical objects. In the case of finite object sets, the packing fraction can be defined with respect to a certain type of container set that accommodates the given set of objects. Here we will primarily discuss the problem of packing spheres into a container sphere, with brief comments on related problem-types. Since the case $d = 1$ is trivial (for all finite sphere packings), we will assume throughout that $d \geq 2$.

The case of packing finite or infinite sets of congruent spheres in $\mathbb{R}^d$ (mostly for $d = 2,3$) has been studied extensively: for reviews and extensive collections of further references cf. e.g. Melissen (1997), Conway and Sloane (1998), Zong (1999), Sloane (2002). Considering first the case of $\mathbb{R}^2$, it has long been known that the best infinite packing is the so-called hexagonal lattice packing: in this configuration each circle is touching six others. This result was proven by Thue (1892, 1910): the corresponding optimal density is approximately 0.9069. References to Thue's original work appear extensively, cf. e.g. Steinby and Thomas (2000).

The famous conjecture by Kepler (1611) stated that the densest infinite configuration of identical size spheres in $\mathbb{R}^3$ is the face-centered-cubic lattice arrangement. The face-centered cubic system is closely related to the hexagonal close packed system, and the two systems differ only in the relative placements of their hexagonal layers: the density of these sphere arrangements is approximately 0.7405. Kepler's long-standing conjecture was finally proven by Hales (2005). For historical context and additional details, consult also Fejes Tóth (1964), Szpiro (2003), with numerous further references.

The topic of packing congruent spheres in higher-dimensional spaces remains attractive for mathematicians, computer scientists and other researchers. To illustrate this point, recent works by Viazovska (2016) and by Cohn *et al.* (2016) prove that specific (E_8 root and Leech) lattice packings give the densest packing of congruent spheres in 8 and 24 dimensions, respectively: consult also Leech (1967) and Griess (2003, 2011) for background. Without going into further details on this line of research, let us remark that the packing density of identical spheres decreases rapidly with the dimension d of the space: the significant gap (factor) between the best known upper and lower bounds grows exponentially as a function of d, consult e.g. Cohn (2010). We also note that sphere packings are related to information theory Shannon (1948) and error-correcting codes (Conway, 1995), with further applications in number theory, approximation theory, algebra, theoretical physics and other areas (Cohn, 2010). The notorious difficulty of (identical) sphere packings optimized for density is partially due to the known fact that such problems have many local maxima.

Castillo *et al.* (2008) and Hifi and M'Hallah (2009) review both uniform and arbitrary size circle packings in $\mathbb{R}^2$ and highlight several areas of their applications: these include circular cutting, container loading, cylinder packing, facility dispersion, communication networks, facility location and dashboard layout.

In the natural sciences and engineering, sphere packings in the "real world" ($\mathbb{R}^3$) are of significant interest, because they capture and reveal some essential structural features of many complex systems such as liquids (Jadrich and Schweizer, 2013a, 2013b), crystals (Cheng *et al.* 1999; Chaikin and Lubensky, 2000), liquid to crystal transition (Chaikin, 2000), glasses (Zallen, 1983), colloids (Torquato, 2002), granular media (de Gennes, 1999), heterogeneous materials (Nesterenko, 2001; Sahimi, 2003a, 2003b), particles and powders (Olmos *et al.*, 2009; Zohdi, 2014a, 2014b). The topical book by Fasano (2014) and the edited volume (Fasano and Pintér, 2015) discuss a range of significant industrial, engineering and scientific applications of real world packings.

In addition to the numerous theoretically and practically important topics highlighted above, object packing problems *per se* frequently lead to interesting model development and numerical optimization challenges. As noted earlier, in full generality, d-dimensional packings lead to difficult optimization problems that cannot be tackled effectively by purely analytical approaches. Next, we highlight some of the topical research focused on the numerical optimization of finite sphere packings.

The 2-dimensional case of packing identical circles inside a circle or a square has received considerable attention in the literature. Due to the inherently symmetric structure of this rather special problem-type, studies dealing with uniform size circle packings often aim to prove the optimality of the configurations found, either theoretically or with the help of rigorous computational approaches. Provably optimal circle packings have been found so far only for a relatively small number of instances (currently, with up to several tens of circles), in spite of the significant effort spent on variants of the problem over several decades. Consult e.g. Szabó *et al.* (2007) for an in-depth discussion of packing identical circles in a square; the reader is referred also to Melissen (1997) for a review of the early circle packing research. The website of Specht (2016) presents best known finite circle packing solutions in various container sets in $\mathbb{R}^2$, with references. We also mention the website maintained by Friedman (2016) that presents a large variety of finite packing and covering "puzzles," predominantly stated in $\mathbb{R}^2$.

The finite circle packing problem, defined by n (in principle) arbitrary size circles in $\mathbb{R}^2$, is a significant generalization of the identical circle packing case. Here generally valid, provably optimal configurations can be found only to model instances in which $n \leq 4$. Therefore studies dealing with general circle packings typically apply efficient generic or tailored global scope numerical solution strategies, but without the proven optimality of the results obtained. This pathway is followed also by our present study.

In this work, we consider the general d-dimensional finite sphere packing problem in $\mathbb{R}^d, d \geq 2$. Our objective is to find a globally optimized, pairwise non-overlapping arrangement of n arbitrary size d-spheres inside a container d-sphere with minimal radius. This problem-type leads to hard computational challenges, since the problem instances are rapidly becoming difficult to solve as the number of spheres increases. The numerical solution approach proposed here is a partially heuristic procedure combined with calls to a global-local nonlinear optimization solver. We re-emphasize that we can not, and hence do not, pursue provably optimal solutions: instead, our objective is to demonstrate the efficiency of the proposed solution strategy to find high-quality packings with a reasonable computational effort. We formulate the general d-dimensional finite sphere packing model in Section 2, followed by the description of our optimization strategy (Section 3), illustrative numerical results and their discussion (Section 4), and conclusions (Section 5).

2 Model Formulation

Given a collection of n (in principle, arbitrary) size d-spheres, our objective is to minimize the radius of the container d-sphere that can accommodate all the given spheres in a non-overlapping arrangement. Instances of this optimization problem-type are defined by d and n, and by the radii of the d-spheres to be packed. The primary decision variables are then the radius of the container d-sphere and the center positions of each of the packed d-spheres. The optimization model constraints fall into two groups. The first (convex, hence "easy") constraint group consists of the constraints that keep the d-spheres inside the container. The second (non-convex, hence more difficult) constraint group consists of the constraints that prevent pair-wise the d-spheres from overlapping.

Let $S_i \subset \mathbb{R}^d$, $i = 1, \dots, n$, denote a given collection of n arbitrary size d-spheres with radii $r_i > 0$. Let S_0 represent the container d-sphere with radius r_0, which is to be minimized. In order to standardize the model setup, we choose $c_0 = 0 \in \mathbb{R}^d$ as the center of the container sphere, and we denote the center position of S_i by $c_i = \{x_{i,1}, x_{i,2}, \dots, x_{i,d}\}$. The Euclidean ($l_2$-norm based) distance between the pair of d-sphere centers c_i and c_j will be denoted by $e(c_i, c_j) = \|c_i - c_j\|$.

