

Finite displacements
measurements.

Generate finite dis-
placements stencils.

Displacement
amplitudes Δ .

The unique jobs to
be computed with
first principles.

First principle
configurations.

Database

Compute finite
displacements..

Inputs for first prin-
ciple calculations.

Extract results from first
principle calculations.

Finite displace-
ments results.

Execute first prin-
ciple calculations.

