The Alloy-Theoretic Automated Toolkit (ATAT): A User Guide

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Chapter 1

Features/Capabilities

The Alloy-Theoretic Automated Toolkit (ATAT) is a generic name that refers to a collection of alloy theory tools:

- Codes to construct cluster expansions from first-principles (maps and mmaps). A cluster expansion is a very compact and efficient expression giving the energy of an substitutional alloy as a function of its configuration (i.e. which type of atom sits where on the lattice).
- Codes to perform Monte Carlo simulation (emc2 and memc2) of lattice models in order to compute thermodynamic properties of alloys, starting from a cluster expansion.
- Codes to perform lattice dynamics calculations (fitfc, fitsvsl, svsl)
- Codes to calculate electronic and magnetic free energy contributions (felec, fmag, fempmag) using simple physical or semiempirical models.
- Utilities to combine all of the above to generate free energies that include configurational, vibrational and electronic contributions (mkteci).
- Codes to generate Special Quasirandom Structures (SQS), to model disordered solid solutions (mcsqs, gensqs) and to enumerate structures (genstr).
- A large library of pre-computed SQS and structure prototypes.
- Extension of the two above tools that allow the construction of so-called reciprocal-space cluster expansion, which are useful to model the energetics of alloys exhibiting a large atomic size mismatch.
- Tensorial cluster expansions (gce).
- Elastic constant calculations (calcelas).
- Structure conversion utilities (subcells, supercells, coordinate system changes, file format, etc.) (cellcvrt, wycked, etc.)
- Scripts to automate tasks (foreachfile, sspp, getvalue, getlines, etc.).
- Codes to generate CALPHAD databases (sqs2tdb).
- Utilities to interface the above tools with first-principles codes, such as VASP (runstruct_vasp, runstruct_abinit, runstruct_gulp, etc.).
- Job control utilities that enable the efficient use of a cluster of workstations to run the first-principles codes that provide the input to the above codes (pollmach).

Chapter 2

Credits and Licence

The Alloy-Theoretic Automated Toolkit (ATAT)[1] is a generic name that refers to a collection of alloy theory tools developped by Axel van de Walle[2], in collaboration with various research groups.

2.1 Collaborators and Credits

The MAPS[3] (MIT Ab-initio Phase Stability) code, which automatically constructs a cluster expansion from the result of first-principles calculations, was developped by Axel van de Walle in collaboration with Prof. Gerd Ceder's group[4] from the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. MAPS consists of the following codes: maps, corrdump, genstr, checkcell, kmesh, cv.

The EMC2 (Easy Monte Carlo Code), which automate the calculation of alloy thermodynamic properties via Monte Carlo simulations of lattice models, were developped by Axel van de Walle in collaboration with Prof. Mark Asta's group[5] from the Department of Materials Science and Engineering at Northwestern University. EMC2 consists of the following codes: emc2, phb.

The CSE (Constituent Strain Extension) to both the MAPS and EMC2 codes, which implement the constituent strain formalism based on a reciprocal-space cluster expansion, was developped by Axel van de Walle in collaboration with Alex Zunger's Solid State Theory Group[6] at the National Renewable Energy Laboratory in Golden, Colorado and in collaboration with Gus Hart[7] from the Department of Physics and Astronomy at Northern Arizona University. CSE conssists of the following files: csfit.cc predcs.cc, predrs.cc, kspacecs.cc.

Mayeul D'Avezac at NREL has provided all the changes needed for ATAT to compile with g++ versions 4.1 and later as well as intel's c++ compiler.

Volker Blum at NREL has contributed to improve the portability of the package by providing a `perl` version of the `chl` utility.

Dongwon Shin at Penn State has converted a large number of common lattices (found at the NRL navy web site[8]) into the `atat` format. See directory `data/str`.

Greg Pomrehn has improved the efficiency of the structure enumeration algorithm and contributed the script `mmapsrep`.

Jesper Kristensen has been quite active on the ATAT forum, helping me answer queries. He also maintains some documentation on his web site[9]

Ruoshi Sun has also answered many queries on the ATAT forum.

Martin Bäker has written a simple and useful tutorial for ATAT's emc2 and phb tools for computing phase diagrams via Monte Carlo.

[1] http://www.its.caltech.edu/~avdw/atat/
[2] http://www.mit.edu/~avdw/
[3] http://www.mit.edu/~avdw/maps
[4] http://burgaz.mit.edu/
[5] http://cms.northwestern.edu/
[6] http://www.sst.nrel.gov/
[7] http://www.phy.nau.edu/~hart/
[8] http://cst-www.nrl.navy.mil/lattice/
[9] http://www.jespertoftkristensen.com/

The FFT routines in the files fftn.cc and fftn.h were obtained from the package go/fft-olesen.tar.gz available from Netlib[10]. The origin of these routines dates back to a FORTRAN code by R. C. Singleton in 1968 [19], later converted to C and subsequently improved by Mark Olesen and John Beale in 1995. These routines are included in the `atat` package for sole purpose of providing users with the convenience of avoiding a separate download. Axel van de Walle does not claim any ownership of them or intellectual credit for them.

Some of the basic numerical routines were inspired by Numerical Recipes in C, although they were completely re-written according to the ATAT code style conventions, for instance to use 0-indexed arrays and make better use of C++ features.

The Perl routines Permutor (written by Tom Phoenix) and PowerSet (written by David Landgren) were downloaded from the free software resource CPAN.org and included in this distribution simply to avoid users a separate download.

Gao Zhe has contributed an interface to PWSCF (aka Quantum Espresso) that can be found in atat/glue/qe

Matt Probert has contributed an interface to CASTEP that can be found in atat/glue/castep/

2.2 Financial Support

The development of MAPS was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under contract no. DE-F502-96ER 45571. Gerbrand Ceder acknowledges support of Union Minière through a Faculty Development Chair. Axel van de Walle acknowledges support of the National Science Foundation under program DMR-0080766 and DMR-0076097 during his stay at Northwestern University.

The development of EMC2 was supported by the NSF under program DMR-0080766.

The development of the CSE is supported by the NSF under program DMR-0080766.

The development of the tensorial cluster expansion (GCE and gencs code) is supported by the Center for the Science and Engineering of Materials at Caltech, an NSF-funded MRSEC and by the NSF CMMT grant DMR-0907669.

The development of the wycked and getproto codes is supported by the NSF CAREER grant DMR-1154895.

The development of the mcsqs code is supported by ONR grants N00014-11-1-0886 and N00014-12-1-0557.

The development of the sqs2tdb, robustrelax_vasp, infdet and of the SQS database is supported by ONR grants N00014-14-1-0055 and N00014-17-1-2202.

2.3 License and Agreements

[10] http://www.netlib.org/go/fft-olesen.tar.gz
[11] http://creativecommons.org/licenses/by-nd/4.0/
[12] http://creativecommons.org/licenses/by-nd/4.0/
[13] https://alum.mit.edu/www/avdw/atat/
[14] mailto:avdw@alum.mit.edu
[15] references.bib

1. A. van de Walle and G. Ceder, "Automating First-Principles Phase Diagram Calculations[16]", *Journal of Phase Equilibria*, **23**, 348, (2002).

2. A. van de Walle and M. Asta, "Self-driven lattice-model Monte Carlo simulations of alloy thermodynamic properties and phase diagrams[17]", *Modelling Simul. Mater. Sci. Eng.* **10**, 521, (2002).

3. A. van de Walle, M. Asta and G. Ceder, "The Alloy Theoretic Automated Toolkit: A User Guide[18]" *CALPHAD Journal*, **26**, 539, (2002).

4. A. van de Walle, "Multicomponent multisublattice alloys, nonconfigurational entropy and other additions to the Alloy Theoretic Automated Toolkit[19]", *Calphad Journal* **33**, 266, (2009).

5. As of version 2.81, the algorithm to generate superstructures has been improved based on the ideas in G. L. W. Hart and R. W. Forcade, "Algorithm for generating derivative structures[20]," *Phys. Rev. B* **77**, 224115, (2008).

6. If the `mcsqs` code is used: A. van de Walle and P. Tiwary and M. M. de Jong and D. L. Olmsted and M. D. Asta and A. Dick and D. Shin and Y. Wang and L.-Q. Chen and Z.-K. Liu, Efficient stochastic generation of Special Quasirandom Structures[21], *Calphad Journal* **42**, 13 (2013).

7. If the constituent strain extension is used: D. B. Laks and L. G. Ferreira and S. Froyen and A. Zunger, *Phys. Rev. B* **46**, p. 12587 (1992).

8. If the robustrelax_vasp command is used: A. van de Walle and S. Kadkhodaei and R. Sun and Q.-J. Hong, "Epicycle method for elasticity limit calculations[22]", *Phys. Rev. B* 95 144113 (2017) and A. van de Walle and Q.-J. Hong and S. Kadkhodaei and R. Sun, "The free energy of mechanically unstable phases[23]", *Nature Commun.* 6 7559 (2015).

9. If the `sqs2tdb` code is used, please cite "Software tools for high-throughput CALPHAD from first-principles data[24]", *Calphad Journal* **58**, 70 (2017).

10. The `wycked` code uses the Wyckoff position database from the Bilbao Crystallographic Server[25]. Accordingly, if you use this code, you should also cite the following papers:

    M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E. Tasci, G. de la Flor, A. Kirov, "Crystallography online: Bilbao Crystallographic Server", *Bulg. Chem. Commun.* **43** 183 (2011).

    M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov and H. Wondratschek, "Bilbao Crystallographic Server I: Databases and crystallographic computing programs", *Z. Krist.* **221**, 15 (2006).

    M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato and H. Wondratschek, "Bilbao Crystallographic Server II: Representations of crystallographic point groups and space groups", *Acta Cryst.* **A62**, 115 (2006).

11. The `getproto` code uses processed data from the index of the Landolt-Börnstein database[26]. This data is available upon request by contacting avdw@alum.mit.edu[27] if you can show that you have access to this database. Also, if using this data, please cite: Villars, P., Cenzual, K., Daams, J., Gladyshevskii, R., Shcherban, O., Dubenskyy, V., Melnichenko-Koblyuk, N., Pavlyuk, O., Stoiko, S., Sysa, L., "Landolt-Börnstein — Group III Condensed Matter: Numerical Data and Functional Relationships in Science and Technology", Edited by Villars, P. and Cenzual, K., SpringerMaterials — The Landolt-Börnstein Database, Volume 43A1-43A10 (2013).

[16] http://arXiv.org/abs/cond-mat/0201511
[17] http://arXiv.org/abs/cond-mat/0201473
[18] http://arxiv.org/abs/cond-mat/0212159
[19] http://arxiv.org/abs/0906.1608
[20] http://link.aps.org/abstract/PRB/v77/e224115
[21] http://dx.doi.org/10.1016/j.calphad.2013.06.006
[22] http://dx.doi.org/10.1103/PhysRevB.95.144113
[23] http://dx.doi.org/10.1038/ncomms8559
[24] http://dx.doi.org/10.1016/j.calphad.2017.05.005
[25] http://www.cryst.ehu.es/
[26] http://www.springermaterials.com/
[27] mailto:avdw@alum.mit.edu

2.4 Beta testers

The following researchers have provided numerous constructive comments that have proven extremely useful to improve the quality of the program.

1. Dane Morgan (University of Wisconsin)
2. Paul Dalach (Northwestern)
3. Dinesh Balachandran (MIT, Gerd Ceder's group)
4. Ben Burton (National Institute of Standards and Technology)
5. Gautam Ghosh (Northwestern University)
6. Nikolai Andreevich Zarkevich (University of Illinois at Urbana-Champaign, Duane Johson's group)
7. Volker Blum (NREL, Alex Zunger's group)
8. Chris Woodward (Northwestern University/Air Force)
9. Zhe Liu (Northwestern University, Mark Asta's group)
10. Yi Wang and Raymundo Arroyave (Pennsylvania State University, Long-Qing Chen and Zi-Kui Liu's group)
11. Elif Ertekin (University of California at Berkeley, Daryl Chrzan's group)
12. Rodrigo Barbosa Capaz (University of California at Berkeley)
13. Sundar Amancherla (General Electric)

Chapter 3

Getting started

3.0.1 Requirements

You need the following utilities installed:

- `g++` version 2.7.2 or later. Type `g++ --version` to verify this. This package can be downloaded from http://www.gnu.org/.
- GNU `make` (any version). Type `make --version` to verify this. On some systems this command may be called `gmake` or `gnumake`. This package can be downloaded from http://www.gnu.org/.
- A first-principle electronic structure calculation code, such as VASP[1]
- You may want to use `gnuplot` to plot the output of the code. Type `gnuplot` and check the program starts (Type `q` to quit). If not, it can be downloaded from http://www.gnuplot.info/.
- You may need `ssh` if you have multiple machines and they are connnected through an unsecure network (e.g. the internet). This package can be downloaded from http://www.openssh.com/.

3.0.2 Installation

If you have an earlier version of `ATAT` installed, please delete or rename the former `atat` directory before proceeding, e.g.,

```
mv atat atatold
```

Then, type

```
gunzip atatX_XX.tar.gz
```

```
tar -xvf atatX_XX.tar.gz
```

where `X_XX` is the current version number. These commands create a directory called atat in the current directory. It contains the whole package. For future reference, I'll call the whole access path to this directory `atat`.

Type

```
cd atat
```

and open the file `makefile` with a text editor and look for the line `BINDIR=$(HOME)/bin/`. Change `$(HOME)/bin/` to point wherever you want to put the executables. Type

```
make
```

If no error message appears, proceed with the next steps, otherwise consult Chapter 8.

```
make install
```

`rehash` (not necessary with bash shell)

[1] http://cms.mpi.univie.ac.at/vasp/

3.0.3 Test MAPS with a simple example

Change to a directory of your choice (preferably empty) and type

```
cp atat/examples/cuau.in lat.in
```

```
maps -d &
```

Maps is running and waiting for a signal. Type

```
touch ready
```

to indicate that you are ready to for maps to generate a structure. Maps replies `Finding best structure...` To find the structure just created, wait for `done` to appear and type:

```
ls */wait
```

to observe that directory `0` has been created. This directory contains a file `str.out` which describes the structure whose energy needs to be calculated. The file `wait` is just a flag that allows you to find the newly created directory. Let's pretend that we have computed the energy of that structure. We need to let maps know about it. Type, for instance:

`echo 1.1 > 0/energy` (If 1.1 is the energy of the structure.)

```
rm 0/wait
```

Maps responds by `Finding best cluster expansion...`, followed by `done`. You can repeat the process (`touch ready`, etc.) to add more structures. Maps will update the current cluster expansion every time a new energy becomes known. (By default, maps checks every 10 sec.). For a description of the output files, type:

```
maps -h | more
```

or refer to section 7 A nice utility called `mapsrep` allows you to plot the results using gnuplot. To stop maps cleanly, type: `touch stop`

Suggestion: to clarify the output of the program, it is recommended that you run `maps` in one terminal window and type all other command in another terminal window.

3.1 Install the interface between MAPS and VASP

Type

```
ezvasp
```

and follow the instructions posted on the screen to configure this command.

To test this interface, change to a directory of your choice and type

```
maps -d &
```

(unless maps is running already in that same directory).

While MAPS automatically create files that describe the geometry of the structures (called`n/str.out`, where `n` is the structure name), we need to provide a file containing all the other parameters needed by the first-principles code. Type:

```
cp atat/glue/vasp/vasp.wrap .
```

to copy an example of such file in the current directory. For a description of these parameters, type:

```
ezvasp -h | more
```

Let's say you have a new structure in directory `0` (created by typing `touch ready`). Type:

```
cd 0
```

`runstruct_vasp`

When the command has terminated, the directory `0` will contain a file `energy` giving the energy of the structure. If error messages appear consult Chapter 8.

If no error messages appear, you can proceed another level up in automation. Type

`cd ..` (to go back into the main directory)

`pollmach runstruct_vasp &`

This script will automatically call the above command repeatedly. To stop it cleanly, type:

`touch stoppoll`

(Disregard the warning message.) If you only have access to one machine, this is as good as it gets, if you have more than one machine, read the next section. If you want to use another code than VASP, read section 3.3.

3.2 Install and test the job control utilities

This section requires some knowledge of UNIX, but it is worth it!

3.2.1 With queueing systems

Let's start with the simple and common case of a computer cluster with a queueing system. We don't give here the specific syntax of the job submission script, because it is highly system-dependent. In a nutshell, one would submit on job containing the following commands, assuming the system is using a standard implementation of MPI:

[some header specifying the number of nodes etc.]

`maps -d &` (note the `&` to run in the background.)

`pollmach runstruct_vasp mpirun` (you may need to specify the number of processors as `mpirun -np [number]`)

If your system does not allow a background commands in the script (or if this would be very inefficient), then you could put each command (without `&`) in a separate script, but making sure they run at the same time. Either way, parallelization occurs at the level of the `vasp` command. If you wish to also parallelize by running multiple vasp commands simultaneously then you should submit yet another job script with

[some header specifying the number of nodes etc.]

`pollmach runstruct_vasp mpirun`

repeating this process as many times as you the number of simultaneous `vasp` processes you want (note that there is still only one copy of `maps` running).

3.2.2 Without queueing systems

We now cover the case where there is no queueing system and the user has full power to run on any of the nodes in the cluster.

Networking problems can be tricky and we will test various thing as we go along. You only need to perform this installation on your "master" machine that will run maps. All other machine (which we be called the "remote" machines) only need to have VASP (or any other ab-initio code).

Before you start, you must first make sure that it is possible to login from the master machine to the remote machines without entering a password. This is essential for the program to be able to run on its own, without your intervention. Don't worry it is generally possible to do this without compromising the security of your system. Two commands allow you to run a command on a remote machine. If the master and remote machines are connected through a secure network (e.g. a beowolf cluster having its own local network) or if you don't care about security (for now), you can use `rsh`. Otherwise, `ssh` provides a secure way to command a machine remotely.

To set up `rsh` so that you can login without typing a password, you must have the appropriate `.rhosts` file on the remote machine. For more information, consult the `rsh` man page. (One important issue, often not mentioned

in the man pages, its that you need to set the file permissions of the `.rhosts` file so that noone else but you has "write" permission: `chmod og-w ~/.rhosts`).

To set up `ssh` so that you can login without typing a password, consult the `ssh` man page, especially the section on "RSA-based host authentication". (This is the feature that makes the login secure even if no password is needed.) In general, setting this up involves creating a `.shosts` file and generating a public key files to be copied onto the remote machines.

If your username is different on the remote machine and if you use `ssh`, use the syntax `node username@host` instead. If you use `rsh`, use the syntax `node -l username host`.

Once you are able to run either `rsh node2 ls` or `ssh node2 ls` and get the content of your home directory on the remote machine (assuming that you have a remote machine called `node2`), you can proceed to the next step. Do you have the same home directory on the master and remote machines and does it have the same access path? To check this, `cd` to some arbitrary subdirectory and type:

```
node node2 ls
```

where `node` is a command provided with ATAT and node2 is the name of the remote machine. If you want to use `ssh` instead, type

```
node -s node2 ls
```

This should print the content of the *current* directory on the master machine (not your home directory). If you get an error message or if you get the content of another directory, you will need to check if the following works. Make sure you are in a directory that does not contain too many files. If you want to use `rsh`, type:

```
node -r node2 ls
```

while if you want to use `ssh`

```
node -s -r node2 ls
```

In either case, you should get the content of the current directory before continuing on. The `node -r` command works by copying the content of the current directory on the remote machine in a temporary directory. Once the command has terminated, the new content is copied back and the remote temporary directory is deleted.

We are now ready to automate the calculations. Type

```
chl
```

and, as indicated on the screen, open the file `~/.machines.rc` with a text editor. This file contains numerous comment lines explaining the format of the file and a few examples.

The commands in the first column (before the `+`) must print a single number indicating the load of the machine. It is a good check to copy and paste each of these command, one at the time, into a shell window to see if the output is a single number. In order to extract a single number out of a complicated output, the command `getvalue` is provided. It extracts the single number following the token given as an argument. The first entry, with the `none` keyword after the `+` indicates the threshold load above which a machine is considered too busy to be usable. Note that the load checking commands may quite elaborate if, for instance, you need to "rescale" the load of some machines because they have a different reporting scheme or if you want to tweak the priority given to each machine.

The second column (after the `+`) give the command prefix needed to run on each remote machine. These prefix will usually consist of the command `node` described above. It is very important that the command prefix be such that the current directory in the remote machine when the command is run is the same as on the local machine. The best way to test that is to try the prefix in front of the `ls` command and verify that what is printed is indeed the content of the current local directory.

Once you are done with entering the information for each of your machines (you can also enter only a few and come back later to add the remaining ones), make sure to comment out the examples provided (placing a `#` at the beginning of the unwanted line). Do not comment out the first line which contains the `none` keyword.

Once you have edited the `~/.machines.rc` file, type `chl`. This should give a list of the load of all machines in the first column and a list of command prefix in the second. Next, try the command `minload`. It should give the command prefix that let you access the machine with the minimum load or `none` if no machine is available. To check, once again, that the command prefix are correct, type `` `minload` ls `` (make sure you use backward quotes!). This should print the content of the current directory (unless there are no machines available).

This approach could also be used with a queueing system, but this is much more advanced and requires good knowledge of scripting languages. You could read the "node list file" the queueing system assigned to the job and create a local `.machine.rc` file on-the-fly. The `-s` option of `pollmach` could prove helpful to ensure two vasp runs do run on the same processors, and avoids the need for load balancing code.

3.3 Interfacing MAPS with other first-principles codes

You need to provide a command (e.g. a shell script) called `runstruct_xxx`, where xxx is any name of your choice. This script should read, from the current directory , the file `str.out` describing the geometry of the structure and create the appropriate input files for the first-principles code. It should then execute the command(s) needed to run the code. If a multiple machine environment is used, the script should use the first argument passed to the script (`$1`) as command prefix to put in front of any command in order for them to be run on a remote machine. That is, if the first-principle code is called "myfp" the script should execute

```
$1 myfp
```

Once the first-principles code has terminated, the script should

- Create a file called `energy` containing the energy of the structure per unit cell of the structure (not the lattice) (this is what first-principles code usually give anyways).
- If the calculation fails, no `energy` file should not be created. Instead, an empty file called `error` should be created.

The above files must all reside in the current directory (from where the script was invoked). To follow the philosophy of the package, the additional input parameters (besides the structure geometry) needed by the first-principles code should be contained in a file called `xxx.wrap` located one (or two) levels up in the directory hierarchy, relative to the current directory.

As a starting point to write this script, have a look at the file `atat/glue/vasp/runstruct_vasp`.

Chapter 4

Version History and Bugs

```
1.50:
constituent strain
allow any structure names
allow new structures to be added at all times

1.66:
unit cell in 'symmetric' form, ready for ab-initio codes
constituent strain fitting code
temperature-dependent ECI in Monte Carlo code
manual in tex/html
reciprocal space Monte-Carlo (BETA)
easy-to-configure job control scripts

2.03:
vibrational and electronic entropy included.

2.50:
mixed canonical/grandcanonical multicomponent monte carlo

2.53:
reciprocal space multicomponent monte carlo (for electrostatics)

2.54:
automated patching system for c++ language qwirks

2.70:
tensorial/generalized cluster expansion (gce utility)

2.71:
fixed bug in multisublattice structure enumeration routine
(only affects cases where a pure translation maps one sublattice onto another:
omits some structures with lattice vector equal to one of the unit cell lattice vectors
cluster expansions not affected, but perhaps missed ground states or SQS, but unlikely)
```

Chapter 5

User guide

5.1 Introduction

First-principles calculations of alloy thermodynamic properties have been successfully employed in a variety of contexts for metallic, semi-conductor and ceramic systems, including the computation of: composition-temperature phase diagrams, thermodynamic properties of stable and metastable phases, short-range order in solid solutions, thermodynamic properties of planar defects (including surfaces or antiphase and interphase boundaries), and the morphology of precipitate microstructures [6, 5, 28, 29, 26, 3, 1].

Although the formalism that allows the calculation of thermodynamic properties from first principles has been known for decades [6, 5, 28], its practical implementation remains tedious. These practical issues limit the accuracy researchers are able to obtain without spending an unreasonable amount of their time writing input files for various computer codes, monitoring their execution and processing their output. These practical difficulties also limit the community of researchers that use these methods solely to those that possess the necessary expertise to carry out such calculations.