Applying these notations, we can formulate the following model-class in $\mathbb{R}^d$ for packing n given spheres in an optimized container.

$$\text{minimize} \quad r_0 \tag{1}$$

$$\text{subject to} \quad \sqrt{\sum_{k=1}^{d} x_{i,k}^2} + r_i \leq r_0 \qquad i = 1, \dots, n.$$

$$r_i + r_j \leq e(c_i, c_j) \qquad i, j = 1, \dots, n; i < j.$$

By simple inspection, the optimization model (1) has $1 + d \cdot n$ decision variables, n convex constraints (the first constraint set), and $n(n-1)/2$ non-convex constraints (the second constraint set). We note that, based on elementary geometric observations, explicit variable lower and upper bound constraints can be also added to this optimization model: the number of bound constraints is $2(1 + d \cdot n)$, including bounds also for r_0.

Due to the non-convex (second) constraint set, model (1) represents a global optimization problem-class which can be instantiated by defining (selecting) d, n, and r_i, $i = 1, \dots, n$. Let us also remark that the number of decision variables increases (only) linearly with dimension d, assuming that all other model descriptor parameters remain the same. Assuming a given dimension d, the number of convex constraints also increases (only) linearly as a function of n; however, the number of non-convex constraints increases quadratically as a function of n.

To illustrate these modeling aspects by a few examples, the packing problem considered with $n = 10$ spheres in $\mathbb{R}^2$ leads to a model-instance with 21 decision variables, 10 convex and 45 non-convex constraints. The same type of problem in 4 dimensions still has only 41 decision variables and 55 constraints (as above). As a second example, we select $n = 50$ and $d = 2,3,4$: these settings lead to models that have 101, 151, 201 decision variables, 50 convex and 1225 non-convex constraints, respectively. Hence, even rather small model instances can be seen as a non-trivial computational challenge.

Both the general theory of global optimization (cf. e.g. Pintér, 1996) and our numerical experience related to solving problems of comparable type and difficulty indicate that traditional local optimization strategies on their own would not be sufficient to aim for the global solution of model (1); thus a proper global scope search is required. At the same time, a theoretically correct "pure" global search approach – implemented in software – may not be sufficiently effective to solve sizeable models in realistic time. Hence our proposed optimization approach is a "hybrid" solution procedure. In this framework we make sequential calls to a global-local nonlinear optimization solver engine, and use local search heuristics to assist and to expedite the theoretically required global scope search.

3 A Hybrid Solution Strategy: Global Optimization + Local Search Heuristics

As we already noted – even when considering far less complicated packing models than the one introduced here – one cannot expect to find analytical (provable) solutions to general finite sphere packing problems. Therefore we have been applying numerical optimization to handle various similar problem types, in order to produce high quality feasible solutions to non-trivial packing model instances: for details, consult e.g. Pintér (2001), Stortelder *et al.* (2001), Riskin *et al.* (2003), Castillo and Sim (2004), Pintér and Kampas (2005, 2006), Kampas and Pintér (2006), Castillo *et al.* (2008), Pintér and Kampas (2013).

In our present study, we apply the Lipschitz Global Optimizer (LGO) solver system for global-local nonlinear optimization, within a hybrid optimization framework. LGO (Pintér, 1996, 1997, 2016) is aimed at finding the numerical global (or local) optimum of model instances from a very general class of constrained global optimization problems – while assuming only a continuous model structure. LGO seamlessly integrates several derivative-free global and local optimization strategies, without requiring higher-order information. In order to use LGO within a theoretically sound framework, the key assumptions are: a finitely bounded, non-empty feasible region; and continuous or (Lipschitz-)continuous model objective and constraint functions. All listed conditions can be directly verified for the model-class (1).

The implementation of LGO with a link to *Mathematica* (Wolfram Research, 2015) – with the software product name *MathOptimizer Professional* (*MOP*) – has been extensively used in our recent benchmarking studies, and it will be used also here. To summarize *MOP* operations: users formulate their optimization model in *Mathematica*;

next (without any further user interaction) this model is automatically translated into C or Fortran code, the converted model is solved by LGO, and the results are seamlessly returned to the calling *Mathematica* (notebook) document. The outlined structure supports the combination of *Mathematica*'s model development, documentation, visualization, and other capabilities with the robust performance and speed of the external LGO solver engine. The current LGO (as well as *MOP*) release supports the numerical solution of nonlinear optimization models with thousands of variables and general constraints. For further details, related to *MOP* and its performance we refer e.g. to Pintér and Kampas (2013, 2015).

Next, we outline our hybrid optimization approach, which is composed of using LGO in combination with procedures *pack*, *add*, and *swap* as described below. In order to add numerical context, we mention that in our illustrative results presented here we use the (d-sphere radii) input data $r_i = i$, $\forall S_i \subset \mathbb{R}^d$.

Procedure *pack*:

Step 1: Use *MOP* with its default global search option to pack a subset containing the largest d-spheres. Specifically, we use the subset $S_i \subset \mathbb{R}^d$, $i = \lceil n/2 \rceil, \ldots, n$, where $\lceil a \rceil$ is the ceiling function (that returns the smallest integer greater than or equal to the real value a). This step will lead to our first global solution estimate (providing a lower bound of the optimal container radius), and the current best approximate (incomplete) solution.

Step 2: Attempt to improve the result obtained in Step 1 using procedure *swap*. Update the current best approximate result whenever possible during the steps of *swap*.

Step 3: Add the remaining d-spheres one-by-one, starting with the current largest remaining d-sphere, using procedure *add*. Update the current best approximate result whenever possible during the steps of *add*.

Step 4: Perform *swap* repeatedly on the result of *add* until one of the related or overall stopping criteria (no improvement iteration limit set in *swap*, function evaluation limit or time limit set in LGO) is met. Update the current best approximate result whenever possible during the steps of *swap*.

Step 5: Return the final result, which is our numerical optimum estimate with a corresponding sphere configuration (but without a formal optimality proof, of course).

Procedure *add*:

Step 1: Find the largest d-dimensional hole (interstice) in the current packing configuration using *MOP* with its default global search method: this hole is found by searching for the maximal radius of a d-sphere that could be inserted in the current configuration, without increasing the radius of the container sphere.

Step 2: Attempt to place the current largest remaining d-sphere inside the hole. If the radius of this d-sphere is greater than the radius of the hole, then use *MOP* (only) with its local search method, in order to find a new feasible packing.

Step 3: Re-optimize the configuration, if possible, applying procedure *swap*.

Procedure *swap*:

Step 1: Swap the positions of all pairs of d-spheres whose radii differ at most by a given threshold value τ. Since $r_i = i$, $\forall S_i \subset \mathbb{R}^d$, we (heuristically) use $\tau = 2$.

