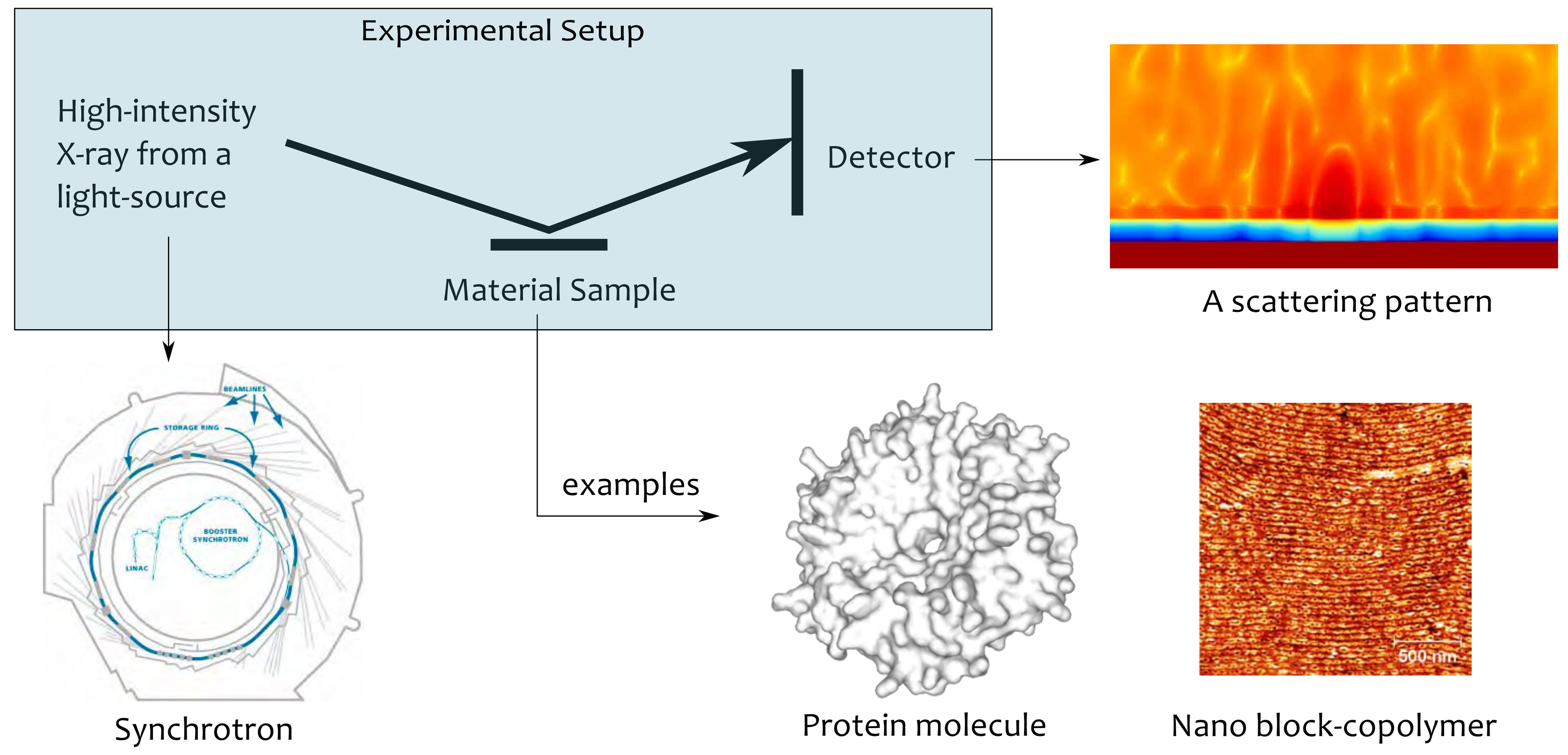
Abstract

We consider the inverse modeling problem of recovering nanostructures from X-ray scattering data obtained through experiments at synchrotrons. This has been a primary bottleneck problem in such data analysis. X-ray scattering based extraction of structural information from material samples is an important tool for the characterization of macromolecules and nano-particle systems applicable to numerous applications such as design of energy-relevant nano-devices. We exploit massive parallelism available in clusters of graphics processors to gain efficiency in the reconstruction process. To solve this numerical optimization problem, here we show the application of the stochastic algorithms of Particle Swarm Optimization (PSO) in a massively parallel fashion. We develop high-performance codes for various flavors of the PSO class of algorithms and analyze their performance with respect to the application at hand. We also briefly show the use of two other optimization methods as solutions.

