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The Computational Analysis of the Radial Distribution Function in a Many Body, Lennard Jones System

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Introduction

- No analytical solution can be found for a stochastic, many bodied system.
- Modeling and computational evaluation is an increasingly facile and successful approach.

Model

- Argon, Lennard Jones Force
- Velocity Verlet in Python
- Periodic, Force Cutoff, Wall BC’s

Radial Distribution Function

Initial Solid Argon (Crystalline)

Liquid 1K

Gas 300K

B.C.’s Vs Temp. vs Size

A Periodic
B Cutoff
C Wall

A
B
C

1K
100K
200K

25
50
75

300K

100

Conclusions

- RDF converges $\rightarrow 1$ as expected.
- RDF varies strongly with T.
- Fast Development time w/ python.
- Liquid to Gas, but no FCC solid (!)

Challenges

- Initial Conditions extreme, $\Delta t$ limit
- Size effect, physics simple.