

Atoms

51.6059	5.3279	5.6240	1	1	1
50.2541	7.4810	7.4995	1	1	2
51.2149	8.0236	8.2322	1	1	3

Set up initial positions
and topology

Find interacting atoms

Provide interatomic
potential
(Forcefield)

Calculate interaction forces:

$$F_{ij} = -\nabla U_{ij}$$

Provide constraints
of integration
(Ensemble)

Solve Newtons equations of motion,
obtain new positions:

$$\ddot{r}_i = \sum_{j=1}^n F_{ij}/m$$

No

Yes

End of time?

Calculate macroscopic
properties (P, T ...)