The Alloy Theoretic Automated Toolkit (ATAT) [23] drastically simplifies the practical use of these methods by implementing decision rules based on formal statistical analysis that free the researchers from a constant monitoring during the calculation process and automatically "glues" together the input and the output of various codes, in order to provide a high-level interface to the calculation of thermodynamic properties from first principles. In order the make this powerful toolkit available to the wide community of researchers who could benefit from it, this article present a concise user guide to this toolkit.

5.2 Theoretical Background

While there exist numerous methodologies that enable the calculation of thermodynamic properties from first principles, we will focus on the following two-step approach (see Figure 5.1). First, a compact representation of the energetics of an alloy, known as the cluster expansion [18, 6, 5, 28], is constructed using first-principles calculations of the formation energies of various atomic arrangements. Second, the cluster expansion is used as a Hamiltonian for Monte Carlo simulations [16, 2, 8, 15] that can provide the thermodynamic properties of interest, such as the free energy of a phase or short-range-order parameters as a function of temperature and concentration. This two-step approach is essential, because the calculation of thermodynamic quantities through Monte Carlo involves averaging the property of interest over many different atomic configurations and it would be infeasible to calculate the energy of each of these configurations from first principles. The cluster expansion enables the prediction of the energy of any configuration from the knowledge of the energies of a small number of configurations (typically between 30 and 50), thus making the procedure amenable to the use of first-principles methods.

Formally, the cluster expansion is defined by first assigning occupation variables σ_i to each site i of the *parent lattice*, which is defined as the set of all the atomic sites that can be occupied by one of a few possible atomic species. In the common case of a binary alloy system, the occupation variables σ_i take the value -1 or $+1$ depending on the type of atom occupying the site. A particular arrangement of these "spins" on the parent lattice is called a *configuration* and can be represented by a vector σ containing the value of the occupation variable for each site in the parent lattice. Although we focus here on the case of binary alloys, this framework can be extended to arbitrary

multicomponent alloys (the appropriate formalism is presented in [18]).

The cluster expansion then parametrizes the energy (per atom) of the alloy as a polynomial in the occupation variables:

$$E(\sigma) = \sum_{\alpha} m_\alpha J_\alpha \left\langle \prod_{i \in \alpha'} \sigma_i \right\rangle \tag{5.1}$$

where α is a cluster (a set of sites i). The sum is taken over all clusters α that are not equivalent by a symmetry operation of the space group of the parent lattice, while the average is taken over all clusters α' that are equivalent to α by symmetry. The coefficients J_α in this expansion embody the information regarding the energetics of the alloy and are called the effective cluster interaction (ECI). The *multiplicities* m_α indicate the number of clusters that are equivalent by symmetry to α (divided by the number of lattice sites).

It can be shown that when *all* clusters α are considered in the sum, the cluster expansion is able to represent any function $E(\sigma)$ of configuration σ by an appropriate selection of the values of J_α. However, the real advantage of the cluster expansion is that, in practice, it is found to converge rapidly. An accuracy that is sufficient for phase diagram calculations can be achieved by keeping only clusters α that are relatively compact (*e.g.* short-range pairs or small triplets). The unknown parameters of the cluster expansion (the ECI) can then be determined by fitting them to the energy of a relatively small number of configurations obtained through first-principles computations. This approach is known as the Structure Inversion Method (SIM) or the Collony-Williams [4] method.

The cluster expansion thus presents an extremely concise and practical way to model the configurational dependence of an alloy's energy. A typical well-converged cluster expansion of the energy of an alloy consists of about 10 to 20 ECI and necessitates the calculation of the energy of around 30 to 50 ordered structures (see, for instance, [25, 9, 17]). Once the cluster expansion has been constructed, the energy of any configuration can be calculated using Equation 5.1 at a very small computational cost. This enables the use of various statistical mechanical techniques such as Monte Carlo simulations [2], the low-temperature expansion (LTE) [11, 6], the high-temperature expansion (HTE) [6], or the cluster variation method (CVM) [10, 6] to calculate thermodynamic properties and phase diagrams. The `atat` software implements Monte Carlo simulations, the LTE and the HTE.

Paralleling the two-step approach described in the previous section, `atat` consists of two main computer programs (see Figure 5.1). The cluster expansion construction is performed by the MIT *Ab initio* Phase Stability (MAPS) code [24], while the Monte Carlo simulations are driven by the Easy Monte Carlo Code (EMC2), developed at Northwestern University [22]. Each of these codes will be discussed in turn.

While the present user guide describes how the `atat` software can be used to carry out all the steps necessary for the calculation of thermodynamic properties from first principles, it must be emphasized that each part of the toolkit can be used as a stand-alone code. For instance, many users may have access to an existing cluster expansion obtained through the SIM or other popular methods, such as concentration-wave-based methods (see, for instance, [7, 6, 21]). It is then staightforward to setup the appropriate input files to run the `emc2` Monte Carlo code. Alternatively, after obtaining a cluster expansion using the `maps` code, users could choose to calculate thermodynamic properties with the cluster variation method (CVM) [10, 6], as implemented in the `IMR-CVM` code [20]. The modularity of the toolkit actually extends below the level of the `maps` and `emc2` codes — many of the subroutines underlying these codes can be accessed through stand-alone utilities [23].

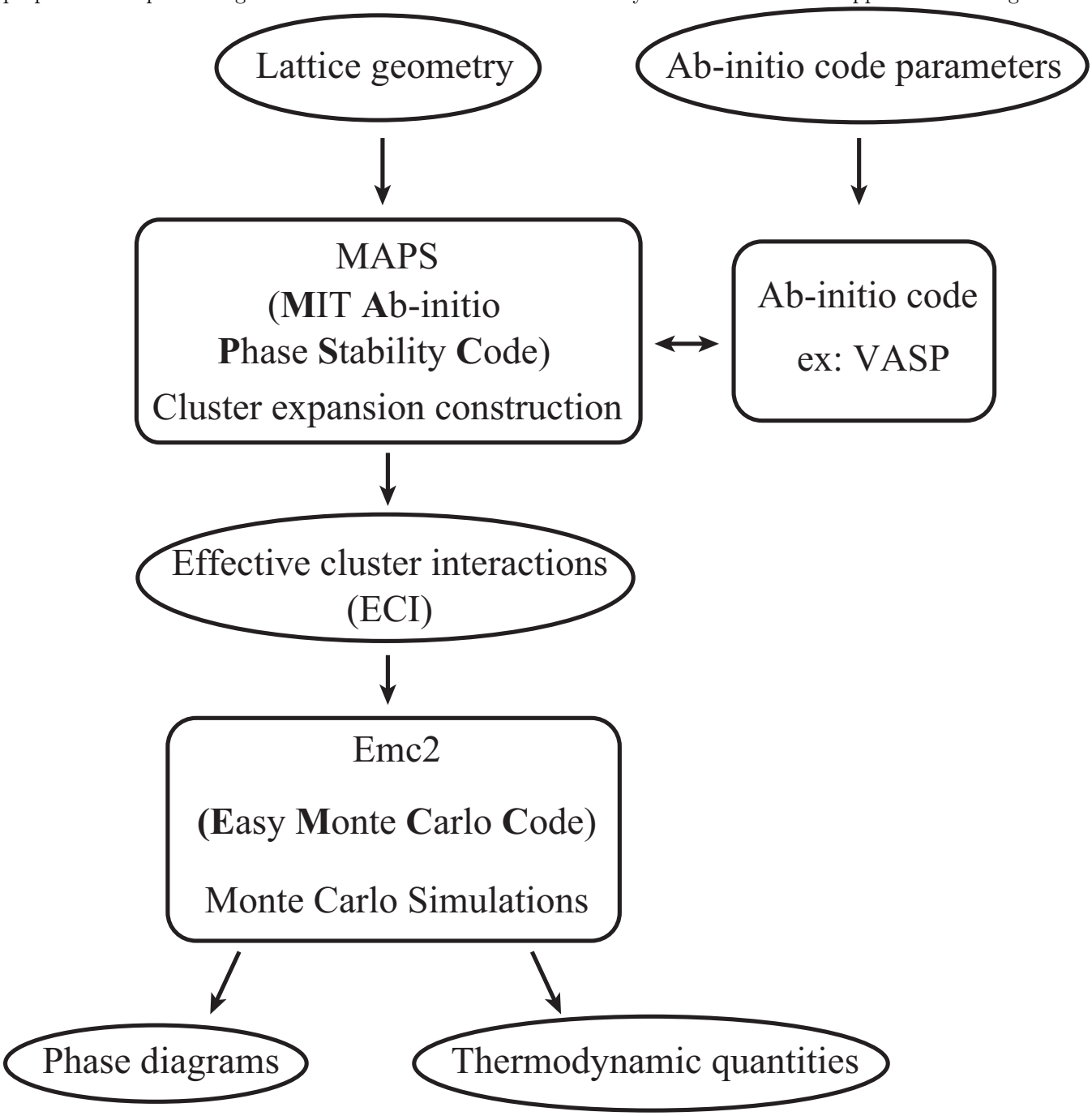
5.3 Cluster expansion construction using the MAPS code

The `maps` code implements the so-called Structure Inversion Method (SIM), also known as the Connolly-Williams method [4]. While the algorithms underlying the `maps` code are described in [24], the present section focuses on its practical use.

5.3.1 Input files

The `maps` code needs two input files: one that specifies the geometry of the parent lattice (`lat.in`) and one that provides the parameters of the first-principles calculations (`xxxx.wrap`, where `xxxx` is the name of the first-principles code used). The clear separation between the thermodynamic and first-principles calculations is a distinguishing feature of `atat` that enables the package to be easily interfaced with any first-principles code. Table 5.1 gives two annotated examples of a lattice geometry input file. The package includes ready-made lattice files for the common lattice types (*e.g.* bcc, fcc, hcp). It also includes an utility that automatically constructs multiple lattice geometry input files for common lattices. For instance,

Figure 5.1: Methodology implemented in `atat` for the computation of thermodynamic properties from first principles. The automated construction of the cluster expansion is performed by the `maps` code. Whenever needed, `maps` requests the calculation of the formation energy of various atomic configurations by a first-principles code (such as `vasp`). The necessary input files are created and the resulting output files are parsed without requiring user intervention. The output of `maps` is a set of effective cluster interactions that define a computationally efficient Hamiltonian that can be used to perform Monte Carlo simulations with the `emc2` code. These simulations provide thermodynamic properties and phase diagrams that can be used to create thermodynamic databases or supplement existing ones.




```
makelat Al,Ti fcc,bcc,hcp
```

creates 3 subdirectories containing the appropriate input files for each specified lattice.

Table 5.1: Examples of lattice geometry input file `lat.in`. Typically, the coordinate system entry is used to define the conventional unit cell so that all other entries can be specified in the normalized coordinates that are the most natural for the symmetry of the lattice. The input lattice parameters do not need to be exact, as the first-principles code will optimize them.

Example 1: hcp Ti-Al system

`3.1 3.1 5.062 90 90 120`	(Coordinate system: $a\ b\ c\ \alpha\ \beta\ \gamma$ notation)
`1 0 0`	(Primitive unit cell: one vector per line
`0 1 0`	expressed in multiples of the above coordinate
`0 0 1`	system vectors)
`0 0 0 Al,Ti`	(Atoms in the lattice)
`0.6666666 0.3333333 0.5 Al,Ti`	

Example 2: rocksalt CaO-MgO pseudobinary system

`4.1 4.1 4.1 90 90 90`	
`0 0.5 0.5`	
`0.5 0 0.5`	
`0.5 0.5 0`	
`0 0 0 Ca,Mg`	("Active" atoms in the lattice)
`0.5 0.5 0.5 O`	("spectator" ion)

The first-principles input file is usually less than 10 lines long, thanks to the dramatic improvements in the user-friendliness of most modern first-principles codes. For instance, in the case of the widely used VASP code [13, 12], a typical input file is given in Table 5.2. Examples of such input files are provided with the package. Note that `atat` contains a utility that enables the automatic construction of k-point meshes from a single parameter defining the desired target k-point density, the number of k-point per reciprocal atom (`KPPRA`).

Table 5.2: Examples of first-principles code input file (example given for the `vasp` code). It is especially important to verify that the `KPPRA` parameter is set sufficiently large for the system under study.

`[INCAR]`	
`PREC = high`	
`ENMAX = 200`	
`ISMEAR = -1`	
`SIGMA = 0.1`	
`NSW=41`	
`IBRION = 2`	
`ISIF = 3`	(See `vasp` manual for a description of the above 6 parameters.)
`KPPRA = 1000`	(Sets the k-point density (K Point Per Reciprocal Atom))
`DOSTATIC`	(Performs a "static run" — see `vasp` manual)

5.3.2 Running the code

The `maps` code is started using the command

```
maps -d &
```

where the option `-d` indicates that all default values of the input parameters should be used, which is what most users will ever need. (The optional parameters can be displayed by typing `maps` by itself and further help is available via the command `maps -h`.) The trailing `&` character cause the command to execute in "background" mode. In this

fashion, `maps` can continuously be on the lookout, responding to various "signals", while the user performs other tasks. (The ongoing discussion assumes that the code is run under a UNIX environment within a shell such as `sh`, `csh`, `tcsh` or `bash`.)

The process of constructing a cluster expansion from first-principles calculations can be summarized as follows.

1. Determine the parameters of the first-principles code that provide the desired accuracy.
2. Let `maps` refine the cluster expansion.
3. Decide when the cluster expansion is sufficiently accurate.

Typically, one calibrates the accuracy of the first-principles calculations using the "pure"[1] structures of the alloy system of interest. To generate the two "pure" structures, type

```
touch ready
```

This creates a file called `ready` which tells `maps` that you are ready to calculate the energy of a structure. Within 10 seconds, `maps` replies with

```
Finding best structure...

done!
```

`maps` has just created a directory called `0` and, within it, a file called `str.out` that contains the geometry of one of the two "pure" structures. If you type `touch ready` once more, the other "pure" structure is written to `1/str.out`. You now need to launch the first-principles code to calculate the energy of each structure. Type

```
cd 0
```

to go into the directory of the first structure. Assuming that your first-principles code is called `xxxx`, type

```
runstruct_xxxx &
```

After this command has successfully terminated, display the energy of that structure and go back to the initial directory

```
cat energy

cd ..
```

and edit the file defining the first-principles code parameters

```
emacs xxxx.wrap &
```

so that the precision of the calculation is increased (*e.g.* increase the k-point density or the cut-off of the plane-wave energy). Then you rerun the calculations to check by how much the calculated energy has changed:

```
cd 0

runstruct_xxxx &

cat energy (After the calculations are completed)

cd ..
```

This process is repeated until the user is satisfied with the precision of the calculation (that is, if the energy has become insensitive to changes in the input parameters within the desired accuracy).[2] A similar study should also be performed for the other "pure" structure (labeled structure `1`) and, if one is really concerned with precision, for a few structures with intermediate concentrations.

Once the appropriate *ab initio* code parameters have been determined, the fully automated process can begin. From within the directory where `maps` was started, type

[1] In the case of pseudobinary alloys with spectator ions (*e.g.* the MgO-CaO system), the "pure" structures would correspond to the structures where the sublattice of interest is entirely filled with a single type of atom.

[2] A key number to keep in mind is that an error of 25meV corresponds to 300K on a temperature scale.

```
pollmach runstruct_xxxx
```

to start the job manager that will monitor the load on your local network of workstations and ask `maps` to generate new structures (*i.e.* atomic arrangements) whenever a processor becomes available. Note that the first time the command is run, instructions will appear on screen that explain how to configure the job dispatching system in accordance to your local computing environment. Once this configuration is complete, the above command should be invoked in the background by appending a "`&`" to it.

5.3.3 Output of MAPS

While the calculations are running, you can check on the status of the best cluster expansion obtained so far. The file `log.out` contains a brief description of the status of the calculations, such as the accuracy of the cluster expansion and various warning messages. Most of the messages pertains to the accurate prediction of the so-called ground states of the alloy system. The ground states, which are the structures that have the lowest energy for each given concentration, are extremely important to predict accurately because they determine which phases will appear on the phase diagram. The four possible messages are described below.

- `Not enough known energies to fit CE.` Before displaying any results, `maps` waits until enough structural energies are known to fit a minimal cluster expansion containing only nearest-neighbor pair interactions and test its accuracy. Thus, the first cluster expansion is typically constructed after at least 4 structural energies have been computed (this number may vary as a function of the symmetry of the lattice).

- `Among structures of known energy, true ground states differ from fitted ground states.` The current cluster expansion incorrectly predicts which structures have the lowest energy for given concentrations, among structures whose first-principles energy is known. The code has built-in checks to avoid this. However, in rare instances, it may be mathematically impossible to satisfy all the constraints that the code imposes for a cluster expansion to be acceptable. This problem becomes increasingly unlikely as the number of calculated structural energies increases, so the user should just wait until the problem fixes itself.

- `Among structures of known energy, true and predicted ground states agree.` Opposite of the previous message. When this message is displayed, `maps` also displays either one of the following two messages.

- `New ground states of volume less or equal to` n `predicted, see predstr.out.` This indicates that the cluster expansion predicts that, at some concentration, there exist other structures that should have an energy even lower than the one of the structures whose energy has been calculated from first principles. In this case, `maps` will investigate the matter by generating those structures and requesting that their energy be calculated. Once again, the user should just wait for the problem to fix itself. The predicted ground states are flagged by a `g` in the `predstr.out` file, so that you can display their energy by typing

  ```
  grep g predstr.out
  ```

- `No other ground states of` n `atoms/unit cell or less exist.` The energies of all ground states predicted by the cluster expansion have been confirmed by first-principles calculations. Because it can be computationally intensive to perform a full ground state search when interactions extend beyond the nearest-neighbor shell [6], `maps` uses a search algorithm that merely enumerates every possible structures having n atoms or less per unit cell and uses the cluster expansion to predict their energies. The upper limit n increases automatically as calculations progress.

The `log.out` file also contains two other pieces of information:

- `Concentration range used for ground state checking:` [a,b] This displays the user-selected range of concentration over which ground state checking is performed (which can be specified as a command-line option of the `maps` command: `-c0=`a `-c1=`b). It may be useful to relax the constraints that ground states be correctly reproduced over the whole concentration range when it is known that other parent lattices are stable in some concentration range. In this fashion, the code can focus on providing a higher accuracy in the concentration range where the user needs it.

- `Crossvalidation score:` s. This provides the predictive power of the cluster expansion. It is analogous to the root mean square error, except that it is specifically designed to estimate the error made in predicting the energy for structures not included in the least-squares fit [24]. It is defined as

$$CV = \left(\frac{1}{n} \sum_{i=1}^{n} \left(E_i - \hat{E}_{(i)} \right)^2 \right)^{1/2}$$

  where E_i is the calculated energy of structure i, while $\hat{E}_{(i)}$ is the predicted value of the energy of structure i obtained from a least-squares fit to the $(n-1)$ other structural energies.

The `maps` code also outputs quantitative data in various output files. The simplest way to analyze this data is by typing

```
mapsrep
```

As illustrated in Figure 5.2, this command displays, in turn

- The `log.out` file described earlier.
- The formation energy of all structures whose energy is known from first-principles calculations, as well as the predicted energy of all structures `maps` has in memory. The convex hull of the ground states among structures of known energy is overlaid while the new predicted ground states (if any) are marked by an "×". (Note that this ground state line is only meaningful if the `log.out` file contains "`Among structures of known energy, true and predicted ground states agree.`")
- The formation energy of all structures calculated from first principles and associated ground state line.
- A plot of the magnitude of the Effective Cluster Interactions (ECI) as a function of the diameter of their associated cluster (defined as the maximum distance between any two sites in the cluster). Pairs, triplets, etc. are plotted consecutively. This plot is useful to assess the convergence of the cluster expansion. When the magnitude of the ECI for the larger clusters has clearly decayed to a negligible value (relative to the nearest-neighbor pair ECI), this is indicative of a well-converged cluster expansion.
- A plot of the residuals of the fit (*i.e.* the fitting error) for each structure. This information is useful to locate potential problems in the first-principles calculations. Indeed, when first-principles calculations exhibit numerical problems, this typically results in calculated energies that are poorly reproduced by the cluster expansion.

When the user is satisfied with the results (which are constantly updated), `maps` can be stopped by creating a file called `stop` in the current directory using the command:

```
touch stop
```

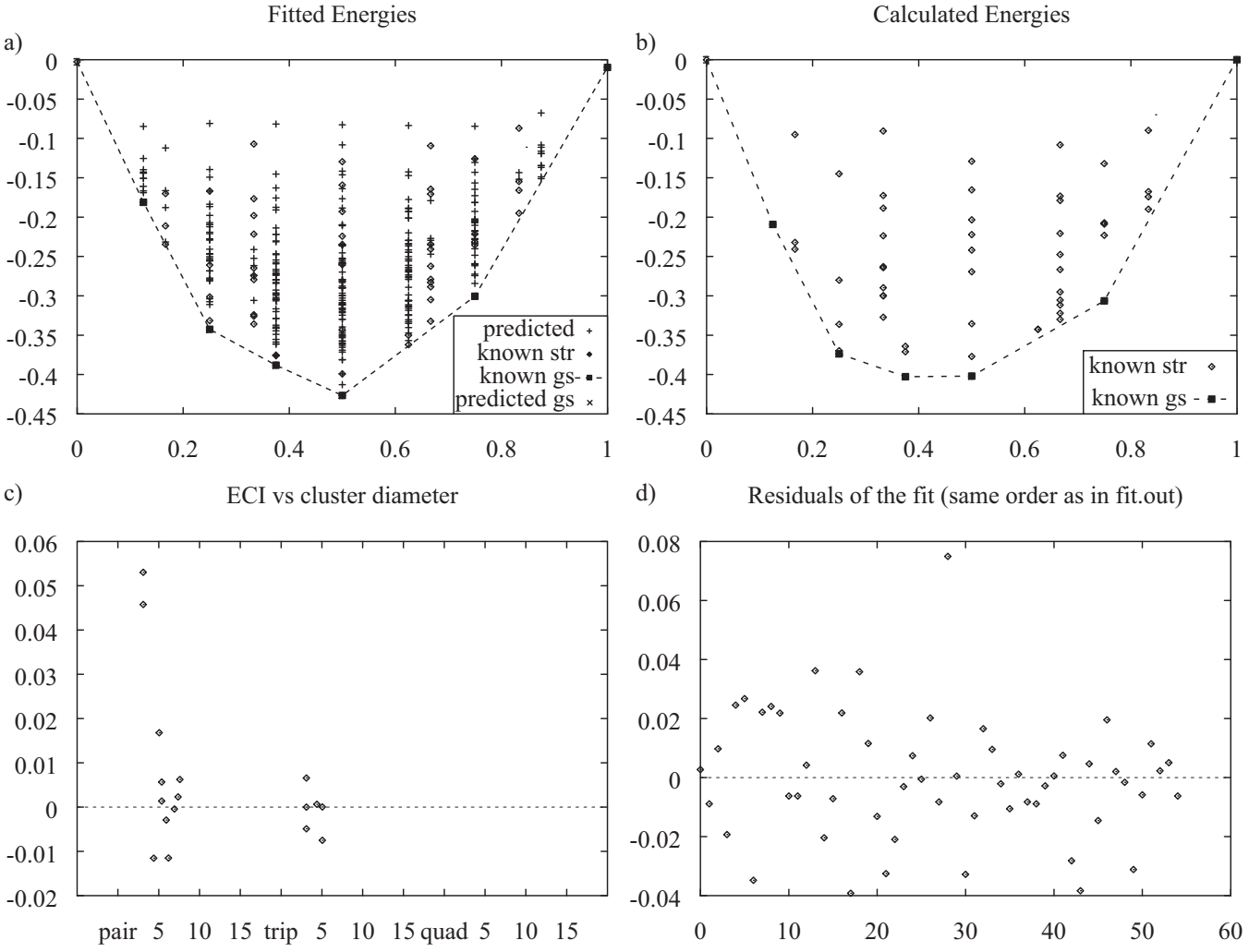
while the job dispatching system can be stopped by typing:

```
touch stoppoll
```

A cluster expansion can be considered satisfactory when

1. All ground states are correctly reproduced and no new ground states are predicted. (The `log.out` file would then indicate that `Among structures of known energy, true and predicted ground states agree. No other ground states of` n `atoms/unit cell or less exist.`)
2. The crossvalidation score, as given in the `log.out` file, is small (typically less than 0.025 eV).
3. Optionally, it is instructive to verify that the magnitude of the ECI decays as a function of the diameter of the corresponding cluster and as a function of the number of sites it contains.

