Packing circles in a square: new putative optima obtained via global optimization

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Abstract

The problem of finding the optimal placement of N identical, non overlapping, circles with maximum radius in the unit square is a well known challenge both in classical geometry and in optimization. A database of putative optima is currently maintained at `www.packomania.com`. Recently, through clever use of an extremely simple global optimization method, we succeeded in finding improved configurations for several instances. The improved configurations are in the range $N \leq 90$, i.e., they improve over relatively small instances (even $N = 53$), an event that some researchers did not believe to be possible. We also improved larger instances using a simpler strategy initialized at the previously known putative optimum.

1 Problem definition

The problem of optimally placing N identical and non overlapping circles inside the unit square has been studied both as a theoretical geometrical problem as well as a hard test for global optimization methods since many years. Among many survey papers we address the reader to the nice survey in [SMC04] and to the references cited in this paper.

Among different possible statements of the problem let us start with the most natural one. Given an integer N the aim is to solve the following global optimization problem:

$$\begin{aligned} \max r & & & (1) \\ \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} & \geq 2r \quad \forall\, i < j \in 1, N & & (2) \\ x_i, y_i & \geq r \quad \forall\, i = 1, N & & (3) \\ x_i, y_i & \leq 1 - r \quad \forall\, i = 1, N & & (4) \end{aligned}$$

In this formulation we have $2N + 1$ variables (the coordinates of the N circle centers and the radius); constraints (2) imply that two different circles will not overlap, while constraints (3–4) state that no circle can have a portion outside $[0, 1]^2$.

Often the problem is transformed into an equivalent one in which only the centers of the circles are contrained to be in $[0, 1]$, and not the circles themselves:

$$\begin{aligned} \max d & & & (5) \\ \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} & \geq d \quad \forall\, i < j \in 1, N & & (6) \\ x_i, y_i & \in [0, 1] \quad \forall\, i = 1, N & & (7) \end{aligned}$$

It is easy to show that from the global optimum of each of these two formulations it is possible to recover the global optimum of the other.

Stated in this way the problem is easily seen to be extremely hard. In fact, while the objective is linear, the non-overlapping constraints are quadratic reverse-convex. Some attempts have appeared in the literature which use deterministic methods with guaranteed accuracy in the solution, but, as N increases their complexity become extremely high. So, as it is quite common when dealing with hard and large scale global optimization problems, heuristici procedures and, in particular, stochastic methods are the only viable solution.

We began our experiments in this field with a very effective, yet quite elementary, global optimization method: Monotonic Basin Hopping (MBH), a simple stochastic method which has been re-discovered several times in the global optimization literature. Under the name Basin Hopping it appears to have been first adopted in the somewhat related problem of minimum energy molecular conformation in [WD97] and [Lea00]. Finding the global minimum conformation in 3-dimensional space of a cluster of N particles interacting through pairwise energy contribution might seem to be a problem in some way related to that one discussed here. However important differences arise: first of all here there is no energy to minimize; moreover, circle packing is a constrained optimization problem and, in particular, it is so complex that even *local* optimization is an hard task. On the contrary, in Lennard-Jones or Morse cluster, local optimization is usually quite easy, at least for moderately sized clusters.

Just for reference, we report here the basic structure of MBH: let $MaxNoImprove$ be an integer constant. Then the algorithm can be schematically described as follows:

MBH(X : **initial local minimum)**
Step 1. Compute $Y := \mathbf{\Phi}(X)$;
Step 2. **if** $f(Y) < f(X)$ **then** set $X := Y$;
else reject $\bar{Y}$;
Step 3. Repeat Steps 1–2 until $MaxNoImprove$ consecutive rejections have occurred;
return X;

The mapping $\mathbf{\Phi}$ is usually defined as the product of two procedure:

1. a random perturbation of the current solution X, which produces a different solution $\tilde{X}$
2. a local optimization performed using $\tilde{X}$ as a starting point.

It is easily seen that the method is extremely simple, but it requires some careful definition. In particular, being the circle packing problem a constrained one, some care has to be taken in order to avoid that a perturbation of the current configuration leads to an infeasible point.

