Memetic Phase Retrieval for Coherent Diffraction Imaging

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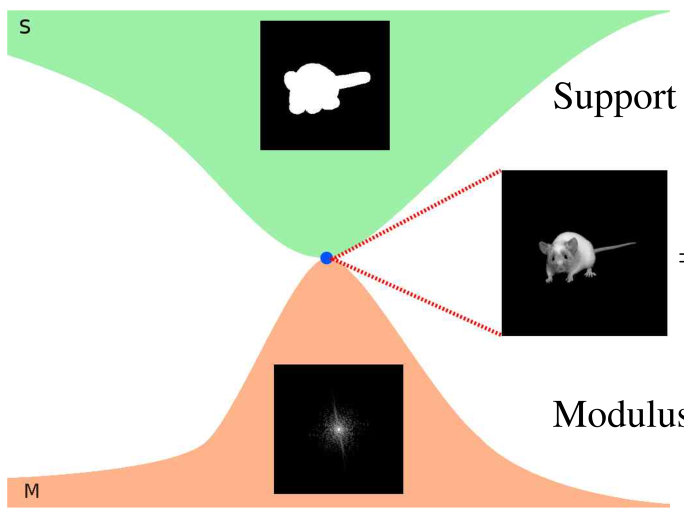
NOXSS The Free-Electron Laser for Ultrafast Imaging at the Nanoscale

Coherent Diffraction Imaging is a lensless technique that allows imaging of matter at a spatial resolution not limited by lens aberrations. This technique exploits the measured diffraction pattern of a coherent beam scattered by periodic and non-periodic objects to retrieve spatial information. The diffracted intensity, for weak-scattering objects, is proportional to the modulus of the Fourier Transform of the object scattering function. Any phase information, needed to retrieve its scattering function has to be retrieved by means of suitable algorithms [1]. Here we present a new approach, called Memetic Phase Retrieval [2], to face the phase problem, which exploits the synergy of deterministic and stochastic optimization methods. Results show that our method outperforms standard approaches, representing a new powerful tool for the study of matter.

The *phase retrieval problem* in Coherent Diffraction Imaging

Experimental data	Scope	Problem
$I(q) = \lvert\mathcal{F}[\rho](q)\rvert^2$	$\rho(x) = \mathcal{F}^{-1}[\sqrt{I(q)}\exp^{i\phi(q)}]$	Retrieve $\phi(q)$



Ideal case

Support constraint: $S = \{\rho(x) : \rho(x) = \Pi(x)\rho(x)\}$

$\Rightarrow \rho_{\text{sol}}(x) = S \cap M$

Modulus constraint: $M = \{\rho(x) : \lvert\mathcal{F}[\rho](q)\rvert = \sqrt{I(q)}\}$

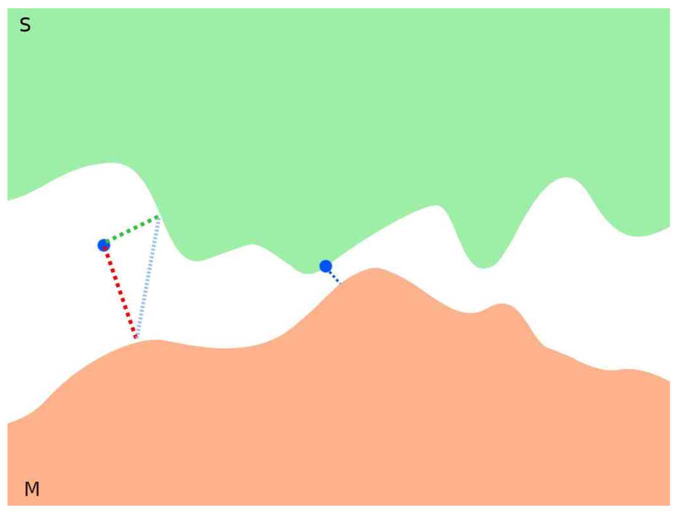
Real data

- Noise
- Partial knowledge on $I(q)$
- Lack of information on the support $\Pi(x)$

$$\Downarrow$$

$$\rho_{\text{sol}}(x) = \min_{\rho(x)} D[P_m\rho(x), P_s\rho(x)]$$

with $P_m\rho(x) = \mathcal{F}^{-1}[\sqrt{I(q)}e^{i\arg(\hat{\rho})}](x)$, $P_s\rho(x) = \Pi(x)\rho(x)$



The *phase retrieval problem* is an **optimization problem** for the *distance* D between the two sets, which can be intended as the *error* of the reconstruction.

