Stony Brook University

Oganov's Lab

COMPUTATIONAL MATERIALS DISCOVERY LABORATORY

Tutorial 8: Introduction to USPEX

Maksim Rakitin
maksim.rakitin@stonybrook.edu

Shengnan Wang
shengnan.wang@stonybrook.edu

Stony Brook University
Department of Geosciences

Useful links:

- References, where the method was exhaustively described: http://uspex.stonybrook.edu/uspex.html

- USPEX manual:
  - HTML: http://han.ess.sunysb.edu/uspex_manual/
  - PDF: http://han.ess.sunysb.edu/uspex_manual/uspex_manual.pdf

- USPEX utilities: http://han.ess.sunysb.edu/

How to start your calculations

1. Prepare INPUT.txt file.
2. Prepare files in `Specific/` directory (for VASP: INCAR_1,…,INCAR_*N*, POTCAR_A, POTCAR_B, etc.)
3. If necessary, prepare additional files, which are described in the manual.
4. Start calculation: `USPEX -r`

Connection information:

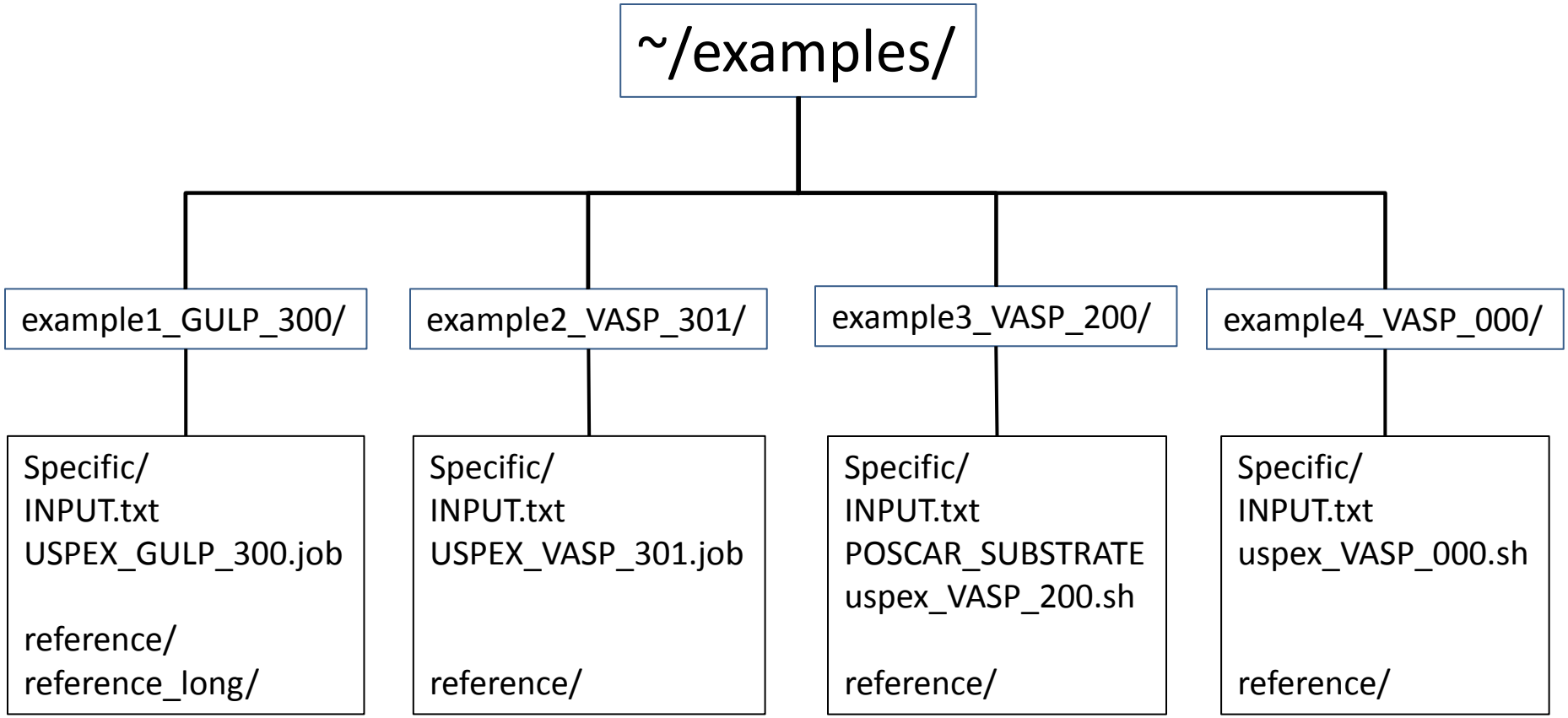
- `ssh USPEXBNL@qsh.ess.sunysb.edu`

  Password: `********` (please enter the password correctly, otherwise we will be blocked)
- `cd ~/workshop`
- `mkdir <your userid on nano.bnl.gov>`
- `cd <your userid on nano.bnl.gov>`
- `USPEX -h`

Examples for today:

- Bulk $Mg_4Al_8O_{16}$ (fixed composition, calculationType=300, GULP)
- Bulk Si-C (variable composition, calculationType=301, VASP)
- O_2 @ Si (100) (fixed composition, calculationType=200, VASP)
- C_{13} nanoparticles (fixed composition, calculationType=000, VASP)

Examples file system



Examples for today:

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- Bulk Si-C (variable composition, calculationType=301, VASP)
- O_2 @ Si (100) (fixed composition, calculationType=200, VASP)
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Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

$MgAl_2O_4$ (28 atoms/cell) at 100 GPa pressure. Variable-cell calculation using Buckingham potentials, GULP code. This test has direct bearing on the physics of the Earth's interior!

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

INPUT.txt:

```
1  ****************************************
2  *      TYPE OF RUN AND SYSTEM          *
3  ****************************************
4  USPEX   : calculationMethod (USPEX, VCNEB, META)
5  300     : calculationType (dimension: 0-3; molecule: 0/1;
6  1       : optType (1=enthalpy, 2=volume, 3=hardness, 4=str
7
8  % symmetries
9  2-230
10 % endSymmetries
11
12 % atomType
13 Mg Al O
14 % EndAtomType
15
16 % numSpecies
17 4 8 16
18 % EndNumSpecies
19
20 % valences
21 2 3 2
22 % endValences
```

▷ *variable* `optType`

Meaning: This variable allows you to specify the qua

Possible values (characters):

- enthalpy (or "1") — to find the stable phases
- volume (or "2") — volume minimization (to fi
- hardness (or "3") — hardness maximization (t
- struc_order (or "4") — maximization of the degr structure)
- aver_dist (or "5") — maximization of average s ation
- diel_sus (or "6") — maximization of the static dielectric susceptibility (only for VASP and GULP)
- gap (or "7") — maximization of the band gap (only for VASP)
- diel_gap (or "8") — maximization of electrical energy storage capacity (only for VASP)
- mag_moment (or "9") — maximization of the magnetization (only for VASP)
- quasientropy (or "10") — maximization of structural quasientropy

▷ *variable* `calculationType`

Meaning: Specifies type of calculation, *i.e.*, whether the structure of a bulk crystal, nanoparticle, or surface is to be predicted. This variable consists of three indices: *dimensionality*, *molecularity*, and *compositional variability*:

- dimensionality:
  - "3" — bulk crystals
  - "2" — surfaces, "–2" — 2D-crystals
  - "1" — polymers
  - "0" — nanoparticles
- molecularity:
  - "0" — non-molecular
  - "1" — molecular calculations
- variability of chemical composition in the calculation:
  - "0" — fixed composition
  - "1" — variable composition

Default: 300

Format:

```
301 :  calculationType
```

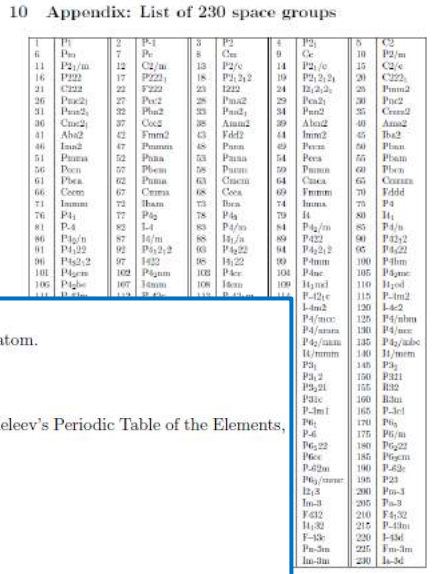
Note: If `calculationType`=310, *i.e.*, a prediction for a molecular crystal is to be performed, then USPEX expects you to provide files `MOL_1`, `MOL_2`, ... with molecular geometries for all types of molecules, and these molecules will be placed in the newly generated structures as whole objects. Available options: 300, 301, 310, 000, 200, 201, –200 (and not yet released: 110, 311.)