2 Preliminary results and new configurations

We implemented a version of Monotonic Basin Hopping using, for the local search, SNOPT 6.0 [GMS02]. For relatively small circle packing problems ($N \leq 86$) we ran MBH, performing 100 independent runs with $MaxNoImprove = 50$. This way we were able to discover 8 new putative globally optima configurations, which are strictly better than those previously known.

For $N > 86$ we just ran a single instance of MBH using the known putative optimum as a starting point. This way we discovered new putative optima for $N = 88, 106, 108, 115, 116, 130, 133, 134, 135, 146, 155, 157$ For the first 8 newly discovered packings the figures in the appendix report the geometry of the new (on the left) versus the previously known (on the right) putative optima.

Acknowledgements

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References

[GMS02] P.E. Gill, W. Murray, and M. A. Saunders. SNOPT: An SQP algorithm for large-scale constrained optimization. *SIAM J. Optim.*, 12:979–1006, 2002.

[Lea00] Robert H. Leary. Global optimization on funneling landscapes. *Journal of Global Optimization*, 18:367–383, 2000.

[SMC04] Péter Gábor Szabó, Mihály Csaba Markót, and Tibor Csendes. *Global Optimization in Geometry - Circle Packing Into the Square.* GERAD, 2004.

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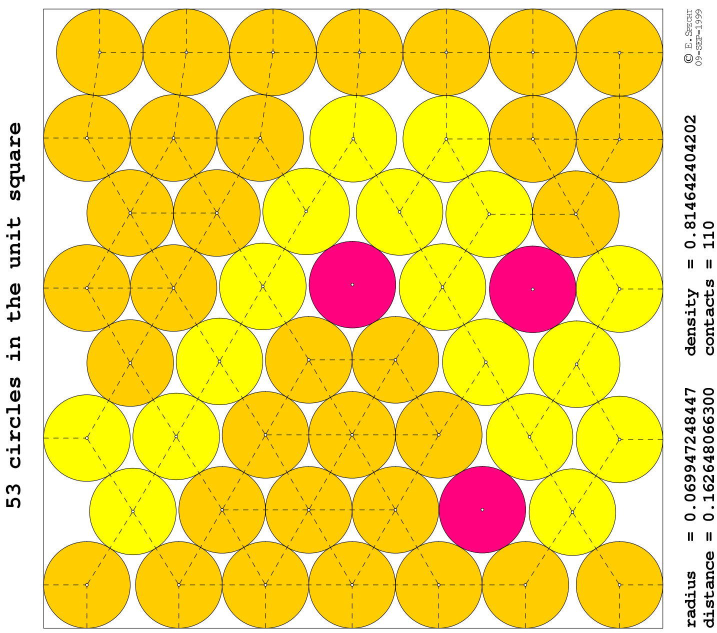
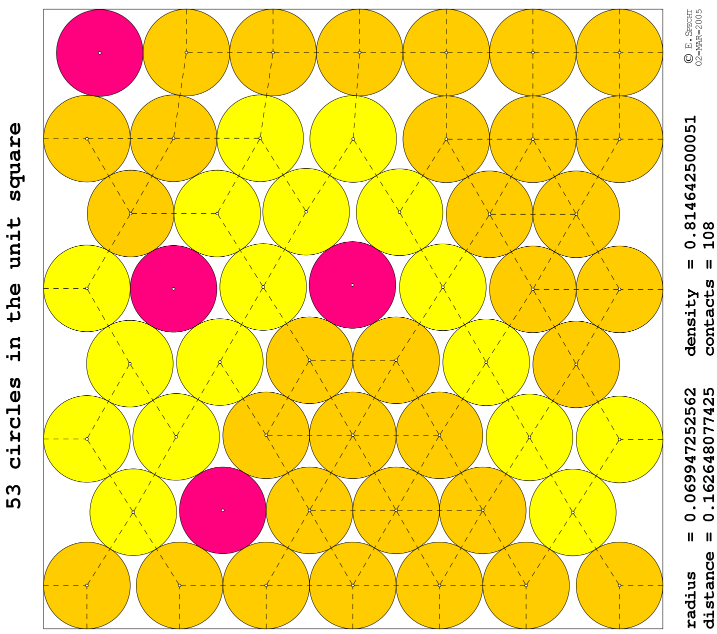
Appendix: Pictures of the new putative optima


