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# Cloud computing in nanoHUB powering education and research

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## ABSTRACT

MiniMol is a minimal molecular statics (MS) and molecular dynamics (MD) program accompanying the book “Modeling Materials: Continuum, Atomistic and Multiscale Techniques” by Ellad B. Tadmor and Ronald E. Miller, Cambridge University Press, 2011. In MS mode, the program performs energy minimization using a conjugate gradient minimization. In MD mode, it can perform dynamical simulations at constant energy or constant temperature using a velocity rescaling, Nose–Hoover or Langevin thermostat. MiniMol is compliant with the Knowledgebase of Interatomic Models (KIM) application programming interface. This means MiniMol can be seamlessly run with any KIM-compliant interatomic model (potential) stored within the OpenKIM repository (http://openkim.org). KIM is a major NSF-funded effort to improve the reliability, gage the accuracy, and enhance the portability of empirical interatomic potentials.