# park\_1d

1D line - full-atomistics - static relaxation

In Park's surface Cauchy-Born paper, final displacement of the end atom (i.e., 31) is presented as 0.0025, which was normalized by the initial spacing (i.e., 1.1196). Un-normalized displacement is 0.0028.

# rectangle\_2d

2D rectangle - full-atomistics - static relaxation

Energy tolerances work differently for LAMMPS and MMM. Therefore, we apply a tolerance of 1e-8 in LAMMPS against a tolerance of 1e-6 in MMM, found by trial and error. Smaller tolerances are eliminated due to long simulation durations.

The details of the LAMMPS simulation are:

* Energy start: 35079.501 eV (33846.565 g/mole-A^2/10fs^2)
* Energy end: 35160.621 eV (33924.834 g/mole-A^2/10fs^2)
* Iteration number: Conjugate gradient with line search 1e-8 471
* Potential cut-off radius 2.3 + bin 0.7

# dynamic\_morse\_1d

1D line - full-atomistics - dynamics

Final total energy is -3.1967 eV (-3.0843 g/mole-A^2/10fs^2).

# dynamic\_force

|  |  |  |  |
| --- | --- | --- | --- |
| **Name** | **Dimension** | **Total energy (g/mole-^2/10fs^2)** | **Last atom (A)** |
| FA initial | 1 | -17.8759 | 20.20431687 |
| FA final | 1 | -17.8628 | 20.23705508 |
| MMM initial | 1 | -17.9058 | 20.20431687 |
| MMM final | 1 | -17.8946 | 20.23241710 |
| FA initial | 2 | -584.027 | 20.20431687 |
| FA final | 2 | -584.048 | 20.17792682 |
| MMM initial | 2 | -643.209 | 20.20431687 |
| MMM final | 2 | -643.24 | 20.17317946 |