53 circles in the unit square
radius = 0.069947248447
distance = 0.162648066300
density = 0.814642404202
contacts = 110
© E. SPECHT
09-SEP-1999


53 circles in the unit square
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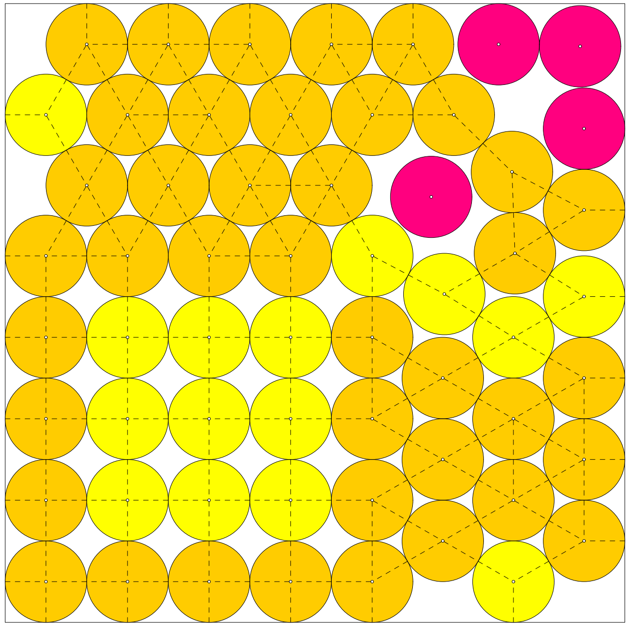
© E. SPECHT
02-MAR-2005

59 circles in the unit square



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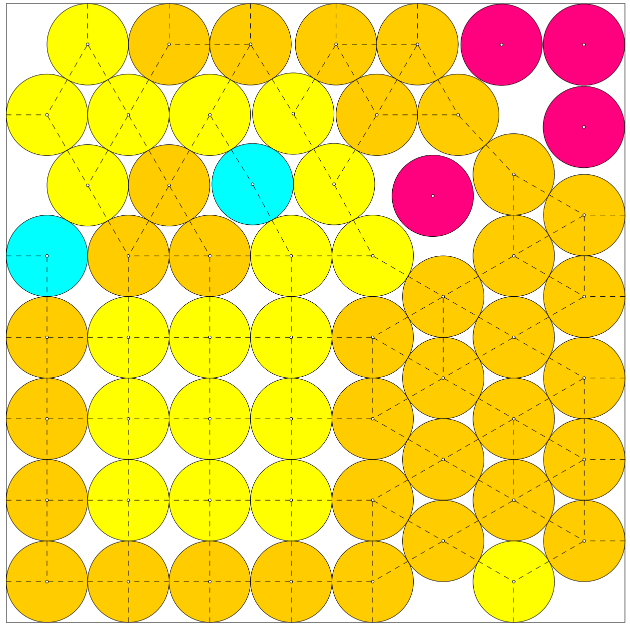
distance = 0.151562950614 contacts = 121

59 circles in the unit square



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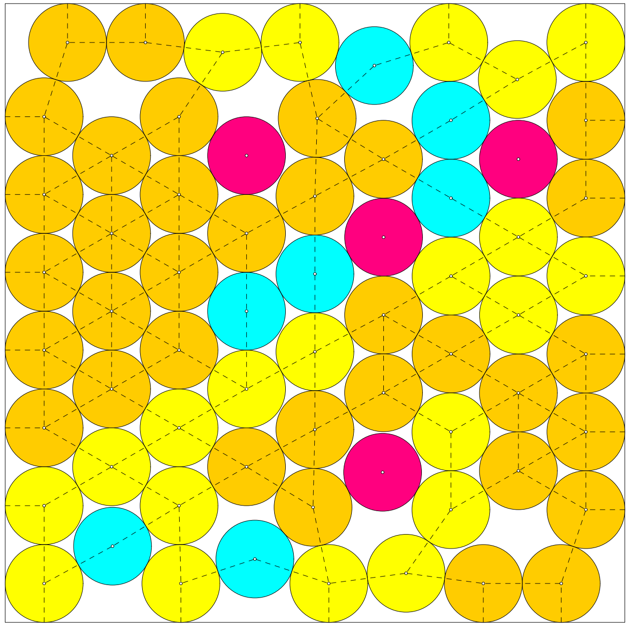