Step 2: For each pair of swapped d-spheres, use *MOP* applying its local search option, in order to find a new feasible packing.

One of the key motivations behind the outlined hybrid optimization strategy is the empirical observation that the best packings appear to be determined by a smaller number of (the larger) d-spheres, with the rest occupying the d-interstices (d-holes). The specific implementation of this heuristic idea could (and, arguably, will) depend on the particular choice of the radius sequence r_i, $i = 1, \dots, n$. We note that d-spheres occupying the interstices often still have freedom for movement inside the container: these loose d-spheres are called "rattlers."

4 Illustrative Numerical Results

Let us denote by $A(n)$ the total volume of the d-spheres to be packed. Since we use the d-sphere radius sequence $r_i = i$, it follows that $A(n) \to \infty$ as $n \to \infty$. In our view, this general property can make the corresponding packing model instances more difficult to handle (as opposed to the case of packing objects into containers with an *a priori* bounded size).

The illustrative calculations reported here were performed mainly on a personal computer running under Windows 7, with an Intel Core i5 processor running at 2.6 GHz, and with 16 Gigabytes of RAM. We used *MOP* running as an add-on application in *Mathematica* version 10, and the GNU Compiler Collection (GCC, version 4.9.2 by the GNU Project, 2015) to automatically generate the necessary (Fortran) model input files for LGO. Again, while we cannot guarantee the optimality of the d-sphere configurations found, our hybrid solution procedure leads to visibly good quality packings in dimensions 2 and 3 (where we can visualize the results obtained).

Tables 1-3 summarize our results for $d = 2,3,4$ dimensions and $n = 5, \dots, 50$ d-spheres. The total number of model-instances solved is 138: the CPU times range from seconds to less than two hours for each problem solved, throughout the entire range of model-instances. (Interestingly, the runtimes reported do not seem to increase with increasing d.) The result summary tables also include the packing fraction (the total volume of the packed d-spheres divided by the container d-sphere volume) and the rattler fraction (the ratio between the number of rattlers and the total number of d-spheres to pack).

While for the cases $d = 3,4$ we are not aware of comparable results to ours, for $d = 2$ we can directly compare our results to the best known results recorded at the website http://www.packomania.com. The fractional difference

$$\frac{\text{our container radius}}{\text{best known container radius}} - 1 \qquad (2)$$

for each solved model-instance is also reported. The average fractional difference for $d = 2$ is 0.00986: that is, on average our results are within 99% of the best known solution. This finding indicates that the results presented here are fairly close to the best known entire solution set, produced by the cumulative effort of dozens of expert researchers, with a corresponding, arguably substantial total effort.

Since for $d = 3,4$ there are no equivalent results available in the literature, we compare to a single call to *MOP* with its global search method. The simple average of all the fractional differences for $d = 3,4$ are -0.00723 and -0.00057, respectively. For $d = 3,4$, the negative average fractional differences are achieved at a lower average computational effort, indicating that our hybrid optimization approach does indeed effectively assist the theoretically required global optimization framework provided by *MOP*. We note that the rattler fraction for $d = 2,3$ has in general a decreasing trend with respect to n, but this decrease is not monotonic. However, the rattler fraction for $d = 4$ has in general an increasing trend with respect to n. Two illustrative packing configurations using our hybrid optimization approach are displayed by Figures 1 and 2 for the model-instances $n = 10, d = 2,3$.

Figures 3-5 capture the positive correlation between the radius r_0 of the container d-sphere and the number of d-spheres to pack for $d = 2,3,4$, respectively. Regression analysis indicates that for $d = 2$ the regression function for the container radius equals $-5.9119 + 2.3802 \cdot n + 0.0445 \cdot n^2$, with *p*-values (observed significance levels) below 0.00001 for all the input parameters. This finding indicates that we have very strong statistical evidence suggesting that the regression coefficients are different from zero (consult e.g. Black *et al*., 2014). For $d = 3$, the regression function for the container radius equals $-2.0559 + 1.9739 \cdot n + 0.0186 \cdot n^2$; for $d = 4$ the regression function for the container radius equals $-1.9944 + 1.9944 \cdot n + 0.0097 \cdot n^2$. In both cases the corresponding *p*-values are again below 0.00001 for all the input parameters.

Figures 6-8 capture the correlation between the packing fraction and the number of d-spheres to pack for $d = 2,3,4$, respectively. Our regression analysis based on the results found indicates that for $d = 2$ the regression function for the packing fraction equals $0.8741 - 0.8611 \cdot (1/n)$, with a *p*-value below 0.00001 for the input parameter. For $d = 3$, the regression function for the packing fraction equals $0.5862 - 1.6230 \cdot (1/n)$, while for $d = 4$ the regression function for the packing fraction equals $0.2914 - 0.7241 \cdot (1/n)$. In both cases, the *p*-values are again below 0.00001, for all input parameters.

5 Summary and Conclusions

The topic of object packings leads to fascinating areas of scientific exploration, as well as to important, interesting and hard numerical optimization challenges. In this work, we introduce a broad class of general d-dimensional finite sphere packing problems that (in general) cannot be tackled by purely analytical approaches. The proper numerical solution of these problems (and of similarly complex other packings) requires the use of global scope – nonlinear and/or combinatorial – optimization tools. Suitable, problem-class dependent heuristic approaches can often greatly enhance the efficiency of automatic global optimization: we believe that this aspect becomes essential in most real-world applications.

In line with the advocated general solution framework, we developed a hybrid optimization strategy to solve instances of finite d-sphere packing problems. This hybrid approach is based on using the LGO solver suite in combination with heuristic steps aimed at finding improved configurations quickly. The quality of our numerical results for a well-studied model-instance with n = 5 to 50 spheres in $\mathbb{R}^2$ is on average better than 99% for the entire set of best known results obtained by expert researchers / teams. We also present optimized (conjectured) packings for previously unexplored generalizations of the same model-class in $\mathbb{R}^d, d = 3,4$. The results obtained support the estimation of the optimized container sphere radii and of the packing fraction as functions of the model instance parameters n and $\frac{1}{n}$, respectively. We believe that our solution approach and the subsequent analysis can be directly applied, *mutatis mutandis*, also to other model-instances defined by given (non-trivial, formula-based) sphere sequences in $\mathbb{R}^d, d \geq 2$.