Standard Approaches

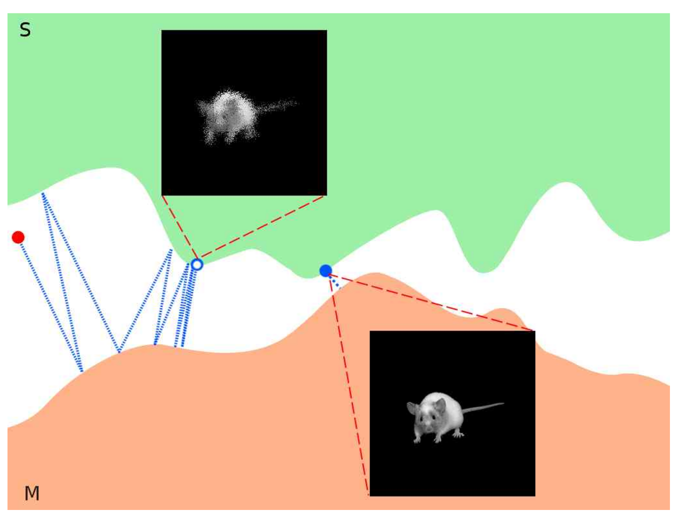
Standard iterative methods [3] are, in most cases, based on the cyclical imposition of constraints:

$$\rho_{i+1}(x) = P_s P_m \rho_i(x)$$

$$\Downarrow$$

Stagnation in local minima

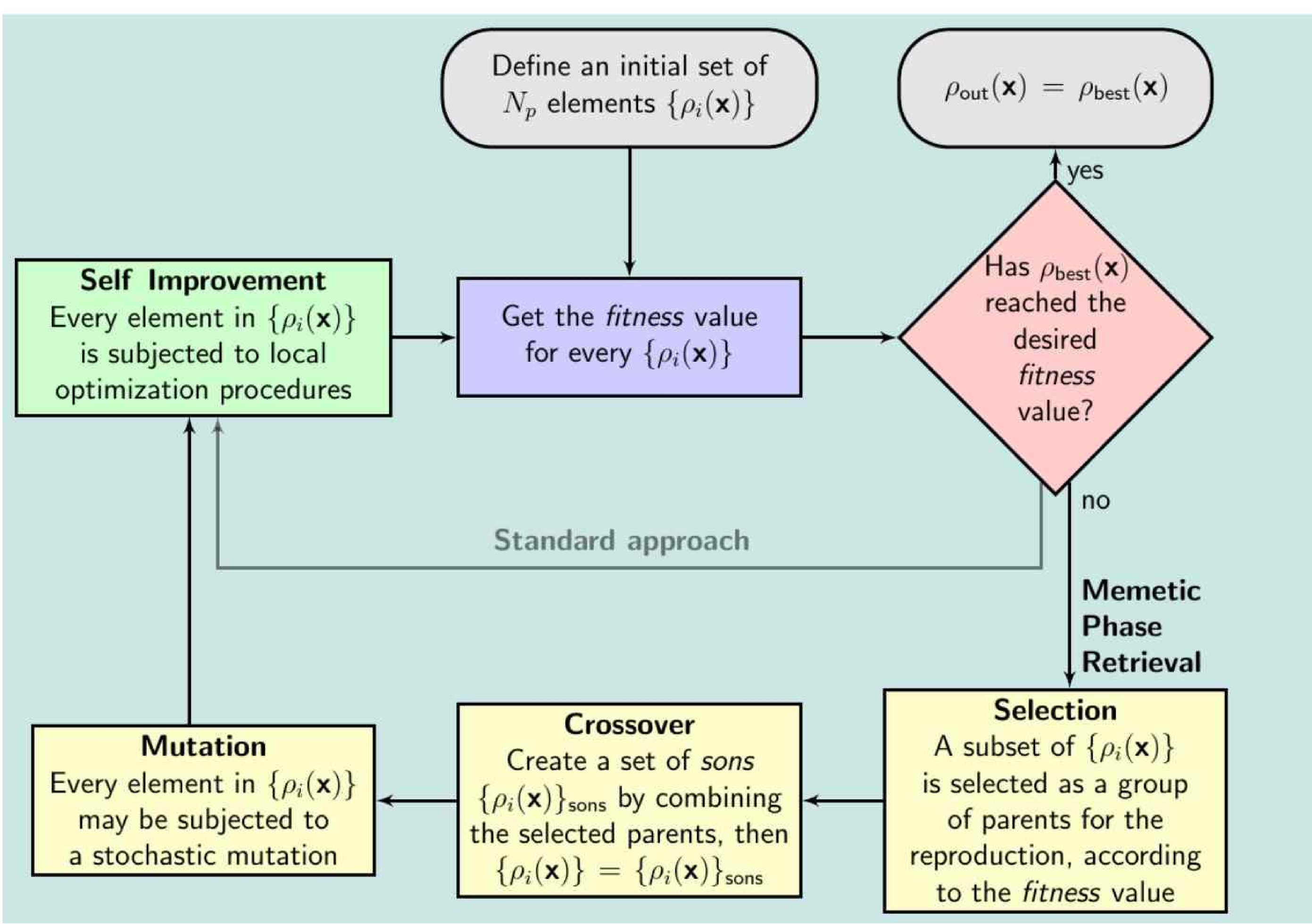
Standard strategy: carry out many parallel retrieval processes from different starting points and choose the ones with the lowest error