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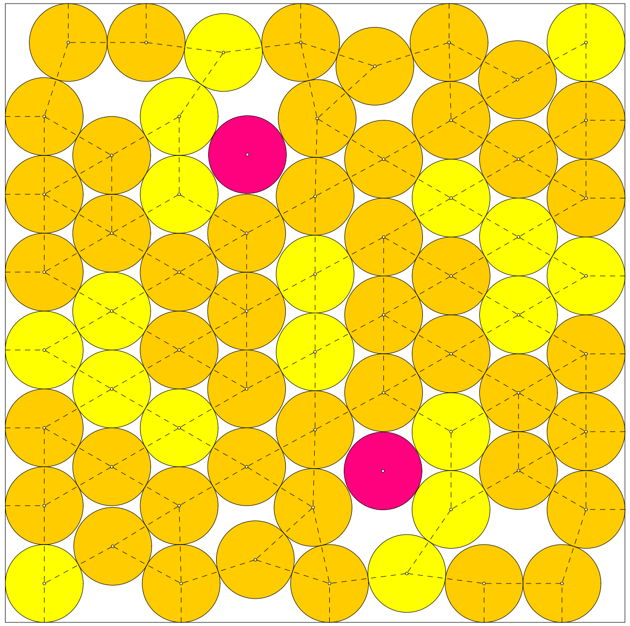
distance = 0.143804230800 contacts = 124

66 circles in the unit square



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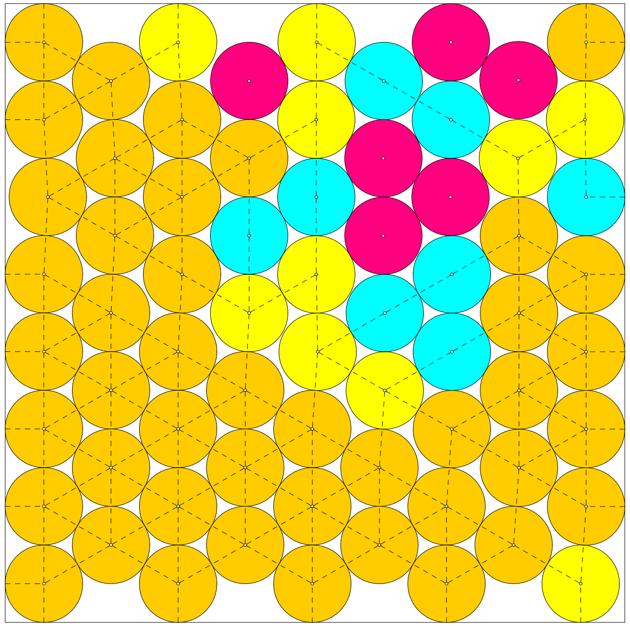
68 circles in the unit square



radius = 0.062520077998 density = 0.835021788293
distance = 0.142909593911 contacts = 139