Table 1. 2-dimensional packing results

n	Best known r_0	Packing fraction	Rattler fraction	Hybrid optimization approach r_0	Packing fraction	Rattler fraction	Time (sec.)	Fractional difference
5	9.00140	0.67880	0.40	9.00140	0.67880	0.40	9.84	0.00000
6	11.05704	0.74433	0.50	11.05700	0.74433	0.50	11.89	0.00000
7	13.46211	0.77251	0.29	13.46210	0.77251	0.29	19.58	0.00000
8	16.22175	0.77524	0.25	16.22170	0.77524	0.25	28.70	0.00000
9	19.23319	0.77045	0.33	19.23320	0.77045	0.33	36.60	0.00000
10	22.00019	0.79544	0.50	22.00020	0.79544	0.50	21.26	0.00000
11	24.96063	0.81216	0.36	24.96060	0.81216	0.36	40.09	0.00000
12	28.37139	0.80752	0.50	28.46380	0.80228	0.25	112.93	0.00326
13	31.54587	0.82300	0.38	31.75710	0.81209	0.38	145.39	0.00670
14	35.09565	0.82406	0.21	35.33360	0.81300	0.50	42.01	0.00678
15	38.83800	0.82207	0.53	39.40760	0.79848	0.40	159.99	0.01467
16	42.45812	0.82987	0.44	42.98300	0.80973	0.38	192.54	0.01236
17	46.29134	0.83299	0.53	46.80550	0.81479	0.41	233.58	0.01111
18	50.11976	0.83957	0.44	50.57340	0.82458	0.28	154.49	0.00905
19	54.24029	0.83956	0.47	54.71920	0.82493	0.26	312.67	0.00883
20	58.40057	0.84149	0.30	59.02270	0.82384	0.25	318.83	0.01065
21	62.55888	0.84602	0.38	63.18950	0.82922	0.24	216.07	0.01008
22	66.76029	0.85148	0.41	67.89780	0.82319	0.27	520.46	0.01704
23	71.19946	0.85297	0.35	71.91150	0.83616	0.22	545.24	0.01000
24	75.74914	0.85397	0.46	77.07610	0.82482	0.33	351.61	0.01752
25	80.28586	0.85714	0.32	81.22670	0.83740	0.28	565.38	0.01172
26	84.97819	0.85871	0.35	85.77710	0.84279	0.27	703.86	0.00940
27	89.75096	0.86031	0.41	90.22820	0.85123	0.37	760.75	0.00532
28	94.52588	0.86333	0.50	95.66040	0.84298	0.32	868.33	0.01200
29	99.48311	0.86441	0.34	100.93000	0.83980	0.24	861.95	0.01454
30	104.54036	0.86515	0.23	105.94500	0.84237	0.23	496.94	0.01344
31	109.62924	0.86666	0.39	111.69300	0.83493	0.29	762.43	0.01882
32	114.79981	0.86805	0.38	116.39200	0.84446	0.19	1312.21	0.01387
33	120.06566	0.86912	0.36	121.67500	0.84628	0.42	1202.54	0.01340
34	125.36694	0.87072	0.50	126.16900	0.85968	0.21	1680.83	0.00640
35	130.84908	0.87084	0.34	132.53500	0.84882	0.23	1609.53	0.01288
36	136.30791	0.87224	0.39	138.61400	0.84346	0.31	1553.17	0.01692
37	141.78373	0.87426	0.46	143.52900	0.85314	0.24	1592.44	0.01231
38	147.45212	0.87475	0.37	149.56600	0.85020	0.21	2118.75	0.01434
39	153.19974	0.87515	0.46	154.91600	0.85587	0.28	2397.07	0.01120
40	159.02158	0.87552	0.45	160.47900	0.85969	0.30	2422.80	0.00916
41	164.80623	0.87703	0.27	167.02300	0.85390	0.34	2673.48	0.01345
42	170.69781	0.87807	0.38	172.43900	0.86043	0.24	3028.64	0.01020
43	176.73266	0.87833	0.56	179.38700	0.85252	0.21	2965.38	0.01502
44	182.77262	0.87919	0.32	185.15800	0.85668	0.23	4381.82	0.01305
45	188.96497	0.87922	0.38	190.55700	0.86459	0.29	4617.60	0.00843
46	195.20390	0.87945	0.37	197.35800	0.86036	0.24	5659.88	0.01104
47	201.48619	0.87987	0.38	203.72200	0.86067	0.21	4887.42	0.01110
48	207.80084	0.88057	0.31	209.83200	0.86361	0.25	4639.94	0.00977
49	214.18093	0.88123	0.49	216.62200	0.86148	0.24	6177.08	0.01140
50	220.56540	0.88234	0.38	224.15900	0.85428	0.20	5583.73	0.01629

Table 2. 3-dimensional packing results

n	Single *MOP* global call r_0	Packing fraction	Time (sec.)	Hybrid optimization approach r_0	Packing fraction	Rattler fraction	Time (sec.)	Fractional difference
5	9.00140	0.30850	2.48	9.00000	0.30864	0.40	12.85	-0.00016
6	11.05700	0.32623	1.15	11.05700	0.32623	0.50	12.53	0.00000
7	13.15510	0.34438	1.31	13.15510	0.34438	0.57	15.02	0.00000
8	15.27270	0.36379	1.48	15.27270	0.36379	0.63	17.49	0.00000
9	17.40110	0.38432	1.75	17.40110	0.38432	0.67	19.75	0.00000
10	19.53610	0.40571	2.11	19.53610	0.40571	0.60	22.99	0.00000
11	21.68330	0.42728	2.43	21.68330	0.42728	0.36	24.70	0.00000
12	23.85240	0.44833	3.12	23.85240	0.44833	0.58	34.24	0.00000
13	26.40690	0.44971	3.96	26.22890	0.45893	0.54	46.30	-0.00674
14	28.85810	0.45875	5.04	28.85810	0.45875	0.43	32.19	0.00000
15	31.14560	0.47662	6.58	31.36620	0.46664	0.53	51.62	0.00708
16	33.94200	0.47301	8.31	33.84520	0.47708	0.50	56.27	-0.00285
17	36.56420	0.47887	11.00	36.20200	0.49338	0.59	69.75	-0.00991
18	39.24170	0.48389	14.15	39.13020	0.48804	0.50	54.48	-0.00284
19	41.79580	0.49443	17.97	41.54430	0.50347	0.47	91.56	-0.00602
20	44.89450	0.48737	22.93	44.43190	0.50275	0.55	172.46	-0.01030
21	47.36920	0.50204	29.62	47.32330	0.50350	0.52	63.98	-0.00097
22	50.53530	0.49597	36.52	50.08440	0.50949	0.59	234.22	-0.00892
23	53.17970	0.50650	47.55	53.31640	0.50262	0.43	86.49	0.00257
24	56.28420	0.50476	58.41	56.18730	0.50738	0.50	62.10	-0.00172
25	59.53380	0.50058	73.59	58.73390	0.52132	0.48	293.41	-0.01344
26	62.46270	0.50554	90.28	61.75510	0.52311	0.50	258.07	-0.01133
27	65.48330	0.50885	111.09	64.79290	0.52529	0.52	232.31	-0.01054
28	68.70220	0.50832	137.11	68.13310	0.52117	0.61	210.74	-0.00828
29	71.78350	0.51157	164.60	71.29800	0.52209	0.45	196.35	-0.00676
30	74.96910	0.51317	202.38	74.29920	0.52717	0.50	232.87	-0.00894
31	78.06340	0.51716	244.87	76.83300	0.54240	0.45	543.59	-0.01576
32	81.30480	0.51870	295.87	80.43980	0.53562	0.56	387.14	-0.01064
33	84.38330	0.52379	353.14	83.30040	0.54448	0.55	538.56	-0.01283
34	87.90600	0.52117	427.10	86.70100	0.54320	0.47	410.46	-0.01371
35	90.92610	0.52798	510.14	90.34260	0.53828	0.49	391.19	-0.00642
36	94.32780	0.52848	607.06	93.18350	0.54819	0.39	547.82	-0.01213
37	97.70920	0.52979	712.81	96.86980	0.54368	0.54	878.44	-0.00859
38	100.99200	0.53306	828.70	100.08500	0.54769	0.47	409.77	-0.00898
39	104.91500	0.52684	971.48	103.47900	0.54907	0.51	707.61	-0.01369
40	108.02800	0.53336	1131.83	106.72900	0.55307	0.50	589.58	-0.01202
41	111.19400	0.53922	1290.89	110.04500	0.55628	0.41	661.79	-0.01033
42	115.32100	0.53167	1518.46	113.40500	0.55909	0.50	915.04	-0.01661
43	118.52200	0.53751	1721.60	117.48700	0.55184	0.42	872.77	-0.00873
44	122.48400	0.53337	1985.85	121.15400	0.55114	0.48	1001.48	-0.01086
45	125.68500	0.53955	2295.61	124.38100	0.55669	0.47	753.85	-0.01038
46	129.15400	0.54240	2675.40	127.79200	0.55993	0.54	1355.07	-0.01055
47	132.63600	0.54530	2916.19	131.46800	0.55996	0.51	1923.79	-0.00881
48	137.42400	0.53287	3345.35	135.00600	0.56203	0.50	1033.61	-0.01760
49	140.52400	0.54078	3733.74	138.60000	0.56362	0.53	1638.57	-0.01369
50	144.31700	0.54084	4231.94	142.83400	0.55786	0.52	1359.97	-0.01028