Memetic Phase Retrieval

A Memetic Algorithm [4] is a particular Genetic Algorithm [5], which is a stochastic optimization method that imitates the *Natural Evolution* of a population, exploiting the processes of **Mutation**, **Selection** and **Crossover**, acting on a set of candidate solutions, in order to optimize a *fitness* function. Memetic Algorithms are characterized by a further step, called **Self Improvement**, where every candidate solution is subjected to a local optimization of the *fitness* function.

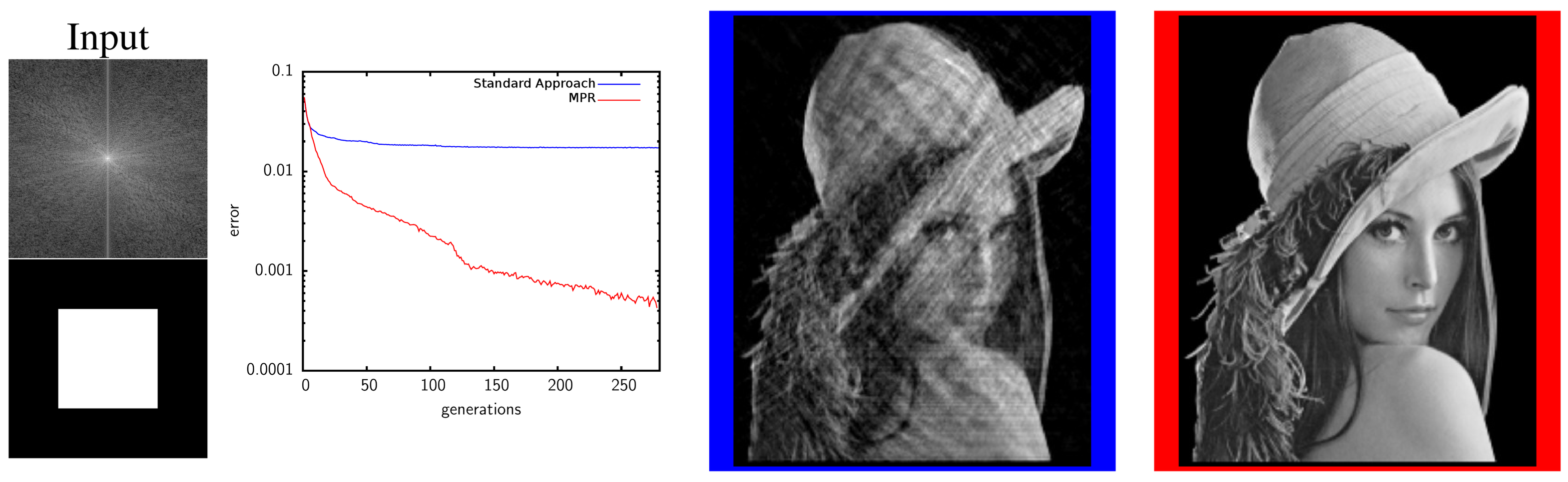
In our Memetic Phase Retrieval (MPR) approach [2], we induce the *genetic dynamic* on a set of densities $\{\rho_i(x)\}_{i...N_{\text{pop}}}$ which represents N_{pop} candidate solutions to the *phase problem*. The **Self Improvement** step is carried out by standard iterative methods based on projections. It's worth noting that the standard approach, consisting in many parallel reconstruction processes, can be intended as MPR without the genetic steps, as depicted in the diagram below.



