Strain Simulations in NEMO 5

- Objective:
  - » Calculate strain in nanostructures using atomistic valence-force-field (VFF) models
  - » Zincblende or Wurtzite lattices

- Results / Impact:
  - » Fast-converging solver that uses exact derivatives
  - » Models easily switchable in input deck
  - » Improved anharmonic model: both physical validity and numerical convergence

- Approach:
  - » Energy functional minimization using Newton's method applied to gradient.
  - » Models for energy functional:
    - Harmonic Keating
    - Anharmonic Keating
    - Zunger
    - Paul