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

INPUT.txt:

```
1  ******************************************
2  *       TYPE OF RUN AND SYSTEM           *
3  ******************************************
4  USPEX   : calculationMethod (USPEX, VCNEB, META)
5  300     : calculationType (dimension: 0-3; molecule: 0/1; varcomp: 0/1)
6  1       : optType (1=enthalpy, 2=volume, 3=hardness, 4=struc_order, 5=aver_dist)
7
8  % symmetries
9  2-230
10 % endSymmetries
11
12 % atomType
13 Mg Al O
14 % EndAtomType
15
16 % numSpecies
17 4 8 16
18 % EndNumSpecies
19
20 % valences
21 2 3 2
22 % endValences
```

Possible space groups for crystals


10 Appendix: List of 230 space groups

1	$P1$	2	$P\bar{1}$	3	$P2$	4	$P2_1$	5	$C2$
6	Pm	7	Pc	8	Cm	9	Cc	10	$P2/m$
11	$P2_1/m$	12	$C2/m$	13	$P2/c$	14	$P2_1/c$	15	$C2/c$
16	$P222$	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	$C222$	22	$F222$	23	$I222$	24	$I2_12_12_1$	25	$Pmm2$
26	$Pmc2_1$	27	$Pcc2$	28	$Pma2$	29	$Pca2_1$	30	$Pnc2$
31	$Pmn2_1$	32	$Pba2$	33	$Pna2_1$	34	$Pnn2$	35	$Cmm2$
36	$Cmc2_1$	37	$Ccc2$	38	$Amm2$	39	$Abm2$	40	$Ama2$
41	$Aba2$	42	$Fmm2$	43	$Fdd2$	44	$Imm2$	45	$Iba2$
46	$Ima2$	47	$Pmmm$	48	$Pnnn$	49	$Pccm$	50	$Pban$
51	$Pmma$	52	$Pnna$	53	$Pmna$	54	$Pcca$	55	$Pbam$
56	$Pccn$	57	$Pbcm$	58	$Pnnm$	59	$Pmmn$	60	$Pbcn$
61	$Pbca$	62	$Pnma$	63	$Cmcm$	64	$Cmca$	65	$Cmmm$
66	$Cccm$	67	$Cmma$	68	$Ccca$	69	$Fmmm$	70	$Fddd$
71	$Immm$	72	$Ibam$	73	$Ibca$	74	$Imma$	75	$P4$
76	$P4_1$	77	$P4_2$	78	$P4_3$	79	$I4$	80	$I4_1$
81	$P\bar{4}$	82	$I\bar{4}$	83	$P4/m$	84	$P4_2/m$	85	$P4/n$
86	$P4_2/n$	87	$I4/m$	88	$I4_1/a$	89	$P422$	90	$P42_12$
91	$P4_122$	92	$P4_12_12$	93	$P4_222$	94	$P4_22_12$	95	$P4_322$
96	$P4_32_12$	97	$I422$	98	$I4_122$	99	$P4mm$	100	$P4bm$
101	$P4_2cm$	102	$P4_2nm$	103	$P4cc$	104	$P4nc$	105	$P4_2mc$
106	$P4_2bc$	107	$I4mm$	108	$I4cm$	109	$I4_1md$	110	$I4_1cd$
111	$P\bar{4}2m$	112	$P\bar{4}2c$	113	$P\bar{4}21m$	114	$P\bar{4}21c$	115	$P\bar{4}m2$
116	$P\bar{4}c2$	117	$P\bar{4}b2$	118	$P\bar{4}n2$	119	$I\bar{4}m2$	120	$I\bar{4}c2$
121	$I\bar{4}2m$	122	$I\bar{4}2d$	123	$P4/mmm$	124	$P4/mcc$	125	$P4/nbm$
126	$P4/nnc$	127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$	130	$P4/ncc$
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nnm$	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	$I4/mmm$	140	$I4/mcm$
141	$I4_1/amd$	142	$I4_1/acd$	143	$P3$	144	$P3_1$	145	$P3_2$
146	$R3$	147	$P\bar{3}$	148	$R\bar{3}$	149	$P312$	150	$P321$
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	$R32$
156	$P3m1$	157	$P31m$	158	$P3c1$	159	$P31c$	160	$R3m$
161	$R3c$	162	$P\bar{3}1m$	163	$P\bar{3}1c$	164	$P\bar{3}m1$	165	$P\bar{3}c1$
166	$R\bar{3}m$	167	$R\bar{3}c$	168	$P6$	169	$P6_1$	170	$P6_5$
171	$P6_2$	172	$P6_4$	173	$P6_3$	174	$P\bar{6}$	175	$P6/m$
176	$P6_3/m$	177	$P622$	178	$P6_122$	179	$P6_522$	180	$P6_222$
181	$P6_422$	182	$P6_322$	183	$P6mm$	184	$P6cc$	185	$P6_3cm$
186	$P6_3mc$	187	$P\bar{6}m2$	188	$P\bar{6}c2$	189	$P\bar{6}2m$	190	$P\bar{6}2c$
191	$P6/mmm$	192	$P6/mcc$	193	$P6_3/mcm$	194	$P6_3/mmc$	195	$P23$
196	$F23$	197	$I23$	198	$P2_13$	199	$I2_13$	200	$Pm\bar{3}$
201	$Pn\bar{3}$	202	$Fm\bar{3}$	203	$Fd\bar{3}$	204	$Im\bar{3}$	205	$Pa\bar{3}$
206	$Ia\bar{3}$	207	$P432$	208	$P4_232$	209	$F432$	210	$F4_132$
211	$I432$	212	$P4_332$	213	$P4_132$	214	$I4_132$	215	$P\bar{4}3m$
216	$F\bar{4}3m$	217	$I\bar{4}3m$	218	$P\bar{4}3n$	219	$F\bar{4}3c$	220	$I\bar{4}3d$
221	$Pm\bar{3}m$	222	$Pn\bar{3}n$	223	$Pm\bar{3}n$	224	$Pn\bar{3}m$	225	$Fm\bar{3}m$
226	$Fm\bar{3}c$	227	$Fd\bar{3}m$	228	$Fd\bar{3}c$	229	$Im\bar{3}m$	230	$Ia\bar{3}d$

▷ *variable* atomType

Meaning: Describes the identities of each type of atom.

Default: none, must specify explicitly

Format:

If you prefer to use the atomic numbers from Mendeleev's Periodic Table of the Elements, specify:

```
% atomType
12 14 8
% EndAtomType
```

Or, if you prefer to use atomic names, specify:

```
% atomType
Mg Si O
% EndAtomType
```

You can alternatively specify the full names of the elements, for example:

```
% atomType
Magnesium Silicon Oxygen
% EndAtomType
```

Number of atoms of each type

Valences of each type of atom

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

INPUT.txt:

```
24  ****************************************
25  *                POPULATION              *
26  ****************************************
27  5      : populationSize (how many individuals per generation)
28  5      : initialPopSize (how many individuals in the first generation)
29  3      : numGenerations (how many generations shall be calculated)
30  3      : stopCrit (max number of generations with the same b
31  0      : reoptOld (should the old structures be reoptimized?
32  0.6    : bestFrac (What fraction of current generation shall
33
34  ****************************************
35  *          VARIATION OPERATORS           *
36  ****************************************
37  0.50   : fracGene (fraction of generation produced by heredi
38  0.20   : fracRand (fraction of generation produced randomly
39  0.05   : fracPerm (fraction of the generation produced by permutations)
40  0.25   : fracAtomsMut (fraction of the generation produced by softmutation)
41
42  ****************************************
43  *             CONSTRAINTS                *
44  ****************************************
45  % IonDistances
46  0.6 0.6 0.6
47  0.0 0.6 0.6
48  0.0 0.0 0.6
49  % EndDistances
```

▷ *variable* numGenerations

Meaning: Maximum number of generations allowed for the simulation. The simulation can terminate earlier, when the same best structure remains unchanged for `stopCrit` generations.

Default: 100

▷ *variable* stopCrit

Meaning: The simulation is stopped if the best structure did not change for stopCrit generations, or when `numGenerations` have expired — whichever happens first.

Default: total number of atoms for fixed-composition runs, maximum number of atoms `maxAt` for variable-composition runs.

▷ *variable* bestFrac

Meaning: Fraction of the current generation that shall be used to produce the next generation.

Default: 0.7

▷ *variable* IonDistances

Meaning: Sets the minimum inter-atomic distance matrix between different atom types.

Default: half of the covalent radii sum (in Å) for a corresponding atom pair.