Figure 5.2: Output of the `maps` Code, as reported by the `mapsrep` command. a) Energies predicted from the cluster expansion as a function of composition for each structure generated. "`known str`" denotes structures whose energy has been calculated from first principles. "`known gs`" indicate the ground states that have so far been confirmed by first-principles calculations and the dashed line outlines the convex hull of the ground states, which serves as a threshold to detect other candidate ground states. "`predicted`" denotes structures whose energy has *not yet* been calculated from first principles. "`predicted gs`" are structures that are predicted by the cluster expansion to be ground states, although this prediction has not yet been confirmed by first-principles calculations. b) Energies calculated from first principles. "`known str`" and "`known gs`" are as in a), except that the energy calculated from first principles is reported. c) Effective Cluster Interaction (ECI) as a function of the diameter of the associated cluster and as a function of the number of sites in the cluster (*i.e.* pair, triplet, etc.). d) Residuals of the fit, that is, the difference between the first-principles energies and the energies predicted from the cluster expansion. (The abscissa refers to the line number within the output file `fit.out` listing all the structures with known energies.)



5.4 Monte Carlo simulations

The `emc2` code implements semi-grand canonical Monte Carlo simulations [16, 2, 8, 15], where the total number of atoms is kept fixed, while the concentration is allowed to adapt to an externally imposed difference in the chemical potential of the two types of atoms. The chemical potential difference will be simply referred to as the "chemical potential" in what follows. This ensemble offers the advantage that, for any imposed chemical potential, the equilibrium state of the system is a single phase equilibrium, free of interfaces.[3] It also simplifies the process of calculating

[3] If the simulation cell is commensurate with the unit cell of the phase under study, a requirement that the code automatically ensures.

free energies through thermodynamic integration. While a detailed description of the algorithm underlying this code can be found in [22], the current section focuses on the practical usage of the code.

5.4.1 General input parameters

The Monte Carlo code needs the following files as an input

1. A lattice geometry file (`lat.in`), which is the same as the input for `maps` (see Table 5.1).
2. Files providing the cluster expansion (the clusters used are listed in the `clusters.out` file while the corresponding ECI are listed in the `eci.out` file.). These files are automatically generated by `maps`, although users can supply their own cluster expansion, if desired. A description of the format of these files is available by typing `maps -h`.
3. A list of ground states (`gs_str.out`), which merely provide convenient starting configurations for the simulations. `maps` also automatically creates this file.

The parameters controlling the simulation are specified as command-line options. The first input parameter(s) needed by the code are the phase(s) whose thermodynamic properties are to be determined. There are two ways to invoke the Monte Carlo simulation code. When the command `emc2` is used, a single Monte Carlo simulation is run to allow the calculation of thermodynamic properties of a single phase for the whole region of chemical potential and temperature where that phase is stable. The phase of interest is specified by a command-line option of the form

`-gs=`n,

where n is a number between -1 and $G-1$ (inclusive), where G is the number of ground states. The value -1 indicates the disordered phase while values ranging from 0 to $G-1$ indicate the phases associated with each ground states (0 denoting the ground state with the smallest composition). When the command `phb` is used, two Monte Carlo simulations are run simultaneously to enable the determination of the temperature-composition phase boundary associated with a given two-phase equilibrium. The two phases are specified by

`-gs1=`n_1 `-gs2=`n_2.

It is possible to compute a two-phase equilibrium between phases defined on a different parent lattice. In this case, the user needs to specify the directories where the cluster expansions of each lattice resides using the options of the form

`-d1=`*directory 1* `-d2=`*directory 2*

The accuracy of the thermodynamic properties obtained from Monte-Carlo simulations is determined by two parameters: The size of the simulation cell and the duration of the simulation.

The size of the simulation cell is specified by providing the radius r of a sphere through the command-line option

`-er=`r.

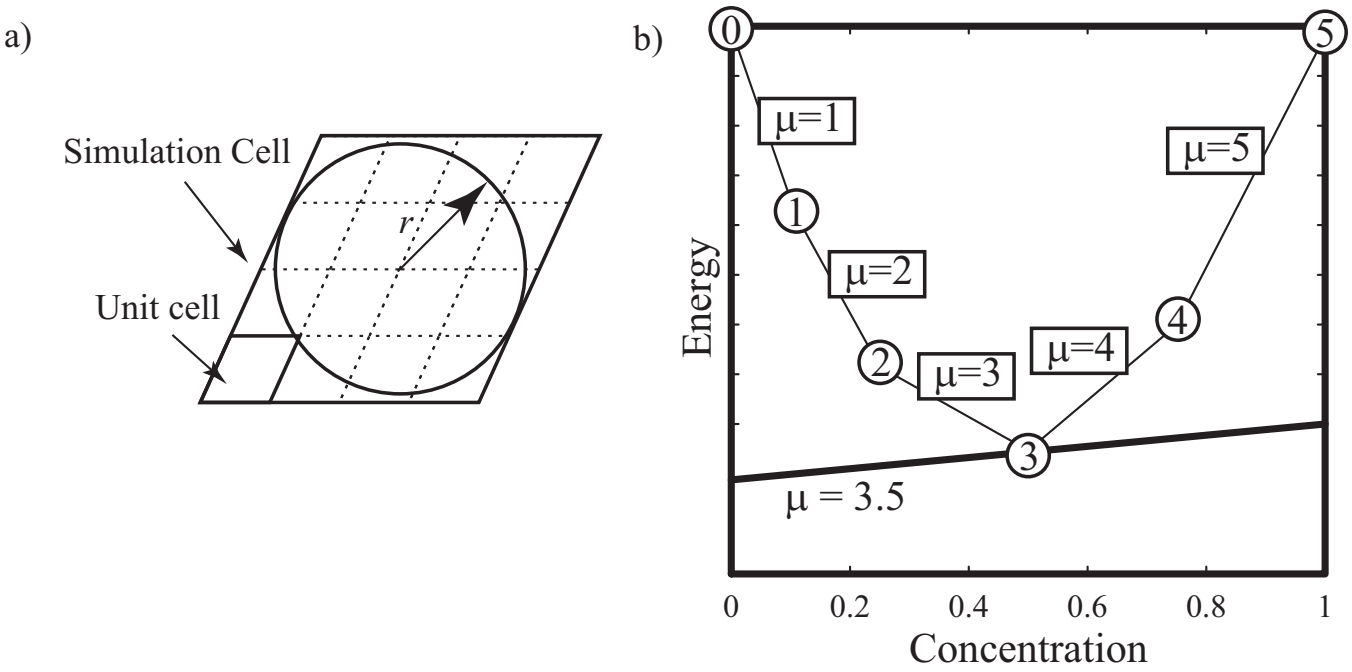
As illustrated in Figure 5.3a, the simulation cell size will be the smallest supercell that both contains that sphere and that is commensurate with the unit cell of the ground state of interest. This way of specifying the simulation cell size ensures that the system size is comparable along every direction, regardless of the crystal structure of the ground state of interest. It also frees the user from manually checking the complicated requirement of commensurability. It is important that the user check that the simulation cell size is sufficiently large for the thermodynamic properties of interest to be close to their infinite-system-size limiting value. This can be done by gradually increasing the system size until the calculated quantities become insensitive to the further increases in system size, within the desired accuracy.

The duration of the simulations is automatically determined by the code from a user-specified target precision on the atomic composition of the phase, indicated by a command-line option of the form

`-dx=`Δx.

Alternatively, the user may also manually set the number n_{eq} of Monte Carlo steps the system is allowed to equilibrate before thermodynamic averages are computed over a certain number n_{avg} of Monte Carlo steps using the options

Figure 5.3: Definitions of the quantities used to specify a) the simulation cell size and b) the chemical potential.



`-eq=`n_{eq} `-n=`n_{avg}.

The Monte Carlo code also needs additional parameters that specify which portion of a phase's free energy surface needs to be computed. With `emc2`, the range of temperatures to be scanned are specified in either one of the following two ways:

`-T0=`T_0 `-T1=`T_1 `-dT=`ΔT (for steps in direct temperature)

or `-T0=`T_0 `-T1=`T_1 `-db=`$\Delta(1/T)$ (for steps in reciprocal temperature).

The temperature steps in reciprocal temperature ($\Delta(1/T)$) can be useful when calculations are started from infinite temperatures down to a finite temperature. The `-T1` and `-dT` (or `-db`) options can be omitted if calculations at a single temperature are desired. Since the program automatically stops when a phase transition is detected, it is not necessary to know in advance the temperature range of stability of the phase. The user only needs to ensure that the initial temperature lies within the region of stability of the phase of interest. An obvious starting point is $T_0 = 0$, since the ground state is then stable, by definition. With the `phb` code, the syntax is

`-T=`T `-dT=`ΔT

If the `-T` option is omitted, calculations start at absolute zero.[4] The energy and temperature units used are set by specifying the Boltzman's constant with the command-line option

`-k=`k_B.

A value of 8.617×10^{-5} corresponds to energies in eV and temperatures in Kelvin.

With `emc2`, the range of chemical potentials to be scanned needs to be specified. Once again, only the starting point really matters, because the code will stop when a phase transition is reached. By default, chemical potentials are given in a dimensionless form, so as to facilitate the link between the value of the chemical potential and the phase that it stabilizes. For instance, a chemical potential equal to 3.0 is such that it would stabilize a two phase equilibrium between phase number 2 and phase number 3 at absolute zero (see Figure 5.3b). A chemical potential between 3.0 and 4.0 stabilizes phase number 3 at absolute zero. While these ranges of stability are no longer exact at finite temperature, this dimensionless chemical potential still provides easy-to-interpret input parameters. The syntax is

[4] Temperature steps in reciprocal temperature are not needed, because a two-phase equilibrium never extents up to infinite temperature.

`-mu0=`μ_0 `-mu1=`μ_1 `-dmu=`$\Delta\mu$

where $\Delta\mu$ is the chemical potential step between each new simulation. Chemical potentials can also be entered in absolute value (say in eV, if the energies are in eV) by specifying the `-abs` option. Note that the output files always give the absolute chemical potentials, so that thermodynamic quantities can be computed from them. With `phb`, the initial chemical potential is optional when starting from absolute zero because the code can determine the required value from the ground state energies. It can nevertheless be specified (in absolute value) with the `-mu=`μ option, if a finite temperature starting point is desired.

A list of the command line options of either the `emc2` or `phb` codes can be displayed by simply typing either command by itself. More detailed help is displayed using the `-h` option.

5.4.2 Examples

We now give simple examples of the usage of these commands. Consider the calculation of the free energy of the phase associated with ground state number 1 as a function of concentration and temperature. Then, the required commands could, for instance, be

```
emc2 -gs=1 -mu0=1.5 -mu1=0.5 -dmu=0.04 -T0=300 -T1=5000 -dT=50 -k=8.617e-5 -dx=1e-3 -er=50 -innerT
-o=mc10.out
```

```
emc2 -gs=1 -mu0=1.5 -mu1=2.5 -dmu=0.04 -T0=300 -T1=5000 -dT=50 -k=8.617e-5 -dx=1e-3 -er=50 -innerT
-o=mc12.out
```

(The only difference in the two command lines is the value of `-mu1` and the output file name, specified by the `-o` option.) These commands separately compute the two "halfs" of the free energy surface, corresponding to the values of the chemical potential below and above the "middle" value of 1.5 which stabilizes ground state 1 at absolute zero. This natural separation allows you to run each half calculation on a separate processor and obtain the results in half the time. The values of `-dmu`, `-dT`, `-dx` and `-er` given here are typical values. The user should ensure that these values are such that the results are converged. Note that, thanks to the way these precisions parameters are input, if satisfying values have been found for one simulation, the same values will provide a comparable accuracy for other simulations of the same system. The option `-innerT` indicates that the inner loop of the sequence of simulations scans the temperature axis while the outer loop scans the chemical potential. In this fashion, the point of highest temperature in the region of stability of the phase will be known early during the calculations. If the user is more interested in obtaining solubility limits early on, this option can be omitted and the inner loop with scan the chemical potential axis. In either cases, the code exits the inner loop (and the outer loop, if appropriate) when it encounters a phase transition.

The `emc2` code thus enables the automated calculation of the whole free energy surface of a given phase, as illustrated in Figure 5.4a. Such free energy surfaces can be used as an input to construct thermodynamic databases or supplement existing ones. To facilitate this process, a utility that converts the output of `emc2` into input files for the fitting module of ThermoCalc is provided.

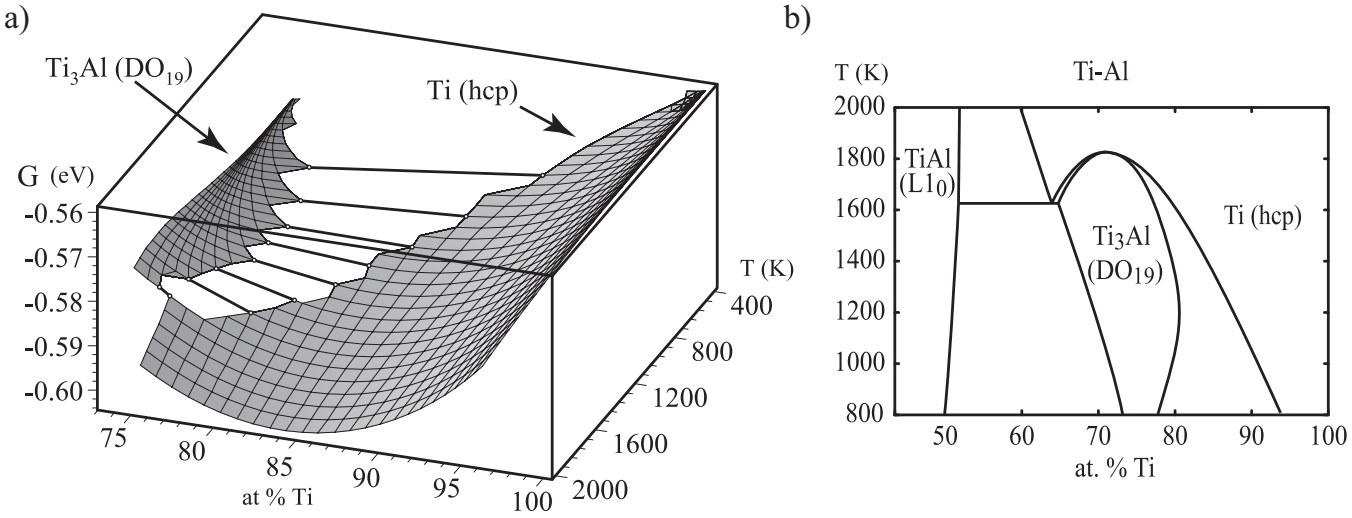
While the above examples focus on the calculation of a phase's thermodynamic properties over its whole region of stability, one may be interested in directly computing the temperature-composition phase boundary without first constructing a full free energy surface. To accomplish this task, a typical command-line for the `phb` program would be

```
phb -gs1=0 -gs2=1 -dT=25 -dx=1e-3 -er=50 -k=8.617e-5 -ltep=5e-3 -o=ph01.out
```

This command computes the two phase equilibrium between phase 0 and phase 1, starting at absolute zero and incrementing temperature in steps of 25 K. (The `-ltep` option indicates that a Low Temperature Expansion (LTE) should be used instead of Monte Carlo simulation whenever its precision is better than 5×10^{-3} eV.) The output file `ph01.out` contains the temperature-composition phase boundary of interest, as well as the chemical potential stabilizing the two-phase equilibrium as a function of temperature. This output can be used to generate phase diagrams, as illustrated in Figure 5.4b.

The program automatically terminates when the "end" of the two-phase equilibrium has been reached. If the two-phase equilibrium disappears because of the appearance of a third phase, two new two-phase equilibria have to be separately calculated. To do so, one uses the final temperature T and chemical potential μ given in the output file as a starting point for two new `phb` runs:

Figure 5.4: Output of Monte Carlo codes. a) The `emc2` provides free energy surfaces as a function of temperature T and composition x. (For clarity, the common tangent construction (thick lines) is drawn over the calculated free energy.) b) The `phb` command generates temperature-composition phase diagrams. The calculational details underlying these results can be found in [24, 22]




```
phb -T=T -mu=μ -gs1=0 -gs2=-1 -dT=25 -dx=1e-3 -er=50 -k=8.617e-5 -o=ph0d.out
```

```
phb -T=T -mu=μ -gs1=-1 -gs2=1 -dT=25 -dx=1e-3 -er=50 -k=8.617e-5 -o=phd1.out
```

In the above example, it is assumed that the new phase appearing is the disordered phase (indicated by the number -1), which will usually be the case. Of course, it is also possible that a given two-phase equilibrium terminates because one of the two phases disappears. In this case, only one new calculation needs to be started, as in the following example:

```
phb -T=T-mu=μ -gs1=0 -gs2=2 -dT=25 -dx=1e-3 -er=50 -k=8.617e-5 -o=phd1.out
```

Note that phase 1 has been replaced by phase 2. Finally, it is also possible that the two-phase equilibrium terminates because the concentration of each phase converges to the same value, a situation which requires no further calculations. The user can easily distinguish these three cases by merely comparing the final composition of each phase.

5.4.3 Interpreting the output files

The output file of `emc2` reports the value of all calculated thermodynamic functions for each value of temperature and chemical potential scanned. The quantities reported include

- Statistical averages over Monte Carlo steps, such as energy, concentration, short-range and long-range order parameters.[5]
- Integrated statistical averages, such as the Gibbs free energy G or the semi-grand-canonical potential $\phi = G - \mu x$.
- The result of common approximations, namely, the low temperature expansion (LTE) [6, 11, 27], the mean-field (MF) approximation and the high temperature expansion (HTE) (see, for instance, [6]).

While quantities obtained from statistical averages over Monte Carlo steps are valid for all temperatures and chemical potentials, caution must be exercised when interpreting the result of the various approximations or when looking at the integrated quantities. The LTE, MF and HTE approximations are only accurate in a limited range of temperature and it is the responsibility of the user to assess this range of validity. Also, the free energy or the semi-grand-canonical potential are obtained from thermodynamic integration and are thus only valid if the starting point of the integration

[5] For efficiency reasons, the long range order parameters are only calculated when starting from an ordered phase.

is chosen appropriately. By default, the low temperature expansion value is used as a starting point whenever the phase of interest is a ground state, while the high temperature expansion is used when the phase of interest is the disordered state. Hence, to obtain absolute values of the semi-grand-canonical potential, one must ensure that the calculations are started at a sufficiently low temperature (or sufficiently high temperature, in the case of the disordered phase). This can be checked by comparing the Monte Carlo estimates with the LTE (or HTE) estimates and verifying that they agree for the first few steps of the thermodynamic integration. A user-specified starting point for ϕ (*e.g.* obtained from an earlier Monte Carlo simulation) can be indicated using the option

`-phi0=`ϕ

Note that, unlike `emc2`, the `phb` code automatically makes use of the low temperature expansion whenever it is sufficiently accurate in order to save a considerable amount of computational time.

By default, the code reports the thermodynamic quantities associated with the semi-grand-canonical ensemble, such as the semi-grand-canonical potential ϕ. The command-line option `-can`, instructs the code to add μx to all appropriate thermodynamic quantities, so that the code outputs the more commonly used canonical quantities, such as the Gibbs free energy G and the internal energy E.

5.5 Recent developments

The multicomponent version of `maps` is `mmaps` and the multicomponent version of `emc2` is `memc2`. The `phb` code does not have a multicomponent version. All other utilities can handle multicomponent systems.

Although the present tutorial does not discuss the topic, `atat` also implements reciprocal space cluster expansions and, in particular, the constituent strain formalism [14], see the command reference for `csfit`. `atat` can also calculate nonconfigurational contributions to the free energy, such as lattice vibrations and electronic excitations, see the command reference for `fitsvsl`, `svsl`, `fitfc` and `felec`.

5.6 Conclusion

The Alloy Theoretic Automated Toolkit (ATAT) drastically simplifies the practical implementation of the Connolly-Williams method, in combination with semi-grand-canonical Monte Carlo simulations, thus providing a high-level interface to the calculation of thermodynamic properties from first principles. This toolkit enables researcher to focus on higher-level aspects of first-principles thermodynamic calculations by encapsulating the intricate details of the calculations under an easy-to-use interface. It also makes these powerful methodologies readily available to the wide community of researchers who could benefit from it.

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Chapter 6

Interfacing with ThermoCalc

A description of the steps necessary to convert the output of the Monte Carlo code `emc2` to input files suitable for the PARROT module of ThermoCalc are described in an online tutorial by Gautam Ghosh available in: `atat/doc/emc2tc.pdf`. These steps are partially automated in the script `atat/glue/tc/emc2tc` included in the `ATAT` distribution.