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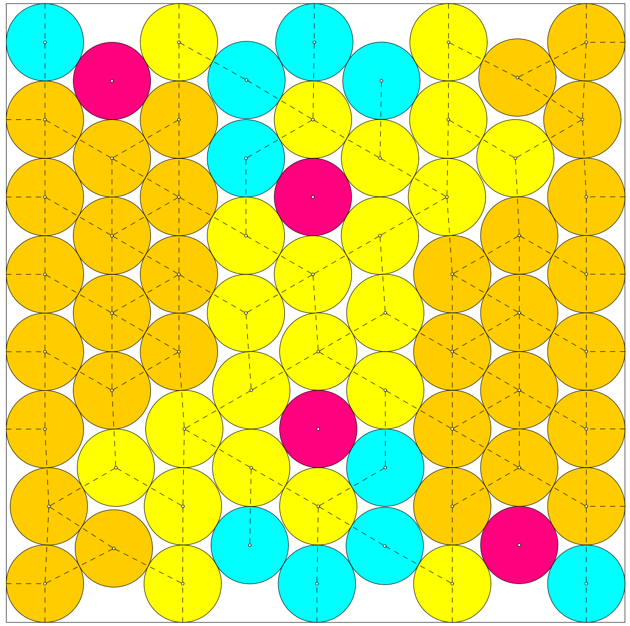
68 circles in the unit square



radius = 0.062520033463 density = 0.835020598672
distance = 0.142909477564 contacts = 121

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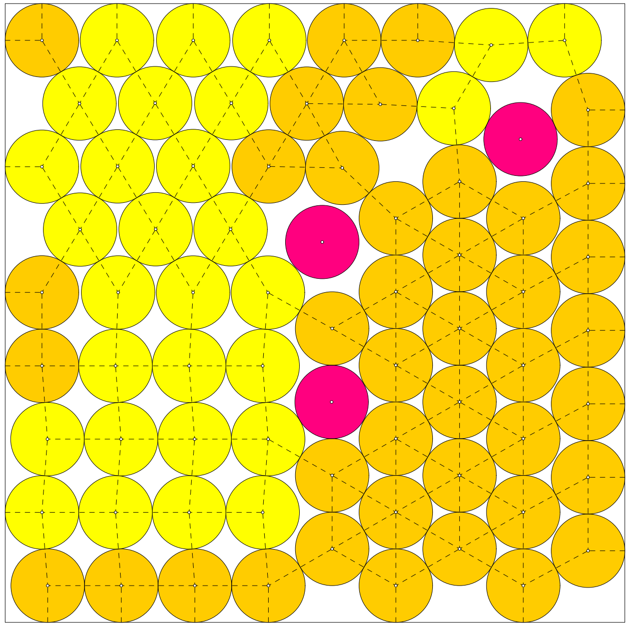
73 circles in the unit square



radius = 0.059366050583 density = 0.808256206863
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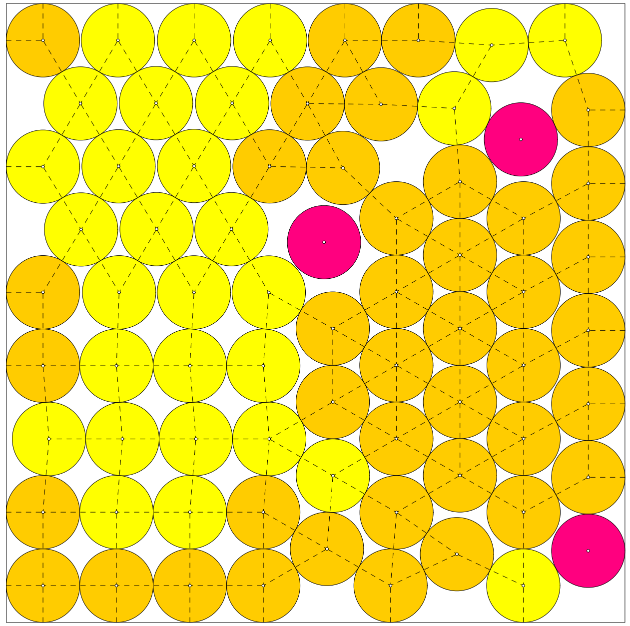
73 circles in the unit square



