Optimization and Simulation for Favourable Plasmonic Detector Development

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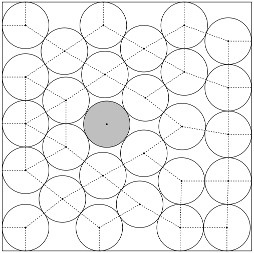
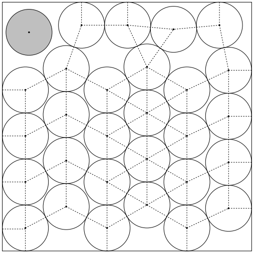
Word cloud of my paper titles

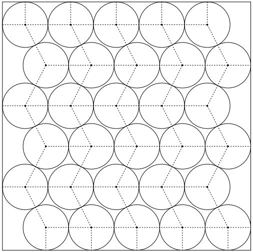
Verified optimal packings for 28-30 circles



n = 28



n = 29



n = 30

The shaded circles can be moved slightly keeping the optimality (the set of global minimizer points is of positive measure).

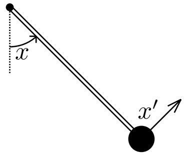
The forced damped pendulum

Consider a forced damped pendulum with these parameters:

- The mass and the length of the pendulum are both unit.
- The friction factor is $b = 0.1$. The friction depends on the speed of the pendulum.
- The degree of forcing is $\cos(t)$, where t is the time.
- The differential equation:

$$x'' = \cos(t) - 0.1x' - \sin(x),$$

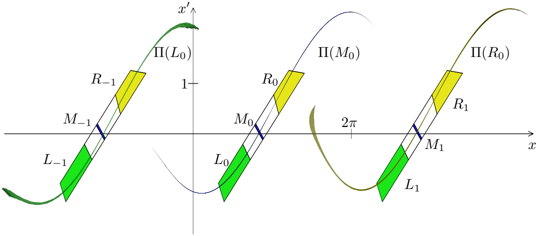
where x is an angle of the pendulum, and x' is speed of the pendulum.



Frame of proof

If we want to prove it, we must solve two subproblems:

- to show a Smale horseshoe between two Poincaré sections, and



- to show what the pendulum does during I_k.

The Wright conjecture on a delay differential equation

Conjecture

The trajectories of the delay differential equation

$$y'(t) = -\alpha \left(e^{y(t-1)} - 1 \right)$$

converge to zero for $1.5 \leq \alpha \leq \pi/2$.

Citations

"My methods, at the cost of considerable elaboration, can be used to extend this result to $\alpha \leq \frac{37}{24}$ and, probably to $\alpha < 1.567...$ (compare with $\frac{\pi}{2} = 1.570796...$). But the work becomes so heavy for the last step that I have not completed it."

"... the authors using a combination of analytic and computational techniques, prove partially the long-standing Wright's conjecture ..."

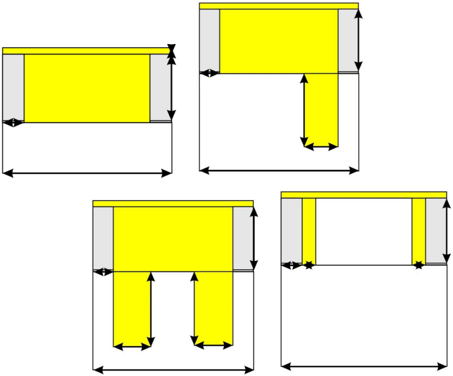
The problem is closely related to the series of

$$y_1(x) = -1 - \sum_{n=1}^{\infty} c_n e^{n\alpha x}, \qquad y_2(x) = -1 - \sum_{n=1}^{\infty} (-1)^n c_n e^{n\alpha x}$$

with $c_1 = 1$, $(n-1)c_n = \sum_{m=1}^{n-1} c_m c_n m e^{-m\alpha}$.

$(1.5706 - 1.5)/(\pi/2 - 1.5) = 99.723\%$

Detector types: NCAI, NCDAI, NCDDAI, NCTAI



The light comes into the (microns size) detectors from below, in several angles.