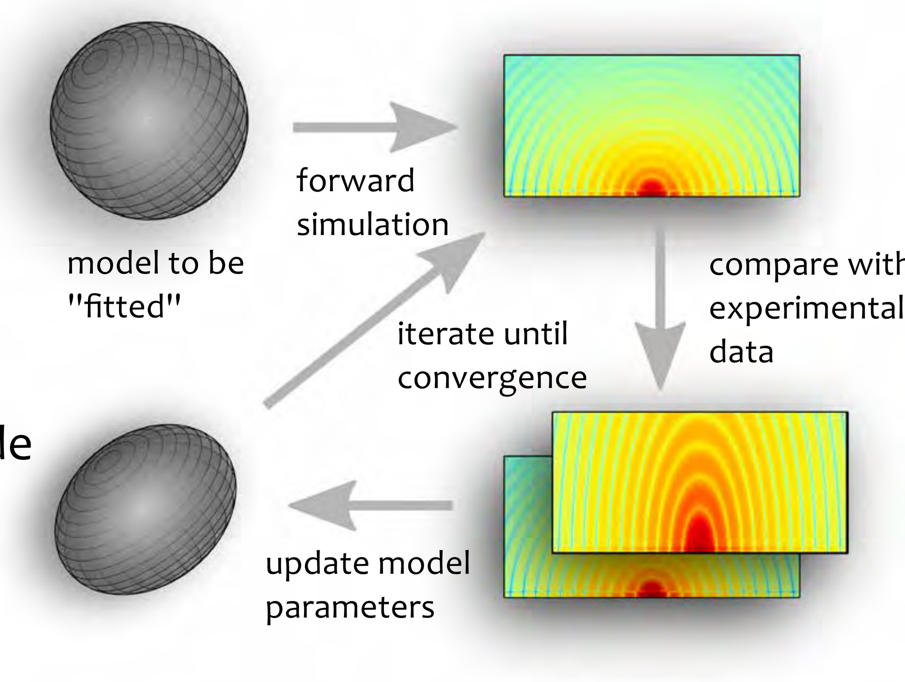
X-Ray Scattering

X-ray scattering comes in various flavors, and here we focus on data obtained using methods from the class of **grazing incidence X-ray scattering**, such as GISAXS (small-angle) and GIWAXS (wide-angle).



Inverse Modeling

The process of recovering physical properties using experimentally measured data is commonly known as inverse modeling and appears in numerous applications. This generally involves minimization of an objective function value iteratively until convergence w.r.t. a set of parameters to be "fitted", or recovered. In our case, this function is a computationally intensive forward simulation of the scattering patterns, which we developed previously, and has been implemented as a massively parallel high-perfomance code utilizing Nvidia graphics processors (GPUs) for kernel computations [1, 2, 3].



Recovering Nanostructures from X-Ray Scattering Data

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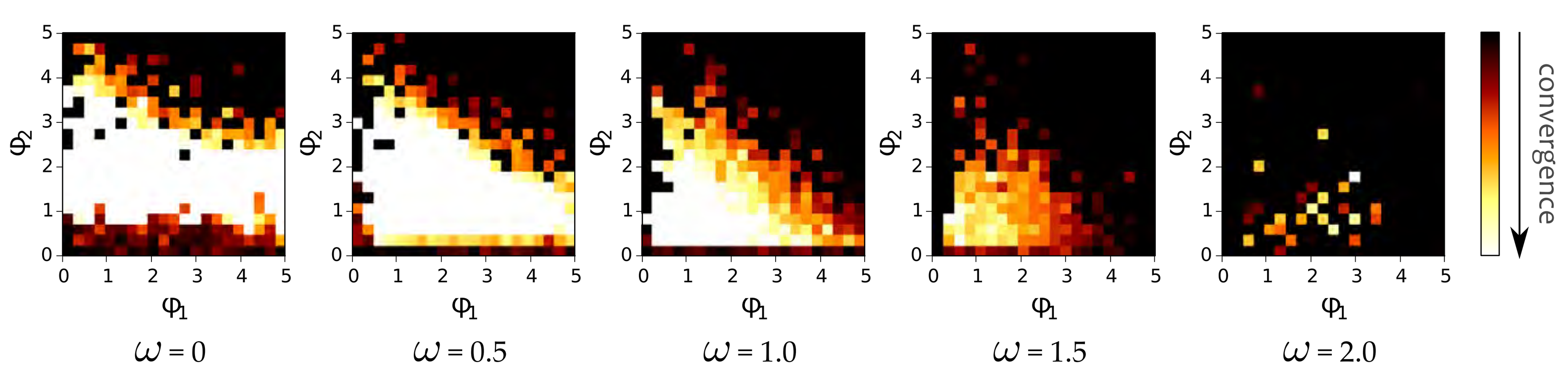
Particle Swarm Optimization