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

INPUT.txt:

```
34  ****************************************
35  *          VARIATION OPERATORS           *
36  ****************************************
37  0.50  : fracGene (fraction of generation produced by heredity)
38  0.20  : fracRand (fraction of generation produced randomly from space groups specified by user)
39  0.05  : fracPerm (fraction of the generation produced by permutations)
40  0.25  : fracAtomsMut (fraction of the generation produced by softmutation)
```

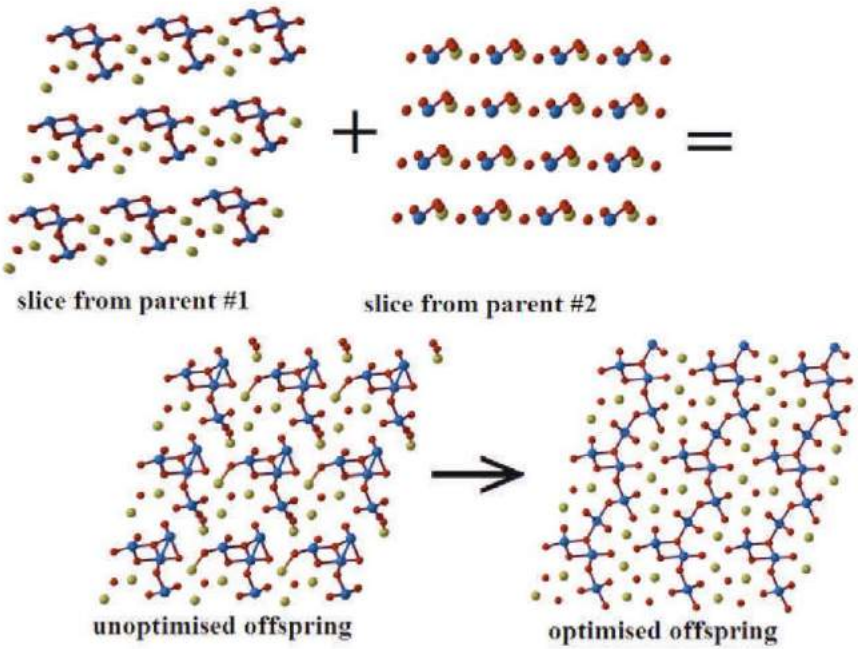


Figure 1. Heredity operator: slices of two parent structures, and the offspring structure before and after local optimization.

Picture from "Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. (2010). Evolutionary crystal structure prediction as a method for the discovery of minerals and materials. *Rev. Mineral. Geochem.* **71**, 271-298"

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

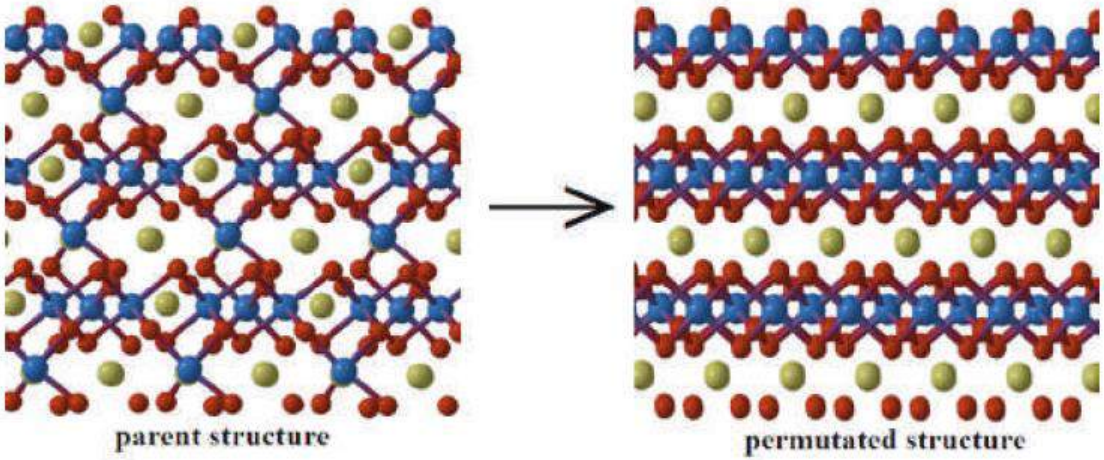
INPUT.txt:

```
34  ****************************************
35  *          VARIATION OPERATORS           *
36  ****************************************
37  0.50  : fracGene (fraction of generation produced by heredity)
38  0.20  : fracRand (fraction of generation produced randomly from space groups specified by user)
39  0.05  : fracPerm (fraction of the generation produced by permutations)
40  0.25  : fracAtomsMut (fraction of the generation produced by softmutation)
```

▷ *variable* `fracPerm`

Meaning: Percentage of structures obtained by permutation; 0.1 means 10%, *etc.*

Default: `0.1` if there is more than one type of atom/molecule; `0` otherwise.



Pictures from "Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. (2010). Evolutionary crystal structure prediction as a method for the discovery of minerals and materials. *Rev. Mineral. Geochem.* **71**, 271-298"

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

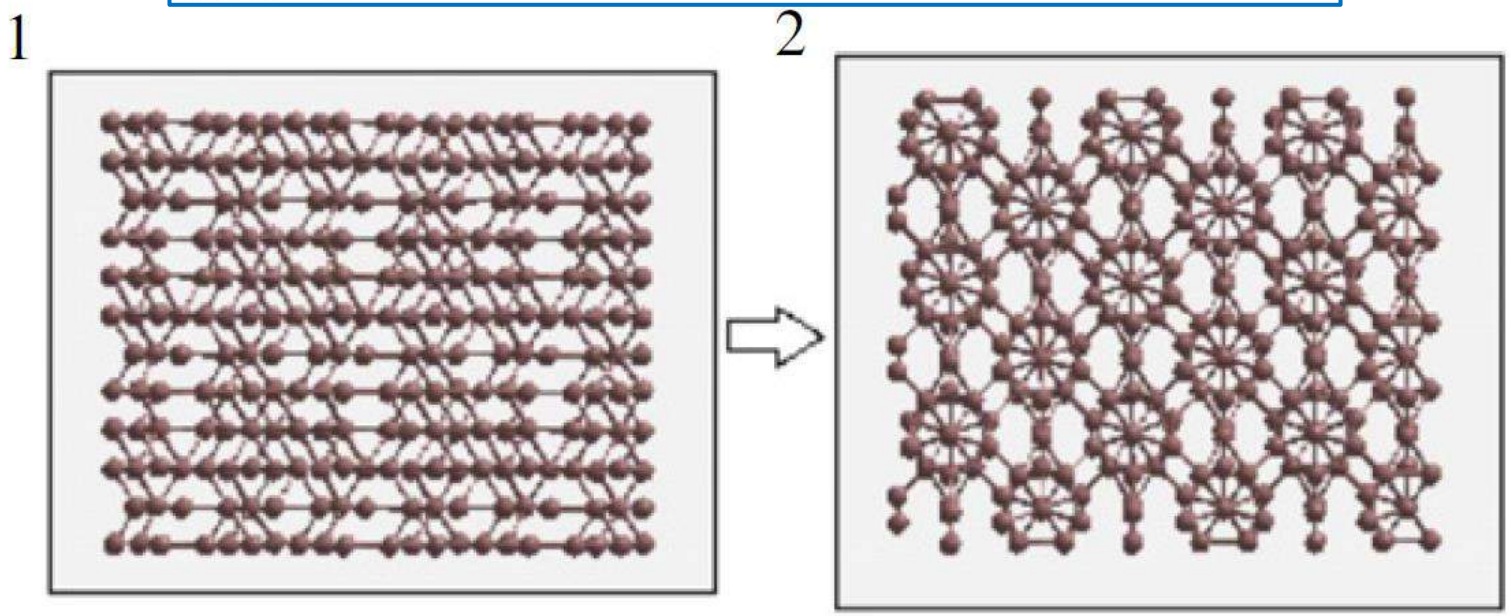
INPUT.txt:

```
34  ****************************************
35  *          VARIATION OPERATORS           *
36  ****************************************
37  0.50  : fracGene (fraction of generation produced by heredity)
38  0.20  : fracRand (fraction of generation produced randomly from space groups specified by user)
39  0.05  : fracPerm (fraction of the generation produced by permutations)
40  0.25  : fracAtomsMut (fraction of the generation produced by softmutation)
```

▷ *variable* fracAtomsMut

Meaning: Specifies the percentage of structures obtained by softmutation or coormutation.

Default: 0.1



Picture from "Lyakhov A.O., Oganov A.R., Stokes H.T., Zhu Q. (2013). New developments in evolutionary structure prediction algorithm USPEX. *Comp. Phys. Comm.* **184**, 1172-1182"

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

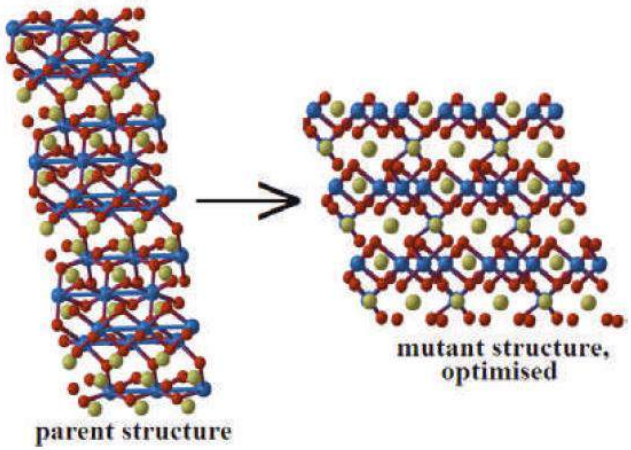
In results1/OUTPUT.txt you will notice:

▷ *variable* `fracLatMut`

Meaning: Percentage of structures obtained from lattice mutations; 0.1 means 10%, *etc.*

