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Fitting of interatomic potentials without using force information: a parallel particle swarm optimization algorithm DIEGO GONZÁLEZ, SERGIO DAVIS, Grupo de Nanomateriales, Departamento de Fisica, Facultad de Ciencias, Universidad de Chile — In this work we present a methodology for fitting interatomic potentials to *ab initio* data, using the particle swarm optimization (PSO) algorithm. The objective function to be minimized is the total prediction error in the energies for the configurations provided, thus the algorithm does not require any information besides the atomic positions for each configuration and their corresponding ab initio energies. In particular it does not require the atomic forces, as in other fitting procedures such as force matching methods. Our procedure has been tested by fitting both pair potentials and embedded atom potentials, up to a prediction error of the order of 10^{-4} eV/atom, using only 10 different configurations. The implementation code is parallelized using message passing interface (MPI) libraries.

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