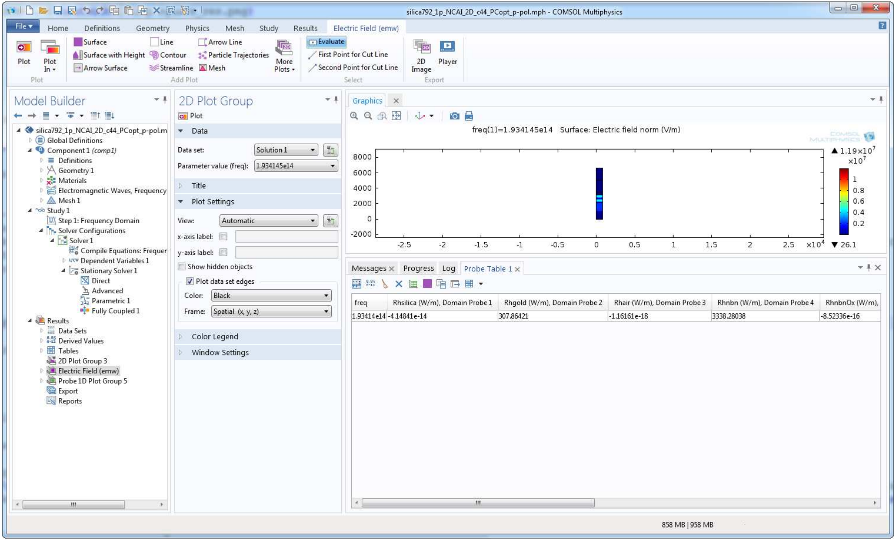
Motivation

- Even a slight improvement on the recognition rate of diverse photons can be very important in military application.
- The parameters of the optimal structure of the detectors sensing quantum information holding infrared one-photons depend much on the wave length.
- 3-4 plasmonic structures have relevant properties for controlling the optic properties of integrated detectors.
- We encounter many diverse optimization problems studying these integrated structures

Comsol

- COMSOL is a Java based Matlab tool for quantum physics simulation
- The RF module of the COMSOL is a well accepted tool for investigating the sensitivity of detectors in nanophotonics.
- It is cooperating well with other platforms such as Matlab, Java, Excel etc.
- Also a server-client type websocket based communication is available between the applications and the simulation engine.

COMSOL control page



Comsol LiveLink (MATLAB)

```
addpath '/n/comsol/COMSOL44/mli';
import com.comsol.model.*
import com.comsol.model.util.*
mphstart(pcName,2036);
model=mphload(mphFileName);
model.sol('sol1').run;
mphmean(model,'var4',1);
```

Comsol LiveLink (JAVA)

```
System.setProperty("cs.root",
      "C:\\Program Files\\COMSOL\\COMSOL44");
ModelUtil.initStandalone(false);
ModelUtil.connect(pcName, 2036);
model = ModelUtil.loadCopy("Model",mphFileName);
model.sol("sol1").run();
model.result().table("tbl1").getTableData(true)[0][0]
```

The global optimization problem

$$\min f(x)$$

$$g(x) \leq 0,$$
$$h(x) = 0,$$
$$a \leq x \leq b,$$

where $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}$, $g(x), h(x) : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are two times continuously differentiable real functions, $a, b \in \mathbb{R}^n$. These are in general nonlinear, and often given only by a subroutine, not by expression.

Optimization problems

- What is the maximal detection rate for a given type detector? The available values in the literature are around 93%.
- What is the maximal detection rate for other property (e.g. different polarization) photons? The information carrying type photon should be absorbed the most – compared to other type photons.
- Can we improve the absorption rate without a major decrease in the detection rate?

A clustering multistart global optimization algorithm: GLOBAL

It is a multistart procedure, that applies local search methods for finding local minimizer points.

Two local search algorithms can be selected: the first is UNIRANDI, a direct search technique. It is a random walk method, that does not assume differentiability of the objective function, and requires only a subroutine for the calculation of the objective function value.

The other method is BFGS, that is readily available in Matlab (even without the optimization packages). This is assumes a smooth objective function, although requires again only a subroutine for the calculation of the objective function value.

The framework multistart algorithm assumes that the relative size of the region of attraction of the global minimizer point(s) is not negligible, i.e. say larger than 0.00001.

The algorithm

Step 1: Draw N points with uniform distribution in X, and add them to the current cumulative sample C. Construct the transformed sample T by taking the γ percent of the points in C with the lowest function value.