Default: `0` for fixed cell prediction; `0.1` otherwise.

```
-------------------------------------------------------------------------------
----------------------------- VARIATION OPERATORS -----------------------------
-------------------------------------------------------------------------------
The fittest 60 percent of the population used to produce next generation
    fraction of generation produced by heredity        :     0.50
    fraction of generation produced by random          :     0.20
    fraction of generation produced by softmutation    :     0.25
    fraction of generation produced by permutation     :     0.05
    fraction of generation produced by latmutation     :     0.10
    fraction of generation produced by rotmutation     :     0.00
    fraction of generation produced by transmutation   :     0.00
-------------------------------------------------------------------------------
------------------------- Variation operators applied -------------------------
-------------------------------------------------------------------------------
          3 structures produced by heredity
          1 structures produced by random
          1 structures produced by softmutation
          0 structures produced by permutation
          0 structures produced by latmutation
          1 structures kept as best from the previous generation
          0 structures imported from the other USPEX Calculations
          0 Seeds structures are added from Seeds/POSCARS
```



Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

INPUT.txt:

```
51  ******************************************
52  *   DETAILS OF AB INITIO CALCULATIONS    *
53  ******************************************
54  % abinitioCode
55  3 3 3
56  % ENDabinit
57
58  % KresolStart
59  0.16 0.14 0.12
60  %  Kresolend
61
62  % commandExecutable
63  gulp < input > output
64  % EndExecutable
65
66  1       : numParallelCalcs (how many parallel calculations shall be performed)
67  0       : whichCluster (0: no-job-script, 1: local submission, 2: remote submission)
68  100     : ExternalPressure (GPa)
69
70  0       : pickUpYN (if pickUpYN~=0, then a previous calculation will be picked up)
71  0       : pickUpGen (at which generation shall the previous calculation be picked up)
72  0       : pickUpFolder (number of the results folder to be used)
```

▷ *variable* abinitioCode

Meaning: Defines the code used for every optimization step.

Default: 1 for every optimization step (VASP)

Format:

```
% abinitioCode
3 2 2 1 1
% ENDabinit
```

Note: Numbers indicate the code used at each step of structure relaxation: 1 — VASP, 2 — SIESTA, 3 — GULP, 4 — LAMMPS, 5 — Neural Networks code, 6 — DMACRYS, 7 — CP2K, 8 — Quantum Espresso, 9 — ASE, 10 — ATK, 11 — CASTEP.

▷ *variable* KresolStart

Meaning: Specifies the reciprocal-space resolution for k-points generation (units: $2\pi\text{Å}^{-1}$).

Default: from 0.2 to 0.08 linearly

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Run the example:

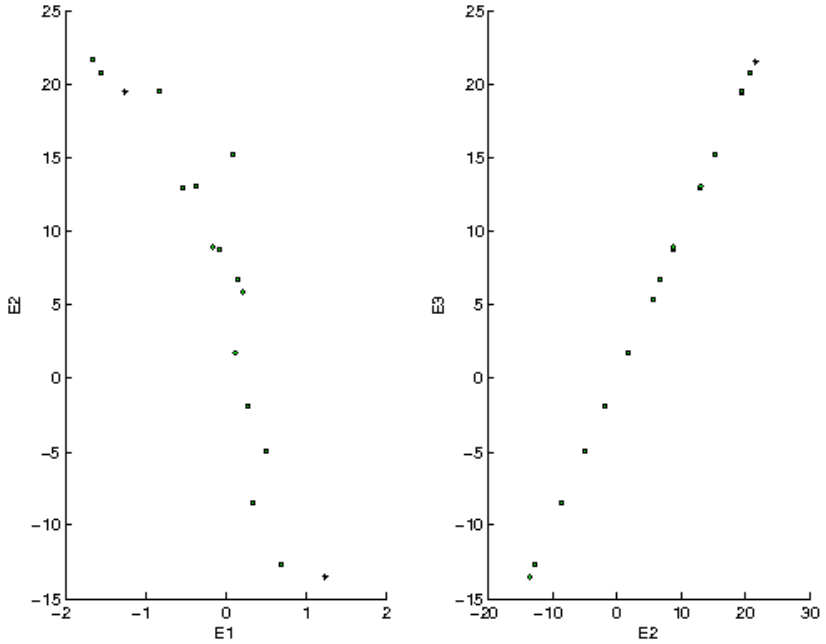
- cp –r ~/examples/example1_GULP_300/ .
- cd example1_GULP_300/
- bsub < USPEX_GULP_300.job

Monitor **log** file, check if **USPEX_IS_DONE** file appeared. Then cd to **results1/** to view results.

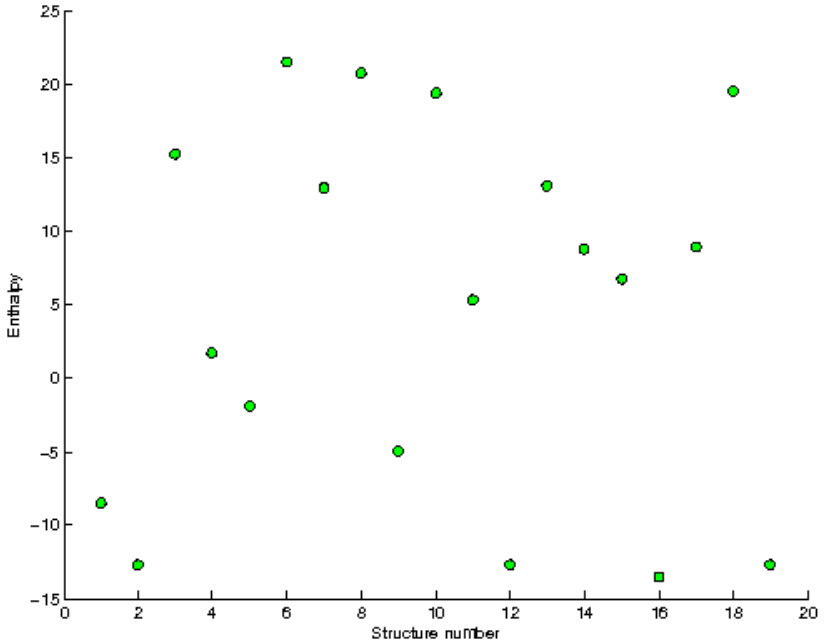
Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Output files:

E_series.tif



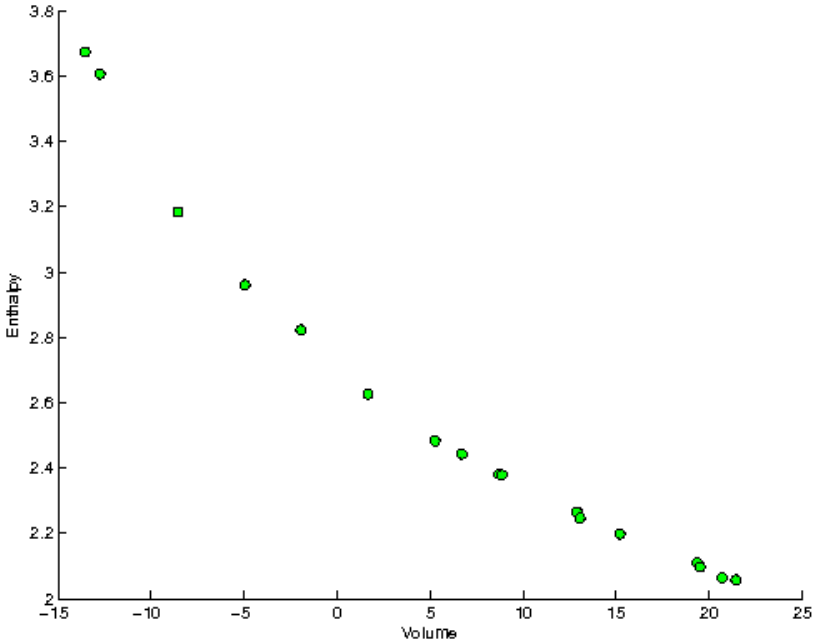
Energy_vs_N.tif



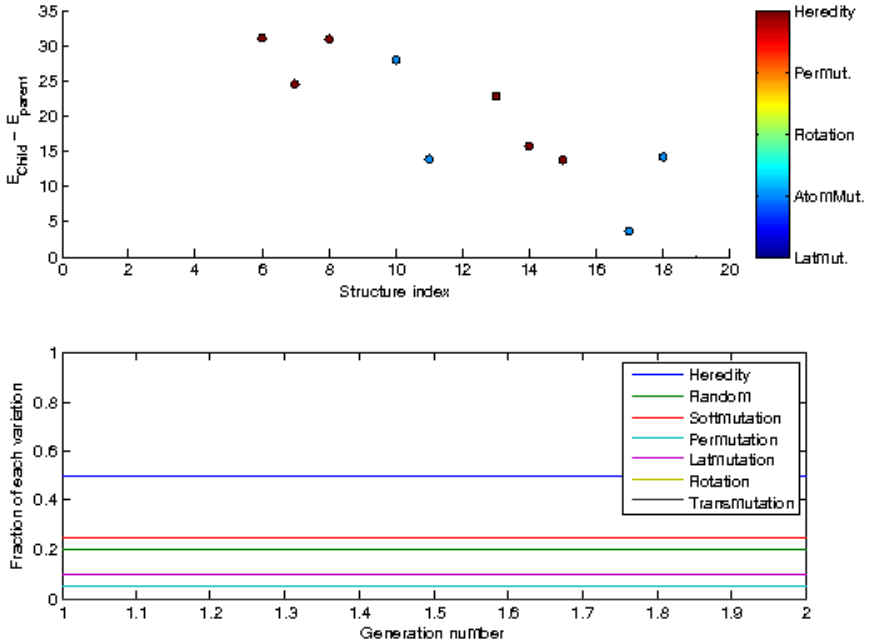
Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Output files:

Energy_vs_Volume.tif



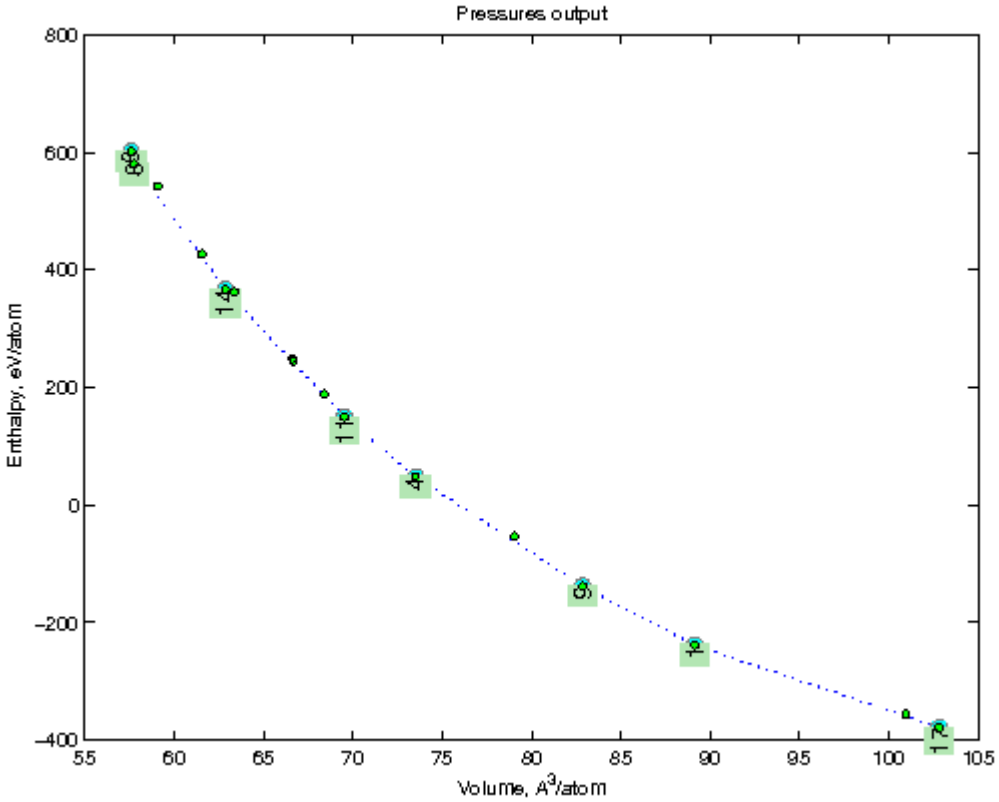
Variation-Operators.tif



Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Output files:

Pressures_output.png



Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Output files:

log – contains console output of USPEX
results1/generation*/ folders – contain results in *.mat files for the generations
results1/OUTPUT.txt – contains detailed information on each generation
results1/Parameters.txt = INPUT.txt
Individuals – summary file where you can find main results:

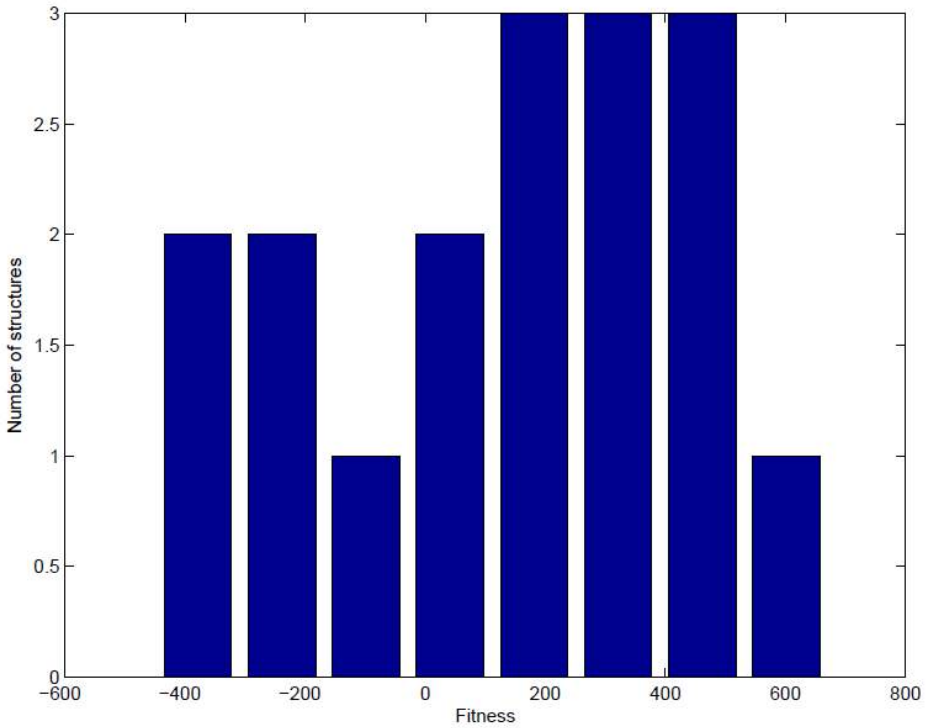
Gen	ID	Origin	Composition	Enthalpy (eV)	Volume (A^3)	Density (g/cm^3)	Fitness	KPOINTS	SYMM	Q_entr	A_order	S_order
1	1	Random	[4 8 16]	-238.872	89.138	10.601	-238.872	[1 1 1]	1	0.207	0.887	1.782
1	2	Random	[4 8 16]	-356.267	100.939	9.362	-356.267	[1 1 1]	1	0.244	0.847	1.547
1	3	Random	[4 8 16]	427.272	61.546	15.354	427.272	[1 1 1]	8	0.227	0.868	1.645
1	4	Random	[4 8 16]	47.898	73.509	12.855	47.898	[1 1 1]	1	0.228	0.831	1.590
1	5	Random	[4 8 16]	-53.740	79.057	11.953	-53.740	[1 1 1]	1	0.221	0.807	1.577
2	6	Heredity	[4 8 16]	601.445	57.609	16.403	601.445	[1 1 1]	1	0.226	0.774	1.504
2	7	Heredity	[4 8 16]	362.394	63.374	14.911	362.394	[1 1 1]	1	0.226	0.801	1.541
2	8	Heredity	[4 8 16]	580.464	57.730	16.368	580.464	[1 1 1]	1	0.207	0.812	1.642

BESTIndividuals – gives this information for the best structures from each generation
gatheredPOSCARS – concatenated POSCAR files
gatheredPOSCARS_order – same as gatheredPOSCARS, but with order parameter
BESTgatheredPOSCARS – the same data for the best structure in each generation
BESTgatheredPOSCARS_order – same as BESTgatheredPOSCARS, but with order parameter

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

Output files:

goodStructures – like Individuals, but ordered by descending of stability
goodStructures_POSCARS – concatenated POSCAR files ordered by descending of stability
enthalpies_complete.dat – gives the enthalpies for all structures in each stage of relaxation
non_optimized_structures – gives all structures produced before relaxation
origin – shows which structures originated from which parents and through which variation operators
fitnessStatistics.pdf:



Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

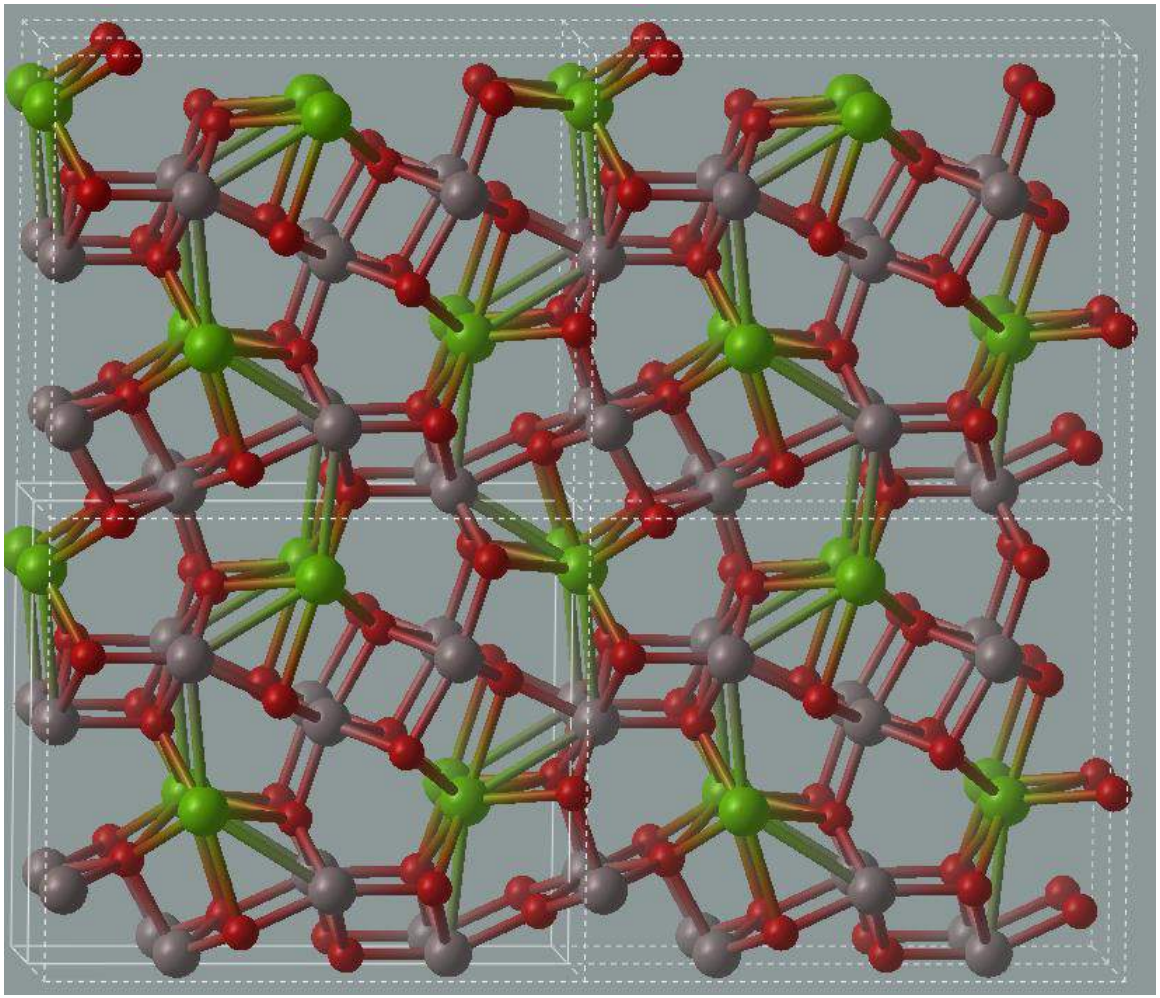
View gatheredPOSCARS:

- cd results1/
- python ~/examples/split_POSCARS.py

This will produce **POSCAR_files/** folder with splitted POSCAR files, which you can download on your computer and visualize using VESTA, VMD, etc.

Bulk $Mg_4Al_8O_{16}$ (example1_GULP_300)

View **gatheredPOSCARS** (from reference_long/):



Examples for today:

- Bulk $Mg_4Al_8O_{16}$ (fixed composition, calculationType=300, GULP)
- **Bulk Si-C (variable composition, calculationType=301, VASP)**
- O_2 @ Si (100) (fixed composition, calculationType=200, VASP)
- C_{13} nanoparticles (fixed composition, calculationType=000, VASP)

Bulk Si-C (example2_VASP_301)

INPUT.txt:

```
% PARAMETERS EVOLUTIONARY ALGORITHM

USPEX : calculationMethod (USPEX, VCNEB, META)
301   : calculationType (dimension: 0-3; molecule: 0/1; va
1     : optType (1=enthalpy, 2=volume, 3=hardness, 4=struc

% symmetries
2-230
% endSymmetries

% atomType
Si C
% EndAtomType

% numSpecies
1 0
0 1
% EndNumSpecies

% valences
4 4
% endValences
```

▷ *variable* calculationType

Meaning: Specifies type of calculation, *i.e.*, whether the structure of a bulk crystal, nanoparticle, or surface is to be predicted. This variable consists of three indices: *dimensionality*, *molecularity*, and *compositional variability*:

- dimensionality:
  - "3" — bulk crystals
  - "2" — surfaces, "–2" — 2D-crystals
  - "1" — polymers
  - "0" — nanoparticles
- molecularity:
  - "0" — non-molecular
  - "1" — molecular calculations
- variability of chemical composition in the calculation:
  - "0" — fixed composition
  - "1" — variable composition

Default: 300

Format:

molecular crystal is to be performed, ...with molecular geometries for all n the newly generated structures as 201, –200 (and not yet released: 110,

Notes: For variable-composition calculations, you have to specify the compositional building blocks as follows:

```
% numSpecies
2 0 3
0 1 1
% EndNumSpecies
```

This means that the first building block has formula A_2C_3 and the second building block has formula BC, where A, B and C are described in the block `atomType`. All structures will then have the formula $xA_2C_3 + yBC$ with x, y = (0,1,2,...) — or $A_{2x}B_yC_{3x+y}$. If you want to do prediction of all possible compositions in the A-B-C system, you should specify:

```
% numSpecies
1 0 0
0 1 0
0 0 1
% EndNumSpecies
```

Bulk Si-C (example2_VASP_301)

INPUT.txt:

```
2      : minAt
4      : maxAt

0.6    : bestFrac

0.40   : fracGene (fraction of generation produced by heredity)
0.20   : fracRand (fraction of generation produced randomly from space groups)
0.20   : fracAtomsMut (fraction of the generation produced by softmutation)
0.20   : fracTrans

2.0    : minVectorLength ( minimal length of any lattice vector)

% IonDistances
1.0 0.9
0.0 0.8
% EndDistances


abinitioCode (which code from CommandExecutable shall be used for calculation? )
1 1
ENDabinit

% KresolStart
0.15 0.12
% Kresolend

1      : numParallelCalcs (how many parallel calculations shall be performed)
0      : whichCluster (0: no-job-script, 1: local submission, 2: remote submission)
0.010  : toleranceFing (tolerance for identical structures)

0      : pickUpYN (if pickUpYN~=0 , then a previous calculation will be picked
0      : pickUpGen (at which generation shall the previous calculation be picked
0      : pickUpFolder (number of the results folder to be used. If = 0 , then

% commandExecutable
vasp > output
% EndExecutable
```

Si Si C
C

▷ *variable* `minAt`

Meaning: Minimum number of atoms in the unit cell for the first generation.

Default: No default

▷ *variable* `maxAt`

Meaning: Maximum number of atoms in the unit cell for the first generation.

Default: No default

Only for variable-composition calculations!

▷ *variable* `minVectorLength`

Meaning: Sets the minimum length of a cell parameter of a newly generated structure.

Default: 1.8 × covalent diameter of the largest atom.

1 for VASP

Bulk Si-C (example2_VASP_301)

Run the example:

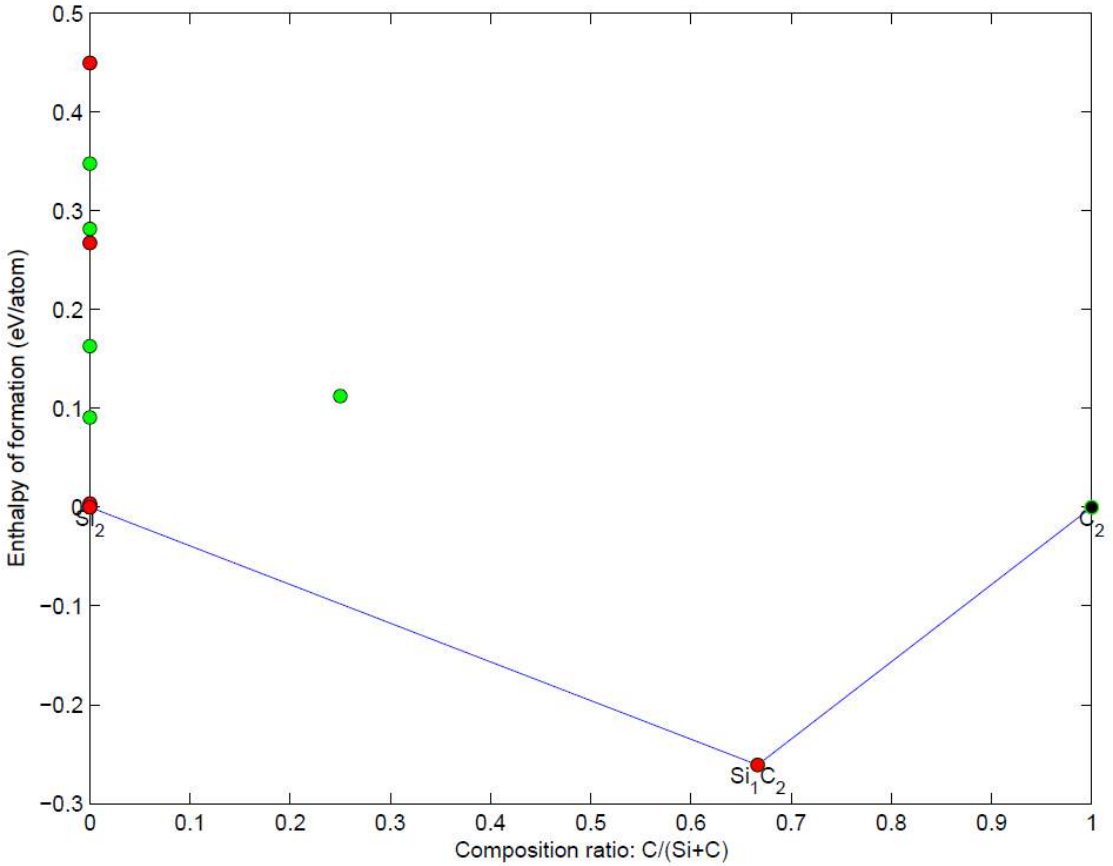
- cd ~/workshop/<your directory>
- cp –r ~/examples/example2_VASP_301/ .
- cd example2_VASP_301/
- bsub < USPEX_VASP_301.job

Monitor **log** file, check if **USPEX_IS_DONE** file appeared. Then cd to **results1/** to view results.

