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# Fitting of interatomic potentials without forces: A parallel particle swarm optimization algorithm

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ABSTRACT

We present a methodology for fitting interatomic potentials to ab initio data, using the particle swarm optimization (PSO) algorithm, needing only a set of positions and energies as input. The prediction error of energies associated with the fitted parameters can be close to 1 meV/atom or lower, for reference energies having a standard deviation of about 0.5 eV/atom. We tested our method by fitting a Sutton–Chen potential for copper from *ab initio* data, which is able to recover structural and dynamical properties, and obtain a better agreement of the predicted melting point versus the experimental value, as compared to the prediction of the standard Sutton–Chen parameters.



## 1. Introduction

In Condensed Matter Physics, the task of obtaining different mechanical properties of materials, simulated atomistically with a large number of atoms under *ab initio* methods, is an almost prohibitive one, in terms of computational effort with the current computer architectures. It might even at times be impossible. Because of this, producing a "classical" interatomic potential as a substitute for the genuine quantum-mechanical interaction of the particles is highly desirable. The usual procedure is to fit some empirical interatomic potential function, depending on $N$ parameters, requiring either agreement with certain macroscopic properties (structural, thermodynamical, etc.) or simply agreement between the predicted and observed energies and atomic forces. A standard algorithm based on force information is the force matching method [1,2].

In this work we present a methodology for fitting interatomic potentials to *ab initio* data, using the particle swarm optimization (PSO) algorithm [3]. 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.

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## 2. Interatomic potential models

We implemented two families of interatomic potentials, pair potentials and embedded atom potentials. Among the former, we tested the well-known Lennard-Jones potential [4], given by

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \tag{1}$$

and the 6-parameters "generic" potential as implemented in Moldy [5],

$$V(r) = A\exp(-Br) + \frac{C}{r}^{12} - \frac{D}{r}^{4} - \frac{E}{r}^{6} - \frac{F}{r}^{8}. \tag{2}$$

From the family of embedded atom potentials [6], having the general form

$$E_i = \frac{1}{2}\sum_{j\neq i}\phi(|\mathbf{r}_i - \mathbf{r}_j|) + F\left(\sum_{j\neq i}\psi(|\mathbf{r}_i - \mathbf{r}_j|)\right) \tag{3}$$

we implemented the Sutton–Chen potential, where the pair functions and the embedding function are given by

$$F(\rho) = \epsilon C\sqrt{\rho} \tag{4}$$

$$\phi(r) = \epsilon(a/r)^n \tag{5}$$

$$\psi(r) = (a/r)^m. \tag{6}$$

## 3. Particle swarm optimization

The particle swarm optimization (PSO) algorithm is based on the idea of distributing the search procedure among a large number of "agents", which act independently of each other. Each agent moves through the search space with a simple dynamics, reacting to fictitious forces drawing it towards its own *current best* solution and the *global best* solution for the whole swarm. In this way, when an agent finds a better solution than the current global best, it becomes the new global best and all the other agents react instantly, the swarm is directed towards the new solution.

For a set of $n$ particles represented by their positions $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, the velocity for the $i$th particle and the $k$th step is

$$\mathbf{v}_i^k = \omega \mathbf{v}_i^{k-1} + c_1 r_1^k (\mathbf{x}_\mathbf{B} - \mathbf{x}_i^{k-1}) + c_2 r_2^k (\mathbf{x}_\mathbf{G} - \mathbf{x}_i^{k-1}) \tag{7}$$

and the position is given by

$$\mathbf{x}_i^k = \mathbf{x}_i^{k-1} + \mathbf{v}_i^k. \tag{8}$$

We employed the following choice of PSO parameters: $\omega = 0.7$, $c_1 = 1.4$ and $c_2 = 1.4$, after a few trial convergence runs.

## 4. Implementation of the fitting algorithm

For a potential function where we wish to find the parameters $a_0, a_1, \ldots, a_m$ from a set of positions $\mathbf{r}_i^j$ and energies $E_j$ satisfying the relation

$$V(\mathbf{r}_1^j, \mathbf{r}_2^j, \ldots, \mathbf{r}_n^j; \mathbf{a}) = E_j \tag{9}$$

with

$$\mathbf{a} = (a_0, a_1, \ldots, a_m),$$

we can define an objective function which is just the total prediction squared error, of the form

$$f(\mathbf{a}) = \sum_j \left( V(\mathbf{r}_1^j, \mathbf{r}_2^j, \ldots, \mathbf{r}_n^j; \mathbf{a}) - E_j \right)^2, \tag{10}$$

and then for the set of parameters $\mathbf{a}^*$ that correctly fit the potential $V$ we have $f(\mathbf{a}^*) = 0$.