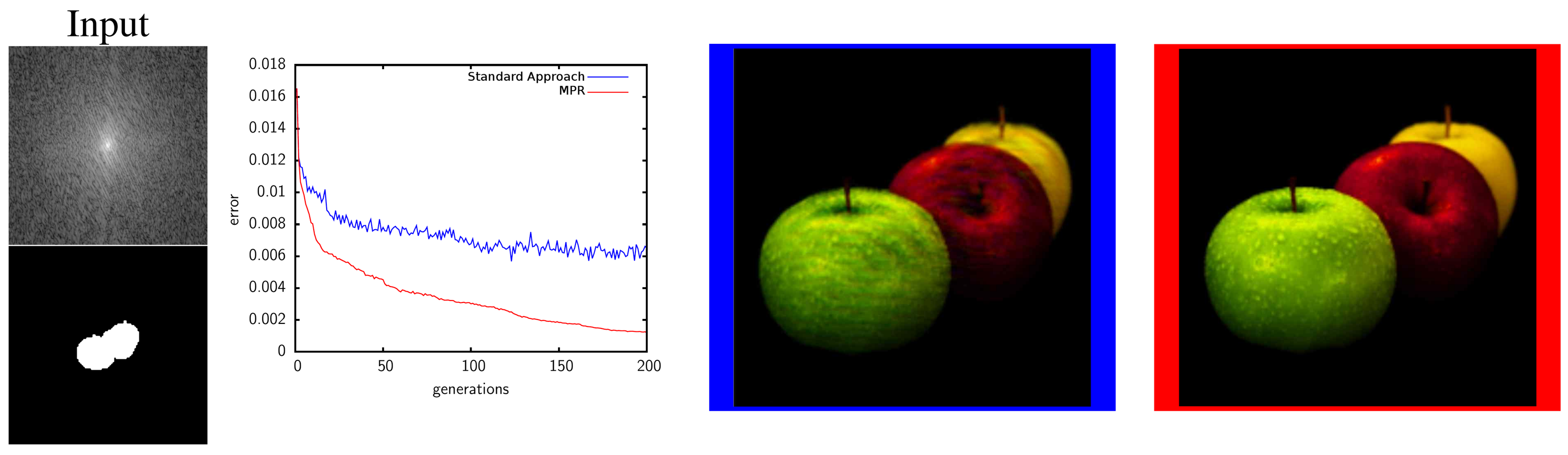
[1]Experimental data: courtesy of Yuriy Chushkin, ESRF.
[2]For more information, see Ref. [2]

Test on Simulated Data

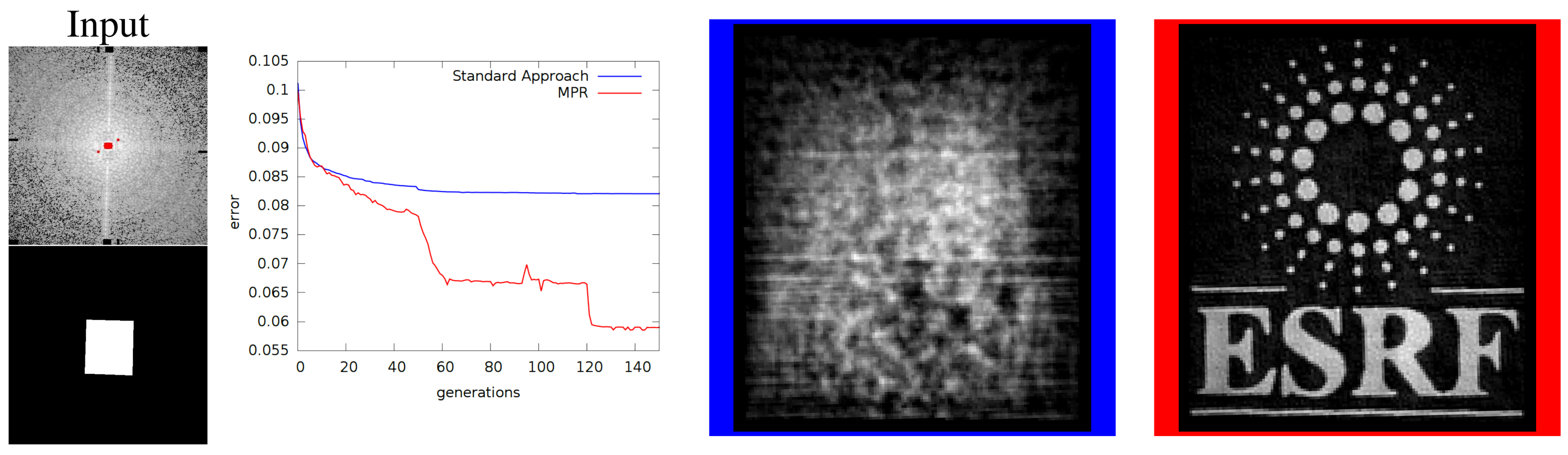
Real-valued phasing test.



