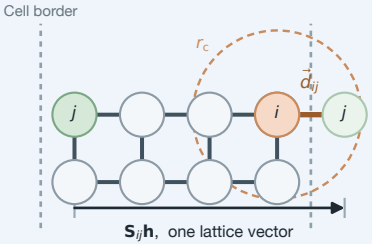
(a) Structure → graph



$$\vec{d}_{ij} = \vec{r}_j - \vec{r}_i + \mathbf{S}_{ij}\mathbf{h}$$

Atoms are nodes; every edge carries a vector

(b) `AtomsData`: unified data object

Graph

`num_atoms` `atomic_numbers` `positions` `cell` `edge_indices` `edge_vectors` `num_edges`

Labels (when training)

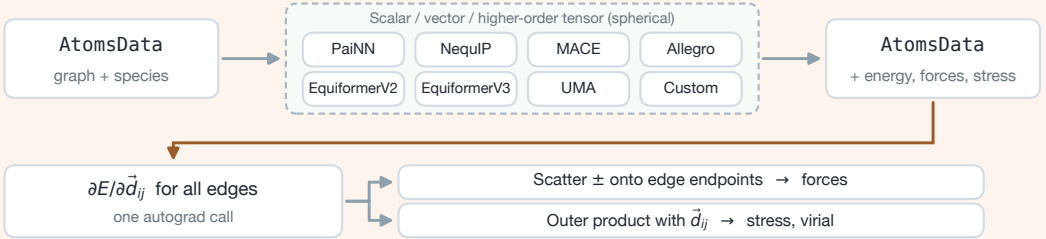
`energy` `forces` `stress` `virial`

Batching

`image_indices` + `edge_indices offset`

Declared statically ⇒ TorchScript-safe

(c) Model-agnostic forward pass and analytic derivatives



$$\vec{F}_i = -\partial E/\partial \vec{r}_i = \sum_{j \in \mathcal{N}(i)} \partial E/\partial \vec{d}_{ij} - \sum_{j\,:\,i \in \mathcal{N}(j)} \partial E/\partial \vec{d}_{ji}$$

exact under periodic boundary conditions, identical in every model