The particle swarm optimization (PSO) method is a stochastic process involving large number of "agents" which move around and explore the parameter search space. For agent *i*, its "velocity" is determined as:

$$\underbrace{\vec{v_i} \leftarrow \omega}_{\text{inertia coefficient}}\vec{v_i} + (\underbrace{\vec{b_i}}_{\text{local best position}} - \vec{x_i})\vec{r_1}\phi_1 + (\underbrace{\vec{b_g}}_{\text{global best position}} - \vec{x_i})\vec{r_2}\phi_2$$

(force coefficients: ϕ_1, ϕ_2)

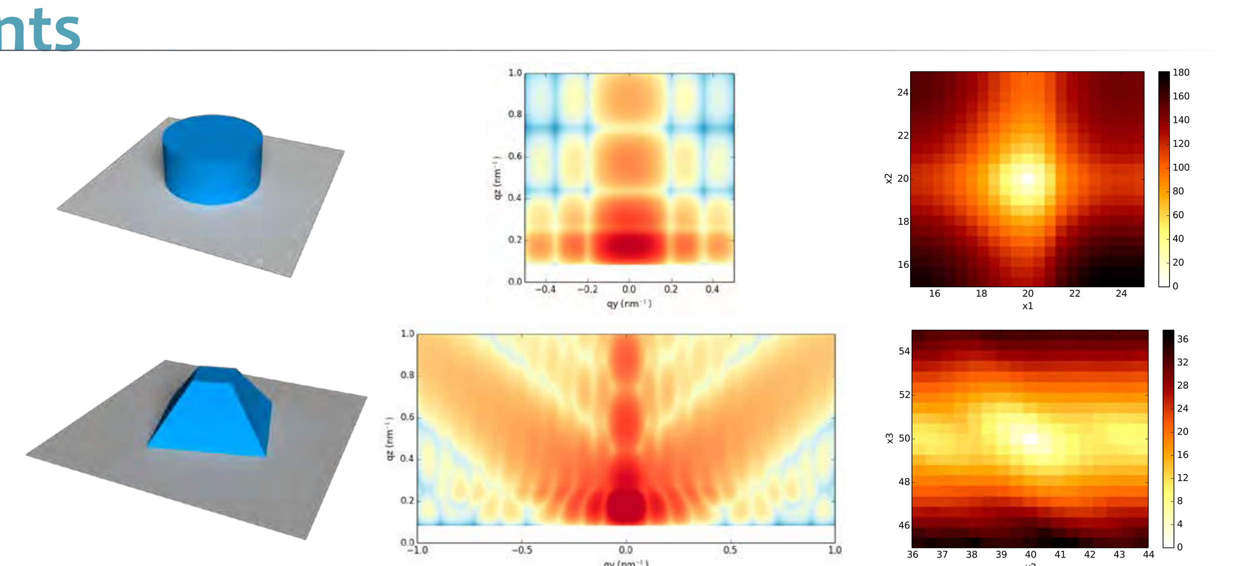
The coefficients, inertia and force, determine how viscous is the search space, and how attractive are the forces towards local and global best found positions, respectively. They affect convergence as follows:



