Memetic Phase Retrieval and HPC for the Imaging of Matter at Atomic Resolution

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Abstract. Memetic Algorithms represent one of the most promising implementation of Evolutionary Algorithms. Their strength resides in the ability to exploit stochastic and deterministic optimization methods at the same time. A Memetic Algorithm has been applied to the *phase retrieval problem* in the field of Coherent Diffraction Imaging, called Memetic Phase Retrieval; it represents a significant improvement in the imaging of matter via coherent diffraction experiments. Memetic Phase Retrieval requires the latest High Performance Computing resources, due to the high dimensionality of the problem and the involvement of the Fourier Transform, requiring an efficient parallel implementation able to fully exploit multi-core and multi-node hardware. The implementation of Memetic Phase Retrieval, which exploits the hybrid OpenMP/MPI parallel programming paradigm, along with MPI Remote Memory Access communications, is presented. Its scaling performances on the recent Intel's Knights Landing hardware are shown.

Keywords. Memetic Algorithms, Phase Retrieval Problem, Coherent Diffraction Imaging, Hybrid Parallelization, Remote Memory Acces, Intel Knights Landing.

1. Introduction

Coherent Diffraction Imaging [1,2] (CDI) is a lensless technique that allows imaging of matter at a spatial resolution not limited by lens aberrations, opening the opportunity to have a look inside matter up to atomic resolution. CDI experiments can be performed where coherent radiation sources are available, for example *Synchrotrons* [3] and *Transmission Electron Microscopes* [4]. CDI is an increasingly growing technique, also thanks to the recent availability of Free Electron Laser facilities [5] like FERMI (Italy), FLASH (Germany), SACLA (Japan) the European X-ray Free Electron Laser[2] (Eu-XFEL).

This technique exploits the measured two-dimensional[3] diffraction pattern I_{ij} of a coherent beam scattered by a sample, in order to retrieve its spatial distribution ρ_{kl}. In the so-called *Fraunhofer diffraction* regime, the experimental diffraction data I_{ij} is the square modulus of the Fourier Transform (FT) of ρ_{kl}, that is $|\mathscr{F}[\rho]_{ij}|^2 = I_{ij}$. In order to retrieve the spatial density ρ_{kl} from the measured data I_{ij}, which are both $N \times N$ matrices,

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[2]For more information visit: `www.xfel.eu`
[3]CDI is performed both in two and three dimensions. In this work we focus on the more common two-dimensional case.