Table 3. 4-dimensional packing results

n	Single *MOP* global call r_0	Packing fraction	Time (sec.)	Hybrid optimization approach r_0	Packing fraction	Rattler fraction	Time (sec.)	Fractional difference
5	8.39048	0.19753	1.26	8.35382	0.20102	0.40	10.19	-0.00437
6	10.35940	0.19754	1.20	10.34000	0.19902	0.00	12.23	-0.00187
7	12.40390	0.19753	1.36	12.33840	0.20176	0.43	14.93	-0.00528
8	14.51660	0.19753	1.59	14.47590	0.19976	0.00	17.47	-0.00280
9	16.69160	0.19753	1.93	16.59440	0.20220	0.00	19.94	-0.00582
10	18.92400	0.19753	2.31	18.85750	0.20033	0.20	22.89	-0.00351
11	21.20980	0.19753	2.89	21.07870	0.20249	0.55	24.99	-0.00618
12	23.54540	0.19753	3.71	23.44990	0.20077	0.67	27.30	-0.00406
13	25.92800	0.19753	4.76	25.76120	0.20270	0.54	30.08	-0.00643
14	28.21150	0.20158	6.36	28.21150	0.20158	0.71	32.06	0.00000
15	30.40390	0.20867	8.19	30.40390	0.20867	0.73	34.64	0.00000
16	32.60130	0.21586	10.81	32.60130	0.21586	0.69	37.67	0.00000
17	34.80250	0.22315	13.88	34.80250	0.22315	0.65	40.54	0.00000
18	37.00980	0.23044	17.75	37.00980	0.23044	0.67	43.48	0.00000
19	39.22480	0.23769	22.50	39.22480	0.23769	0.42	45.60	0.00000
20	41.47750	0.24417	28.36	41.48580	0.24397	0.55	74.32	0.00020
21	44.14480	0.24150	35.90	44.08090	0.24291	0.62	52.61	-0.00145
22	46.43240	0.24771	45.15	46.51820	0.24589	0.64	113.47	0.00185
23	49.00430	0.24819	56.80	48.76860	0.25302	0.74	120.39	-0.00481
24	51.11170	0.25833	71.67	51.17170	0.25712	0.71	64.79	0.00117
25	53.85740	0.25597	95.02	53.52990	0.26229	0.60	83.65	-0.00608
26	56.27170	0.26037	121.10	56.44490	0.25718	0.65	111.29	0.00308
27	58.96450	0.25993	135.60	58.79620	0.26292	0.52	77.92	-0.00285
28	61.47400	0.26305	165.31	61.45510	0.26338	0.32	87.06	-0.00031
29	63.88110	0.26806	203.37	64.09150	0.26456	0.69	111.24	0.00329
30	66.51280	0.26948	246.70	66.64490	0.26735	0.53	102.67	0.00199
31	69.01790	0.27313	303.25	69.32200	0.26837	0.65	155.40	0.00441
32	71.83510	0.27212	358.04	71.82060	0.27234	0.66	121.37	-0.00020
33	74.29750	0.27672	430.61	74.50370	0.27367	0.61	180.67	0.00278
34	77.13570	0.27593	501.60	77.17460	0.27538	0.62	199.31	0.00050
35	79.74440	0.27867	612.27	79.80400	0.27783	0.60	135.88	0.00075
36	82.52710	0.27915	724.37	82.43700	0.28037	0.56	156.44	-0.00109
37	85.09130	0.28274	830.89	85.31860	0.27974	0.54	164.22	0.00267
38	87.63950	0.28661	976.64	87.97920	0.28221	0.53	204.21	0.00388
39	90.59950	0.28529	1118.02	90.66850	0.28442	0.59	204.35	0.00076
40	93.39760	0.28625	1307.31	93.44840	0.28563	0.53	227.87	0.00054
41	96.06090	0.28898	1542.52	96.04750	0.28915	0.59	932.44	-0.00014
42	99.08060	0.28762	1761.17	99.03550	0.28814	0.57	368.12	-0.00046
43	101.61800	0.29202	2058.28	101.98200	0.28786	0.58	257.26	0.00358
44	104.71400	0.29015	2378.76	104.44600	0.29315	0.57	293.65	-0.00256
45	107.43400	0.29265	2725.74	107.48100	0.29213	0.36	341.61	0.00044
46	110.34300	0.29319	3266.79	110.28200	0.29384	0.48	419.98	-0.00055
47	113.04100	0.29607	3467.08	112.98500	0.29666	0.57	352.38	-0.00050
48	116.04000	0.29591	3910.97	116.22500	0.29402	0.63	618.98	0.00159
49	118.88900	0.29740	4581.53	119.08200	0.29548	0.51	476.89	0.00162
50	121.82000	0.29817	5056.86	121.80600	0.29831	0.62	552.60	-0.00011

