

VASTOS


Crystal Structures Classifier for an Evolutionary Algorithm Structure Predictor

Mario Valle – Swiss National Supercomputing Centre (CSCS)
Artem Oganov – ETH Zürich


(Excerpts from the conference talk)

The problem to solve

USPEX is a crystal structure predictor based on an evolutionary algorithm

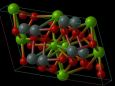


Each run produces hundred of putative crystal structures...
...but many of them are equal

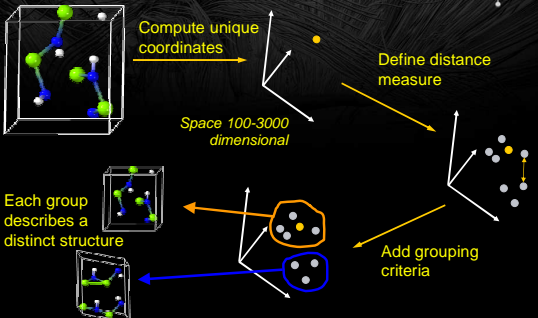


Project: to develop a (semi)automatic way to extract unique structures from the USPEX output

So an intensive manual labor is needed to prune duplicated structures



Proposed solution: use methods and ideas from multidimensional spaces



Compute unique coordinates

Space 100-3000 dimensional

Define distance measure

Add grouping criteria

Each group describes a distinct structure

Visual diagnostics: scatterplot

The scatterplot tries to map High-D space points to 2D preserving their relative distances

Colored by "stress" to detect local minima traps

Colored by group

Diagnostic chart: distances in 2D vs. distances in High-D space

Various visual diagnostics tools

- 2D maps
- Charts
- Picking for details
- 2D data export

Visual diagnostic tools

Grouping quality: silhouette coefficients

Scatterplot

Diagnostic charts

Distance matrix