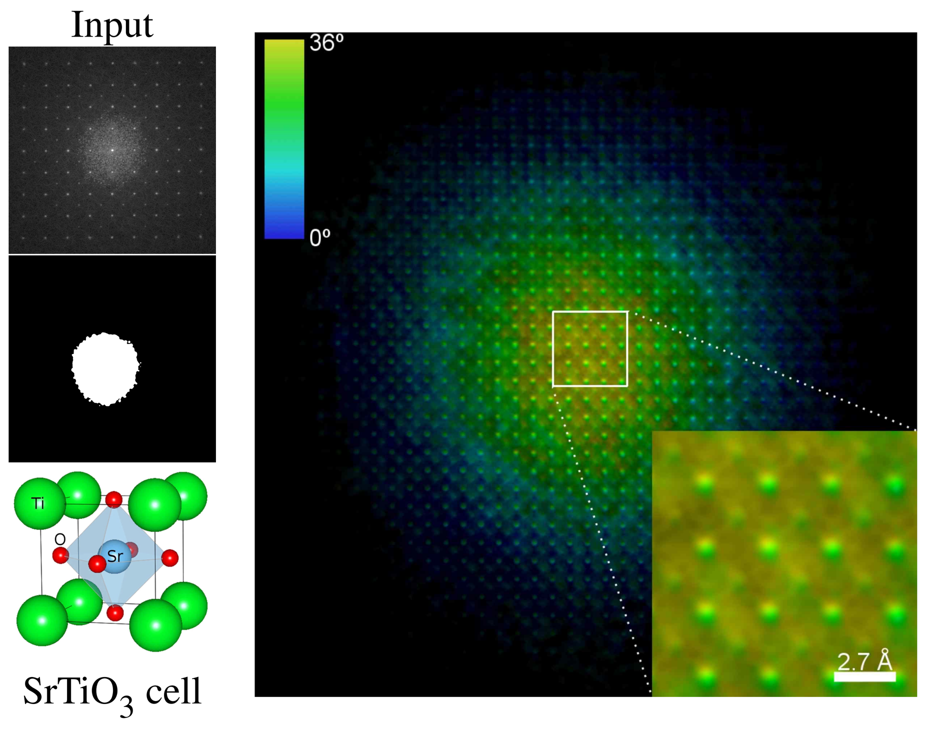
Complex-valued phasing test. The hue of the retrieved scattering function represents the phase, while the lightness is proportional to the retrieved module.



Test on X-Ray Diffraction Data[1]

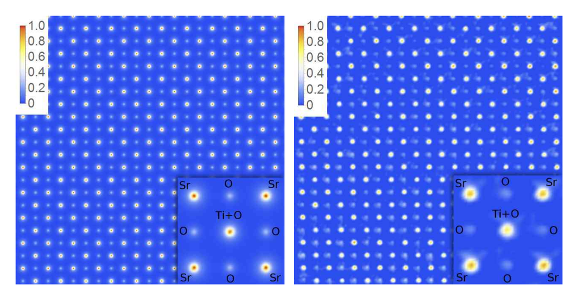


Results on Electron Diffraction Data[2]



$SrTiO_3$ cell

Scope: retrieve quantitative spatial information of a $SrTiO_3$ nanocrystal.



Theoretical (left) and retrieved (right) projected potential of the $SrTiO_3$ nanocrystal.

Comments

- Memetic Phase Retrieval reaches an error value lower than the Standard approach, with the same computational cost and same initial conditions

  $\Rightarrow$ **better exploitation of information/resources, results less dependent on initial conditions**
- Our approach is based on standard algorithms

  $\Rightarrow$ **Every improvement in standard iterative methodologies can be easly included in MPR**
- MPR can be easily tuned to optimize any *fitness* function

  $\Rightarrow$ **better identification of the optimal solution**
- Our approach requires high-level computational resources

  $\Rightarrow$ **Execution on High Performance Computing (HPC) hardware is needed**

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