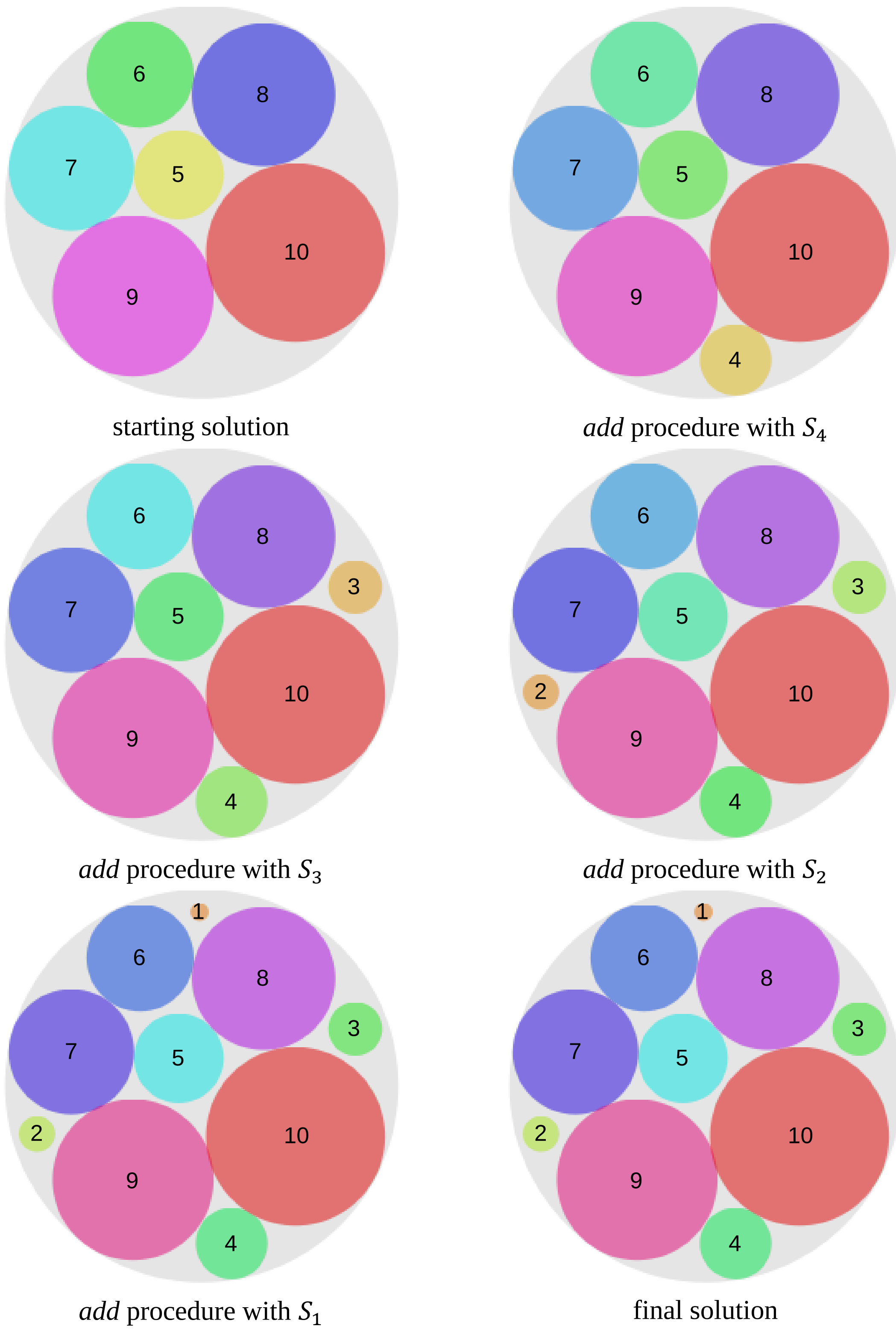
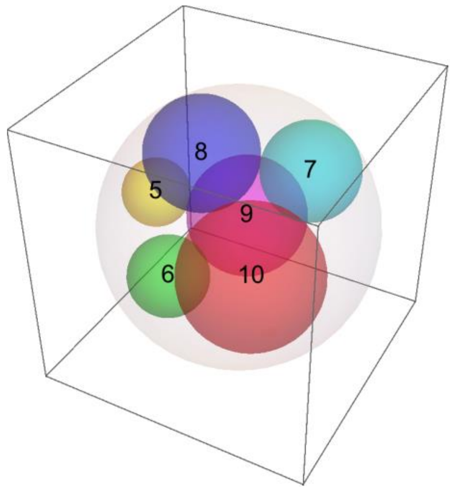
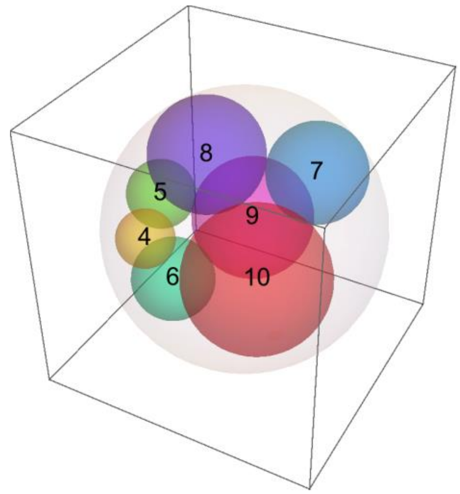


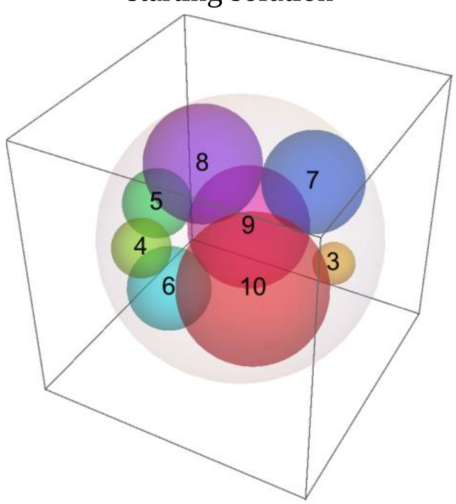
Figure 1. Hybrid optimization approach based configurations for $d = 2$ and $n = 10$