Chapter 7

Command Reference

7.1 Man pages

7.1.1 apb

```
This code creates an APB from a given structure file and computes its APB
energy using ECIs.

Reference:
R. Sun and A. van de Walle.
Automating impurity-enhanced antiphase boundary energy calculations from
ab initio Monte Carlo.
Calphad 53, 20 (2016).

* The structure file is assumed to have the following form.
  Orient the cell such that the APB plane is defined by T1 x T2:

       a   0   0
       0   b   0
       0   0   c
      T1x T1y T1z
      T2x T2y T2z
      T3x T3y T3z

* The APB structure is generated by duplicating atoms along T3 and shifting
  them by the slip vector.

* To obtain the APB energy, the user should first perform a cluster expansion
  on the system and provide clusters.out and eci.out as input.

* In Monte Carlo mode, the concentration of the initial structure is fixed in
  conccons.in. The temperature and number of averaging steps are used to write
  control.in. The file name of the perfect and defective structures MC snapshot
  is str????.out and str????_apb.out, respectively. After MC, the APBs are
  generated and their energies are computed.

* The output format is:
      [id] e0 e1 gamma
  where
       [id] = structure ID (only shown in Monte Carlo mode)
         e0 = total energy (eV/atom) of perfect cell
         e1 = total energy (eV/atom) of defective cell
      gamma = APB energy (mJ/m^2)
```

7.1.2 corrdump

```
->What does this program do?

1) It reads the lattice file (specified by the -l option).
```

```
2) It determines the space group of this lattice and
   writes it to the sym.out file.

3) It finds all symmetrically distinct clusters that satisfy the
   conditions specified by the options -2 through -6.
   For instance, if -2=2.1 -3=1.1 is specified,
   only pairs shorter than 2.1 units and triplets containing
   no pairs longer than 1.1 will be selected.

4) It writes all clusters found to clusters.out.
   If the -c option is specified, clusters are read from clusters.out instead.

5) It reads the structure file (specified by the -s option).

6) It determines, for that structure, the correlations associated with all
   the clusters chosen earlier.
   This information is then output on one line, in the same order as in the
   clusters.out file. See below for conventions used to calculate correlations.

7) It writes the files corrdump.log containting the list of all adjustements
   needed to map the (possibly relaxed) structure onto the ideal lattice.

->File formats

Lattice and structure files

Both the lattice and the structure files have a similar structure.
First, the coordinate system a,b,c is specified, either as
[a] [b] [c] [alpha] [beta] [gamma]
or as:
[ax] [ay] [az]
[bx] [by] [bz]
[cx] [cy] [cz]
Then the lattice vectors u,v,w are listed, expressed in the coordinate system
just defined:
[ua] [ub] [uc]
[va] [vb] [vc]
[wa] [wb] [wc]
Finally, atom positions and types are given, expressed in the same coordinate system
as the lattice vectors:
[atom1a] [atom1b] [atom1c] [atom1type]
[atom2a] [atom2b] [atom2c] [atom1type]
etc.

In the lattice file:
-The atom type is a comma-separated list of the atomic
 symbols of the atoms that can sit the lattice site.
-In a binary, the first symbol listed is assigned a spin of -1.
 In general, ordering of the atom symbol corresponds to value of s=0,1,... in the table
 'Convention used to calculate the correlations' below.
-When only one symbol is listed, this site is ignored for the purpose
 of calculating correlations, but not for determining symmetry.
-The atomic symbol 'Vac' or 'Va' is used to indicate a vacancy.

In the structure file:
-The atom type is just a single atomic symbol
 (which, of course, has to be among the atomic symbols given in the
 lattice file).
-Vacancies do not need to be specified.

Examples

The fcc lattice of the Cu-Au system:
1 1 1 90 90 90
0   0.5 0.5
0.5 0   0.5
0.5 0.5 0
0 0 0 Cu,Au
```

```
The Cu3Au L1_2 structure:
1 1 1 90 90 90
1 0 0
0 1 0
0 0 1
0   0   0   Au
0.5 0.5 0   Cu
0.5 0   0.5 Cu
0   0.5 0.5 Cu

A lattice for the Li_x Co_y Al_(1-y) O_2 system:
0.707 0.707 6.928 90 90 120
 0.3333  0.6667 0.3333
-0.6667 -0.3333 0.3333
 0.3333 -0.3333 0.3333
 0       0      0       Li,Vac
 0.3333  0.6667 0.0833  O
 0.6667  0.3333 0.1667  Co,Al
 0       0      0.25    O

Symmetry file format (sym.out)

[number of symmetry operations]

3x3 matrix: point operation

1x3 matrix: translation

repeat, etc.

Note that if you enter more than one unit cell of the lattice,
sym.out will contain some pure translations as symmetry elements.

Cluster file format (clusters.out)

for each cluster:
[multiplicity]
[length of the longest pair within the cluster]
[number of points in cluster]
[coordinates of 1st point] [number of possible species-2] [cluster function]
[coordinates of 2nd point] [number of possible species-2] [cluster function]
etc.

repeat, etc.

(Multiplicity and length are ignored when reading in the clusters.out file.)
For each 'point' the following convention apply
-The coordinates are expressed in the coordinate system given in
 the first line (or the first 3 lines) of the lat.in file.
-The 'number of possible species' distinguishes between binaries, ternaries, etc...
 Since each site can accomodate any number of atom types,
 this is specified for each point of the cluster.
-In multicomponent system, the cluster function are numbered from 0 to number of possible species-2.
In the simple of a binary system [number of possible species-2] [cluster function] are just 0 0.
For a ternary, the possible values are 1 0 and 1 1.
All the utilities that are not yet multicomponent-ready just ignore the entries [number of possible species-2] [cluster function].

Convention used to calculate the correlations:
  The cluster functions in a m-component system are defined as
   function '0' : -cos(2*PI*  1  *s/m)
   function '1' : -sin(2*PI*  1  *s/m)
                              .
                              .
                              .
                -cos(2*PI*[m/2]*s/m)
                -sin(2*PI*[m/2]*s/m)   <--- the last sin( ) is omitted if m is even
  where the occupation variable s can take any values in {0,...,m-1}
  and [...] denotes the 'round down' operation.
  Note that, these functions reduce to the single function (-1)^s in the binary case.
```

```
Special options:

-sym:  Just find the space group and then abort.
-clus: Just find space group and clusters and then abort.
-z:    To find symmetry operations, atoms are considered to lie on
       top of one another when they are less than this much apart.
-sig:  Number of significant digits printed.


->Cautions

When vacancies are specified, the program may not be able to warn
you that the structure and the lattice just don't fit.
Carefully inspect the corrdump.log file!

If the structure has significant cell shape relaxations, the program
will be unable to find how it relates to the ideal lattice.
The problem gets worse as the supercell size of the structure gets
bigger.

There is no limit on how far an atom in a structure can be from
the ideal lattice site. The program first finds the atom that can
be the most unambiguously assigned to a lattice site. It then
finds the next best assignement and so on. This is actually a
pretty robust way to do this. But keep in mind that the -z option
does NOT control this process.
```

7.1.3 cv

```
Help for cv

Command-line options:

-g: Favor cluster choices where the ground state line is correct.
    (It is suggested to turn this feature on if you have trouble getting the
    right ground states).
-w: Weight structures by w/(struct_energy-gs_energy+w)
    (recommended value: start with 1. and decrease down to about 0.010 (eV)
    if you have trouble getting the correct ground states.
    Default: all structure have equal weight)
-p: Penality for structures that lie below the ground state line.
    (recommended value: start with 1. and increase up to about 20.
    if you have trouble getting the correct ground states.
    Default: 0)

-> corr.in

table of correlations, one structure per line
(exactly the output of corrdump)

-> energy.in
column of energy values, one per line, in the same order as in the corr.in file.
If energy is unknown, put 'x'.

-> include.in

This file can be omitted.
It gives a list of clusters than must be part of the cluster expansion.
(Each number in this file indicates a column in the corr.in file.)

-> weight.in

This file can be omitted.
It indicates the weight that must be given to each structure.
Usually this file is copied from the weight_sug.out file obtained from a previous run.
Each weight in this file is multiplied by
  gs_prec/(structure_energy-ground_state_energy+gs_prec)
(see above).
```

```
-> clusters.out

A list of the clusters (in the same format as generated by either maps
or corrdump)

OUTPUT FILES

-> fit.out

Contains the results of the fit, one structure per line and each line
has the following information:
  concentration energy fitted_energy weight index
'concentration' lies between 0 and 1.
'energy' is the true formation energy.
'fitted_energy' is the predicted formation energy.
'weight' is the weight of this structure in the fit.
'index' is the structure number (not counting structure of unknown energies)

-> predstr.out
Contains the predicted energy of all structures whose true energy is unknown.
Format: one structure per line, and each line has the following information:
  concentration predicted_energy -1 status
the '-1' is for compatibility with maps.
status is 'u' (for compatibility with maps) and a 'g' is appended to status if
 that structure is predicted to be a ground state.
 To list all predicted ground states, type
 grep 'g' predstr.out

-> gs.out

The ground states, as determined by energies given in energy.in.
Each line is a concentration, energy pair.

-> gs_fitted.out

The ground states, as determined by energies predicted from
the cluster expansion. (Structures for which the true energy is
unknown are omitted.)
Each line is a concentration, energy pair.

-> weight_sug.out

If the ground states are incorrectly predicted by the cluster expansion,
this file contains suggested weight that should correct the problem.
just type
cp weight_sug.out weight.in
and rerun the program.

-> weight_used.out

Weights actually used to do the fit.

-> fit.gnu

A gnuplot script that display all the relevant information.
Just type:
gnuplot fit.gnu

-> eci.out

The values of the fitted eci, in the same order as in the corr.in file.
```

7.1.4 emc2

```
Easy Monte Carlo Code (emc2)
by Axel van de Walle

Command line parameters:
```

```
-T0 : initial temperature
-T1 : final temperature
-dT : temperature step
-db : inverse temperature step

Temperatures are given in units of energy unless the -k option is set.
-dT and -db are mutually exclusive. Which option you use determines
whether T or 1/T are unformly spaced. The output file always shows T.
Avoid setting -T0 or -T1 to 0: The output will be nonsensical.

-k : Sets boltman'z constant (default k=1). This only affects how
     temperatures are converted in energies.  -k=8.617e-5 lets you enter
     temperatures in kelvins when energies are in eV.
     (You can also select this value by using the -keV option.)

-mu0 : initial chemical potential
-mu1 : final chemical potential

  By default, these are input as dimensionless values defined as
  follows: If x is integer, x is the chemical potential that
  stabilizes a two phase equilibrium between ground state x-1 and
  x. (Ground states are numbered starting at 0.) Fractional values
  interpolate linearly between these integer values.  Negative values
  or values larger than the number of ground states - 1 are allowed.
  The values of mu are found by linear extrapolation.  If the -abs
  option is specified, the value of mu are in units of energy per spin
  value (as in the output file).  (The ground states are read in from
  the file gs_str.out .)

  If there are only two ground states, the only correction performed is
  to shift mu so that mu=0 stabilizes a two-phase equilibrium between
  the two ground states.
  If there are less than 2 ground states (!), no correction is made.

-dmu : chemical potential step (expressed in the same units as mu0 and mu1).

NOTE: If mu1 is omitted, only a scan through T is performed keeping mu=mu0.
      If T1 is omitted, only scan through mu is performed keeping T=T0.

-gs : Gives the index of the ground state to use as an initial spin
      configuration (the leftmost pure element is numbered 0).  If the
      index is -1, the disordered state with an average spin of zero
      is used as the starting configuration.

-phi0 : value of the grand canonical potential at the initial point of
        the run.  If left unspecified, it is set to the grand canonical
        potential of given by either the 1-spin Low Temperature Expansion
        or the High Temperature Expansion, depending whether the initial
        state is an ordered or a disordered phase.

-er : enclosed radius. The Monte Carlo cell will the smallest possible
    supercell of unit cell of the initial configuration such that a
    sphere of that radius fits inside it.  This allows you to specify
    the system size in a structure-independent fashion.

-innerT : by default, the inner loop is over values mu while the outer
          loop is over values of T. This flag permutes that order.

-eq : number of equilibration passes. (Equilibration is performed at
      the beginning of each step of the outer loop.)

-n : number of Monte Carlo passes performed to evaluate thermodynamic
     quanties at each step of the inner loop.

-dx: instead of specifying -eq and -n, you can ask the code to equilibrate
     and run for a time such that the average concentration is accurate
     within the target precision specifified by -dx=.
```

```
-tstat : Critical value of the test for discontinuity. The code is
         able to catch phase transformations (most of the time) when
         going from an ordered phase to another or to the disordered
         state. This involves a statistical test which a
         user-specified confidence level. The default, 3, corresponds
         to a 0.4% chance of finding a transition where there is
         none. (Refer to a standard normal table.)  -tstat=0 turns off
         this option.  Suggestion: if a phase transition is
         undetected, first try to reduce dT or dmu or increase n or decrease dx
         before toying around with this parameter.  Also: beware of
         hysteresis.

-sigdig : Number of significant digits printed. Default is 6.

-o:       Name of the output file (default: mc.out).

Tricks:

   To read parameters from a file, use:
    emc2 `cat inputfile`
   where inputfile contains the commands line options.

   To selectively display a few of the output quantities, use:
    emc2 [options] | cut -f n1,n2,n3,...
   where n1,n2,n3,... are the column number desired (see below).

Input files:

lat.in       : description of the lattice.
clusters.out : describes the clusters.
eci.out      : provides the ECI.
gs_str.out   : a list of ground states, in increasing order of concentration.

   These 4 files can be created by maps.
   See maps documentation (maps -h) for a description of the formats.

Optional input file:

teci.out     : if present, provides temperature-dependent eci (overrides eci.out)
               (Note that, even when the teci.out file is used, column 6 of the output file
                reflects only the configurational contribution to the heat capacity.)

The format this file is:
[maximum temperature: Tm]
[number of temperatures where eci are provided: nT]
[ECIs for temperature 0]
[ECIs for temperature Tm/(nT-1)]
[ECIs for temperature 2*Tm/(nT-1)]
...
[ECIs for temperature Tm]

Note that these numbers can be seperated by blanks or newlines, as desired.

Format of the output file:

Each line contains, in order:

 1) T:  Temperature
 2) mu: chemical potential (derivative of the free energy wrt to average spin)
 3) E-mu*x:  Average energy (per spin)
 4) x:  Average Concentration [ranges from -1 to 1]
 5) phi: grand canonical potential per spin (F-mu*x, where F is the Helmholtz free energy)
 6) E2: Variance of the energy (proportional to heat capacity)
 7) x2: Variance of the concentration (proportional to susceptibility)
 8) E_lte-mu*x_lte: calculated with a one spin Low Temperature Expansion
 9) x_lte
10) phi_lte
11) E_mf-mu*x_mf:  calculated with the Mean Field approximation
12) x_mf
```

```
13) phi_mf
14) E_hte-mu*x_hte: calculated with a High Temperature Expansion (ideal solution + polynomial in x)
15) x_hte
16) phi_hte
17) lro: Long Range Order parameter of the initial ordered phase (=0 if initial phase is disordered).
18-) corr: the average correlations associated with each cluster.

NOTE: to obtain 'canonical' rather than grand canonical quantities,
use the -g2c option. This has the effect of adding mu*x to columns
3,5,8,10,11,13,14,16.
Then, for instance, column 5 gives F, the Helmholtz free energy while column 3 gives E, the energy.
```

7.1.5 epic

```
Summary

This code find a saddle using a modification of the dimer method called the epicycle method.
An epicycle differs from a dimer in that one of the system images lies in the center and the
other one is rotating around it while in a dimer the two images lie symmetrically about the center.
The algorithm is described in:
A. van de Walle, S. Kadkhodaei, R. Sun, and Q.-J. Hong., 'Epicycle method for elasticity limit calculations.',
Phys. Rev. B, 95:144113, 2017. http://dx.doi.org/10.1103/PhysRevB.95.144113

It is implemented as two nested optimization problems:
an inner optimization problem to find the softest phonon mode using a modification of the dimer method
(called the epicycle method) and an outer optimization problem to find the actual atomic geometry.

All options that pertain to the inner 'epicycle' optimization start with '-e' while
those that control ionic (and cell parameter) movement start with '-i'.
Both optimization are implemented via a conjugate gradient algorithm.

Parameters controlling the optimization

-el  (Epicycle Length, in Angstrom) specifies the distance between the two images of the epicycle.
-egt (Epicycle Gradient Tolerance, in eV/Ang^2) is the stopping criterion for the soft mode search algorithm.
-ets (Epicycle Trial Step, in radiant) trial step for the line minimizations.
     If this trial step fails to bracket the minimum, the step is size multiplied by the...
-eml (Epicycle Multiplier in Line minimization) until the minimum is bracketed.
     But the step size will never exceed the...
-ems (Epicycle Maximum Step multiplier).
     The actual maximum step is equal to trial step times the multiplier.
     Bracketing stops when a bracket is found or the
-ebl (Epicycle maximum number of Bracketing steps in Line minimizations) is reached.
     Once the bracketing step is done, the algorithm does a sequant search, finding the point most likely to have zero derivative
     based on the derivatives at the end points of the bracket. If the predicted point falls too close to the endpoints
     (not in the middle half of the bracket) a bisection step is taken instead, except the first 't' times this occurs,
     where 't' is the...
-ebf (Epicycle motion Bad step Forgiveness).
     This is repeated until either the gradiant tolerance is met (-egt divided by sqrt(number of degrees of freedom ) or the...
-eil (Epicycle maximum number of Iterations in Line minimizations) is reached.
     The line minimizations are embedded in a conjugate gradient proceedure which is repeated until the gradient
     tolerance (-egt) is met or the ...
-eic (Epicycle maximum number of Iterations in Conjugate gradient) is reached.
     As in any conjugate gradient method, the conjugate direction reset to steepest descent every...
-eir (Epicycle iterations between conjugate gradient reset) steps.

For the outer optimization problem (ion motion), the same parameters are available: with the initial '-e' replaced by '-i':
-igt,-its,-iml,-ims,-ibl,-ibf,-iil,-iic,iir.
     One difference is that -igt is in eV/Ang and -its and -ims are in Angstrom.
     In addition, the outer optimization start with a few steps of steepest descent, indicated by the
-isi (Ion motion Steepest maximum number of Iterations) parameter.
     This helps because the outer optimization problem can be far from quadratic in behavior initially.
     The step size is equal to the force times the
-ism (Ion motion Steepest descent Multiplier, in Angstrom^2/eV).
     The outer optimization problem also optimizes cell shape in addition to ionic coordinates.
     To make cell degress of freedom comparable to atomic coordinates, the following scaling is used:
     The 'force' on the cell is Omega^(2/3) * (stress tensor) * f where Omega is the average atomic volume for the
     initial configuration and f is a constant set with:
 -ff (Force scale Factor, dimensionless).
```

```
     The cell shape is parametrized by n*Omega^(1/3)*strain/f where n is the number of atoms.
     This convention ensures that stress and cell parameters scale approriately with cell size and have units and magnitudes
     comparable to the atomic coordinates. Note that the atomic coordinates are stored internally as the coordinates for the
     initial cell shape (and are distorded according the strain acting on the cell).
-ds  indicates whether and how to relax the cell shape. 0 (the default) means no cell relaxations,
     3 means fully general 3d strains are allowed, 2 means means fully general 2d strains, etc.
     The unique axis is x be default but can be changed by adding 4 (for y axis) or 8 (for z axis).
-st (Sleep Time between read access) is the time between each attempt to check if the calculation lauched has completed.

Input files
  str.in  The initial structure geometry in standard ATAT format (see mmaps -h)
 Optionally the following files can be read to continue a previous run (see below for a description):
  epidir.out
  epipos.out

Final output files
  cstr_relax.out  The optimized inflection point geometry at the end of the calculations.
  cenergy.out     The corresponding final energy.
  stdout          Log file (written to infdet.log if called by robustrelax_xxxx)

A few notes about the log file (assuming it is redirected to infdet.log):
  -The inner optimization problem output is bracketted by the phrases 'begin on_sphere' and 'end on_sphere'.
  -For a quick overview of the progress, use:      grep curv infdet.log
  -For a more detailed view (each c.g. step), use: grep norm infdet.log
   The inner optimization steps are indicated by s_gnorm while the outer by l_gnorm.
  -To see each function evaluation, use:           grep dfx infdet.log
  -To see the whole history of epicycle positions and directions:
                                                   grep -e epipos -e epidir infdet.log

Intermediate input/output files
 The infdet code relies on an external program to obtain its energy and force data. At each optimization step, it writes:
  busy            A semaphore file indicating that the external program should run now.
  str.out         The current geometry to be run by the external code
 When done, the external program deletes the busy file and infdet knows it has to read:
  force.out       the forces acting on each atom (one 3d vector per line)
  stress.out      the stress tensor acting on the cell
  energy          the total energy
  str_relax.out   the atomic coordinate (same as str.out but perhaps re-ordered - forces will be re-ordered accordingly)

 As the optimization progresses, the current status is written to various files:
  str_current.out   the current best approximation to the inflection point (in standard ATAT format)
  epipos.out        the current best approximation to the inflection point (as a vector, in internal format)
  epidir.out        the current direction of the epicycle (softest phonon mode)
                    Note that the whole history of these values are available in the log file, prefixed by
                    epipos= and epidir= , which can be used to restart an aborted or misbehaving run.
```

7.1.6 felec

```
This code calculates the electronic free energy within the one-electron
and temperature-independent bands approximations.

It needs an dos.out input file (whose name can be changed with -dos option) that
has the following format:
 [number of electron in unitcell]
 [energy width of each bins used to calculate the dos]
 [a multiplicative scale factor to adjust units]
 [the density in each bin, in states/unit cell/energy] <- repeated

The code calculates the electronic free energy from temperature T0 to T1 in steps of dT.
  a) The defaults are T0=0 T1=2000 dT=100.
  b) If a file Trange.in exists in the upper directory, it is used to set T0,T1,dT:
     Trange.in must contain two numbers on one line separated by a space: T1 (T1/dT+1).
     Note that T0=0 always.
     For phase diagram calculations, you must use this method to specify the temperature range.
  c) These defaults can be overridden by the -T0, -T1 and -dT options.

The output files contain the free energy per unit cell.
  felec.log contain temperature and corresponding free energy on each line.
  felec contains the free energies only.
```

```
  plotdos.out contains the dos (col 1: energy normalized so that Ef=0 , col 2: DOS)

-> For including electronic entropy in phase diagram calculations

 You are likely to use this code as follow:

  #first create the Trange.in file for up to 2000K in intervals of 100K:
  echo 2000 21 > Trange.in

  #This executes the svsl code in each subdirectory containing dos.out but no error file.
  foreachfile -e dos.out pwd \; felec [options if desired]

  #constructs a cluster expansion of the electronic free energy (eci are in felec.eci)
  clusterexpand felec

  #add the energetic eci from eci.out to the electronic eci from felec.eci and create the teci.out
  #file that will be read by the Monte Carlo code.
  mkteci felec.eci

  #you can even combine vibrational and electronic eci:
  mkteci fvib.eci felec.eci
```

7.1.7 fempmag

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I. Ohnuma et al., Phase equilibria in the Fe-Co binary system, Acta Materialia 50 (2002) 379.
```

7.1.8 fitfc

```
Calculates vibrational properties by fitting a spring model to
reaction forces resulting from imposed atomic displacements.

The examples below are given assuming that one uses the vasp code,
although other ab initio codes would work as well.

The calculations proceed as follows:

1) You first need to fully relax the structure of interest.  The code
   expects the relaxed geometry in the file str_relax.out. It also
   expects a str.out file containing the unrelaxed geometry (which may be
   the same as the relaxed geometry, if you wish). The unrelaxed geometry
   will be used to determine the neighbor shells and measure distances
   between atoms.  Typically the user would specify the str.out file,
   then obtain the str_relax.out file by runing an ab initio code with a
   command of the form
       runstruct_vasp
   (making sure the vasp.wrap file indicates that all degrees of freedom
   must be relaxed).

2) Generation of the pertubations.
2a) A typical command line is as follows:
    fitfc -er=11.5 -ns=3 -ms=0.02 -dr=0.1
-er specifies how far apart the periodic images of the displaced atom must be.
    The code then finds the size of the supercell satisfying this constraint.
    Distances are measured according to the atomic positions given in str.out
    and in the same units.
-ns specifies the number of different strain at which phonon calculations
    will be performed.
    (-ns=1 implies a purely harmonic model, the default while values greater
    than 1 will invoke a quasiharmonic model)
-ms specifies the maximum strain (0.02 signifies a 2% elongation along
    every direction).
-dr the magnitude of the displacement of the perturbed atom.
The above command writes out a series of subdirectories vol_*, one for
each level of strain.
If the structure has cubic symmetry or if you are willing to assume that
thermal expansion is isotropic or if you only which to use the harmonic
approximation, the fitfc command should be invoked with the -nrr option
```

```
(do Not ReRelax) and you can now skip to step 3).

2b) Each volume subdirectory now contains a str.out file which is
    stretched version of the main str_relax.out file provided.
    You then need to run the ab initio code to rerelax the geometry at
    the various levels of imposed strain and obtain the energy as a
    function of strain. Typically, this is acheived by typing:
      pollmach runstruct_vasp &
    (make sure that the vasp.wrap file is modified so that all degrees
    of freedom except volume are allowed to relax.)
    After this command each subdirectory will contain an energy and
    a str_relax.out file.
    Type
      touch stoppoll
    after all energies have been calculated.
    The runstruct_vasp command can also be executed manually in each
    subdirectory or as follows:
       foreachfile wait runstruct_vasp \; rm wait

2c) Now you need to reinvoke fitfc to generate perturbations of the
    atomic position for each level of strain.
      fitfc -er=11.5 -ns=3 -ms=0.02 -dr=0.1
    This is exactly the same commmand as before but the code notices
    the presence on the new files and can proceed further.

3) At this point the files generated are arranged as follows.
   At the top level, there is one subdirectory per level of strain
   (vol_*, where * is the strain in percent), and in each
   subdirectory, there are a number of subsubdirectories,
   each containing a different perturbation. The pertubation
   names have the form p<+/-><dr>_<er>_<index>, where
   <pertmag> is the number given by the -dr option,
   <er> by the -er option and <index> is a number used to distinguish
   between different pertubations. Two perturbations that differ only
   by their signs are sometimes generated and are distinguished
   by a + or - prefix.
   If you want to ensure that the third-order force constants
   cancel out exactly in the fit, you need to consider both
   perturbations.
   Otherwise, only the 'positive' perturbation will be sufficient.
   Note that whenever the third-order terms cancel out by
   symmetry, only the 'positive' perturbation will be generated.

   You then need to use the ab initio code to calculate reaction
   forces for each perturbation.
   This will typically be accomplished by typing
     pollmach runstruct_vasp &
   (make sure that the vasp.wrap file indicates that no degrees of
   freedom are allowed to relax and the smearing is used
   for Brillouin zone integration. Do not use the DOSTATIC option.)
   For added efficiently, use the 'lookup up' option:
     pollmach -lu runstruct_vasp &
   This will reuse the WAVECAR and CHGCAR from prior runs to speed up
   convergence of later ones. This works better if -dr is small (e.g. -dr=0.05).
   Make sure to set ICHARG=1 in the vasp.wrap file.

4) Fitting the force constants and phonon calculations.
   This mode is invoked with the -f option.
   In addition, you need to specify the range of the springs included
   in the fit using the -fr=... option.
   Usually, the range specified with -fr should be not more than
   half the distance specified with the -er option ealier.
   Distances are measured according to the atomic positions given
   in str.out and in the same units.
   It is a good idea to try different values of -fr (starting with
   the nearest neighbor bond length) and check that
   the vibrational properties converge as -fr is increased.

