Molecular Dynamics (MD) Protocol

Eamonn Healy

Abstract

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Protocol

Solvation

Step 1.

Solvation Model Explicit Periodic Boundary

Cell Shape : Orthorhombic

Minimum Distance From Boundary 7.0

Add Counterion: True

Salt Concentration 0.145

Cation Type Sodium

Anion Type Chloride

Random Seed 314159

Minimization

Step 2.

First

Algorithm Steepest Descent

Max Steps 20000

RMS Gradient 1.0

Second

Algorithm Conjugate Gradient

Max Steps 20000

RMS Gradient 0.1

Heating

Step 3.

Simulation Time (ps) 100

Time Step (fs) 2

Initial Temperature 50.0

Target Temperature 300.0

Adjust Velocity Frequency 50

Save Results Interval (ps) 20

Equilibriation

Step 4.

Simulation Time (ps) 500

Time Step (fs) 2

Target Temperature 300.0

Adjust Velocity Frequency 50

Save Results Interval (ps) 20

Constant Pressure True

PMass 1000.0

PGamma 25.0

Reference Pressure 1.0

Production

Step 5.

Simulation Time (ps) 2000

Time Step (fs) 2

Target Temperature 300.0

Temperature Coupling Decay Time 5.0

Save Results Interval (ps) 20

Save Restart File True

Type NPT

TMass 1000.0

Miscellaneous Parameters

Step 6.

Nonbond List Radius 14.0

Nonbond Higher Cutoff Distance 12.0

Nonbond Lower Cutoff Distance 10.0

Electrostatics Automatic

Kappa 0.34

Order 4

Dynamics Integrator Leapfrog Verlet

Apply SHAKE Constraint True

Random Number Seed 314159 314159 314159 314159