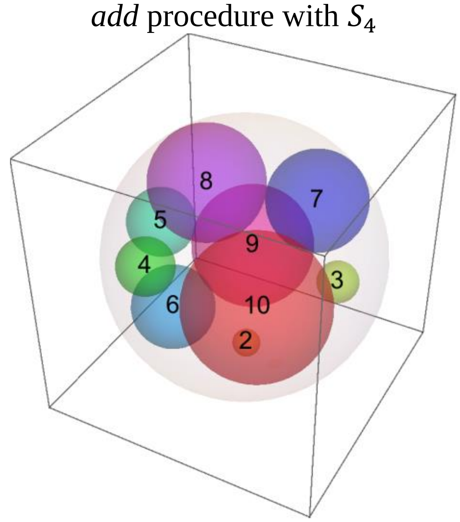
starting solution



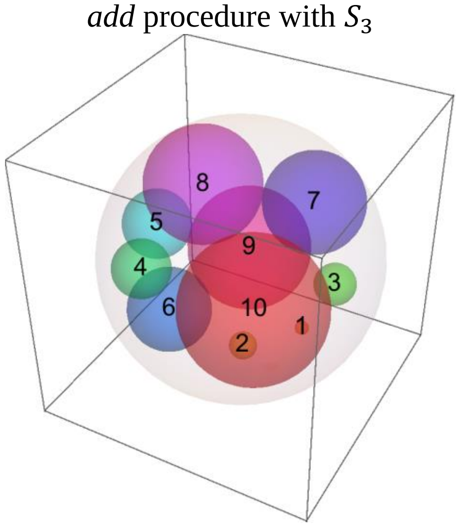
add procedure with S_4



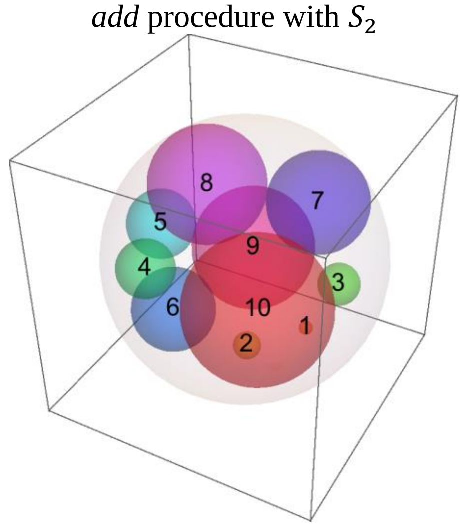
add procedure with S_3



add procedure with S_2



add procedure with S_1



final solution

Figure 2. Hybrid optimization approach based configurations for $d = 3$ and $n = 10$