5) Sometimes you will get the message 'Unstable modes found. Aborting.'
```

```
   This indicates that the structure considered may be mechanically unstable.
   If, in addition, you see the warning 'Warning: p... is an unstable mode.',
   then the structure is certainly unstable. Otherwise, it may be a artifact
   of the fitting procedure.
   To find out, you can tell the code to generate perturbations along the unstable
   directions and let your ab initio code calculate the reaction forces
   which can then be included in the fit to settle this issue.
   First, to view the unstable modes, use the -fu option: the output is in
   vol_*/unstable.out and has the form:
     u [index] [nb_atom] [kpoint] [branch] [frequency]
     [displacements...]
   where [index] is a reference number, nb_atom is the size of the supercell
   needed to represent this mode (the other entries are self-explanatory).
   (If this file contains only entries with nb_atom=too_large,
   you need to increase the -mau option beyond its default of 64.)
   You can pick one of these modes to written out to disk with the option
   -gu=[index] where [index] is the one reported in the unstable.out file.
   Using a negative index gives the sine instead of cosine phase of the mode.
   You can run your ab initio code in the subdirectory generated (named vol_*/p_uns_<dr>_<kmesh>_<number>)
   and rerun fitfc -f -fr=...
   If you see 'Warning: p... is an unstable mode.' then you have found a true
   instability. If you only see 'Unstable modes found. Aborting.' you may repeat the
   process until the message disappear or a truly unstable mode is found.

   Note: If you want to generate a phonon DOS even if there are unstable modes,
   use the -fn option. The unstable modes will be shown as negative frequencies.

-> Phonon Dispersion curves
The -df=inputfile option invokes the phonon dispersion curve module.
The syntax of the input file is:
[nb of points] [kx1] [ky1] [kz1] [kx2] [ky2] [kz2]
repeat...

Each line of input defines one segment (kx1,ky1,kz1)-(kx2,ky2,kz2)
along which the dispersion curve is to be calculated.
[nb of points] specifies the number of points sampled along the segment.
The coordinates are in multiple of the reciprocal cell defined by the axes in the
file specified by the -si option (or, by default, in the str.out file).
(The k-point coordinates are appropriately strained
by the amount needed for the str.out file to be identical to the str_relax.out file.)
The phonon frequencies are output in the eigenfreq.out file,
in the vol_* subdirectories.

Output files:
   fitfc.log       : A general log file.
   vol_*/vdos.out  : the phonon density of states for each volume considered
   vol_*/fc.out    : The force constants.
                     For each force constant a summary line gives:
                         (i)   the atomic species involved
                         (ii)  the 'bond length'
                         (iii) the stretching and bending terms
                     Then, each separate component of the force constant is
                     given and, finally, their sum.
  vol_*/svib_ht    : gives the high-temperature limit of the vibrational
                     entropy (in units of kB/atom) in the harmonic approximation,
                     excluding the configuration-independent contribution at each
                     unit cell volume considered (so, this just -3 times the
                     average log phonon frequency).
  vol_*/fvib       : gives the harmonic vibrational free energy (in eV) at that volume
                     as a function of temperature.

The following 3 files give the output of the quasiharmonic approximation if ns>1 and
the harmonic approximation if ns=1:

  fitfc.out        : gives along each row, the temperature, the free energy,
                     and the linear thermal expansion
                      (e.g. 0.01 means that the lattice has expanded by 1%
                       at that temperature).
  fvib             : gives only the free energy
```

```
  svib             : gives only the entropy (in energy/temperature, by default, eV/K)

  eos0.out         : equation of state at 0K (one strain,energy pair per line)
  eos0.gnu         : gnuplot script to plot polynomial & data

Caution:
  When using fitfc as part of a cluster expansion, make sure you use the -me0 option to
  ensure that the static energy (included in eci.out) is not double-counted.
```

7.1.9 fitsvsl

```
This code determines bond stiffness vs bond length relationship for the purpose
of calculating vibrational properties (with the svsl code).

It requires the following files as an input.
1) A lattice file (by default, lat.in, but this can be overridden with the -l option) which
   allows the code to determine what chemical bonds are present in the system.
   The format is as described in the maps documentation (see maps -h).
2) A list of directories containing structures that will be used to calculate force constants
   (by default strname.in, but this can be overridden with the -dn option).
   Each of the listed directory must contain
   a) a str.out file containing an ideal unrelaxed structure that will be used to automatically
      determine the nearest neighbor shell,
   b) a str_relax.out file containing the relaxed structure that will be used to calculate
      bond lengths and that the code will perturb in various ways to determine the force constants.

The code can operate in two modes: a structure generation mode and a fitting mode (indicated by the
-f option).

In structure generation mode:

  All the above input files are needed and the option
  -er must be specified in order to indicate the size of the supercells generated.
  The -er option indicates how far from each other a displaced atom must be from
  its periodic images, the code will infer the smallest supercell satisfying this constraint.
  Typically, -er should be 3 or 4 times the nearest neighbor distance. All of these distances
  are measured using the ideal structures (*/str.out).

  The following parameters have reasonable default values which can be overridden:
   -dr specifies the displacement of the perturbed atom, which is 0.2 Angstrom by default.
   -ms specifies the maximum (linear) expansion of the structures for the purpose of
       lengthing the bond lenght. For instance -ms=0.01 (the default) indicates that the
       supercells will be stretched by up to 1% isotropically.
   -ns indicates the number of intermediate lattice parameters sampled (by default 2, which is
       the minimum in order to be able to determine the length dependence of bond stiffness).

After the structure generation step:

  Each of the directory specified in strname.in will contain multiple subdirectories,
  each of which contains
    a) the ideal unrelaxed supercell in a str_ideal.out file.
    b) the relaxed but unperturbed supercell in a str_unpert.out file.
    c) the actual geometry of perturbed supercell calculation in a str.out file.
  The appropriate first-principles calculations can be performed using the other utilities in the atat
  package, such as runstruct_vasp. Of course a corresponding vasp.wrap file must given
  in order to provide the input parameters for the first-principles calculations.
  Make sure that these parameters indicate a static run (no relaxations!).
  After all (or some) of these calculations are done, each subdirectory will contain
    a force.out file containing the forces acting on each atoms
    a str_relax.out file containing the atomic positions (in the same order as in force.out)

The fitting mode (-f option) of ftsvsl then needs to be used.
  The lattice file (e.g. lat.in) must be present and the code will look for all files of the form
  */force.out and */*/force.out   and the corresponding files */str*.out and */*/str*.out .
  The code will then use that information to create the length-dependent force constants
  (this may take a few minutes) and ouputs them in
     slspring.out
  Here is an example of the format of this file:
    Al Al         (gives the type of bond)
```

```
    2            (2 parameters: linear fit is used)
    50.28971     \  polynomial coeficients of the stiffness vs length relationship for stretching term
    7.88973      /  (typically, stiffness is in eV/Angstrom^2 and length is in Angstrom)
    2            \
    6.12722       | idem for bending term
    -1.01641     /
    Ti Al         (repeat for each type of chemical bond)
    3
    etc.
  The only option controling this process is -op, which specifies the order of the polynomial
  used to fit the length dependence (by default -op=1 and a linear fit is used).
  (Contact the author for information about the -sf option.)

Diagnostic files are also output:
  fitsvsl.log                    (a log file)
  fitsvsl.gnu and f_*.dat        (to plot the s vs l relationship)
```

7.1.10 gce

```
->What does this program do?

1) It reads the lattice file (specified by the -l option). (See format below.)

2) It determines the space group of this lattice and
   writes it to the sym.out file.

3) It finds all symmetrically distinct clusters-'object' pairs that satisfy the
   conditions specified by the options -2 through -6.
   For instance, if -2=2.1 -3=1.1 is specified,
   only pair clusters shorter than 2.1 units and triplet clusters containing
   no pairs longer than 1.1 will be selected.
   This produces a generalized cluster expansion (GCE) representating a relationship
   between a property of type 'object' and a crystal structure.
   The 'object' can be anything obeying well-defined symmetry rules.
   By default the 'object' is a tensor of rank defined in the file gcetensor.in (see below for format).

4) It writes all clusters found to clusters.out.
   If the -c option is specified, clusters are read from clusters.out instead.

5) It reads the structure file (specified by the -s option).

6) It determines, for that structure, the correlations associated with all
   the clusters chosen earlier.
   This information is then output on one line, in the same order as in the
   clusters.out file. See below for conventions used to calculate correlations.

7) It writes the files corrdump.log containting the list of all adjustements
   needed to map the (possibly relaxed) structure onto the ideal lattice.

->File formats

Lattice and structure files

Both the lattice and the structure files have a similar structure.
First, the coordinate system a,b,c is specified, either as
[a] [b] [c] [alpha] [beta] [gamma]
or as:
[ax] [ay] [az]
[bx] [by] [bz]
[cx] [cy] [cz]
Then the lattice vectors u,v,w are listed, expressed in the coordinate system
just defined:
[ua] [ub] [uc]
[va] [vb] [vc]
[wa] [wb] [wc]
Finally, atom positions and types are given, expressed in the same coordinate system
as the lattice vectors:
[atom1a] [atom1b] [atom1c] [atom1type]
```

```
[atom2a] [atom2b] [atom2c] [atom1type]
etc.

In the lattice file:
-The atom type is a comma-separated list of the atomic
 symbols of the atoms that can sit the lattice site.
-The first symbol listed is assigned a spin of -1.
-When only one symbol is listed, this site is ignored for the purpose
 of calculating correlations, but not for determining symmetry.
-The atomic symbol 'Vac' is used to indicate a vacancy.

In the structure file:
-The atom type is just a single atomic symbol
 (which, of course, has to be among the atomic symbols given in the
 lattice file).
-Vacancies do not need to be specified.

Examples

The fcc lattice of the Cu-Au system:
1 1 1 90 90 90
0   0.5 0.5
0.5 0   0.5
0.5 0.5 0
0 0 0 Cu,Au

The Cu3Au L1_2 structure:
1 1 1 90 90 90
1 0 0
0 1 0
0 0 1
0   0   0   Au
0.5 0.5 0   Cu
0.5 0   0.5 Cu
0   0.5 0.5 Cu

A lattice for the Li_x Co_y Al_(1-y) O_2 system:
0.707 0.707 6.928 90 90 120
 0.3333  0.6667 0.3333
-0.6667 -0.3333 0.3333
 0.3333 -0.3333 0.3333
 0       0      0       Li,Vac
 0.3333  0.6667 0.0833  O
 0.6667  0.3333 0.1667  Co,Al
 0       0      0.25    O

File format of gcetensor.in

[rank]
[list of pairs of indices indicating which simultaneous index permutations leave the tensor invariant]
[next list, etc...]

Examples
  for strain or stress:
  2
  0 1

  for elastic constants:
  4
  0 1
  2 3
  0 2 1 3

Symmetry file format (sym.out)

[number of symmetry operations]

3x3 matrix: point operation
```

```
1x3 matrix: translation

repeat, etc.

Note that if you enter more than one unit cell of the lattice,
sym.out will contain some pure translations as symmetry elements.

Cluster file format (clusters.out)

for each cluster:
[multiplicity]
[length of the longest pair within the cluster]
[number of points in cluster]
[coordinates of 1st point] [number of possible species-2] [cluster function]
[coordinates of 2nd point] [number of possible species-2] [cluster function]
etc.
[keyword describing type 'object' in the GCE, for instance: tensor]
['object' data]

repeat, etc.


When the 'object' is a tensor the 'object' data is:
[rank]
[3's repeated 'rank' times]
[3^rank]
[elements of the tensor]


(Multiplicity and length are ignored when reading in the clusters.out file.)
For each 'point' the following convention apply
-The coordinates are expressed in the coordinate system given in
 the first line (or the first 3 lines) of the lat.in file.
-The 'number of possible species' distinguishes between binaries, ternaries, etc...
 Since each site can accomodate any number of atom types,
 this is specified for each point of the cluster.
-In multicomponent system, the cluster function are numbered from 0 to number of possible species-2.
In the simple of a binary system [number of possible species-2] [cluster function] are just 0 0.
For a ternary, the possible values are 1 0 and 1 1.
All the utilities that are not yet multicomponent-ready just ignore the entries [number of possible species-2] [cluster function].

Convention used to calculate the correlations:
  The cluster functions in a m-component system are defined as
   function '0' : -cos(2*PI*  1  *s/m)
   function '1' : -sin(2*PI*  1  *s/m)
                              .
                              .
                              .
                 -cos(2*PI*[m/2]*s/m)
                 -sin(2*PI*[m/2]*s/m)   <--- the last sin( ) is omitted if m is even
  where the occupation variable s can take any values in {0,...,m-1}
  and [...] denotes the 'round down' operation.
  Note that, these functions reduce to the single function (-1)^s in the binary case.

Special options:

-sym:  Just find the space group and then abort.
-clus: Just find space group and clusters and then abort.
-z:    To find symmetry operations, atoms are considered to lie on
       top of one another when they are less than this much apart.
-sig:  Number of significant digits printed.


->Cautions

When vacancies are specified, the program may not be able to warn
you that the structure and the lattice just don't fit.
Carefully inspect the corrdump.log file!
```

```
If the structure has significant cell shape relaxations, the program
will be unable to find how it relates to the ideal lattice.
The problem gets worse as the supercell size of the structure gets
bigger.

There is no limit on how far an atom in a structure can be from
the ideal lattice site. The program first finds the atom that can
be the most unambiguously assigned to a lattice site. It then
finds the next best assignement and so on. This is actually a
pretty robust way to do this. But keep in mind that the -z option
does NOT control this process.
```

7.1.11 gensqs

```
IMPORTANT NOTE: Please see mcsqs command for a better, easier-to-use SQS generator.

This code requires 3 input files:
1) A lattice file (by default lat.in) in the same format as for
   maps or corrdump.
2) A cluster file (by default clusters.out), as generated with
    the corrdump utility.
3) A target correlation file (by default tcorr.out) which
   contains the value of desired correlations for each of
   the clusters listed in the cluster file.

A typical caling sequence would be:

# the following command can be used to generate the target correlation file tcorr.out

corrdump -noe -2=maxradius -rnd -s=conc.in > tcorr.out

# where maxradius is the length of the longest pair desired
# and where conc.in contains an (ordered) structure having the
# desired concentration.
# The geometry of the structure in the conc.in file is not crucial -
# only the average concentration on each sublattice will be used.
# CAUTION: Here, a 'sublattice' is a set of symmetrically equivalent point clusters.
# If your system contains multiple sublattices (as evidenced by multiple
# point clusters in clusters.out, make sure that your conc.in file sets
# the composition of each sublattice correctly! This can be verified
# by looking at the point correlations output.

#this looks for possible sqs of 8 atoms/ cell
gensqs -n=8 > sqs8.out

corrdump -2=anotherradius -3=anotherradius  -noe -s=sqs8.out
# this helps you decide which sqs is best based on other correlations
# associated with clusters (pairs and triplets) of diamter less than
# anotherradius.

Caution:
 gensqs only generates structures containing exactly the number of atoms per unit cell specified by the -n option.
 (If an SQS with a smaller unit cell exists, it will not be listed.)
 If you give too many correlations to match, the code may not
 output anything.
 Finding an 8-atom sqs takes a few minutes, an 16-atom sqs, a few hours
 and a 32-atom sqs, a few days!
 The exact speed depends on the symmetry of the lattice and on your
 computer.
```

7.1.12 infdet

```
Summary

This code seeks to find the geometry that has the minimum energy under the constrain that its softest phonon mode(s)
has zero frequency.

The algorithm is described in:
```

```
A. van de Walle, S. Kadkhodaei, R. Sun, and Q.-J. Hong., 'Epicycle method for elasticity limit calculations.',
Phys. Rev. B, 95:144113, 2017. http://dx.doi.org/10.1103/PhysRevB.95.144113

A theoretical motivation for using such a quantity can be found in:
A. van de Walle, Q. Hong, S. Kadkhodaei, and R. Sun., 'The free energy of mechanically unstable phases',
Nature Commun. 6, 7559 (2015). http://dx.doi.org/10.1038/ncomms8559

This is code often invoked automatically within the script robustrelax_xxxx with the -id option. In this case,
all options are passed with -idop \"[any of the options described below]\". Also, all files described below
then reside in the 01 subdirectory and the log file is 01/infdet.log .

It is implemented as two nested optimization problems:
-an inner optimization problem to find the softest phonon mode using a modification of the dimer method
(called the epicycle method) and
-an outer optimization problem to find the actual atomic geometry.
An epicycle differs from a dimer in that one of the system images lies in the center and the other one
is rotating around it while in a dimer the two images lie symmetrically about the center.

All options that pertain to the inner 'epicycle' optimization start with '-e' while
those that control ionic (and cell parameter) movement start with '-i'.
Both optimization are implemented via a conjugate gradient algorithm.

Parameters controlling the optimization

-el  (Epicycle Length, in Angstrom) specifies the distance between the two images of the epicycle.
-egt (Epicycle Gradient Tolerance, in eV/Ang^2) is the stopping criterion for the soft mode search algorithm.
-ets (Epicycle Trial Step, in radiant) trial step for the line minimizations.
     If this trial step fails to bracket the minimum, the step is size multiplied by the...
-eml (Epicycle Multiplier in Line minimization) until the minimum is bracketed.
     But the step size will never exceed the...
-ems (Epicycle Maximum Step multiplier).
     The actual maximum step is equal to trial step times the multiplier.
     Bracketing stops when a bracket is found or the
-ebl (Epicycle maximum number of Bracketing steps in Line minimizations) is reached.
     Once the bracketing step is done, the algorithm does a sequant search, finding the point most likely to have zero derivative
     based on the derivatives at the end points of the bracket. If the predicted point falls too close to the endpoints
     (not in the middle half of the bracket) a bisection step is taken instead, except the first 't' times this occurs,
     where 't' is the...
-ebf (Epicycle motion Bad step Forgiveness).
     This is repeated until either the gradiant tolerance is met (-egt divided by sqrt(number of degrees of freedom ) or the...
-eil (Epicycle maximum number of Iterations in Line minimizations) is reached.
     The line minimizations are embedded in a conjugate gradient proceedure which is repeated until
     the gradient tolerance (-egt) is met or the ...
-eic (Epicycle maximum number of Iterations in Conjugate gradient) is reached.
     As in any conjugate gradient method, the conjugate direction reset to steepest descent every...
-eir (Epicycle iterations between conjugate gradient reset) steps.

For the outer optimization problem (ion motion), the same parameters are available: with the initial '-e' replaced by '-i':
-igt,-its,-iml,-ims,-ibl,-ibf,-iil,-iic,iir.
     One difference is that -igt is in eV/Ang and -its and -ims are in Angstrom.
     Since the outer optimization takes into account two criteria (curvature and energy), it needs
     one multiplier to convert curvature gradient into force (so they can be combined into a single force):
-ics (Ion motion Curvature constraint Stiffness) If this is set to zero, the multiplier is automatically set to make
     the curvature gradient and the force equal at the first step and then kept constant thereafter.
     In addition, the outer optimization start with a few steps of steepest descent, indicated by the
-isi (Ion motion Steepest maximum number of Iterations) parameter.
     This helps because the outer optimization problem can be far from quadratic in behavior initially.
     The step size is equal to the force times the
-ism (Ion motion Steepest descent Multiplier, in Angstrom^2/eV).
     The outer optimization problem also optimizes cell shape in addition to ionic coordinates.
     To make cell degress of freedom comparable to atomic coordinates, the following scaling is used:
     The 'force' on the cell is Omega^(2/3) * (stress tensor) * f where Omega is the average atomic volume for the
     initial configuration and f is a constant set with:
 -ff (Force scale Factor, dimensionless).
     The cell shape is parametrized by n*Omega^(1/3)*strain/f where n is the number of atoms.
     This convention ensures that stress and cell parameters scale approriately with cell size and have units and magnitudes
     comparable to the atomic coordinates. Note that the atomic coordinates are stored internally as the coordinates for the
     initial cell shape (and are distorded according the strain acting on the cell).
-ds  indicates whether and how to relax the cell shape. 3 (the default) means fully general 3d strains are allowed,
```

```
     2 means means fully general 2d strains, etc.
     0 means no cell relaxations are allowed.
     The unique axis is x be default but can be changed by adding 4 (for y axis) or 8 (for z axis).
-st (Sleep Time between read access) is the time between each attempt to check if the calculation lauched has completed.

Input files
  str.in  The initial structure geometry in standard ATAT format (see mmaps -h)
 Optionally the following files can be read to continue a previous run (see below for a description):
  epidir.out
  epipos.out

Final output files
  cstr_relax.out  The optimized inflection point geometry at the end of the calculations.
  cenergy.out     The corresponding final energy.
  stdout          Log file (written to infdet.log if called by robustrelax_xxxx)

A few notes about the log file (assuming it is redirected to infdet.log):
  -The inner optimization problem output is bracketted by the phrases 'begin on_sphere' and 'end on_sphere'.
  -For a quick overview of the progress, use:      grep curv infdet.log
  -For a more detailed view (each c.g. step), use: grep norm infdet.log
   The inner optimization steps are indicated by s_gnorm while the outer by l_gnorm.
  -To see each function evaluation, use:           grep dfx infdet.log
  -To see the whole history of epicycle positions and directions:
                                                   grep -e epipos -e epidir infdet.log

Intermediate input/output files
 The infdet code relies on an external program to obtain its energy and force data. At each optimization step, it writes:
  busy            A semaphore file indicating that the external program should run now.
  str.out         The current geometry to be run by the external code
 When done, the external program deletes the busy file and infdet knows it has to read:
  force.out       the forces acting on each atom (one 3d vector per line)
  stress.out      the stress tensor acting on the cell
  energy          the total energy
  str_relax.out   the atomic coordinate (same as str.out but perhaps re-ordered - forces will be re-ordered accordingly)

 As the optimization progresses, the current status is written to various files:
  str_current.out   the current best approximation to the inflection point (in standard ATAT format)
  epipos.out        the current best approximation to the inflection point (as a vector, in internal format)
  epidir.out        the current direction of the epicycle (softest phonon mode)
                    Note that the whole history of these values are available in the log file, prefixed by
                    epipos= and epidir= , which can be used to restart an aborted or misbehaving run.
```

7.1.13 maps

```
-> What does this program do?

It gradually constructs a increasingly more accurate cluster expansion.
A user-provided script running concurrently is responsible for notifying
maps when computer time is available. maps creates files describing
structures whose energy should be calculated. The user-provided script
sets up the runs needed to calculate the energy of these structures.
As maps becomes aware of more and more structural energies, it gradually
improves the precision of the cluster expansion, which is continously
written to an output file.
The code terminates when a stop file is created by typing, for instance,
touch stop

NOTE: Fully functional scripts are included with the package:
pollmach and runstruct_vasp.
For for more information type
  pollmach
  runstruct_vasp -h

-> Format of the input file defining the lattice (specified by the -l option)

First, the coordinate system a,b,c is specified, either as
[a] [b] [c] [alpha] [beta] [gamma]
or as:
[ax] [ay] [az]
```

```
[bx] [by] [bz]
[cx] [cy] [cz]
Then the lattice vectors u,v,w are listed, expressed in the coordinate system just defined:
[ua] [ub] [uc]
[va] [vb] [vc]
[wa] [wb] [wc]
Finally, atom positions and types are given, expressed in the same coordinate system
as the lattice vectors:
[atom1a] [atom1b] [atom1c] [atom1types]
[atom2a] [atom2b] [atom2c] [atom2types]
etc.

-The atom type is a comma-separated list of the atomic
 symbols of the atoms that can sit the lattice site.
-The first symbol listed is assigned a spin of -1 and the second, a spin of 1.
-When only one symbol is listed, this site is ignored for the purpose
 of calculating correlations, but not for determining symmetry.

Examples:

The fcc lattice of the Cu-Au system:
3.8 3.8 3.8 90 90 90
0   0.5 0.5
0.5 0   0.5
0.5 0.5 0
0 0 0 Cu,Au

A lattice for the Li_x Co_y Al_(1-y) O_2 system:
 0.707 0.707 6.928 90 90 120
 0.3333  0.6667 0.3333
-0.6667 -0.3333 0.3333
 0.3333 -0.3333 0.3333
 0       0      0       Li,Vac
 0.3333  0.6667 0.0833  O
 0.6667  0.3333 0.1667  Co,Al
 0       0      0.25    O
Running the above example requires the multicomponent version of maps,
called mmaps.