Bulk Si-C (example2_VASP_301)

Output files:

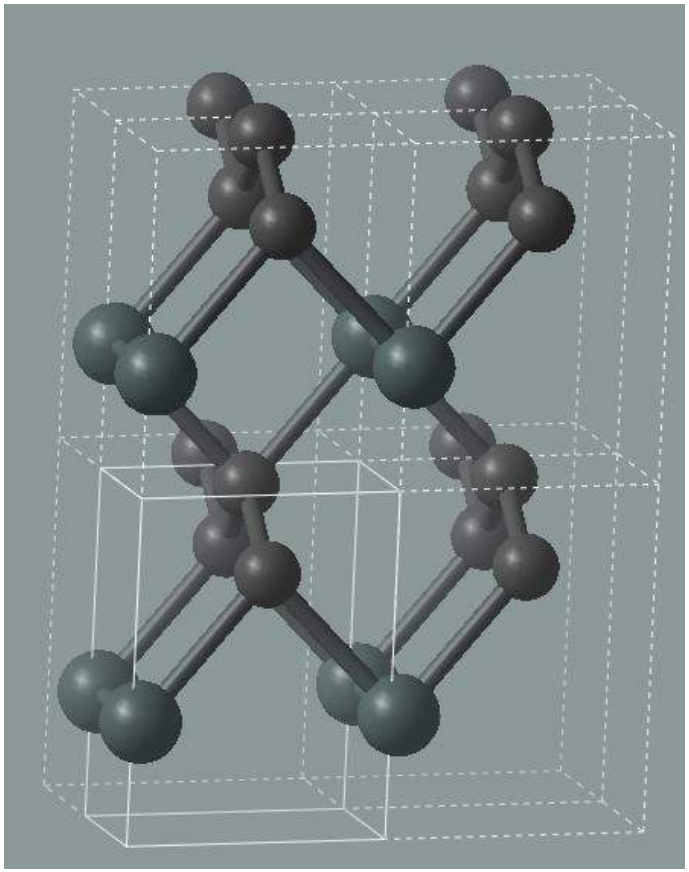
extendedConvexHull.pdf



Bulk Si-C (example2_VASP_301)

Output files:

convex_hull – gives all thermodynamically stable compositions, and their enthalpies (per atom)
extended_convex_hull, extended_convex_hull_POSCARS – all unique low-energy compositions and structures



Your structures may be different!

Examples for today:

- Bulk $Mg_4Al_8O_{16}$ (fixed composition, calculationType=300, GULP)
- Bulk Si-C (variable composition, calculationType=301, VASP)
- **O_2 @ Si (100) (fixed composition, calculationType=200, VASP)**
- C_{13} nanoparticles (fixed composition, calculationType=000, VASP)

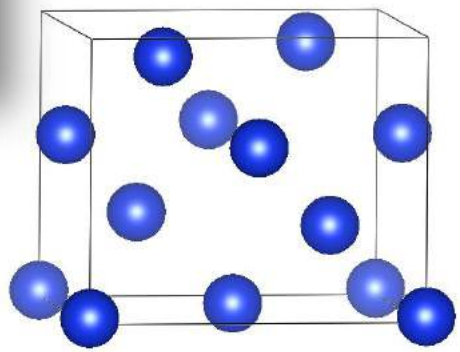
O_2 @ Si (100) (example3_VASP_200)

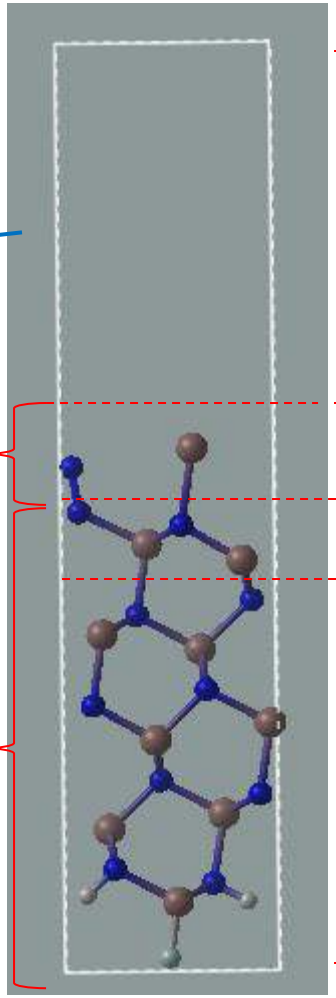
INPUT.txt:

```
1  ****************************************
2  *      TYPE OF RUN AND SYSTEM          *
3  ****************************************
4  ****************************************
5  USPEX   : calculationMethod (USPEX, VCNEB, META)
6  200     : calculationType (dimension: 0-3; molecule: 0/1; varcomp: 0/1)
7  1       : optType (1=enthalpy, 2=volume, 3=hardness, 4=struc_order, 5=aver_dist)
8  2.0     : thicknessS (thickness of surface region, 2 A by default)
9  3.0     : thicknessB (thickness of buffer region in substrate, 3 A by default)
10 1       : reconstruct (only used in surface)
11
12 % vacuumSize
13 5
14 % endVacuumSize
15
16 % atomType
17 Si O
18 % EndAtomType
19
20 % numSpecies
21 0 2
22 % EndNumSpecies
23
24 % symmetries
25 2-17
26 % endSymmetries
27
28
29 ****************************************
30 *               POPULATION             *
31 ****************************************
32 5     : populationSize (how many individuals per
33 5     : initialPopSize
34 4     : numGenerations (how many generations shal
35 4     : stopCrit
36 1     : AutoFrac
```

11 Appendix: List of plane groups

Number	Group
1	Group p1
2	Group p2
3	Group pm
4	Group pg
5	Group cm
6	Group pmm
7	Group pmg
8	Group pgg
9	Group cmm
10	Group p4
11	Group p4m
12	Group p4g
13	Group p3
14	Group p3m1
15	Group p31m
16	Group p6
17	Group p6m





O_2 @ Si (100) (example3_VASP_200)

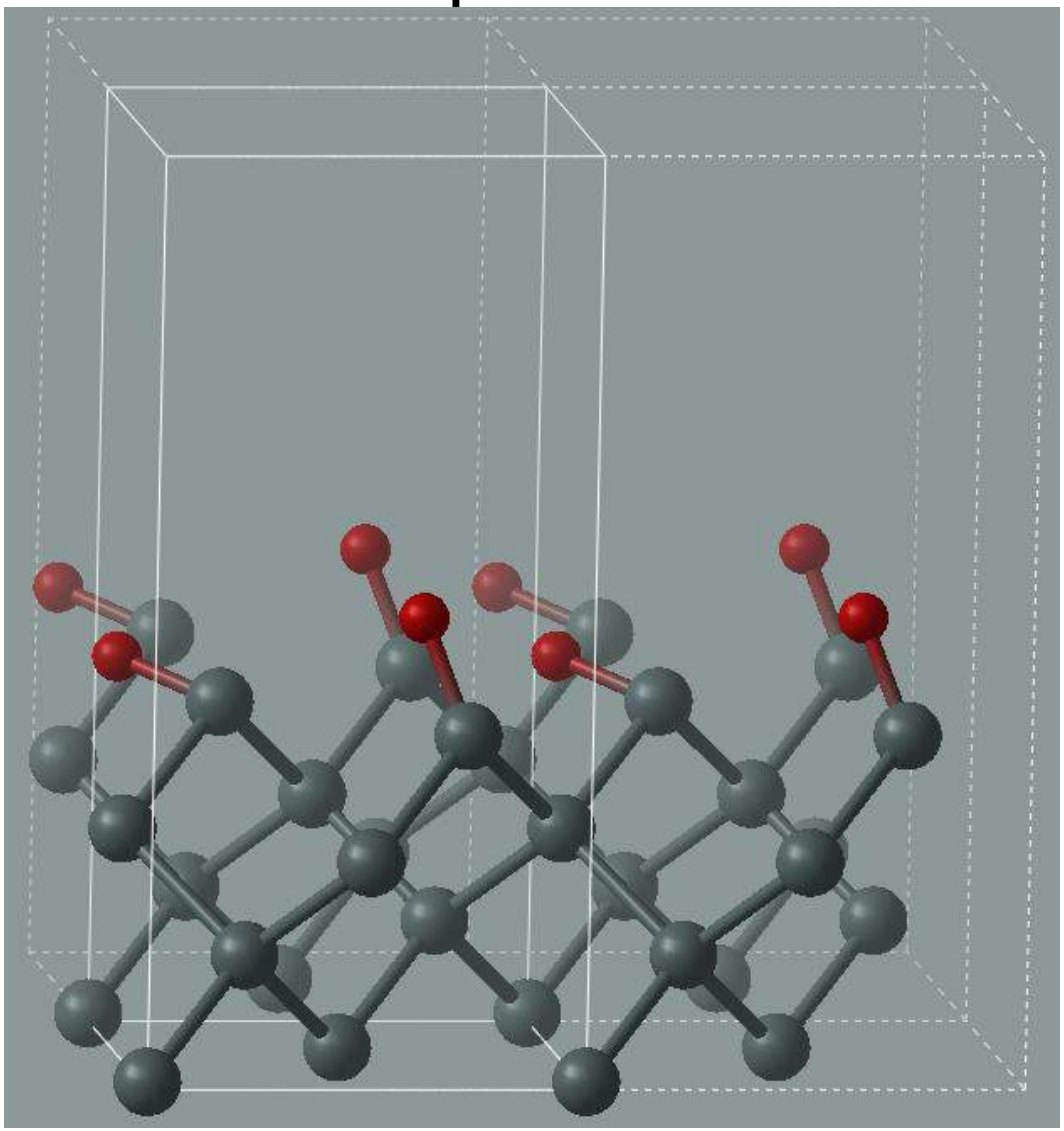
Run the example:

- cd ~/workshop/<your directory>
- cp –r ~/examples/example3_VASP_200/ .
- cd example3_VASP_200/
- nohup ./uspex_VASP_200.sh > out 2>&1 &

Monitor **log** file, check if **USPEX_IS_DONE** file appeared. Then cd to **results1/** to view results.