Then the problem may be solved numerically with the PSO algorithm minimizing the function $f(\mathbf{a})$.

### 4.1. Optimization of the algorithm

We have included some improvements on the PSO implementation, particular to our problem. For instance, we perturbed the swarm every time the procedure gets stuck in a minimum for $N_S$ steps ($N_S$ proportional to the number of parameters $d$ in the potential, usually $N_S = 50d$), completely randomizing their positions.

On the other hand, we exploit the fact that for several families of potentials there is a scale parameter for the interatomic distance, let us call it $\sigma$, such that the potential depends on $r$ only through $r/\sigma$. This is the case for the $\sigma$ parameter in the Lennard-Jones potentials, for the $C$, $D$, $E$, $F$ and $1/B$ parameters in the generic potential from Moldy, and also for the $a$ parameter in the Sutton–Chen variant of the embedded atom potentials. This distance scale parameter can be constrained to be between the minimum observed distance and a multiple of this value (typically 10 times), which considerably reduces the search space.

Parallelization was achieved simply by distributing the PSO particles evenly among the different processors using the message passing interface (MPI) framework, at each step sharing the global best between all processors.

## 5. Results

### 5.1. Lennard-Jones potential

In order to test the consistency of our procedure, we randomly generate [7] a set of 20 configurations and we compute their energy according to the standard Lennard-Jones parameters for argon, $\epsilon = 0.0103048$ eV and $\sigma = 3.41$ Å.

The resulting set has a standard deviation of energy of 0.41063 eV. Then, with the information of positions and energies (in a parallel run using an AMD Opteron 6272, 2.1 GHz, shared-memory machine with 64 cores and 500 PSO particles), the time needed to find the minimum prediction error was 212.6 s. We can see that the algorithm converge quickly for each parameter, recovering their exact values at 1300 steps (the prediction error reached is below $10^{-27}$ meV/atom, see Figs. 1 and 2).

### 5.2. 6-parameter generic potential

For the 6-parameters pair potential using the same set of positions and energies obtained for the previous Lennard-Jones test, the time needed to find the minimum prediction error was 3159.9 s, using the same 64-core machine and 500 PSO particles. In this case the error for the converged set of parameters falls below $8 \times 10^{-2}$ meV/atom at 9000 steps.

### 5.3. Embedded atom potential

We repeated the same approach for the embedded atom potential, this time using the standard Sutton–Chen parameters for copper, $\epsilon = 0.0123820$ eV, $a = 3.61$ Å, $n = 9$, $m = 6$ and $C = 39.432$. We used 4 configurations as input, and we stopped the minimization procedure after 193 015 steps (execution time was 23 h using the same 64-core machine as the section before, and using 800 PSO particles), when we reached a prediction error of about 0.8 meV/atom and the following fitted parameters: $\epsilon = 0.0145749$ eV, $a = 3.5834$ Å, $n = 8.82683$, $m = 5.67465$, and $C = 37.028$ (see Figs. 3 and 4).

As in this case the fitting error in energies is not negligible, we assessed the ability of the potential for reproducing atomic forces on each individual atom. We found an average error of 4.64%, where the average was taken over the individual relative (in percentage) errors for each atom. However, if we manually correct the magnitude of each force to match the correct one, the average error falls to 1.36%. This means about 3% of the total error in the forces is just a propagation of the error in reproducing the correct energy scale (the parameter $\epsilon$ in this case).

## 6. Application: an embedded atom potential for copper from *ab initio* data

In order to test our procedure on a more realist scenario and assess the quality of the fitted potentials we performed *ab initio* microcanonical molecular dynamics simulations of copper at different temperatures (covering its solid, liquid and superheated phases) but at the same room pressure (lattice constant $a = 3.61$ Å). All molecular dynamics calculations were performed using Density Functional Theory (DFT) as implemented in VASP [8]. We used Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) pseudopotentials [9] with an energy cutoff of 204.9 eV and $k$-point expansion around the $\Gamma$ point only.

From these simulations, we generated 13 229 different atomic configurations with their respective energies, mixed from solid ($T = 738$ K), liquid ($T = 2716$ K) and superheated state ($T = 2058$ K) simulations. Among them we chose a subset of 30 with maximum standard deviation of the energy (namely 0.24