Optional input file: ref_energy.in

  Contains the reference energy (per site) to be subtracted to get formation energies.
  The first line is the c=0 energy, the second line is the c=1 energy.
  If this file is omitted, the energies of leftmost and rightmost structures
  (on the concentration axis) are taken.

Optional input file: nbclusters.in
  Allows the user to manually select which clusters to include in the fit.
  This file should contains:
    number of pairs to include
    number of triplets to include
    etc.
  This file can be changed while maps is running. However, you must type
   touch refresh
  to tell maps to reread it.

-> Output files

maps.log
Contains possible warnings:
  'Not enough known energies to fit CE'
  'True ground states not = fitted ground states'
  'New ground states predicted, see predstr.out'

These warning should disappear as more structural energies become available
and the following messages should be displayed:
  'Among structures of known energy, true and predicted ground states agree.'
  'No other ground states of xx atoms/unit cell or less exist.'
```

```
This file also gives the crossvalidation score (in eV/atom) of the current fit
(before the weighting is turned on in order to get the correct ground states).

fit.out
Contains the results of the fit, one structure per line and each line
has the following information:
  concentration energy fitted_energy (energy-fitted_energy) weight index
'concentration' lies between 0 and 1.
'energy' is per site (a site is a place where more than one atom type can lie)
'weight' is the weight of this structure in the fit.
'index' is the name of the directory associated with this structure.

predstr.out
Contains the predicted energy (per site) of all structures maps has in memory but
whose true energy is unknown or has been flagged with error.
Format: one structure per line, and each line has the following information:
  concentration energy predicted_energy index status
index is the structure number (or -1 if not written to disk yet).
energy is the calculated energy (or 0 if unknown).
status is either
   b for busy (being calculated),
   e for error,
   u for unknown (not yet calculated) or
   g if that structure is predicted to be a ground state (g can be combined with the above).
To list all predicted ground states, type
grep 'g' predstr.out

gs.out
Lists the ground state energies, one structure per line and each line
has the following information:
  concentration energy fitted_energy index

gs_str.out
Lists the ground state structures, in the same format as the n/str.out files
(see below). Each structure is terminated by the word 'end' on a line by itself,
followed by a blank line.

eci.out
Lists the eci. (They have already been divided by multiplicity.)
The corresponding clusters are in clusters.out

clusters.out
For each cluster, the first line is the multiplicity, the second line is the
cluster diameter, and the third line is the number of points in the cluster.
The remaining lines are the coordinates of the points in the cluster
(in the coordinate system specified in the input file defining the lattice).
A blank line separates each cluster.

n/str.out
Same format as the lattice file, except that
-The coordinate system is always written as 3x3 matrix
-Only one atom is listed for each site.

ref_energy.out
Reference energies used to calculate formation energies.
(Usually: energy of the pure end members OR values given in
ref_energy.in if provided.)

The standard output reports the current progress of the calculations.
During the fit of the cluster expansion, each line of numbers displayed has the following meaning:
1) The current number of point, pair, triplet, etc. clusters
2) An indicator of whether the predicted ground states agree with the true ones (1) or not (0)
3) The CV score.

-> Communication protocol between maps and the script driving the
   energy method code (e.g. ab initio code)
   (Only those who want to customize the code need to read this section.
   The scripts described in this section are provided with the atat
   distribution in the glue/ subdirectory.)
```

```
Unless otherwise specified all files mentioned reside in the directory where
maps was started. All paths are relative to the startup directory.

+The script should first wait for computer time to be available before creating
 a file called 'ready'.
-Upon detecting that the 'ready' file has been created,
 maps responds by creating a subdirectory 'n' (where 'n' is a number) and a file
 'n/str.out' containing a description of a structure whose energy needs to be
 calculated.
-maps creates a file called 'n/wait' to distinguish this directory
 from other ones created earlier.
-maps deletes the 'ready' file.
+Upon detecting that the 'ready' file has disappeared,
 the script should now look for the 'n/wait' file, start the calculations
 in the directory 'n' and delete file 'n/wait'.
+If anything goes wrong in the calculations, the script should create a file
 'n/error'.
+When the calculations terminate successfully, the energy per unit cell of the structure
 should be copied to the file 'n/energy'.
 (NOTE: use energy per unit cell of the structure NOT per unit cell of the lattice).
-maps continuously scans all the subdirectories 'n' for 'n/energy' or 'n/error'
 files and updates the cluster expansion accordingly.
-maps updates the cluster expansion whenever a file called 'refresh' is created
 (maps then deletes it).
-maps terminates when a 'stop' file is created.

Note that the script can ask maps to create new structure directories even before
the energy of the current structure has been found.
Note that human intervention is allowed: an 'n/error' file can be
manually created if an error is later found in a run.
Users can also manually step up all runs if they wish so, as long
as they follow the protocol.

Example of script
(portions in /* */ have to be filled in with the appropriate code):

#!/bin/csh

while (! -e stop)
  /* check machine load here */
  if ( /* load low enough */ ) then
    touch ready
    while (-e ready)
      sleep 30
    end
    cd `ls */wait | sed 's+/.*++g' | head -1`
    rm -f wait
    /* convert str.out to the native format of ab initio code */
    /* in background: run code and create either energy file or error file */
    cd ..
  endif
  sleep 180
end

-> Using maps with vasp

The script runstruct_vasp, when run from within directory 'n',
1) converts 'vasp.wrap' and 'n/str.out' into all the necessary files to run vasp,
2) runs vasp
3) extract all the information from the output files and writes in a format
   readable by maps.

An example of vasp.wrap is:
[INCAR]
PREC = high
ISMEAR = -1
SIGMA = 0.1
NSW=41
```

```
IBRION = 2
ISIF = 3
KPPRA = 1000
DOSTATIC

See ezvasp documentation for more information.

-> Importing structures into maps

MAPS continuously scans all the first-level subdirectories containing
a file called str.out and tries to map them onto superstructures of the
lattice provided. This lets you 'import' structures from another source
into MAPS. A word of caution: the imported structures must be
unrelaxed and no effort is made to rotate or scale them in order to
match the lattice (aside from space group symmetry operations).
```

7.1.14 mcsqs

```
This code uses a Monte Carlo algorithm to find a Special Quasirandom Structure (SQS).
In writing this code, Axel van de Walle benefited from the input of
Alexey Dick, Dongwon Shin and Yi Wang.

If you use this code in a publication, please cite:
A. van de Walle, P. Tiwary, M. de Jong, D.L. Olmsted, M. Asta, A. Dick, D. Shin, Y. Wang, L.-Q. Chen, Z.-K. Liu,
Efficient stochastic generation of special quasirandom structures, Calphad Journal 42, pp. 13-18 (2013)

-> This code requires 2 input files:
1) A file defining the random state (by default rndstr.in) in a format similar to the lat.in that
   is needed for maps or corrdump but with partial occupation of the sites (see below).
2) A cluster file (by default clusters.out), generated, for instance, with the command line:
   mcsqs -2=... -3=... etc.
   where -2=... -3=... indicate the range of pairs, triplets etc.
   The code display the clusters found (format: nb of points, diameter, multiplicity).

   Internally, this actually calls the command
   corrdump -l=rndstr.in -ro -noe -nop -clus -2=... -3=...  ; getclus
      Note that the (new) -ro option allows corrdump to read the same input file as mcsqs (here rndstr.in)
      The -noe and -nop skip the empty and point clusters that are not used by mcsqs
      -clus indicates to generate clusters only
      -2=... -3=... indicate the range of pairs, triplets etc.
      getclus just indicates to write out the clusters (nb of points, length, multiplicity)
      See corrdump -h for more info.

When generating SQS, one typically needs to specify the -n=[number of atoms per cell] parameter on the command line.

-> Output files:
  bestsqs.out
The best SQS found so far (in stardard ATAT structure file format - see mmaps -h for a description)
  bestcorr.out
For each of the clusters selected,
its number of pointd (1st column)
its diameter (2nd column)
the correlations of the best SQS found so far (3rd column)
along with the target disordered state correlation (4th column)
and the difference between the two (5th column).
  rndstrgrp.out
A file containing the same info as the input file defining the random state (rndstr.in),
but with symmetrically equivalent sites grouped together and separated by blank lines.
(This helps determine which sites can have the same occupations.)
  mcsqs.log
A log file.

The code stops if a perfect match is found (all correlations requested match the disordered state),
but this may never happen if there are too many clusters in clusters.out or -n (the number of atoms) is too small.
In any case, the bestsqs.out and bestcorr.out always contain the best solution found so far.
Stopping the code prematurely if the solution is satisfactory is fine.

-> Optional files:
  Creating a file called stopsqs stops the code cleanly.
```

```
  Creating a file called sqsparam.in (or as specified by the -pf option)
  with 4 numbers in it allows you to set the -wr, -wn, -wd and -T options during runtime.
  (for backward compatibility, if 2 numbers are specified, they set the -wr and -T options
   while the remaining options are set to their defaults.)

  The -rc option lets you specify supercells to use (via a sqscell.out file).
  Useful if brute force enumeration takes too long.
  The  sqscell.out usually comes from a previous mcsqs run but you can create it yourself.
  Note that the sqscell.out file must start with the number supercells you will provide
  and that supercells must be expressed in multiple of the axes defined in the rndstr.in file
  (in particular, all numbers entered would typically be integers).
  [If your are using a version prior to  3.07, these should be entered in cartesian coordinates.]

-> Format of the input file defining the lattice (specified by the -l option)

First, the coordinate system a,b,c is specified, either as
[a] [b] [c] [alpha] [beta] [gamma]
or as:
[ax] [ay] [az]
[bx] [by] [bz]
[cx] [cy] [cz]
Then the lattice vectors u,v,w are listed, expressed in the coordinate system just defined:
[ua] [ub] [uc]
[va] [vb] [vc]
[wa] [wb] [wc]
Finally, atom positions and types are given, expressed in the same coordinate system
as the lattice vectors:
[atom1a] [atom1b] [atom1c] [atomtype11]=[occupation11],[atomtype12]=[occupation12],...
[atom2a] [atom2b] [atom2c] [atomtype21]=[occupation21],[atomtype22]=[occupation22],...
etc.

Examples:

The fcc lattice of the Cu-Au system; request for an SQS at composition 0.5:
3.8 3.8 3.8 90 90 90
0   0.5 0.5
0.5 0   0.5
0.5 0.5 0
0 0 0 Cu=0.5,Au=0.5

A lattice for the Li_x Co_y Al_(1-y) O_2 system; request for an SQS
with different composition on each sublattice:
 0.707 0.707 6.928 90 90 120
 0.3333  0.6667 0.3333
-0.6667 -0.3333 0.3333
 0.3333 -0.3333 0.3333
 0       0      0       Li=0.75,Vac=0.25
 0.3333  0.6667 0.0833  O
 0.6667  0.3333 0.1667  Co=0.25,Ni=0.25,Al=0.5
 0       0      0.25    O

Please note that sites that are equivalent by symmetry must have the same occupation.
The file rndstrgrp.out can help you figure out which sites are equivalent.
If you want override this, you can simply use slightly different species labels (e.g. Fe_a,Fe_b) on the
sites whose occupation must differ, even though these sites are a priori equivalent.
Using different labels forces the code to consider the sites as inequivalent.

-> The objective function used is:

(sum (absolute difference from the disordered state correlations)*exp(-wd*(diameter of cluster))*(wn^(nb of points in cluster-2)))
/
(normalization for weights to sum up to 1 over clusters bigger than the smallest nonmatching cluster)

-sum over p wr* wn^(p-2)*(diameter of smallest cluster of p points or less whose correlation does not match the disordered state)

The wr, wn and wd are set through the -wr,-wn and -wd options respectively (or as the 3 first numbers of in the sqsparam.in file).
The diameter of a cluster is the length of the longest pair contained in a cluster (normalized by nearest-neighbor distance).
```

```
See routine calc_objective_func in mcsqs.c++ for a more precise description.

This objective function reflect researchers' desire to perfectly match all correlation up to some range.
Adding the absolute difference serves to guide the algorithm in the right direction to extend the range
of perfect match.

This objective function is a generalization of the one found in the Calphad paper cited above
(reduces to it for wn=1 and wd=0, the defaults).

-> Post-processing

If you have obtained an SQS and would like to see how good/bad the correlations you have NOT included
in the objective function are, you can use a command of the form:
   corrdump -l=rndstr.in -ro -noe -2=... -3=... -s=bestsqs.out
and compare to the output (for a perfectly random solid solution) of
   corrdump -l=rndstr.in -ro -noe -2=... -3=... -s=bestsqs.out -rnd

Beware that the above commands overwrite the clusters.out file.
Make sure to NOT include the -nop option (which is incompatible with the -rnd option).

The getclus command is useful to get a summary of what the clusters are (number of points, diameter, multiplicity).

<
```

7.1.15 memc2

```
MultiComponent Easy Monte Carlo Code (emc2)
by Axel van de Walle

Command line parameters:

-er : enclosed radius. The Monte Carlo cell will the smallest possible
      supercell of unit cell of the initial configuration such that a
      sphere of that radius fits inside it.  This allows you to specify
      the system size in a structure-independent fashion.

-cf : Control file specifying the ranges of temperature and chemical potentials
      scanned (default: control.in). See file format below.

-eq : number of equilibration passes. (Equilibration is performed at
      the beginning of each step of the outer loop.)

-n  : number of Monte Carlo passes performed to evaluate thermodynamic
      quanties at each step of the inner loop.

-tp : instead of specifying -eq and -n, you can ask the code to equilibrate
      and run for a time such that the average energy is accurate
      within the target precision specifified by -tp=.

-aq : Alternative quantity that must meet the tolerance specified by -tp.
      0: energy (default), 1: long-range order, 2-: concentations, correlations

-gs : Gives the index of the ground state to use as an initial spin
      configuration (starting at 0). The ground states are listed in
      gs_str.out.
      If the index is -1, the disordered state with equiatomic composition is used.
      (If -gs=-1, the LTE and MF approximations are not calculated.
      If you want the LTE and MF ouputs, use one of the 'pure' end members as a starting point.)

-tstat : Critical value of the test for discontinuity. The code is
         able to catch phase transformations (most of the time) when
         going from an ordered phase to another or to the disordered
         state. This involves a statistical test which a
         user-specified confidence level. The default, 3, corresponds
         to a 0.4% chance of finding a transition where there is
         none. (Refer to a standard normal table.)  -tstat=0 turns off
         this option.  Suggestion: if a phase transition is
         undetected, first try to reduce temperature or chem. pot. steps
         or increase n or decrease tp before toying around with this parameter.
```

```
         Also: beware of hysteresis.

-sigdig : Number of significant digits printed. Default is 6.

-o:       Name of the output file (default: mc.out).

-k : Sets boltzman's constant (default k=1). This only affects how
     temperatures are converted in energies.  -k=8.617e-5 lets you enter
     temperatures in kelvins when energies are in eV.
     (You can also select this value by using the -keV option.)

 -mft : Mean field threshold. If the grand canonical potential obtained via
        the mean field approximation and the low temperature expansion are
        less than this threshold, Monte Carlo simulation are skipped
        and mean field values are used instead. (They replace the MC values
        in the output file.
        The column labelled use_mf is equal to 1 when this substitution is made.
        Note: When use_mf=1, the correlations in the output file are incorrectly
              set to their values in an ideal fully ordered structure.
              All other columns are reliable.

 -mftq: Quantity that must meet the tolerance specified by -mft.
        0: phi (default) , 1: energy , 2: long-range order, 3-: concentrations

Tricks:

   To read parameters from a file, use:
    memc2 `cat inputfile`
   where inputfile contains the commands line options.

   To selectively display a few of the output quantities, use:
    memc2 [options] | cut -f n1,n2,n3,...
   where n1,n2,n3,... are the column number desired (see below).

-> Input files:

control.in   : range of temperature and chemical potentials to scan.

 The first line of this file specifies the initial conditions and has the format:
   temperature chemical_potentials_1 ... chemical_potentials_n
 where the chemical potentials are for each specie.
 Each subsequent line of this file indicates one of the axes along which to scan and has the format:
   temperature chemical_potentials_1 ... chemical_potentials_n number_of_steps
 where number_of_steps is the the number of steps made between the initial conditions
 and the final conditions given on the line.
 Example: to scan the region in (T,mu1,mu2,mu3)-space defined by
          100 <= T < 200  and 0 <= mu1 < 1.0 and 0 <= mu2 < 0.5 and mu3 == 0.0
          with a 10x5x5 grid
 the control.in file should be
 100 0.0 0.0 0.0
 200 0.0 0.0 0.0 10
 100 0.0 0.5 0.0 5
 100 1.0 0.0 0.0 5
 Note: Temperatures are given in units of energy unless the -k or -eV options are set.
       By default, the finals conditions are excluded from the scan (in the example above
       the chemical potentials scanned in the last line are 0.0 0.2 0.4 0.6 0.8)
       This behavior can be changed with the -il option, to give: 0.0 0.25 0.5 0.75 1.0)
       Alternatively, the -hf option gives: 0.1 0.3 0.5 0.7 0.9 .

NOTE: The mmaps code generates a file called chempot.out which contains special values of the
chemical potential that stabilize various types of equilibria. These values are useful guidelines
to select relevant regions in mu-space to scan.

-> Other input files:

lat.in       : description of the lattice.
clusters.out : describes the clusters.
eci.out      : provides the ECI.
gs_str.out   : a list of ground states, in no particular order.
```

```
   These 4 files can be created by maps.
   See maps documentation (maps -h) for a description of the formats.

-> Optional input files:

teci.out     : if present, provides temperature-dependent eci (overrides eci.out)
               (Note that, even when the teci.out file is used, column 6 of the output file
                reflects only the configurational contribution to the heat capacity.)

The format this file is:
[maximum temperature: Tm]
[number of temperatures where eci are provided: nT]
[ECIs for temperature 0]
[ECIs for temperature Tm/(nT-1)]
[ECIs for temperature 2*Tm/(nT-1)]
...
[ECIs for temperature Tm]

Note that these numbers can be seperated by blanks or newlines, as desired.

conccons.in : Specifies linear constraints on the composition that spin flips must obey.
              (The code will generate multi-spin flips if necessary.)
              Here is an example of such file:
                     1.0*Al -1.0*Li +0.1*Co = 0.5
              Please use rational numbers only - infinite loop will result otherwise.
              Composition is determined by the user-supplied initial configuration
              (via the -g or -is options).

-> Format of the output file

The file mcheader.out gives the content of column of the output file.
The following abreviations are used:
 T:     temperature
 mu(A): chemical potentials of specie A
 x(A):  concentration of specie A
 E:     energy (per active site)
 Egc:   grand canonical energy (per active site) , i.e., E - sum_i mu(i)*x(i)
 lro:   long Range Order parameter of the initial ordered phase
        (=0 if initial phase is disordered)
 F:     Helmholtz free energy (per active site)
 phi:   grand canonical potential: F - sum_i mu(i)*x(i)
 use_mf: flag that is 1 if mf values have been used instead of mc values
 corr_n_d:  the average correlations associated with each cluster
            n is the number of points in the cluster
            d is the diameter of the cluster

Suffixes:
  _lte: obtained with low temperature expansion
  _mf:  obtained with mean field approximation
  _mc:  obtained with Monte Carlo simulations

NOTE: to obtain 'canonical' rather than grand canonical quantities (adding mu*x),
      to all (free) energies use the -g2c option.

NOTE: an 'active site' is one that can host more than one possible atom type.
Energy and free energy are reported per 'active site' not per total sites.
```

7.1.16 mindist

```
Returns 1 if some atoms are within r of each other and returns 0 otherwise.
This convention allows one to write:
  mindist -r=1.5 -s=str.out && runstruct_xxxx
to mean that the command runstruct_xxxx will run only if the minimum distance
between atoms is at least r.
```

7.1.17 mmaps

```
-> What does this program do?

This is the multicomponent version of the maps code.

It gradually constructs a increasingly more accurate cluster expansion.
A user-provided script running concurrently is responsible for notifying
maps when computer time is available. maps creates files describing
structures whose energy should be calculated. The user-provided script
sets up the runs needed to calculate the energy of these structures.
As maps becomes aware of more and more structural energies, it gradually
improves the precision of the cluster expansion, which is continously
written to an output file.
The code terminates when a stop file is created by typing, for instance,
touch stop

NOTE: Fully functional scripts are included with the package:
pollmach and runstruct_vasp.
For for more information type
  pollmach
  runstruct_vasp -h

-> Format of the input file defining the lattice (specified by the -l option)

First, the coordinate system a,b,c is specified, either as
[a] [b] [c] [alpha] [beta] [gamma]
or as:
[ax] [ay] [az]
[bx] [by] [bz]
[cx] [cy] [cz]
Then the lattice vectors u,v,w are listed, expressed in the coordinate system just defined:
[ua] [ub] [uc]
[va] [vb] [vc]
[wa] [wb] [wc]
Finally, atom positions and types are given, expressed in the same coordinate system
as the lattice vectors:
[atom1a] [atom1b] [atom1c] [atom1types]
[atom2a] [atom2b] [atom2c] [atom2types]
etc.

-The atom type is a comma-separated list of the atomic
 symbols of the atoms that can sit the lattice site.
-When only one symbol is listed, this site is ignored for the purpose
 of calculating correlations, but not for determining symmetry.

Examples:

The fcc lattice of the Cu-Au system:
3.8 3.8 3.8 90 90 90
0   0.5 0.5
0.5 0   0.5
0.5 0.5 0
0 0 0 Cu,Au

A lattice for the Li_x Co_y Al_(1-y) O_2 system:
 0.707 0.707 6.928 90 90 120
 0.3333  0.6667 0.3333
-0.6667 -0.3333 0.3333
 0.3333 -0.3333 0.3333
 0       0      0       Li,Vac
 0.3333  0.6667 0.0833  O
 0.6667  0.3333 0.1667  Co,Al
 0       0      0.25    O

Optional input file: ref_energy.in

  Contains the reference energy (per active site, i.e. those that can host more than one specie)
   to be subtracted to get formation energies.
```

```
  The atomic reference energies must be in the same order as in the atoms.out file.
  If this file is omitted, the energies of the structures with the most
  extreme compositions are used to determine the reference energies,
  which are then output to the ref_energy.out file.

Optional input file: nbclusters.in
  Allows the user to manually select which clusters to include in the fit.
  This file should contains:
    number of pairs to include
    number of triplets to include
    etc.
  This file can be changed while maps is running. However, you must type
   touch refresh
  to tell maps to reread it.

Optional input file: crange.in  (or as specified by the -cr option)
  If present, this file
  selects the range of concentration over which the cluster expansion
  is to be fitted. This controls both where the correct ground states
  are inforced in the fitting process and the range of concentration
  of the generated structures. Occasionally, a structure outside that
  range is generated, to verify the ground state hull.
  Here is an example of such file:
   1.0*Al -1.0*Li +0.1*Co >= 0.5
  Multiple constraints can be listed (on separate lines).
  Make sure to include a numerical prefactor for each species even
  if it is 1.0. Do not put a space between '-' and a number.
  Note that the crange.in file is read (if present) even if the -cr option is
  not specified.

Optional input file: weights.in
  Forces specific weights to assign to each structure when fitting its energy.
  These weights may be updated by the code internally to better reproduce the ground state line.
  Format: one weight per line, in the same order as in fit.out
  This should only be used to fine-tune the fit at the end when
  no new structures will be added (since weights.in would have
  to change every time a new structure us added).

-> Output files

maps.log
Contains possible warnings:
  'Not enough known energies to fit CE'
  'True ground states not = fitted ground states'
  'New ground states predicted, see predstr.out'

These warning should disappear as more structural energies become available
and the following messages should be displayed:
  'Among structures of known energy, true and predicted ground states agree.'
  'No other ground states of xx atoms/unit cell or less exist.'