O_2 @ Si (100) (example3_VASP_200)

Output files:



Your structures may be different!

Examples for today:

- Bulk $Mg_4Al_8O_{16}$ (fixed composition, calculationType=300, GULP)
- Bulk Si-C (variable composition, calculationType=301, VASP)
- O_2 @ Si (100) (fixed composition, calculationType=200, VASP)
- **C_{13} nanoparticles (fixed composition, calculationType=000, VASP)**

C_{13} nanoparticles (example4_VASP_000)

INPUT.txt:

```
PARAMETERS EVOLUTIONARY ALGORITHM
****************************************
****************************************
*      TYPE OF RUN AND SYSTEM          *
****************************************
****************************************
USPEX : calculationMethod (USPEX, VCNEB, META)
000   : calculationType (dimension: 0-3; molecule: 0/1; varcomp: 0/1)
1     : optType (optimise by: 1=enthalpy, 2=volume, 3=hardness, 4=struc_order, 5=aver_dist, 6=mag_moment)

% vacuumSize
5
% endVacuumSize

% What symmetry(s) have to be satisfied by the randomly created structures
% symmetries
E C2 D2 C4 C3 C6 T S2 Ch1 Cv2 S4 S6 Ch3 Th Ch2 Dh2 Ch4 D3 Ch6 O D4 Cv3 D6 Td Cv4 Dd3 Cv6 Oh Dd2 Dh3 Dh4 Dh6 Oh C5 S5 S10 Cv5 Ch5 D5 Dd5 Dh5 I Ih
% endSymmetries

%%%%%%%%%%%%%%%%%%%
% Here come the atomic numbers of the atoms involved
% atomType
C
% EndAtomType

% numbers of species (ions/molecules/blocks) of each type
% numSpecies
13
% EndNumSpecies


****************************************
*              POPULATION              *
****************************************
5    : populationSize (how many individuals per generation)
5    : initialPopSize
4    : numGenerations (how many generations shall be calculated)
4    : stopCrit
```

```
****************************************
*                 CELL                 *
****************************************
% The following is what you know about the lattice. If you know the lattice
% vectors, type them in as 3x3 matrix. If not, type the estimated volume.
% For variable composition - type the estimated atomic volume for each element.
% Latticevalues (this word MUST stay here, type values below)
200
% Endvalues (this word MUST stay here)
```

C_{13} nanoparticles (example4_VASP_000)

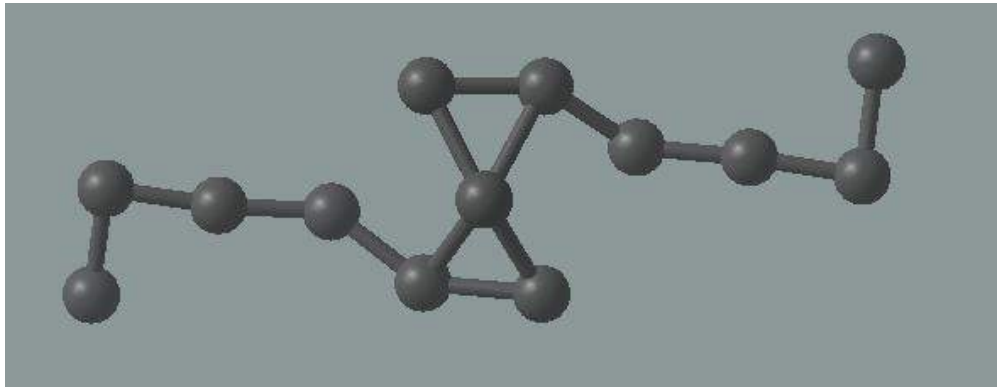
Run the example:

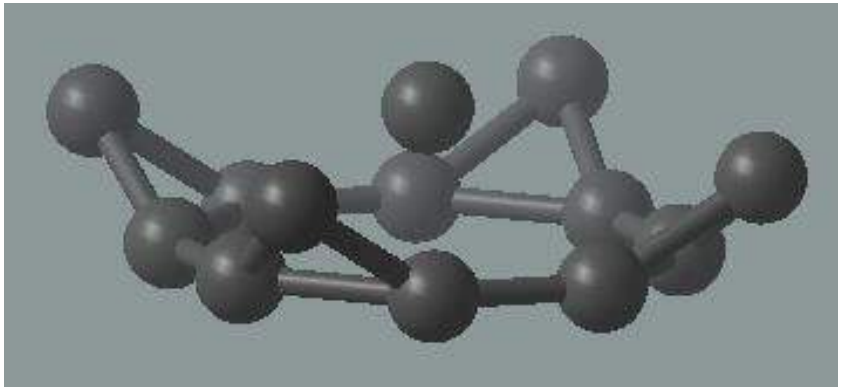
- cd ~/workshop/<your directory>
- cp –r ~/examples/example4_VASP_000/ .
- cd example4_VASP_000/
- nohup ./uspex_VASP_000.sh > out 2>&1 &

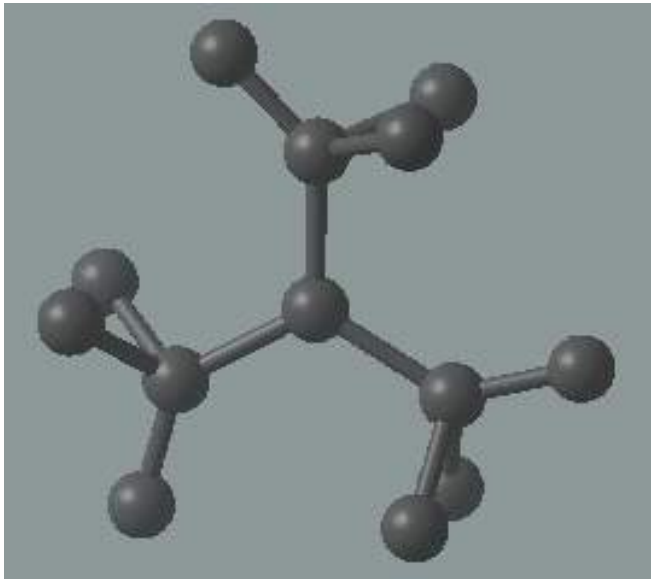
Monitor **log** file, check if **USPEX_IS_DONE** file appeared. Then cd to **results1/** to view results.

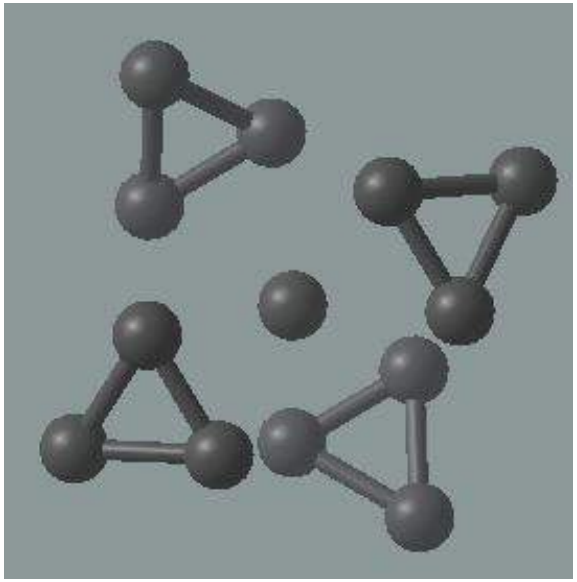
C_{13} nanoparticles (example4_VASP_000)

Results:










Dank u wel
Mahalo
Juspaxar
Khawp khun
Spasibo
Efcharisto
Salamat
Thank
Toda raba
Cám ơn
Dhanyawaad
Köszi
Pidamayado
Dankon
Tusen takk
Terima kasih
Merci
Doh je
Shukria
Grazie mille
Kamsahamnida
Shukuria
Tashakkur
Makasi
Paldies
bolzïn
you
Gracias
suksama
Biyan
Maake
Donkaaja
Tingki
Komapsumnida
gozaimashita
atu
Fakaaue
Sposibo
Tesekkurler
Ekhmet
Mehrbani
Yaqhanyelay
Efcharisto
Arigato
Obrigado
Dankscheen