Step 2: Apply the clustering procedure to T one by one. If all points of T can be assigned to an existing cluster, go to Step 4

Step 3: Apply the local search procedure to the points in T not yet clustered. Repeat Step 3 until every point has been assigned to a cluster.

Step 4: If a new local minimizer has been found, go to Step 1.

Step 5: Determine the smallest local minimum value found, and stop.

Java version of GLOBAL

- The code was earlier available in Fortran, C, and Matlab.
- The reasons for the Java implementation:
  - More efficient optimization, an object oriented version is also welcome.
  - This language supports our parallelization aims well, both the multi-machine and the multi-core versions (CUDA was neglected in the first row).
  - Fits well our present problems.

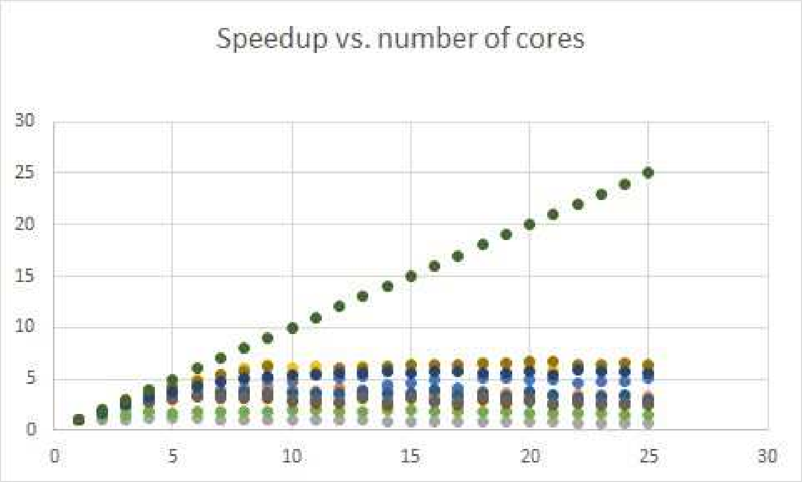
Object oriented GLOBAL

- GLOBAL has three main components: sample generation, clustering, and local minimization.
- All the three are equipped with an interface class
- All of them can be applied in a stand-alone way, other combinations can be formed.
- They have build methods.

Parallelization results: runtime (ms.) vs. # cores

	Number of cores			
Name of problem	1	2	3	4
bra	484.5	288.5	218.6	183.0
eas	865.5	521.1	381.4	312.0
gpr	96.2	96.3	86.7	86.1
hm3	12467.7	6396.3	4263.4	3587.6
hm6	29665.8	14688.0	10451.9	8752.6
ros2	560.9	412.7	351.6	315.2
ros3	4706.4	2904.3	1908.3	1624.6
sh5	2180.2	1149.2	889.8	774.7
sh7	2352.5	1247.3	946.5	799.0
shu	2835.7	1489.0	1017.8	816.9
zakh5	2535.7	1372.6	973.7	767.0

Sublinear speedup



Efficiency results

NCDAI

Optimization method	Period (nm)	Absorbtion
Original (792, optA)	792.46	78.22%
GLOBAL (792, optC)	792.46	79.52%

NCDDAI

Optimization method	Period (nm)	Absorbtion
Original (792, optA)	792.46	86.84%
GLOBAL (792, optC)	792.46	89.90%

NCTAI

Optimization method	Period (nm)	Absorbtion
Original (792, optA)	792.46	89.92%
GLOBAL (792, optC)	792.46	92.07%
GLOBAL (500-600, optG)	600.00	94.49%
GLOBAL (1000-1100, optI)	1056.24	95.05%

Contrast results

System	Original	Optimized	90%	93%
NCAI	146.8800	219.9831	219.9679	199.461
NDAI	1.3420E+03	6.0424E+10	6.3289E+05	3.2113E+03
NCDDAI	1.9468E+03	4.6787E+11	2.1718E+08	1.9135E+07
NCTAI	49.9800	366.4346	69.8521	69.9753

The applied phantom

We used the following simple model for the computational tests:

The tumorous tissue to be treated is a sphere with center at the origin, and radius 2.5.

The tissues to be saved from the radiation are outside the sphere, and a vertical cylinder around the axe z with a radius of 1.

