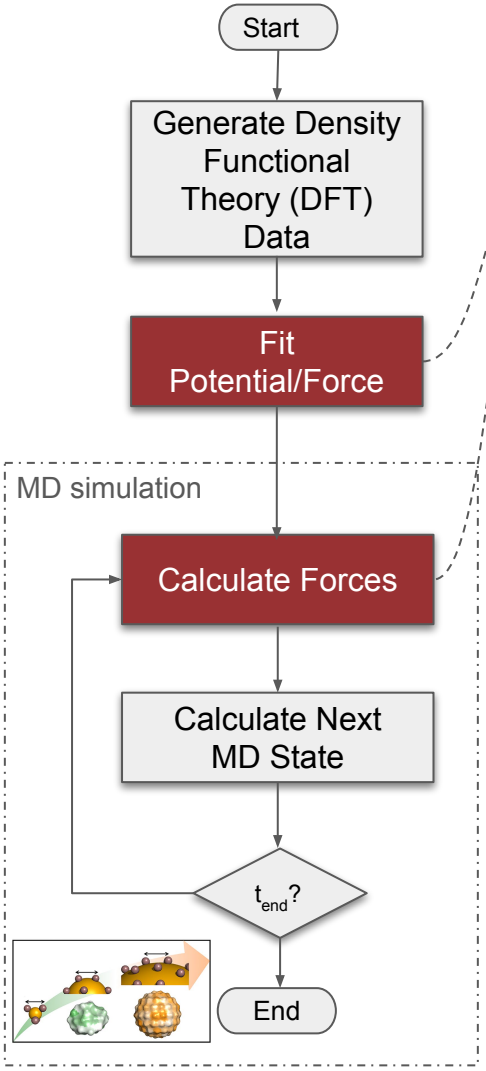


MDP.jl the julia library of Molecular Dynamics (MD) Potentials

"Providing fast and accurate potentials for classical MD simulations on exascale supercomputers."

- Provide a comprehensive library of coupled Empirical and Machine Learning (ML) potentials

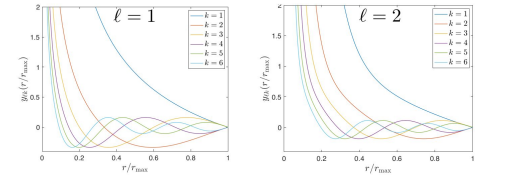
  Fit DFT forces to $F = F_{Empirical} + F_{Machine\ Learning}$

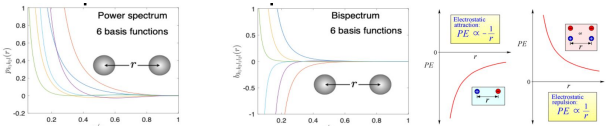
  where $F_{Empirical} = F_{Power\ Spectrum} + F_{Bispectrum}$

- Quantify uncertainties for the trained potentials
- Increase MD simulation performance by implementing and auto-tuning new algorithms for force calculation
- Open Source

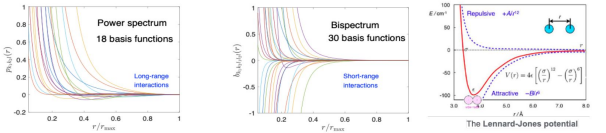
The descriptors are based on products of spherical harmonics $Y_{lm}(\theta,\phi)$ and spherical Bessel functions $y_{lk}(r)$

$$u_{klm}(\boldsymbol{r}) = y_{lk}(r)Y_{lm}(\theta,\phi), \quad 1 \le k \le K, 0 \le l \le L, -l \le m \le l$$





Radial basis functions for $K = 2$ and $L = 1$ (first-order)



Radial basis functions for $K = 3$ and $L = 2$ (second-order)