radius = 0.059358711984 density = 0.808056392279
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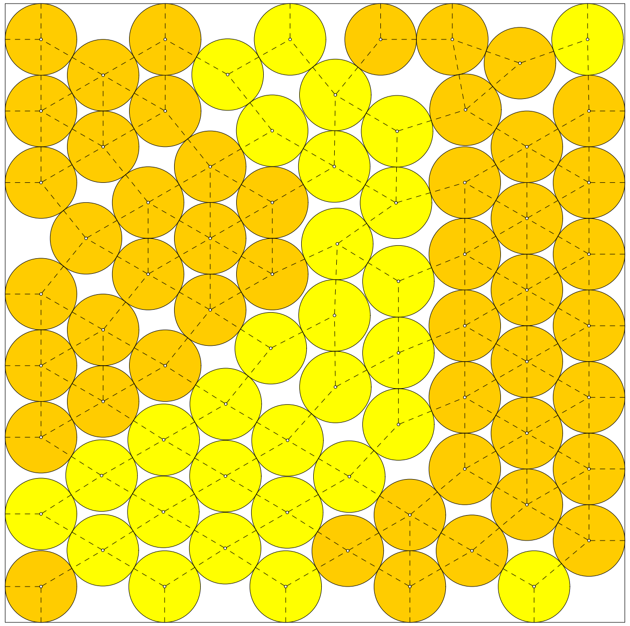
77 circles in the unit square



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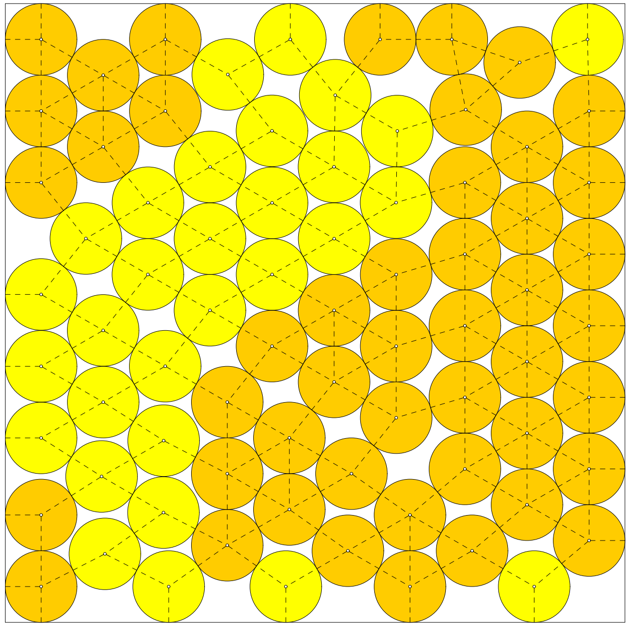
77 circles in the unit square



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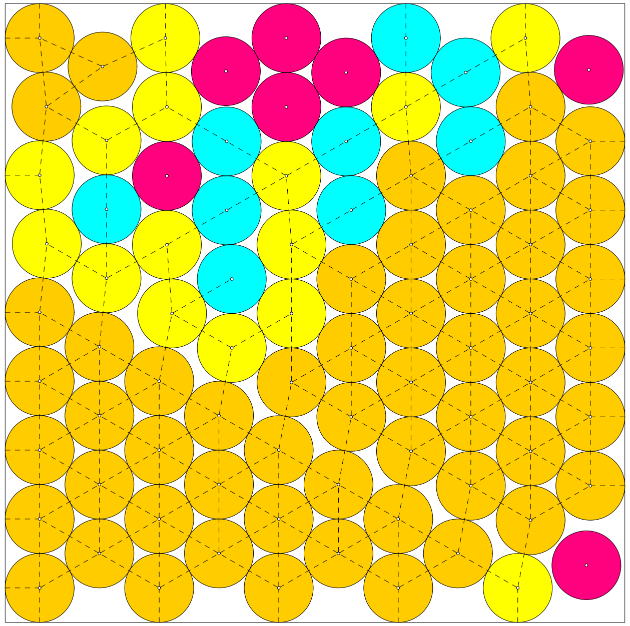
85 circles in the unit square



radius = 0.055680181768 density = 0.827885139567
distance = 0.125315548584 contacts = 179