The radiation dose is assumed to be the same within each cube of side length 5/30, and the dose is calculated in its center. Only those cubes were considered that belong exclusively to one of the mentioned two tissues.

A surgical operation design is regarded to be acceptable, if at least 90% the tumorous tissue obtains radiation dose of 110 units, and at least 90% of the tissues to be saved gets at most 90 units of radiation.

The optimization problem

Let $S_{in} = \{(x,y,z) \mid x^2 + y^2 + z^2 \leq 2.5^2, z^2 \geq 1\}$ be the tissue to be treated, and $S_{out} = [-3,3]^3 \backslash S_{in}$ that to be saved. Then the optimization problem is

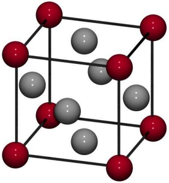
$$\max_{x_i, y_i, z_i \in [-3,3]^3} \frac{(\mathrm{vol}(\{s \in S_{in} \mid D(s) \geq 110\}) + \mathrm{vol}(\{s \in S_{out} \mid D(s) \leq 90\}))}{(\mathrm{vol}(S_{in}) + \mathrm{vol}(S_{out}))},$$

where $D(s)$ is the cumulative dose obtained at point s from all seeds, and $\mathrm{vol}(S)$ is the volume of the set S.

The function $D(s)$ that calculates the summed up dose from the point-like radiation sources, is proportional with the reciprocal of the square of the distance to the seed.

Face centered cubic lattice

The least dense covering of space by spheres is unknown. The best mesh covering is the face centered cubic lattice:



The idea is to generate good starting points for the optimization by finding good step length and shifts of our mesh in such a way, that the objective function value for those mesh points that are inside of the target region is favorable.

The best found face centered cubic mesh

500 sample points per iteration, 16 significant digits, at most 5 local minima allowed. The result after 7 minutes CPU time (87 seeds):

```
>> [x0,f0,NC,NFE] = GLOBAL(FUN, LB, UB, OPTS);
*** TOO MANY CLUSTERS ***
NORMAL TERMINATION AFTER 5015 FUNCTION EVALUATIONS
LOCAL MINIMUM FOUND: 4
F0 =
-0.8603
-0.8589
-0.8575
-0.8575
X0 =
1.2473 1.2297 1.2420 1.2102
0.0049 0.2793 0.0133 0.0853
0.2212 0.0425 0.4352 0.3209

0.4074 0.1400 0.1298 0.1335
```

72% of the target region and closely 100% of the outside region fulfill the dose conditions. The result has the 86.03% summed quality.

References

T. Csendes, L. Pál, J.O.H. Sendín, and J.R. Banga: The GLOBAL Optimization Method Revisited. Optimization Letters 2(2008) 445-454.

L. Pál, T. Csendes, M.Cs. Markót, and A. Neumaier: Black-box optimization benchmarking of the GLOBAL method. Evolutionary Computation 20(2012) 609-639.

T. Csendes, B.M. Garay, and B. Bánhelyi: A verified optimization technique to locate chaotic regions of Hénon systems. J. of Global Optimization 35(2006) 145-160.

P.G. Szabó, M.Cs. Markót, T. Csendes, E. Specht, L.G. Casado, and I. García: New Approaches to Circle Packing in a Square – With Program Codes Springer, Berlin, 2007.

References 2

M. Csete, G. Szekeres, A. Szenes, B. Bánhelyi, T. Csendes, and G. Szabó: Optimized Superconducting Nanowire Single Photon Detectors to Maximize Absorptance. Progress In Electromagnetics Research B, Vol. 65, 81-108, 2016, http://www.jpier.org/PIERB/pierb65/06.15090904.pdf

A. Szenes, B. Bánhelyi, L.Zs. Szabó, G. Szabó, T. Csendes, and M. Csete: Enhancing diamond color center fluorescence via optimized plasmonic nanorod configuration Plasmonics 11:(6), 2016, Paper 10.1007/s11468-016-0384-1

M Csete, A Szenes, D Maráczi, B Bánhelyi, T Csendes, G Szabó: Plasmonic structure integrated single-photon detectors optimized to maximize polarization contrast IEEE Photonics Journal 1(2016): Paper 1609.04850.

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