MedeA Forcefield Optimizer

Efficient Forcefield Parameter Optimization using First-Principles Data

At-a-Glance

The *MedeA*®[1] *Forcefield Optimizer* enables you to determine optimum forcefield parameters for energy minimization (EM), molecular dynamics (MD), and Monte Carlo (MC) simulations.

The *MedeA Forcefield Optimizer* adjusts forcefield parameters to reproduce *ab initio* quantum mechanical data. With the *MedeA Forcefield Optimizer*, enable forcefield based simulation techniques to compute properties that require extensive sampling of configurational space. Then, carry out simulations that employ accurate forcefields with LAMMPS and GIBBS to compute the properties and behavior of systems, even those comprised of large numbers of atoms, for many configurations.

This capability significantly expands the range of properties that can be obtained using simulation, to large scale cooperative atomic motions and diffusive properties, for example.

Key Benefits

Productivity

- Extends *ab initio* results to larger length and time scales
- Automates forcefield fitting
- Searches parameter space using evolutionary methods

Accuracy

- Validates parameter quality using standard least squares methods
- Provides access to all calculation details and information
- Analyses fit quality automatically with generated reports and plots

Forcefields employ simple mathematical expressions and carefully optimized numerical parameters to describe the energetic behavior of atomic and molecular systems. The *MedeA Forcefield Optimizer* allows you to compute forcefield parameters by accurately reproducing supplied target first-principles data for systems of interest.

The *MedeA Forcefield Optimizer* employs first-principles derived information as the desired target behavior which is to be reproduced, using the selected forcefield. Configuration dependent energy, force, and stress data can be employed in the fitting process. The *MedeA Forcefield Optimizer* has been developed in active research and development projects over a number of years and has been thoroughly validated[2,3,7,8].

'. . . force fields will improve as their application in chemistry and molecular biology will advance, and that Darwinian natural selection and survival of the fittest will lead to better force fields which will be gradually accepted according to agreed-upon standards.'

Shneior Lifson, Forcefield Pioneer, in 1981

The desired target data for a given system are collected using a *MedeA* structure list. This compendium of information can contain configurations obtained from high temperature *ab initio* molecular dynamics simulations. These configurations sample the energy surface of the desired system, and the *MedeA Forcefield Optimizer* adjusts all or selected forcefield parameters to optimally reproduce the supplied target information.

Supply weights for the supplied data types. Spec-

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] Asahi, R., et al., *Modelling and Simulation in Materials Science and Engineering*, **22(7)**, p.075009 (2014)

[3] Christensen, M., et al., *Journal of Nuclear Materials*, **445(1-3)**, pp.241-250 (2014)

[7] France-Lanord, A., et al., *The Journal of chemical physics*, **144(10)**, p.104705 (2017)

[8] Christensen, M., et al., *Integrating Materials and Manufacturing Innovation*, **6(1)**, pp.92-110 (2017)

ify whether energies are handled in a relative or absolute manner (which is useful for some forcefield forms such as the embedded atom method). An interactive user interface allows you to select the parameters included in the fitted procedure and to set up any desired bound limits for parameters.

An evolutionary algorithm can be employed to search the forcefield parameter space thoroughly for any given system. Control the parameters of search using a variety of options, including the population size and the number of generations employed by the genetic algorithm. Similarly, least squares optimization algorithm parameters, such as the maximum number of least squares cycles, can be adjusted for specific system needs.

The *MedeA Forcefield Optimizer* provides considerable analytical output, including automated graphical analysis of the degree of fit of the optimized forcefield and supplied target information.

Forcefield optimization is often an iterative process, as the appropriate compromises are determined to efficiently account for a broad range of desired targets. In order to support the entire process of forcefield optimization the *MedeA Forcefield Optimizer* supports the use of validation and training set input, and retains all input and output (including forcefield files which are entirely open and accessible), using the *MedeA JobServer* system.

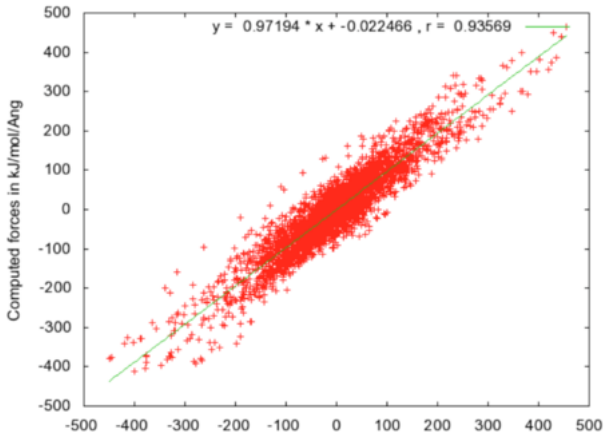

Figure 1: Comparison of target and forcefield derived forces. A range of comparison plots like this are automatically generated by the MedeA Forcefield Optimizer *to allow the rapid assessment of optimized forcefield parameter sets.*

User Interface

- Selection of training data
- Selection of validation data
- Specification of terms for optimization
- Handling of relative and absolute energies
- Selection of evolutionary and least squares parameters
- Report and plot creation for analysis

Supported Target Data

- Energies
- Forces
- Stress tensors

Supported Forcefield Types

- PCFF+ (class II forcefields)
- Buckingham[2]
- Morse with Coulomb terms
- EAM (embedded atom method)[38]
- Tersoff (three body + two body)[4]
- REBO[5]
- Stillinger-Weber **[#Stillinger]**
- COMB3 (Charge-Optimized Many-Body)[7]

Key Features

- Uses VASP derived DFT results
- Interactive selection and control
- Automated results analysis
- Efficient handling of optimization

Required Modules

- *MedeA Environment*
- *MedeA LAMMPS*
- *MedeA VASP*

Find Out More

Learn more about the *MedeA Forcefield Optimizer* by watching the webinar Classical Forcefields for Modeling Materials on Atomic Scale.

[4] Tersoff, J., *Physical Review B*, **37**, 6991-7000 (1988)
[5] Humbird, D. and Graves, D.B., *J. Chem. Phys.*, **120**, 2405 (2004)

Technical Features

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