Experiments

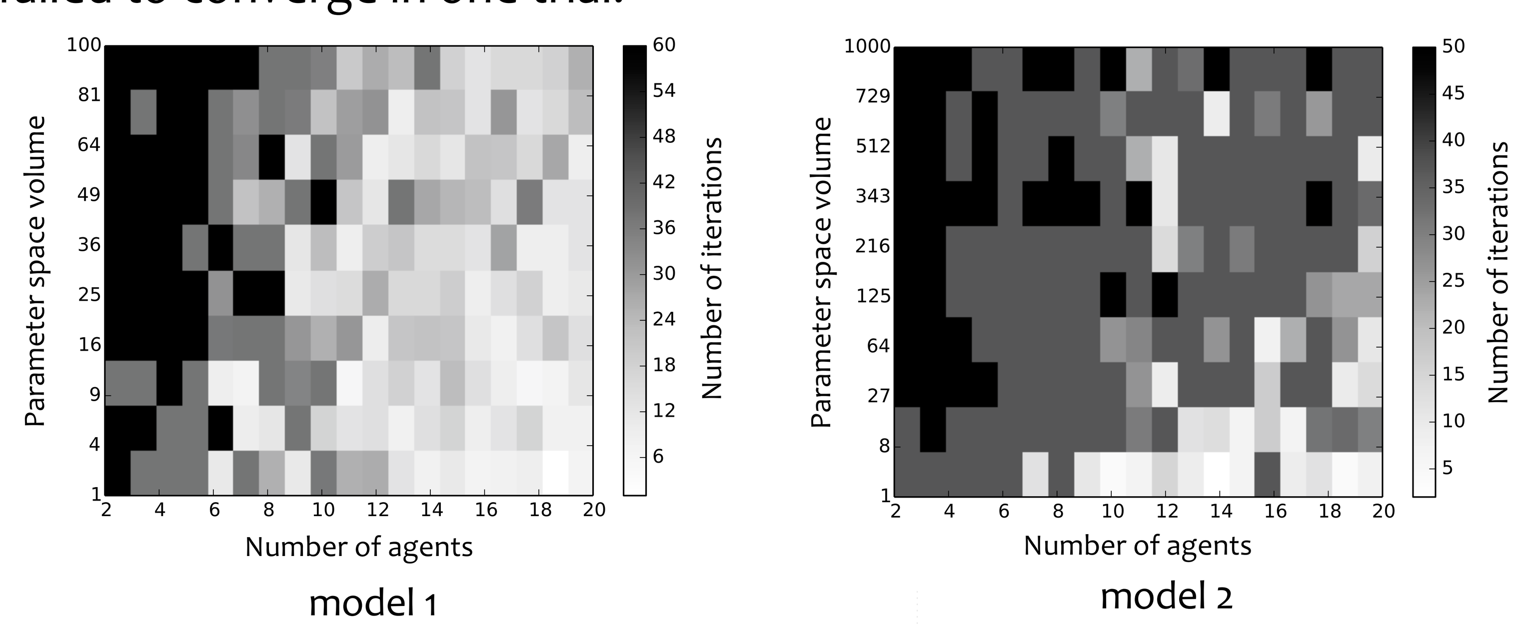
Consider two models to fit:

1. Cylinder (2 parameters)
2. Truncated Pyramid (3 parameters)



Inverse Modeling with PSO

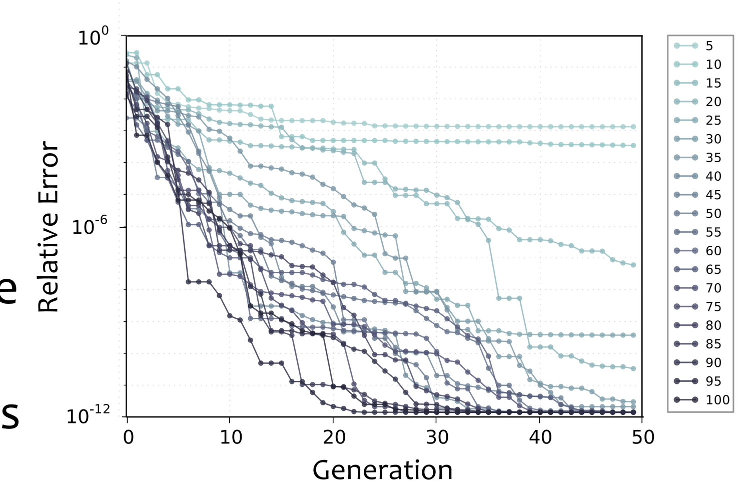
The results for convergence for the two models are shown below. These are shown with respect to varying number of agents, and varying volume of the search space. Black spots represent those configurations which failed to converge in one trial.

