**How to use the GEAM.py code**

This file needs VASP output files: CONTCAR and OUTCAR. From CONTCAR files, the coordinates and elements informations are obtained. From OUTCAR files, the energies and forces are obtained. The Generalized EAM framework contains three different interaction potentials. The two-body potential, the three body two bond potential and the three body three bond potential. Each potentials contain coefficient parameters and gaussian parameters. Two different methods are used to find the optimized parameters. Nelder-Mead algorithm is used to find the gaussian parameter and L-BFGS-B method is used to find the coefficient parameters for the three body two bond and the three body three bond parameters. The algorithm and equations to find the potentials are listed below.

**GEAM equations and algorithms**





To find *β* we optimize the equation, *r = (E – V2)2*

res = minimize(*r*, *β\_initial, method=”nelder-mead”)*

*β =* res.x

From *β* we obtain 

Considering *β* constant we obtain and 



res = minimize(*r, c32\_initial, method = “BFGS”, J*)

*c32* = res.x









Iterating for 100 steps





res = minimize(*r, c33\_initial, method=”BFGS”, J*)







Iterating for 100 steps

Final c2, c32 and c33 parameters are obtained.

There is sample **GEAM\_energy\_force.py** code which actually calculates the energy and forces due to the two body and three body interactions. The code confirms that the forces generated from the code is equal to the forces calculated from the first principles calculations. There are some sample perturbed CONTCAR files which proves the calculations. The data used to fit the generalized EAM interatomic potentials are strictly confidential due to DOE restrictions. We used the GEAM.py code to fit potentials for metal alloy systems.