Übungen zur

Computational Nanoscience

– Blatt 1 –

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Aufgabe 1) EOM

Solve the Equation of Motion (EOM) for a 1-dimensional particle moving in potential:
$U(x) = Cx$,
where C is a constant. Sketch a phase-space plot.

Aufgabe 2) Predictor-Corrector

Determine the order of Predictor-Corrector scheme or Euler-Richardson algorithm.

Aufgabe 3) Verlet

Schow that the Verlet algorithm for Molecular Dynamics is symplectic.