ReaxFF parameterization using Metropolis Monte Carlo algorithm

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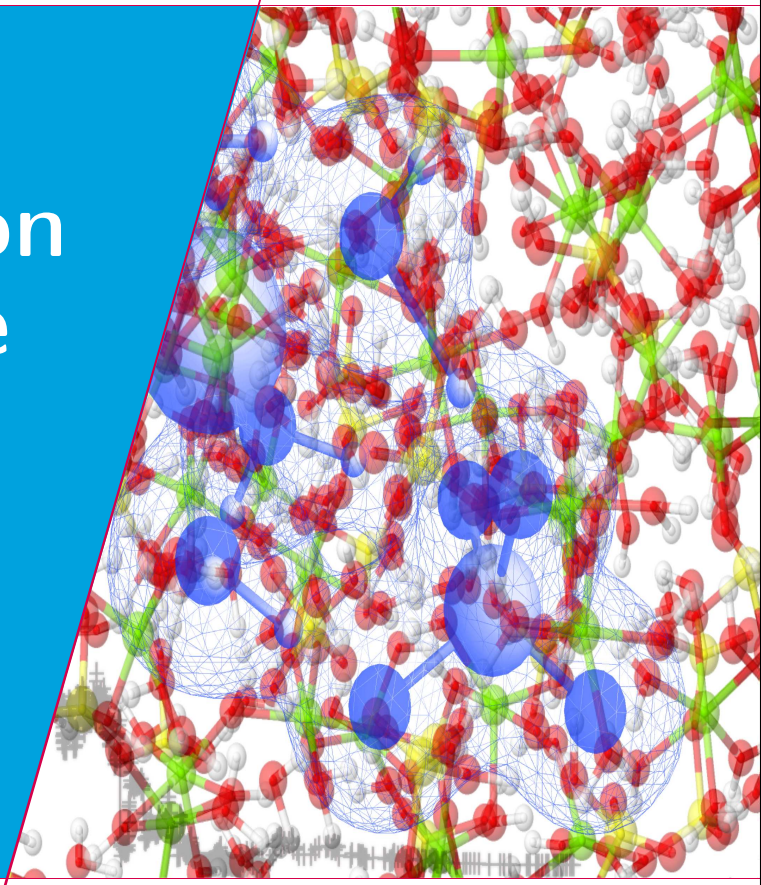

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Where innovation starts

Parameterization of Reax force field

- Quantum Chemical (DFT) data is used to parameterize the force field
- A training data set is prepared which contains the following informations
  - Atomic charges (Mulliken)
  - Equilibrium bond lengths
  - Equilibrium bond angles
  - Torsion angles
  - Energies of the DFT optimized geometries
  - *Heat of formation*
- Error in the force field is then calculated

$$Err(p_1, p_2, \cdots p_n) = \sum_{i=1}^{n} \left[\frac{x_{i,QM} - x_{i,ReaxFF}}{\sigma_i} \right]^2$$

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Metropolis Monte Carlo (MMC) method

- Calculate the error of the starting force field, Err_{old}
- Make a new proposition (move) for the parameters
- Calculate the error of the new force field, Err_{new}
- Calculate the difference in the Error, i.e.

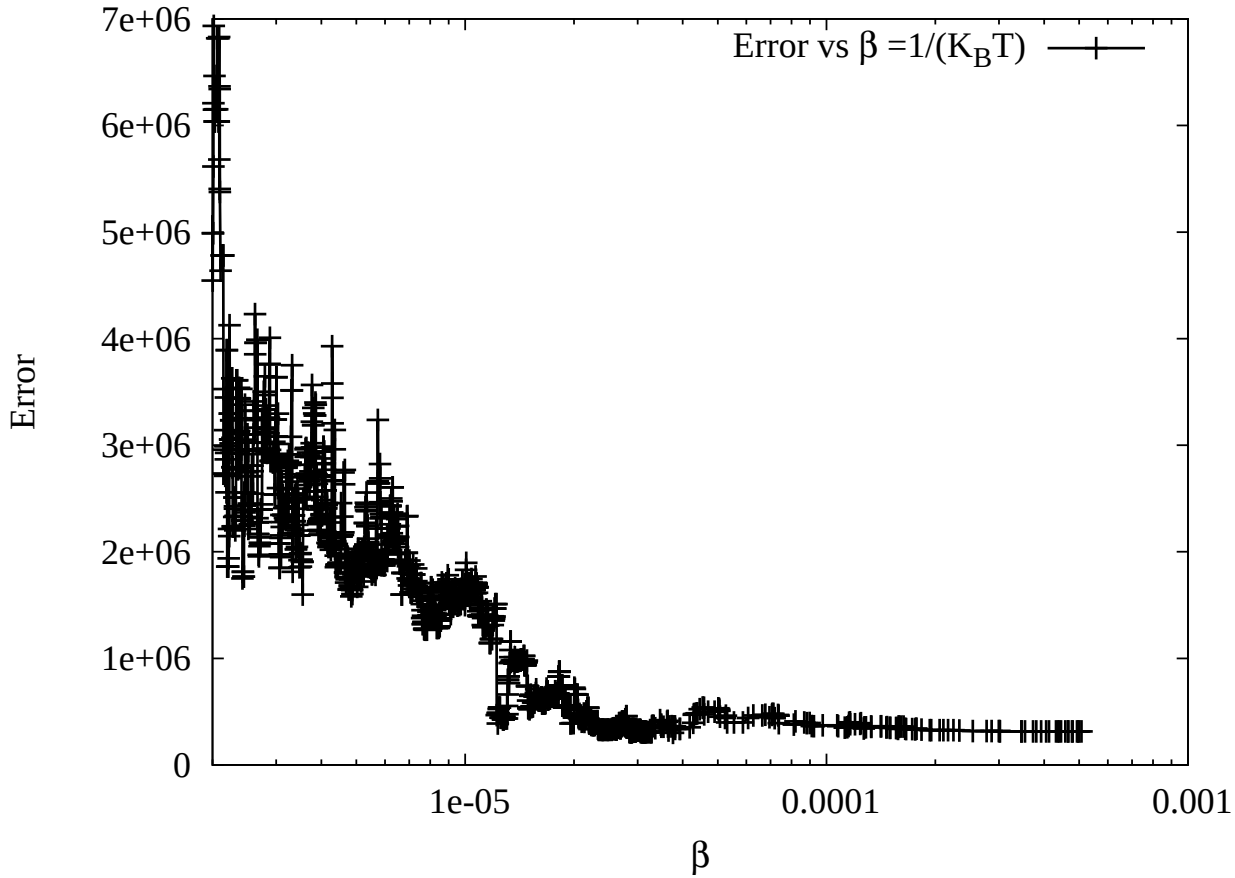
$$\Delta Err = Err_{new} - Err_{old}$$

- Accept the move with a probability given by,

$$P = min\left[1, exp\left(-\beta \Delta Err\right)\right], where, \beta = \frac{1}{k_B T}$$

- Repeat the algorithm

Error vs β for a Simulated Annealing run



Overview

- How to set-up input files (geo,trainset.in)?
- Optimizing water force field, MMC at low temperature
- Simulated annealing

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