This file also gives the crossvalidation score of the current fit
(before the weighting is turned on in order to get the correct ground states).

atoms.out
Lists all atomic species given in the input files.

fit.out
Contains the results of the fit, one structure per line and each line
has the following information:
  concentration energy fitted_energy (energy-fitted_energy) weight index
'concentration' a vector of the atom fraction of all species (in the same
                order as in atoms.out).
'energy' is per site (a site is a place where more than one atom type can sit)
'weight' is the weight of this structure in the fit.
'index' is the name of the directory associated with this structure.

predstr.out
Contains the predicted energy (per site) of all structures maps has in memory but
```

```
whose true energy is unknown.
Format: one structure per line, and each line has the following information:
  concentration predicted_energy index status
index is the structure number (or -1 if not written to disk yet).
status is either
   b for busy (being calculated),
   e for error,
   u for unknown (not yet calculated) or
   g if that structure is predicted to be a ground state (g can be combined with the above).
To list all predicted ground states, type
grep 'g' predstr.out

gs.out
Lists the ground state energies, one structure per line and each line
has the following information:
  concentration energy fitted_energy (energy-fitted_energy) index

gs_connect.out
Indicates which ground states touch each face of the ground state convex hull.

gs_str.out
Lists the ground state structures, in the same format as the n/str.out files
(see below). Each structure is terminated by the word 'end' on a line by itself,
followed by a blank line.

chempot.out
This file contains
(i) the values of the chemical potentials that stabilize all
    fixed-composition multiphase equilibria of the system at 0K.
    (e.g. in a n-nary system, all the n-phase equilibria)
(ii) values of the chemical potentials that stabilize each of the ground states at 0K.
This data is useful to set up Monte Carlo simulations with the memc2 code.

eci.out
Lists the eci. (They have already been divided by multiplicity.)
The corresponding clusters are in clusters.out

clusters.out
For each cluster, the first line is the multiplicity, the second line is the
cluster diameter, and the third line is the number of points in the cluster.
The remaining lines are the coordinates of the points in the cluster
(in the coordinate system specified in the input file defining the lattice).
A blank line separates each cluster.

n/str.out
Same format as the lattice file, except that
-The coordinate system is always written as 3x3 matrix
-Only one atom is listed for each site.

ref_energy.out
Reference energies used to calculate formation energies.
(Usually: energy of the pure end members OR values given in
ref_energy.in if provided.)

The standard output reports the current progress of the calculations.
During the fit of the cluster expansion, each line of numbers displayed has the following meaning:
1) The current number of point, pair, triplet, etc. clusters
2) An indicator of whether the predicted ground states agree with the true ones (1) or not (0)
3) The CV score (per atom, as of version 2.88; per cell earlier).

-> Communication protocol between maps and the script driving the
   energy method code (e.g. ab initio code)
   (Only those who want to customize the code need to read this section.
   The scripts described in this section are provided with the atat
   distribution in the glue/ subdirectory.)

Unless otherwise specified all files mentioned reside in the directory where
maps was started. All paths are relative to the startup directory.
```

```
+The script should first wait for computer time to be available before creating
 a file called 'ready'.
-Upon detecting that the 'ready' file has been created,
 maps responds by creating a subdirectory 'n' (where 'n' is a number) and a file
 'n/str.out' containing a description of a structure whose energy needs to be
 calculated.
-maps creates a file called 'n/wait' to distinguish this directory
 from other ones created earlier.
-maps deletes the 'ready' file.
+Upon detecting that the 'ready' file has disappeared,
 the script should now look for the 'n/wait' file, start the calculations
 in the directory 'n' and delete file 'n/wait'.
+If anything goes wrong in the calculations, the script should create a file
 'n/error'.
+When the calculations terminate successfully, the energy per unit cell of the structure
 should be copied to the file 'n/energy'.
 (NOTE: use energy per unit cell of the structure NOT per unit cell of the lattice).
-maps continuously scans all the subdirectories 'n' for 'n/energy' or 'n/error'
 files and updates the cluster expansion accordingly.
-maps updates the cluster expansion whenever a file called 'refresh' is created
 (maps then deletes it).
-maps terminates when a 'stop' file is created.

Note that the script can ask maps to create new structure directories even before
the energy of the current structure has been found.
Note that human intervention is allowed: an 'n/error' file can be
manually created if an error is later found in a run.
Users can also manually step up all runs if they wish so, as long
as they follow the protocol.

Example of script
(portions in /* */ have to be filled in with the appropriate code):

#!/bin/csh

while (! -e stop)
  /* check machine load here */
  if ( /* load low enough */ ) then
    touch ready
    while (-e ready)
      sleep 30
    end
    cd `ls */wait | sed 's+/.*++g' | head -1`
    rm -f wait
    /* convert str.out to the native format of ab initio code */
    /* in background: run code and create either energy file or error file */
    cd ..
  endif
  sleep 180
end

-> Using maps with vasp

The script runstruct_vasp, when run from within directory 'n',
1) converts 'vasp.wrap' and 'n/str.out' into all the necessary files to run vasp,
2) runs vasp
3) extract all the information from the output files and writes in a format
   readable by maps.

An example of vasp.wrap is:
[INCAR]
PREC = high
ISMEAR = -1
SIGMA = 0.1
NSW=41
IBRION = 2
ISIF = 3
KPPRA = 1000
DOSTATIC
```

```
See ezvasp documentation for more information.

-> Importing structures into maps

MAPS continuously scans all the first-level subdirectories containing
a file called str.out and tries to map them onto superstructures of the
lattice provided. This lets you 'import' structures from another source
into MAPS. A word of caution: the imported structures must be
unrelaxed and no effort is made to rotate or scale them in order to
match the lattice (aside from space group symmetry operations).
```

7.1.18 phb

```
This is Monte Carlo code which automatically follows a given phase boundary.

Input files: (see maps documentation)
  lat.in         (describes the lattice)
  gs_str.out     (lists the ground states)
  eci.out        (ECI)
  clusters.out    (clusters)

You have to provide, on the command line, the following parameters:

-The two phases which are in equilibrium.
  For instance,
    -gs1=0 -gs2=1
  If there are n ground states, phases are numbered from 0 to n-1 .
  These ground states are read in from gs_str.out
  The disordered state is labelled by the number -1.

  If the two phases are on different lattices, you need to specify
  the path that give access to the files
    lat.in
    gs_str.out
    eci.out
    clusters.out
  for each lattice. For instance
   -d1=../fcc/ -d2=../hcp/
  If either or both options are omitted, the files are read from the
  current directory.

-The starting temperature and chemical potential
  for instance,
  -T=100 -mu=0.125
  (Make sure to set blotzmann's constant appropriately.)
  (If you tracing the phase boundary between two ordered phases, starting from
  OK, you do not need to specify a starting T and mu.)

-The temperature step
  for instance -dT=50

-The 'enclosed radius', which sets the system size
  for instance, -er=35
  (see emc2 documentation for more information)

-The precision of the calculation
 This is expressed as the desired precision of the average concentration.
  For instance, -dx=1e-3
 The code automatically finds the equilibration time and the number
 Monte Carlo steps needed to obtain the target standard deviation
 of the average concentration.

There are a number of optional parameters as well.

 -ltep: The low temperature expansion is used to find the free energy
  at low temperature. -ltep gives the maximum error allowed before
  Monte Carlo is used instead of LTE.
```

```
 -dmu: The step in chemical potential used when scanning in search
  of the phase boundary.
  for instance, -dmu=0.005
  Sometimes, the algorithm looses track of the phase boundary
  (because of statistical errors). When that happens, it scans
  a range of values of the chemical potential in search of the
  boudary of the hysteresis loop associated with the first
  order transition of interest. It then position itself in the
  middle of it. dmu is the step size used for that search.
  Note that the code will automatically shrink dmu if needed.
  By default, dmu is automaticaly set to the formation energy
  of a disordered alloy times 0.01.

  -mug lets you specify a small difference in chemical potential
  between the phases, to make the code less sensitive to accidental
  phase transition.

  -k sets boltzman's constant (see emc2 documentation)
  -keV

  -dn indicates that the boundary must be folowed downward
   (decreasing  T)

Output file:

  Column      Value
  1           temperature
  2           chemical potential
  3           concentration of phase 1 in [-1,1]
  4           concentration of phase 2 in [-1,1]
  5           energy-mu*x for phase 1
  6           energy-mu*x for phase 2
```

7.1.19 predcs

```
This code fits a reciprocal-space cluster expansion of the constituent strain
energy for binary systems with cubic symmetry.

USAGE:

csfit needs, as an input, 4 files.

1) A lat.in file defining the geometry of the lattice (same format as maps).
2) Two str_relax.out residing in given directories (-pa and -pb options, or, by
   default 0/ and 1/ ) and providing the relaxed geometry of the two pure
   end members for the system.
3) A dir.in file listing the directions along which to compute epitaxial
   deformation energy in order to fit the expansion.
   Directions are specified as miller indices in the coordinate system
   defined in lat.in .
   Each index must be separated by a space and
   each direction must be on a separate line.

The code then generates subdirectories (in 0/ and 1/ or any other directory
you specify) with deformed structures whose energy will be used to fit the
expansion. The -np and -nl options let you control the number of structures
generated: -np provides the number of intermediate epitaxial strain
(perpendicular to specified directions) considered between the lattice parameters
of the 2 pure elements while -nl provides the number of different values of
strain along the directions specified. The range of strains spanned is
given by the -ml option (+/- that value, 0 strain being the strain that
keeps volume constant). The -ns option controls the numerical energy
minimization (it is the number of mesh points used in the search for a
minimum) and has no effect of the number of generated structures.

All default values are very reasonable. You may want to increase -ml and
-nl for systems with a large size mismatch.

The files generated are compatible with the 'pollmach'
```

```
automatic job control utility. If you use vasp, you would
typically type
  csfit -d &
  pollmach runstruct_vasp -w csvasp.wrap &

where the csvasp.wrap contains the parameters needed for a vasp run
that does not relax the structure geometry (see atat/examples directory).

WARNING: you are free to rerun csfit many times, adding new lines in dir.in
but you CANNOT rerun it with different -ml -np -nl settings without first
deleting the subdirectories generated.

The csfit programs waits until all calculations are done and then fits
the expansion and writes the results to the cs.in file.
The cs.log contains the constituent strain as a function of concentration (rows)
for long period superlattices along the specified directions (columns).

You can use the resulting expansion in maps by using the -p=cs option
and in emc2 or phb by using the -ks=cs option.

CONVENTIONS:

We expand the concentration-dependent reciprocal space ECI associated with
constituent strain as:

  J_{CS}(x,k) = sum_{l=0,2,4,... } a_{l}(x) K_{l}(k)

where |K_{l}(k)|^2 is normalized to integrate to one over the unit spherical
shell |k|=1.
By combining Equations (12) and  (19) in V. Ozolins, C. Wolverton, and A. Zunger,
Phys. Rev. B, 57, 6427 (1998), we see that the coefficients a_{l}(x) are
related to the c_{l}(x) coefficients defined in this paper through:

  a_{l}(x)=c_{l}(x)/(4x(1-x))

The configuration-dependent constituent strain energy is given by

 Delta E_{CS}(sigma) = sum_{k} Delta J_{CS}(x,k) |S(sigma,k)|^2 exp(-|k|^2/k_c^2)

(see Equation (22) in C. Wolverton, V. Ozolins, A. Zunger, J. Phys: Condems. Matter, 12, 2749 (2000)).

The S(sigma,k) is computed according to the following convention:

  S(sigma,k)=sum_{j in unit cell of structure} S_j exp(i 2 pi k . R_j) *
     * (number of atom in unit cell of parent lattice)/
       (number of atom in unit cell of structure)

Delta E_{CS}(sigma) is thus given per unit cell of the parent lattice.

1/kc is given in the same unit of length as in the lat.in file (for instance, Angstroms).

The ouput file cs.in contains:

[1/k_c, set to 0 to turn off 'attenuation']
[Number of kubic harmonic to use, e.g. 2 to use K_0 and K_4]
[Number n of mesh point in concentration grid, including x=0 and x=1]

a_{0}(0)
a_{0}(1/(n-1))
a_{0}(2/(n-1))
.
.
.
a_{0}(1)

a_{4}(0)
a_{4}(1/(n-1))
a_{4}(2/(n-1))
.
```

```
.
.
a_{4}(1)

a_{6}(0)
a_{6}(1/(n-1))
a_{6}(2/(n-1))
.
.
.
a_{6}(1)

etc.


Additional output files

cs.log

Contains the constituent strain energy (cse) of superstructures along
the specified directions as a function of concentration.
Format:
[concentration] [cse along direction 1 of dir.in] [cse along direction 2 of dir.in] etc.
repeat for each concentration

csdebug.out

Contains the raw energies for each calculation.
The outer loop is on the directions of the dir.in file.
The middle loop is on the element (which pure end member).
The inner loop is on the stretching perpendicular to the k-vector.
Each line contains the energy for various amount of stretching along the
direction parallel to the k-vector.
```

7.1.20 svsl

```
This code calculates the vibrational free energy of a structure
using the Stiffness VS Length method.

Before using this code, you will probably first need to use the fitsvsl code, which
generates the length-dependent force constants that the present needs as an input.

It requires, as an input, 3 files:
1) A 'relaxed' structure (the default file name is str_relax.out,
   but it can be overridden with the -rs option).
   This provides the actual atomic positions used in the calculations.
   The format of this file is as described in the maps documentation (see maps -h).
2) An 'unrelaxed' structure (the default file name is str.out,
   but it can be overridden with the -us option).
   This provides the ideal atomic positions that are used to automatically determine which atoms
   lie in the nearest neighbor shell. This file can be the same as the relaxed structure
   but then the determination of the nn shell may be less reliable.
3) A spring constant file (the default is to lookup in slspring.out and ../slspring.out but
   this can be overridden with the -sp option).
   This file provides the bond stiffness vs bond length relationships that are
   used to determine the force constants of the springs joining neighboring atoms.
   The format of this file is described in the documentation of the fitsvsl code, which is
   a utility that fits such spring constants.

A number of optional files can be given as well.
4) An input file defining the atomic masses. By default, the code looks up in the
   ~/.atat.rc file to determine the directory where atat is installed and then
   loads the file data/masses.in. This behavior can be overridden with the -m option.
5) By default, the bulk modulus is calculated from the force constants but it
   can also be read from a file (whose name is specified with the -bf option) or
   specified on the command line with the -b option.

The parameters that govern the accuracy of the calculations are as follows.
The default values are all reasonable.
```

```
   The code uses the quasiharmonic approximation account for thermal expansion.
   For this purpose, it calculates the vibrational free for a range of lattice parameters
   from the 0K value to the (1+ms) larger, where ms is the number specified in the -ms option.
   The -ns option gives the number of volumes considered.
   Setting -ns=1 selects the harmonic (instead of the quasiharmonic) approximation.

   The code calculates the vibrational free energy from temperature T0 to T1 in steps of dT.
   a) The defaults are T0=0 T1=2000 dT=100.
   b) If a file Trange.in exists in the upper directory, it is used to set T0,T1,dT:
      Trange.in must contain two numbers on one line separated by a space: T1 (T1/dT+1).
      Note that T0=0 always.
      For phase diagram calculations, you must use this method to specify the temperature range.
   c) These defaults can be overridden by the -T0, -T1 and -dT options.

   The kpoint sampling is specified with the -kp option. The actual number of kpoints used
   is the number give divided by the number of atoms in the cell.

-> Phonon Dispersion curves
The -df=inputfile option invokes the phonon dispersion curve module.
The syntax of the input file is:
[nb of points] [kx1] [ky1] [kz1] [kx2] [ky2] [kz2]
repeat...

Each line of input defines one segment (kx1,ky1,kz1)-(kx2,ky2,kz2)
along which the dispersion curve is to be calculated.
[nb of points] specifies the number of points sampled along the segment.
The coordinates are in multiple of the reciprocal cell defined by the axes in the
file specified by the -us option (or, by default, in the str.out file).
(The k-point coordinates are appropriately strained
by the amount needed for the str.out file to be identical to the str_relax.out file.)
The phonon frequencies are output in the eigenfreq.out file.

Other parameters can be altered, if needed.
   The physical constants are set by default for
         force constants input in eV/Angstrom^2
         temperature in K
         free energy in eV
         frequencies in Hz
         masses      in a.u.
   They can be altered by the -hb, -kb, -cfk and -mu options.

   By default the code give free energies per unit cell, but the -pa option gives them per atom.
   The -sc option can provide a multiplicative factor for other conventions (e.g. per formula unit).

   By default, the code aborts whenever unstable modes are found, unless the -fn option is specified.

   Contact the author for information about the -df and -sf options.

The output files are as follows:

svsl.log :  a log file giving some of the intermediate steps of the calculations
vdos.out:   the phonon density of states for each lattice parameter considered (unstable modes appear
            as negative frequencies).
svsl.out:   gives along each row, the temperature, the free energy, and the linear thermal expansion
            (e.g. 0.01 means that the lattice has expansion by 1% at that temperature).
fvib:       gives only the free energy

-> For including vibrations in phase diagram calculations

 You are likely to use this code as follow:

  #first create the Trange.in file for up to 2000K in intervals of 100K:
  echo 2000 21 > Trange.in

  #This executes the svsl code in each subdirectory containing str_relax.out but no error file.
  foreachfile -e str_relax.out pwd \; svsl [options if desired]

  #constructs a cluster expansion of the vibrational free energy (eci are in fvib.eci)
  clusterexpand fvib
```

```
  #add the energetic eci from eci.out to the vibrational eci from fvib.eci and create the teci.out
  #file that will be read by the Monte Carlo code.
  mkteci fvib.eci
```

7.2 Command line options

7.2.1 apb

```
AntiPhase Boundary 3.41, by Ruoshi Sun and Axel van de Walle
Automating impurity-enhanced antiphase boundary energy calculations from ab initio Monte Carlo,
 Calphad 53, 20 (2016)

File options:
 -l=[string]   Input file: lattice   (Default: lat.in)
 -s=[string]             : structure (Default: str.out)
 -o=[string]   Output file: APB structure (Default: str_apb.out)
-og=[string]              : energies      (Default: gamma_apb.out)

APB options:
 -f            Generate APB structure file and exit; do not compute APB energy (Default: Off)
-sx=[real]     APB slip vector: x-component (Default: 0)
-sy=[real]                    : y-component (Default: 0)
-sz=[real]                    : z-component (Default: 0)

Monte Carlo options:
-mc            Run Monte Carlo (Default: Off)
-eq=[int]      Number of: equilibration passes (Default: -1)
 -n=[int]               : averaging passes     (Default: -1)
 -T=[real]     Temperature (Default: 0)

Other options:
 -d            Use all default values (Default: Off)
 -h            Display more help (Default: Off)
```

7.2.2 cellcvrt

```
cellcvrt 3.41, by Axel van de Walle
Performs various conversions/changes on structure (or lattices).
Reads from stdin, writes to stdout.
    -c            Use cartesian coordinates (Default: Off)
    -f            Use fractional coordinates (Default: Off)
   -cc            Find conventional cell and use it as coordinate system (Default: Off)
  -abc            Use a b c alpha beta gamma format to specify axes (Default: Off)
-noabc            Use cartesian format to specify the axes (the default) (Default: Off)
   -ro            Read fractional Occupation (Default: Off)
    -u=[string]   User-specified coordinate system input file (optional) (Default: )
  -uss=[string]   User-specified supercell (Default: )
   -ss=[int]      Simple supercell (multiple of axes in all directions) (Default: 0)
   -fc            Fix cell (to make it as symmetric as possible) (Default: Off)
    -s            Look for smaller unit cell (Default: Off)
   -sh=[string]   Shift all atoms (default 0,0,0).
   -ja=[real]     Jitter all atoms positions by a random amount less than specified (Default: 0)
   -jc=[real]     Jitter all cell parameters by a random amount less than the fraction specified
                     (Default: 0)
   -sd=[int]      Seed for random number generation (default: use clock)
   -sg=[string]   Space group file (Default: )
  -gsg            Generate Space Group (Default: Off)
   -wi            Wrap all atoms inside unit cell (Default: Off)
  -wiu            Wrap all atoms inside unit cell and undo shift (Default: Off)
   -rr            Remove redundant atoms (Default: Off)
  -rra            Remove redundant atoms and average (Default: Off)
   -ar            Add redundant atoms (Default: Off)
  -osf=[string]   Original setting file (optional) (Default: )
  -fsf=[string]   Final setting file (optional) (Default: )
    -r            Print reciprocal unit cell (Default: Off)
   -fs=[int]      Index of first structure to process (default: 1)
```

```
   -ns=[int]      Number of structures to process (Default: 2147483647)
  -slf=[string]   Structure list file (Default: )
   -pn            Print the number of atoms in the structure only (Default: Off)
   -pv            Print volume of cell only (Default: Off)
  -sym            Print spacegroup (Default: Off)
  -ppg            Print point group name (Default: Off)
  -pbv            Print Bravais Lattice name (Default: Off)
   -sc=[real]     Scale factor (default: 1)
  -sig=[int]      Number of significant digits to print in output files (Default: 6)
    -z=[real]     Tolerance for checking overlap (Default 1e-3)
```

7.2.3 checkcell

```
check cell distortion 3.41, by Axel van de Walle
-d            default (Default: Off)
-q            be quiet (Default: Off)
-p            print strain (Default: Off)
```

7.2.4 corrdump

```
CORRelation DUMPer 3.41, by Axel van de Walle
    -h            Display more help (Default: Off)
    -2=[real]     Maximum distance between two points within a pair (Default: 0)
    -3=[real]     Maximum distance between two points within a triplet (Default: 0)
    -4=[real]     Maximum distance between two points within a quadruplet (Default: 0)
    -5=[real]     Maximum distance between two points within a quintuplet (Default: 0)
    -6=[real]     Maximum distance between two points within a sextuplet (Default: 0)
    -l=[string]   Input file defining the lattice   (default: lat.in)
    -s=[string]   Input file defining the structure (default: str.out)
   -pc            Print composition only (Default: Off)
  -pcm            Print composition matrix only (Default: Off)
 -fast            Use fast algo to calculate correlations of 'simple' supercells (Default: Off)
-skipr            Skip algorithm robust to relaxations (Default: Off)
  -sym            Just find space group (Default: Off)
 -clus            Just find clusters (Default: Off)
    -c            Read cluster file instead of writing it (Default: Off)
   -cf=[string]   File name of the cluster file (default: clusters.out)
    -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
  -sig=[int]      Number of significant digits printed (default: 5)
  -noe            Do not include empty cluster (Default: Off)
  -nop            Do not include point cluster(s) (Default: Off)
  -noc            Do not include any cluster(s) (Default: Off)
  -eca            Calculate Energy of Clusters of Atoms (Default: Off)
   -wu=[string]   Write Unrelaxed structure into specified file (Default: )
  -rnd            Print correlation of the random state of the same composition as the input
                     structure (Default: Off)
  -eci=[string]   Predict quantity using ECI in specified file (Default: )
   -mi            Multiplicities are already included in ECI file (Default: Off)
  -crf=[string]   Select correlation functions (default: trigo)
   -nb            Print structure number (Default: Off)
   -ro            Read lattice file containing occupation variables (this code does not make use of
                     them) (Default: Off)
```

7.2.5 csfit

```
Constituent Strain FITter 3.41, by Axel van de Walle
  -h            Display more help (Default: Off)
 -nc=[int]      Number of points in concentration mesh (default 50)
 -ns=[int]      Number of points in mesh used to look for energy minimum (default 100)
 -np=[int]      Number of points in stretching mesh in the direction perpendicular to the
                     k-vector(default 5)
 -nl=[int]      Number of points in stretching mesh in the direction parallel to the k-vector
                     (default 3)
 -ml=[real]     Maximum parallel stretching (default 0.05)
  -l=[string]   Input file defining the lattice (default: lat.in)
 -pa=[string]   Directory containing the pure A calculations (default 0/)
 -pb=[string]   Directory containing the pure B calculations (default 1/)
```

```
 -ds=[string]   File containing a list of stretching directions (default: dir.in)
  -t=[int]      Time between disk reads in sec (default: 10 sec)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
  -d            Use all default values (Default: Off)
```

7.2.6 cv

```
Cross-Validation code 3.41, by Axel van de Walle
-g            Favor cluster choices where the ground state line is correct (Default: Off)
-w=[real]     Weight structures by w/(struct_energy-gs_energy+w) (Default: 1000)
-p=[real]     Penality for structures that lie below the ground state line (Default: 0)
-d            Use all default values (Default: Off)
-h            Display Help (Default: Off)
```

7.2.7 emc2