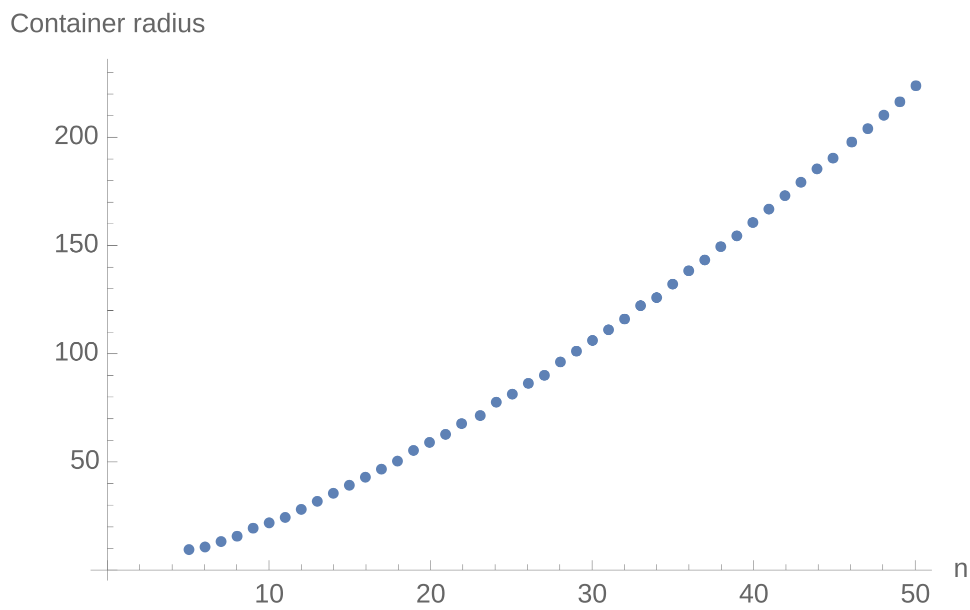


Figure 3. Container radius *vs.* number of d-spheres for $d = 2$

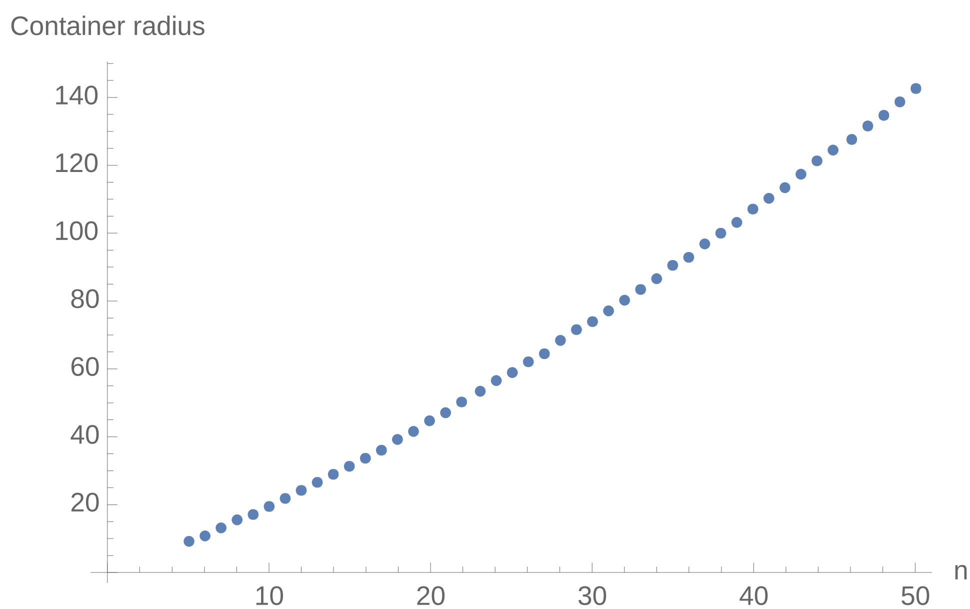


Figure 4. Container radius *vs.* number of d-spheres for $d = 3$

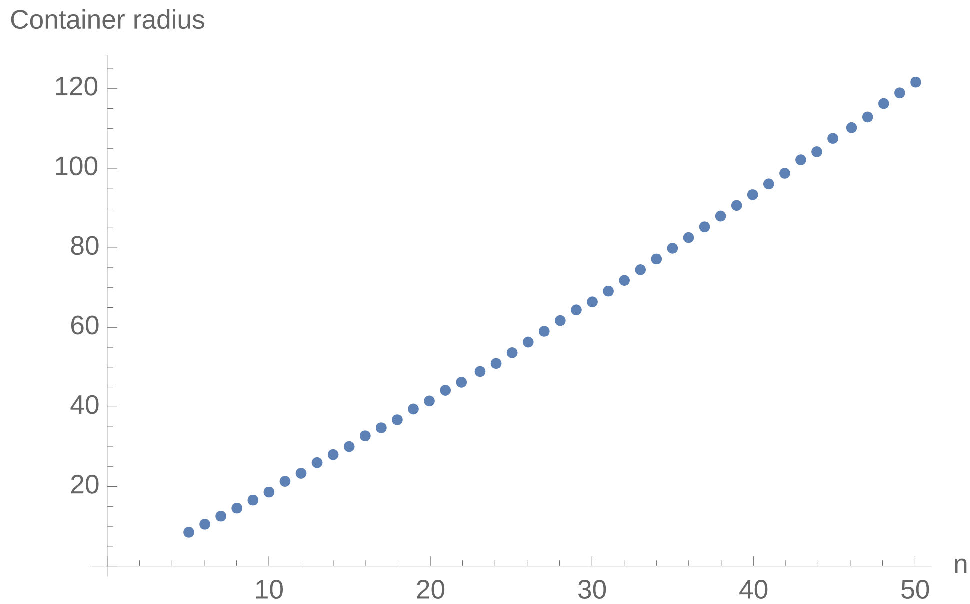


Figure 5. Container radius *vs.* number of d-spheres for $d = 4$

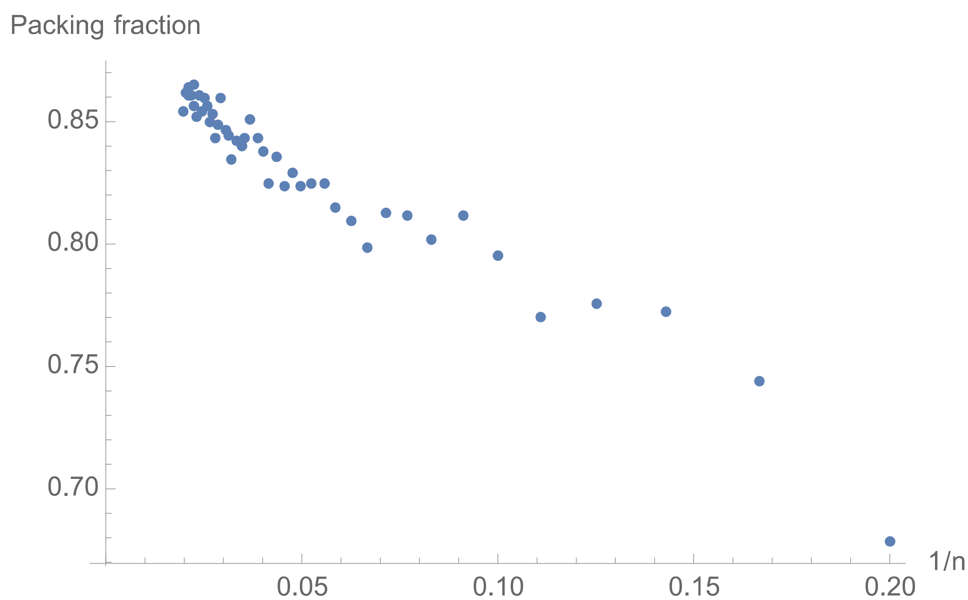


Figure 6. Packing fraction *vs.* $^1/_n$ for $d = 2$

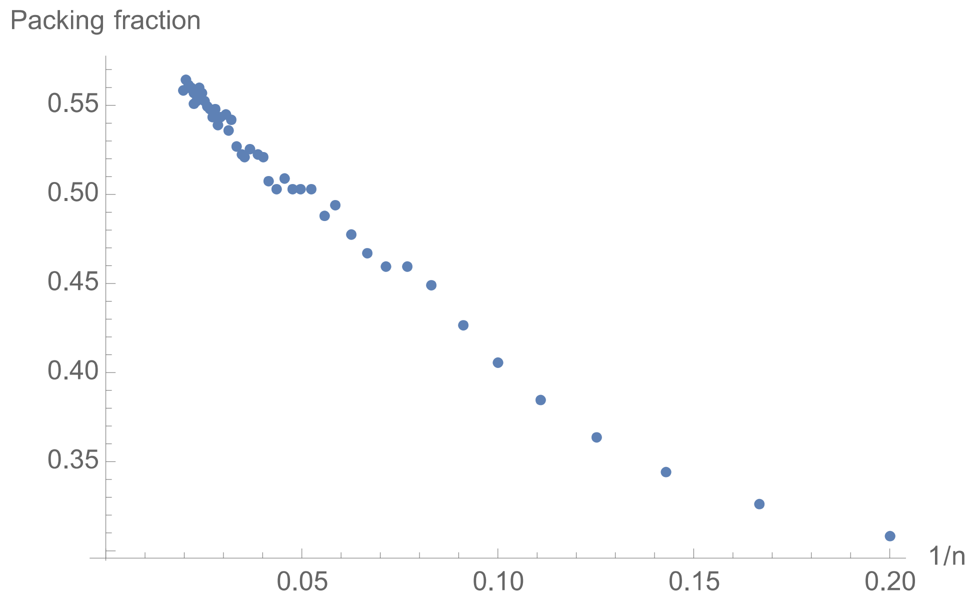


Figure 7. Packing fraction *vs.* $1/n$ for $d = 3$

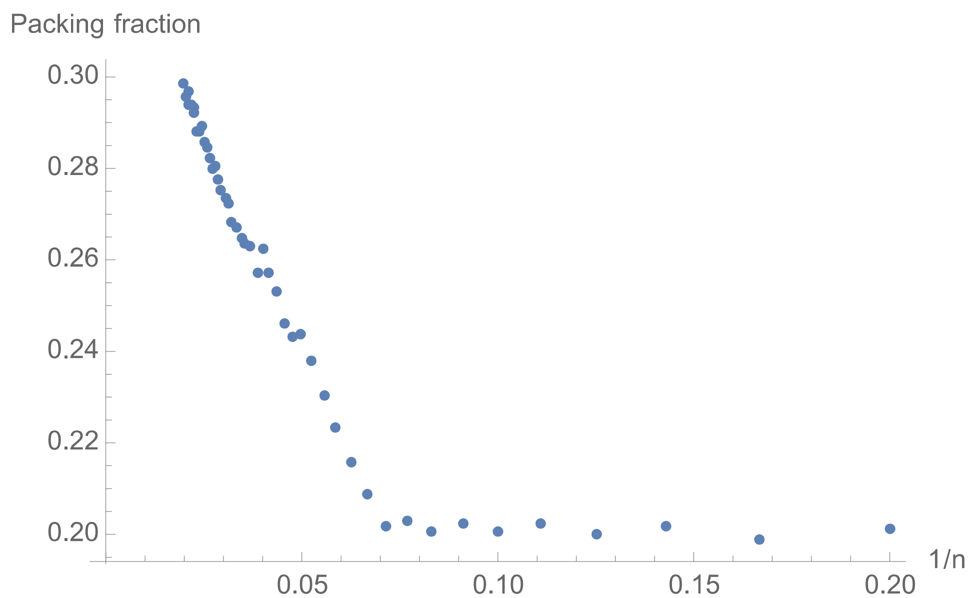


Figure 8. Packing fraction *vs.* $1/n$ for $d = 4$

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