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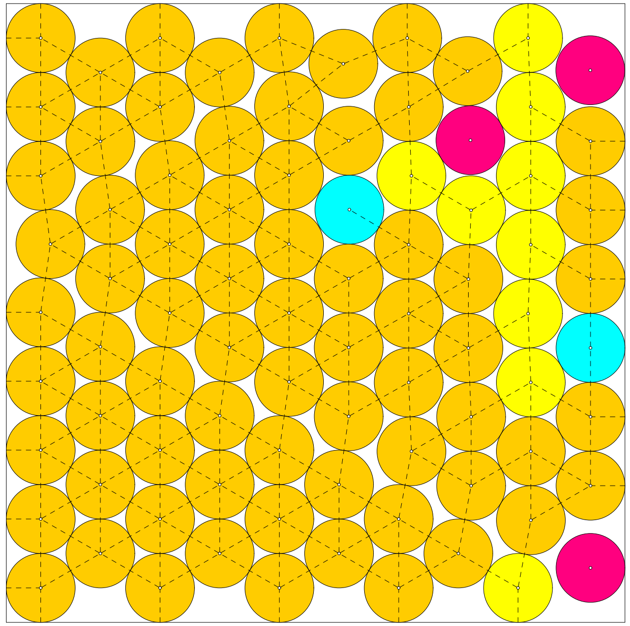
85 circles in the unit square



radius = 0.055678405372 density = 0.827832315434
distance = 0.125311049576 contacts = 192

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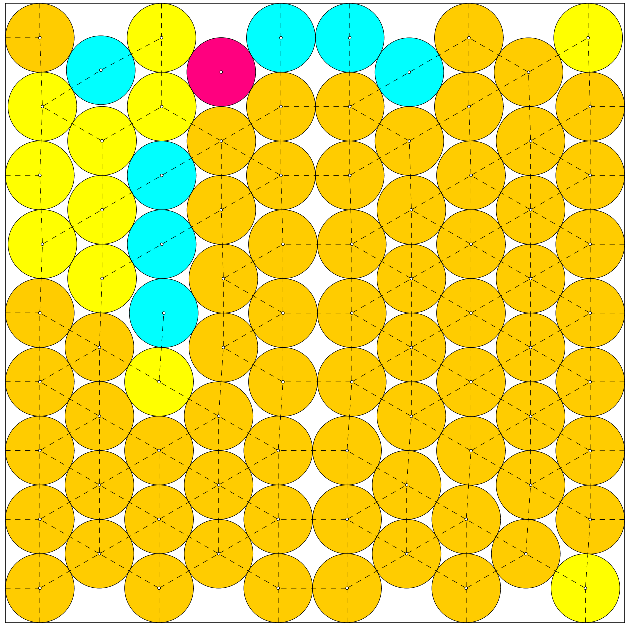
86 circles in the unit square



radius = 0.055572999121 density = 0.834403263688
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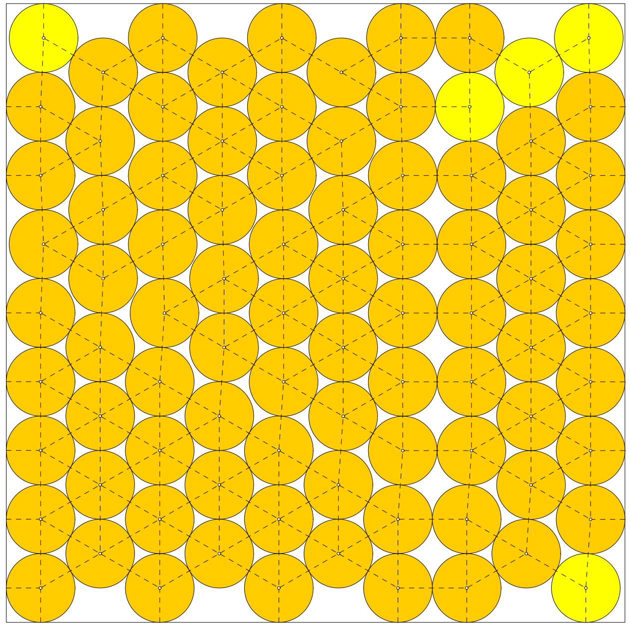
86 circles in the unit square



radius = 0.055572358492 density = 0.834384026280
distance = 0.125042534041 contacts = 216