Molecular Dynamics in Dyalog APL

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- What is Molecular Dynamics?
- In what ways is APL useful?
  - Teaching MD
  - Developing MD

What is MD?

- Modelling atomic and molecular systems using classical (Newtonian) mechanics

$$\vec{F} = m\vec{a}$$

$$F = -\frac{dV(x)}{dx}$$

Numerical Integration

- Insoluble ODEs
- Step from state to state using numerical approximations
- Velocity Verlet

What MD codes are there?

- LAMMPS
- GROMACS
- HOOMD
- + many more…

https://lammps.sandia.gov/other.html

APL for MD

- Teaching MD
  - Explanation
  - Visualisation

The Lennard-Jones fluid

Link to Jupyter notebook in the description ↓
https://nbviewer.jupyter.org/github/rikedyp/APLPhys/blob/master/Jupyter/LJmelt.ipynb

$$V_{LJ} = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

```
LJ ← {4×-/ω∘.*¯12 ¯6}
```

The Lennard-Jones fluid

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$$\mathbf{F} = -\frac{1}{r}\nabla V(\mathbf{r})$$

$$\mathbf{F} = -\frac{1}{r}\nabla V_{LJ}(\mathbf{r}) = -\frac{1}{r}\frac{dV_{LJ}}{d\mathbf{r}} = -24\left[2\left(\frac{\sigma}{\mathbf{r}}\right)^{14} - \left(\frac{\sigma}{\mathbf{r}}\right)^{8}\right]$$

Thermostats: TempRescale

$$\Delta T = \frac{1}{2}\sum_{i=1} 2\frac{m_i\left(\lambda v_i\right)^2}{N_{df}k_B} - \frac{1}{2}\sum_{i=1} 2\frac{m_i v_i^2}{N_{df}k_B}$$

$$\Delta T = \left(\lambda^2 - 1\right)T(t)$$

$$\lambda = \sqrt{T_0/T(t)}$$

```
{ω×0.5*⍨fixtemp÷⍺}
```

Thermostats: Berendsen

$$T = T_0 - Ce^{-t/\tau}$$

$$\lambda^2 = 1 + \frac{\Delta t}{\tau_T}\left(\frac{T_0}{T} - 1\right)$$

APLPhys

https://github.com/rikedyp/APLPhys

- Jupyter notebooks
- Key ⌸ and rank ⍤
- MiServer GUI (MiPhys)

Future

https://github.com/rikedyp/APLPhys

- Scalability: Isolates
- More thermostats
- More models
- Graphs on MiPhys