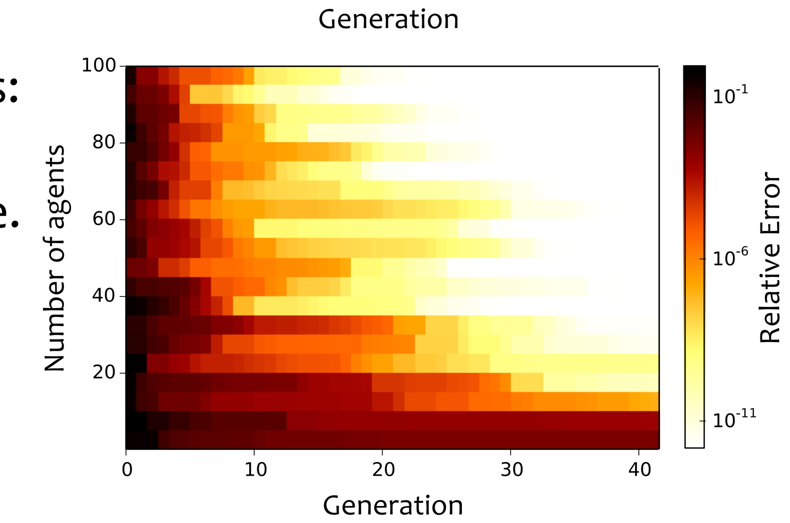


What is better for convergence: fewer agents run for a long time, or, a larger number of agents run for short time?

The plots on the right demonstrate the answer to this question. Each run was performed on a total of 100 GPU nodes in parallel. There are three main advantages of large number of agents:

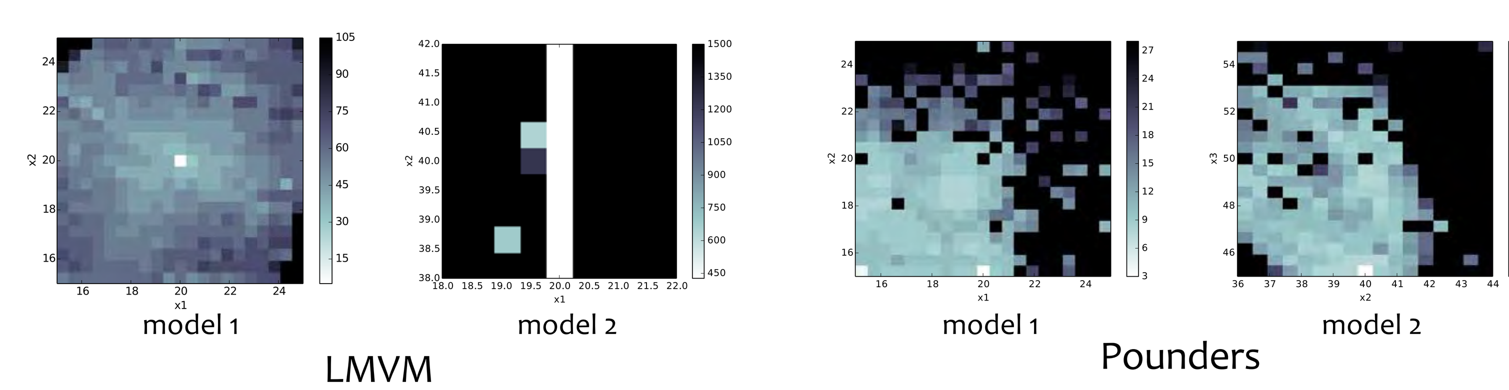
1. **Guarantee:** It provides a higher probability of reaching convergence.
2. **Efficiency:** Available massive parallelism can be effectively exploited.
3. **Speed:** Convergence is reached in fewer generations, i.e. faster.





Conclusions

For the problem of recovering nanostructures from X-ray scattering patterns, the method of particle swarm optimization has proven to be highly effective. The convergence maps for two other sophisticated methods, a quasi-Newton method (LMVM) and a derivative-free trust-region based mothod (Pounders), are shown below w.r.t. initial guess. Although both methods perform well with the first model, they, LMVM in particular, are less effective for the second model. Compared to these, PSO has an additional advantage of not requiring an initial guess.



Acknowledgements

The authors thank Nvidia for providing us with several GPU cards which were used as the primary development platform for this work.
This work was supported by the Director, Office of Science, U.S. Department of Energy (DoE) under contract no. DE-AC02-05CH11231. This work was also supported by DoE Early Career Research Program grant awarded to Alexander Hexemer.
This research used resources of the National Energy Research Scientic Computing Center (NERSC), which is supported by the Office of Science, U.S. DoE, under contract no. DE-AC02-05CH11231, and of the Oak Ridge Leadership Computing Facility (OLCF), which is supported by the Office of Science, U.S.

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