

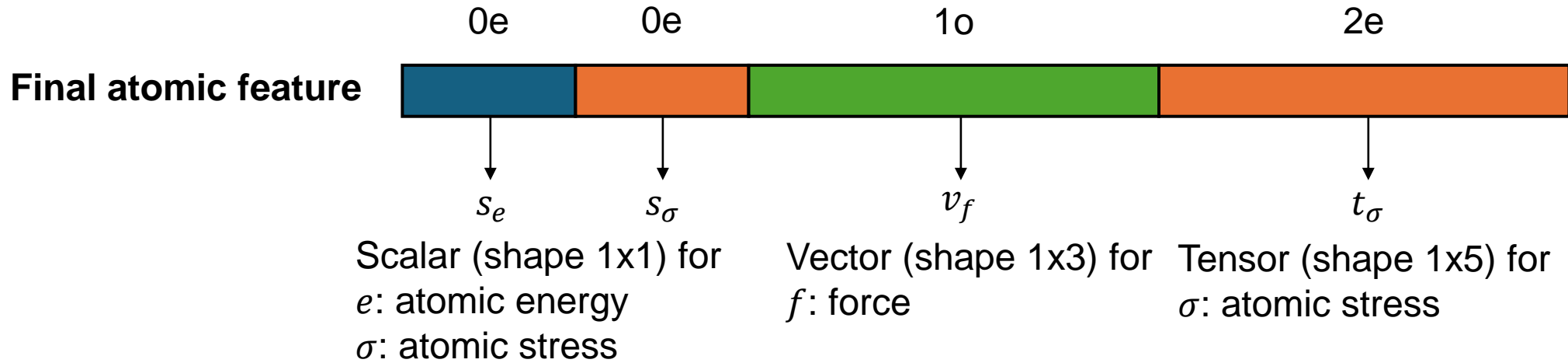
SevenNet-dFS

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SevenNet-dFS



$$\sigma = \frac{1}{V} \sum_i \left\{ \begin{bmatrix} s_\sigma^i \\ s_\sigma^i \\ s_\sigma^i \\ 0 \\ 0 \\ 0 \end{bmatrix} \cdot a_{\sigma,iso} + A t_\sigma \cdot a_{\sigma,aniso} \right\} + \begin{pmatrix} b_\sigma \\ b_\sigma \\ b_\sigma \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$A = \begin{bmatrix} 0 & 0 & -\frac{1}{\sqrt{6}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \end{bmatrix}$$

b_σ : atomic stress shift, mean of $\sigma[:3]V$

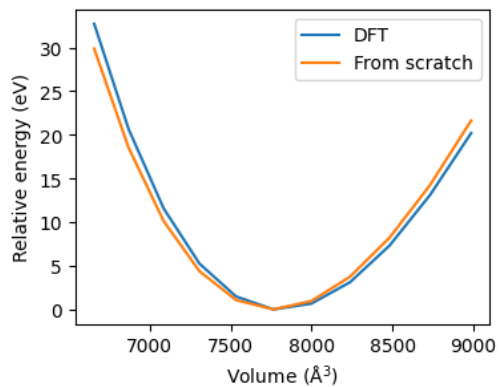
$a_{\sigma,iso}$: atomic stress scale for isotropic, rms of $(\sigma[:3] - \sigma[3:])V$

$a_{\sigma,aniso}$: atomic stress scale for anisotropic, rms of $(\sigma[3:])V$

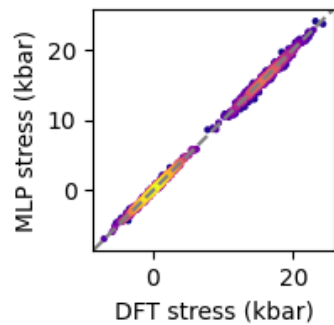
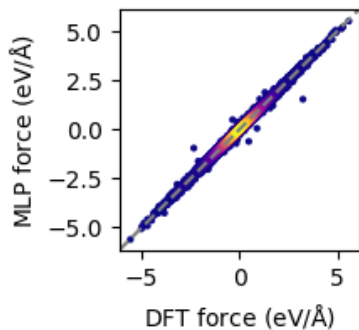
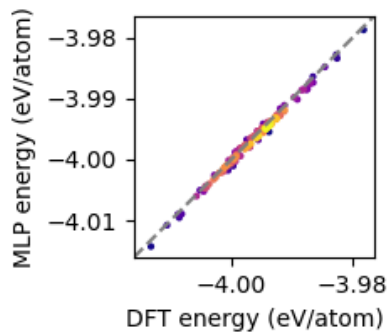
SevenNet-dFS

- Li-argyrodite ($\text{Li}_6\text{PS}_5\text{Cl}$)

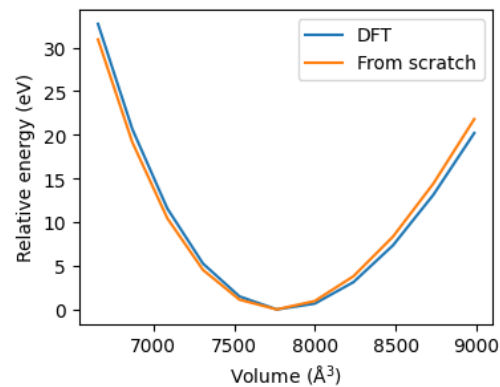
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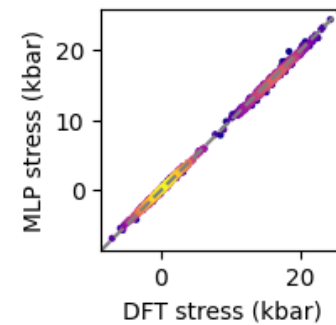
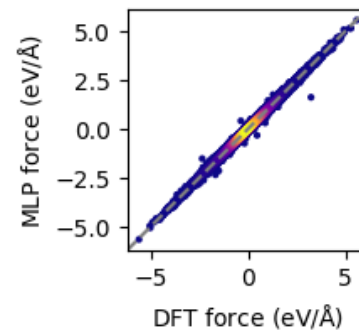
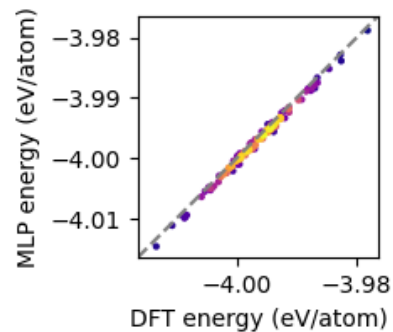
Energy_RMSE (eV/atom): 0.001
Force_RMSE (eV/ \AA): 0.074
Stress_RMSE (kbar): 0.641



SevenNet



Energy_RMSE (eV/atom): 0.001
Force_RMSE (eV/ \AA): 0.069
Stress_RMSE (kbar): 0.691



SevenNet-dFS

- **Training**

- **SevenNet-0**: 302 s
- **SevenNet-dFS** : 480 s
- **1.59x slower**

- **Inference**

- **SevenNet-0**: 130.15 s
- **SevenNet-dFS**: 26.51 s
- **4.91x acceleration**

- **MD simulation**

- **SevenNet-0**: 755.63 s
- **SevenNet-dFS**: 2.96 s
- **255.28x acceleration**