```
Eazy Monte Carlo Code 3.41, by Axel van de Walle
     -h            Help (Default: Off)
   -mu0=[real]     initial chemical potential (Default: Off)
    -T0=[real]     initial temperature (Default: Off)
   -mu1=[real]     final chemical potential (Default: Off)
    -T1=[real]     final temperature (Default: Off)
   -dmu=[real]     chemical potential step (Default: Off)
    -dT=[real]     temperature step (Default: Off)
    -db=[real]     inverse temperature step (Default: Off)
    -cm            Set Canonical mode (Default: Off)
     -x=[real]     Set concentration (Default: Off)
   -abs            take chemical potentials as absolute quantities (as in mc.out) (Default: Off)
  -phi0=[real]     initial (grand) canonical potential (Default: Off)
    -er=[real]     set the system  size so that a sphere of that radius must fit inside the
                     simulation cell (Default: 0)
    -eq=[int]      number of equilibration passes (Default: -1)
     -n=[int]      number of averaging passes (Default: -1)
    -dx=[real]     Target precision for the average concentration (optional, replaces -n and -eq)
                     (Default: 0)
    -aq=[int]      Alternative quantity that must meet the tolerance specified by -dx. 0: energy, 1:
                     concentration (default), 2: long-range order, 3- correlations
    -gs=[int]      which ground state to use as initial config (-gs=-1 to use random state, c=1/2)
                     (Default: -2)
-innerT            inner loop over T (Default: Off)
 -tstat=[real]     Critical value of the test for discontinuity (Default: 3)
-sigdig=[int]      Number of significant digits printed (Default: 6)
     -q            Quiet (do not write to stdout) (Default: Off)
     -o=[string]   Output file (default: mc.out)
   -oss=[string]   Output snapshot file (default: mcsnapshot.out)
  -opss=[string]   Output periodic snapshot files (default: do not write)
     -k=[real]     Boltzman's constant (conversion factor from T to energy) (Default: 1)
   -keV            Set Boltzman's constant to 8.617e-5 so that temperature is in K when energy is in
                     eV (Default: Off)
    -sd=[int]      Seed for random number generation (default: use clock)
    -dl            Drop the last data point of each inner loop (after the phase transition occured)
                     (Default: Off)
   -g2c            Convert output to canonical rather than grand-canonical quantities (Default:
                     Off)
    -is=[string]   File name containing a user-specified initial configuration (replaces -gs)
                     (Default: )
    -ks=[string]   Specify how k space ECI are calculated (e.g. -ks=cs). (Default: )
```

7.2.8 felec

```
Electronic free energy calculator 3.41, by Axel van de Walle
-dos=[string]   DOS input file name (default: dos.out)
 -T0=[real]     Minimum temperature (default: 0)
 -T1=[real]     Maximum temperature (default: 2000)
 -dT=[real]     Temperature step (default: 100)
 -kb=[real]     Boltzman's constant (default: in eV/K)
 -pa            Output free energy per atom instead of per unit cell (Default: Off)
```

```
 -sc=[real]     Correction factor if spectator ion are present (Default: 1)
 -sd=[real]     Smooth DOS with a Gaussian this width (Default: 0)
 -nf            Do not calculate free energy (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 5)
  -h            Display more help (Default: Off)
  -d            Use all default values (Default: Off)
```

7.2.9 fitfc

```
FIT Force Constants 3.41, by Axel van de Walle
   -f            Fit force constants (otherwise, generate pertubations) (Default: Off)
  -si=[string]   Input file defining the ideal structure (default: str.out)
  -sr=[string]   Input file defining the relaxed structure (default: str_relax.out)
  -er=[real]     Minimum distance between displaced atoms (Default: 0)
-ernn=[real]     Minimum distance between displaced atoms in multiple of nearest neighbor distance
                     (Default: 0)
  -fr=[real]     Force constant range (Default: 0)
-frnn=[real]     Force constant range (in multiple of nearest neighbor distance) (Default: 0)
  -dr=[real]     Displacement of the perturbed atom (default: 0.2)
  -ms=[real]     Strain of the maximum volume sampled (default: 0.01)
  -dv            Specified strain above is volumetric (Default: Off)
  -ns=[int]      Number of volume sample (default: 2)
  -iu            Include Unperturbed structure in generated structures (Default: Off)
 -nrr            Do not rerelax structures at each new volume (Default: Off)
  -cs            Check for Singular matrix in fit (Default: Off)
 -ncs            No check for singular matrix in fit (this is the default, option included for
                     backward compatibility) (Default: Off)
  -wm            Write fitting Matrices (Default: Off)
  -sf=[string]   Extra strain file (Default: )
   -m=[string]   Input file defining the atomic masses (default: ${atatdir}/data/masses.in)
  -T0=[real]     Minimum temperature (default: 0)
  -T1=[real]     Maximum temperature (default: 2000)
  -dT=[real]     Temperature step (default: 100)
   -P=[real]     Pressure (in GPa, default: 0)
  -kp=[real]     Number of k-points per reciprocal atom (default: 1000)
  -kx=[int]      k-point mesh (along 1st recip lat. vect.) if <>0 then overrides -kp=... (Default:
                     0)
  -ky=[int]      k-point mesh (along 2nd recip lat. vect.) (Default: 0)
  -kz=[int]      k-point mesh (along 3rd recip lat. vect.) (Default: 0)
  -fp=[int]      Power of polynomial to fit free energy (Default: -1)
  -s0            Use a gamma-centered k-point mesh (default shift: 1/2 1/2 1/2) (Default: Off)
  -sx=[real]     k-point shift (along 1st recip lat. vect.) (Default: 0.5)
  -sy=[real]     k-point shift (along 2nd recip lat. vect.) (Default: 0.5)
  -sz=[real]     k-point shift (along 3rd recip lat. vect.) (Default: 0.5)
  -df=[string]   Phonon dispersion curve calculation input file. (Default: )
  -hp=[real]     Planck's constant (default in (eV s))
  -kb=[real]     Boltzman's constant (default in eV/K)
 -cfk=[real]     Conversion factor for force constants into energy/dist^2 (default: converts eV/A^2
                     into J/m^2)
  -mu=[real]     Mass units (default: converts a.u. mass into kg)
  -rl=[real]     Robust Length algorithm parameter for soft modes (beta) (Default: 0)
 -rls=[real]     Quadratic strain-dependence of robust length for positive strain (beta) (Default:
                     0)
  -cP=[real]     Conversion factor from pressure*volume into eV (Default: 0.00624151)
  -pa            Output free energy per atom instead of per unit cell (Default: Off)
  -pe            Print energy in 3rd column of fitfc.out (Default: Off)
  -sc=[real]     Correction factor if spectator ion are present (default: 1)
 -me0            Subtract energy at 0K (Default: Off)
  -no            Print number of atom in supercell only (Default: Off)
  -w1            Flag first perturbation wait1 instead of wait file (Default: Off)
  -w2            Flag negative perturbation directions with wait2 instead of wait file (Default:
                     Off)
  -fn            Force continuation of calculations even if unstable (Default: Off)
  -fu            Find unstable modes (Default: Off)
  -gu=[int]      Generate unstable modes number n (Default: 0)
  -gn            Also Generate Negative displacements for mode specified by -gu=... (Default: Off)
 -mau=[int]      Maximum number of atom per supercell for unstable mode generation (Default: 64)
 -sfc=[int]      Simplify force constants: 1=streching+bending, 2=symmetric (Default: 0)
 -apd            Atom-Projected DOS (Default: Off)
```

```
 -sig=[int]      Number of significant digits printed (default: 5)
   -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
   -h            Display more help (Default: Off)
```

7.2.10 fitsvsl

```
Fit Stiffness VS Length transferable force constants 3.41, by Axel van de Walle
  -f            Fit force constants (otherwise, generate pertubations) (Default: Off)
  -l=[string]   Input file defining the lattice (default: lat.in)
 -dn=[string]   Input file listing the directories containing the structures used to calculate force
                    constants (default: strname.in)
 -er=[real]     Minimum distance between displaced atoms (Default: 0)
 -dr=[real]     Displacement of the perturbed atom (default: 0.2)
 -ms=[real]     Strain of the maximum volume sampled (default: 0.01)
 -ns=[int]      Number of volume sample (default: 2)
 -op=[int]      Order of the polynomial used to fit stiffness vs length (Default: 1)
 -dd            Use direction-dependent force constants (Default: Off)
 -pc=[int]      Maximum power of composition used in fit (default: no composition dependence)
-msl=[real]     Maximum spring length (Default: Off)
 -sf=[string]   Extra strain file (Default: )
-eqt=[real]     Tolerance for excluding force constants in plots. (Default: 2)
-sig=[int]      Number of significant digits printed (default: 5)
  -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
-ncs            No check for singular matrix in fit (Default: Off)
 -od            Use older 1-level only directory tree (Default: Off)
  -h            Display more help (Default: Off)
```

7.2.11 fixcell

```
fixcell 3.41, by Axel van de Walle
  -d            Use all default values (Default: Off)
  -c            read and print cell in cartesian only (no axes specified) (Default: Off)
  -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
  -b            print bravais lattice type only and conventional (potentially not primitive) cell
                    (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
```

7.2.12 gce

```
Generalized Cluster Expansion 3.41, by Axel van de Walle
   -h           Display more help (Default: Off)
   -2=[real]    Maximum distance between two points within a pair (Default: 0)
   -3=[real]    Maximum distance between two points within a triplet (Default: 0)
   -4=[real]    Maximum distance between two points within a quadruplet (Default: 0)
   -5=[real]    Maximum distance between two points within a quintuplet (Default: 0)
   -6=[real]    Maximum distance between two points within a sextuplet (Default: 0)
   -l=[string]  Input file defining the lattice   (default: lat.in)
   -s=[string]  Input file defining the structure (default: str.out)
  -pc           Print composition only (Default: Off)
 -sym           Just find space group (Default: Off)
-clus           Just find clusters (Default: Off)
   -c           Read clusters.out file instead of writing it (Default: Off)
   -z=[real]    Tolerance for finding symmetry operations (default: 1e-3)
 -sig=[int]     Number of significant digits printed (default: 5)
 -noe           Do not include empty cluster (Default: Off)
 -nop           Do not include point cluster(s) (Default: Off)
 -rnd           Print correlation of the random state of the same composition as the input
                    structure (Default: Off)
 -eci=[string]  Predict quantity using ECI in specified file (Default: )
  -mi           Multiplicities are already included in ECI file (Default: Off)
 -crf=[string]  Select correlation functions (default: trigo)
 -gce=[string]  Select type of Generalized Cluster Expansion (default: tensor)
  -nb           Print structure number (Default: Off)
```

7.2.13 gencs

```
Generalized Constituent Strain 3.41, by Axel van de Walle
```

```
  -h            Display more help (Default: Off)
  -l=[string]   Input file defining the lattice   (default: lat.in)
  -s            Specify point group directly via generator (in sym.in) (Default: Off)
  -z=[real]     Tolerance for finding symmetry operations (default: 2e-4)
  -r=[int]      Maximum Rank of the harmonic (Default: 1)
 -mr=[int]      Minimum Rank of the harmonic (default 1)
-sig=[int]      Number of significant digits printed (default: 5)
```

7.2.14 gensqs

```
GENerate Special Quasirandom Structures 3.41, by Axel van de Walle
  -n=[int]      nb of atom/unit cell (Default: 0)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
 -cf=[string]   Input file defining the clusters (default: clusters.out)
 -tc=[string]   Input file defining the target correlations (default: tcorr.out)
-tol=[real]     Tolerance for matching correlations (default: 1e-3)
  -l=[string]   Input file defining the lattice (default: lat.in)
 -rc            Read unit cells from file (Default: Off)
 -pc            Print number of supercells only, and quit (Default: Off)
 -tp=[int]      Total number of processes (for parallel operation) (Default: 1)
 -ip=[int]      Index of current process (0,...,tp-1) (for parallel operation) (Default: 0)
-crf=[string]   Select correlation functions (default: trigo)
  -h            Display more help (Default: Off)
```

7.2.15 genstr

```
GENerate STRuctures 3.41, by Axel van de Walle
  -n=[int]      maximum nb of atom/unit cell (Default: 0)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
 -2d            Find supercells along a and b axes only (Default: Off)
  -l=[string]   Input file defining the lattice (default: lat.in)
```

7.2.16 infdet

```
INFlection DETection method 3.41, by Axel van de Walle
  -h            Display more help (Default: Off)
-egt=[real]     Epicycle Gradient Tolerance (Default: 0.04)
-ets=[real]     Epicycle Trial Step (Default: 0.1)
-ems=[real]     Epicycle Maximum Step multiplier (Default: 5)
-eml=[real]     Epicycle Multiplier in Line minimization (Default: 2)
-ebl=[int]      Epicycle maximum number of Bracketing steps in Line minimizations (Default: 5)
-eil=[int]      Epicycle maximum number of Iterations in Line minimizations (Default: 3)
-eic=[int]      Epicycle maximum number of Iterations in Conjugate gradient (Default: 20)
-ebf=[int]      Epicycle motion Bad step Forgiveness (Default: 2)
-eir=[int]      Epicycle iterations between conjugate gradient reset (Default: 5)
 -el=[real]     Epicycle Length (Default: 0.1)
-ism=[real]     Ion motion Steepest descent Multiplier (Default: 0.003)
-isi=[int]      Ion motion Steepest maximum number of Iterations (Default: 0)
-igt=[real]     Ion motion Gradient Tolerance (Default: 0.1)
-its=[real]     Ion motion Trial Step (Default: 0.005)
-ims=[real]     Ion motion Maximum Step multiplier (Default: 5)
-iml=[real]     Ion motion Multiplier in Line minimization (Default: 2)
-ibl=[int]      Ion motion maximum number of Bracketing steps in Line minimizations (Default: 5)
-iil=[int]      Ion motion maximum number of Iterations in Line minimizations (Default: 3)
-iic=[int]      Ion motion maximum number of Iterations in Conjugate gradient (Default: 40)
-ibf=[int]      Ion motion Bad step Forgiveness (Default: 2)
-iir=[int]      Ion motion iterations between conjugate gradient reset (Default: 5)
-ics=[real]     Ion motion Curvature constraint Stiffness (0=automatic) (Default: 30)
 -ff=[real]     Force scale Factor (Default: 3)
 -ds=[int]      Dimension of the strain relaxation allowed (0: none, 1: along x, 2: along y,z, 3:
                     along x,y,z (default))
 -ns            Do Not Scale tolerance with number of atoms (Default: Off)
 -st=[int]      Sleep Time between read access (Default: 5)
  -d            Use all default values (Default: Off)
 -os            Output Structure defined by epipos.out into str.out (Default: Off)
  -r            Relax to minimum (Default: Off)
For debugging only:
```

```
 -db            debug (Default: Off)
-aex            Analytical Example (for debugging) (Default: Off)
 -t1=[real]     Temp param 1 (Default: 1.9)
 -t2=[real]     Temp param 2 (Default: -2)
```

7.2.17 kmesh

```
-d            Use all default options (Default: Off)
-q            Quiet! (Default: Off)
-r            Round output to next largest integer (Default: Off)
-e            Force nb of kpoints to be an even number (Default: Off)
```

7.2.18 lsfit

```
Least-Square FIT 3.41, by Axel van de Walle
    -x=[string]   x file (Default: )
    -y=[string]   y file (Default: )
    -w=[string]   weight file (Default: )
    -r=[string]   regularization parameters file (Default: )
   -pf            Perfect Fit algorithm (Default: Off)
   -pw=[string]   number of powers of each column to regress on (Default: )
    -s=[string]   select columns to regress on (one number by column, 0: ignore, 1: use) (Default:
                    )
    -1            add a column of ones as regressor (Default: Off)
-colin            Ignore colinear columns in x file (Default: Off)
   -cv            Print crossvalidation score (Default: Off)
   -se            Print standard errors (Default: Off)
   -ty            Print trues values of y (Default: Off)
    -p            Print predicted values of y (Default: Off)
    -e            Print prediction error (Default: Off)
  -sig=[int]      Number of significant digits printed (default: 5)
```

7.2.19 maps

```
MIT Ab initio Phase Stability (MAPS) code 3.41, by Axel van de Walle
  -h            Display more help (Default: Off)
  -l=[string]   Input file defining the lattice (default: lat.in)
  -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
  -c=[real]     Exponent of the order of complexity (default: 3)
  -t=[int]      Time between disk reads in sec (default: 10 sec)
  -m=[int]      Maximum number of points in cluster (default 4)
  -g=[int]      Extend ground state search up to structures having at least that many atoms.
                    (Default: 0)
 -c0=[real]     [c0,c1] is the concentration range where ground states must be correct. (Default:
                    0)
 -c1=[real]      (Default: 1)
 -mv=[int]      Maximum volume (number of atom per unit cell) allowed when generating structures
                    (default: no limit)
 -mw=[real]     Maximum weight allowed when try to match ground states (Default: 16)
 -2d            Find supercells along a and b axes only (Default: Off)
  -p=[string]   Predictor plugins to use (examples: -p=cs or -p=cs_es) (Default: )
 -ks=[string]   same as -p (Default: )
 -fa=[string]   Select fitting algorithm (default: built-in)
  -q            Quiet mode (do not print status to stderr) (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
  -d            Use all default values (Default: Off)
```

7.2.20 mcsqs

```
Monte Carlo generator of Special Quasirandom Structures 3.41, by Axel van de Walle
   -n=[int]      nb of atom/unit cell (Default: 0)
If -n is not specified, generate clusters of the following sizes:
   -2=[real]      Maximum distance between two points within a pair (Default: 0)
   -3=[real]      Maximum distance between two points within a triplet (Default: 0)
   -4=[real]      Maximum distance between two points within a quadruplet (Default: 0)
   -5=[real]      Maximum distance between two points within a quintuplet (Default: 0)
   -6=[real]      Maximum distance between two points within a sextuplet (Default: 0)
```

```
   -l=[string]   Input file defining the random structure (default: rndstr.in)
  -cf=[string]   Input file defining the clusters (default: clusters.out)
 -tcf=[string]   Input file defining the target multibody correlations (default: internally
                     calculated values for fully disordered state)
 -tol=[real]     Tolerance for matching correlations (default: 1e-3)
  -wr=[real]     Weight assigned to range of perfect correlation match in objective function
                     (default 1)
  -wn=[real]     Multiplicative decrease in weight per additional point in cluster (default 1)
  -wd=[real]     Exponent of decay in weight as function of cluster diameter (default 0)
   -T=[real]     Temperature (default 1)
  -pf=[string]   Input file defining the optimization parameters (default: sqsparam.in)
  -rc            Read supercells from file sqscell.out (default: generate internally and write to
                     sqscell.out) (Default: Off)
  -ip=[int]      Index of current process (for parallel operation) (Default: -1)
-best            Collect best SQS among the outputs of prior parallel runs (Default: Off)
 -crf=[string]   Select correlation functions (default: trigo)
  -sd=[int]      Seed for random number generation (default: use clock)
  -rt=[int]      Read parameter file every (rt) step (default:10000)
  -2d            Generate only supercells in the plane of a,b axes (Default: Off)
 -sig=[int]      Number of significant digits to print in output files (default: 6)
   -h            Display more help (Default: Off)

Perhaps missing -n=[nb of atom/cell] option?
```

7.2.21 memc2

```
Multicomponent Eazy Monte Carlo Code 3.41, by Axel van de Walle
     -h            Help (Default: Off)
    -er=[real]     Set the system  size so that a sphere of that radius must fit inside the
                     simulation cell (Default: 0)
    -cf=[string]   Control file specifying the ranges of temperature and chem. pot. scanned
                     (default: control.in)
    -eq=[int]      Number of equilibration passes (Default: -1)
     -n=[int]      Number of averaging passes (Default: -1)
    -tp=[real]     Target precision (optional, replaces -n and -eq) (Default: 0)
    -aq=[int]      Quantity that must meet the tolerance specified by -tp. 1: energy (default), 2:
                     long-range order, 3-: point correlations
    -gs=[int]      which ground state to use as initial config (-gs=-1 to use random state)
                     (Default: -2)
     -k=[real]     Boltzman's constant (conversion factor from T to energy) (Default: 1)
   -keV            Set Boltzman's constant to 8.617e-5 so that temperature is in K when energy is in
                     eV (Default: Off)
   -g2c            Convert output to canonical rather than grand-canonical quantities (Default:
                     Off)
  -phi0=[real]     initial (grand) canonical potential (default: from mean field approx.)
 -tstat=[real]     Critical value of the test for discontinuity (Default: 3)
   -mft=[real]     Mean field threshold (if |lte-mf|<mft, use mf values instead of mc) (Default:
                     -1)
  -mftq=[int]      Quantity that must meet the tolerance specified by -mft.0: phi (default) , 1:
                     energy , 2: long-range order, 3-: concentrations
-sigdig=[int]      Number of significant digits printed (Default: 6)
     -q            Quiet (do not write to stdout) (Default: Off)
     -o=[string]   Output file (default: mc.out)
   -oss=[string]   Output snapshot file (default: mcsnapshot.out)
  -opss=[string]   Output periodic snapshot files (default: do not write)
    -sd=[int]      Seed for random number generation (default: use clock)
    -dl            Drop the last data point of each inner loop (after the phase transition occured)
                     (Default: Off)
    -is=[string]   File name containing a user-specified initial configuration (replaces -gs)
                     (Default: )
    -hf            Shift all coordinates by half a grid point in scan (e.g. 2 steps in [0,1] give
                     0.25,0.75 instead of 0,0.5) (Default: Off)
    -il            Include last coordinate in scan (e.g. 3 steps in [0,1] gives 0,0.5,1 instead of
                     0,0.333,0.666) (Default: Off)
    -ts=[string]   Triangular scanning. Specify list of composition axes (e.g. -ts=1,2). (Default:
                     )
   -crf=[string]   Select correlation functions (default: trigo)
    -df=[int]      Max distance between flips (in unit cells) in grand-canonical mode (Default: -1)
    -mf=[int]      Minimum number of flips in grand-canonical mode (experimental) (Default: 0)
```

```
    -rw            Use random walk algorithm (experimental) (Default: Off)
   -fdT=[real]     Temperature step for finite differences (Default: 0.01)
  -fdmu=[real]     Chemical potential step for finite differences (Default: 0.01)
    -ks=[string]   Specify how k space ECI are calculated (e.g. -ks=cs). (Default: )
```

7.2.22 mindist

```
Test if MINimum DISTance between two atoms is less than a given threshold, version 3.41, by Axel van
                    de Walle
-s=[string]   Input file defining the structure (Default: stdin)
-r=[real]     Threshold radius (Default: 0)
-e            Create error file atoms are too close (Default: Off)
-h            Display more help (Default: Off)
```

7.2.23 mkaxes

```
MaKe Axes 3.41, by Axel van de Walle
     -h            Display more help (Default: Off)
 -trans            Transform to coordinate system (Default: Off)
   -tri            Gibbs triangle (Default: Off)
 -tetra            Gibbs tetrahedron (Default: Off)
 -hidim=[int]      Dimension (Default: 3)
   -col=[real]     Color (Default: 0)
   -rgb=[real],... RGB Color (Default: )
    -vl=[string]   Vertices labels (Default: )
  -zmax=[real]      (Default: 1000)
  -zmin=[real]      (Default: 0)
-zscale=[real]      (Default: 1000)
    -cs            Cross-Section (Default: Off)
    -cf=[string]   Cross section input File (Default: cut.in)
  -font=[string]   font file (Default: )
    -ef=[string]   Export format (default: vtk)
   -sig=[int]      Number of significant digits printed (Default: 5)
     -d            Use all default values (Default: Off)
```

7.2.24 mmaps

```
MIT Ab initio Phase Stability (MAPS) code 3.41, by Axel van de Walle
  -h            Display more help (Default: Off)
  -l=[string]   Input file defining the lattice (default: lat.in)
  -z=[real]     Tolerance for finding symmetry operations (default: 1e-3)
  -c=[real]     Exponent of the order of complexity (default: 3)
  -t=[int]      Time between disk reads in sec (default: 10 sec)
  -m=[int]      Maximum number of points in cluster (default 4)
  -g=[int]      Extend ground state search up to structures having at least that many atoms.
                     (Default: 0)
 -cr=[string]   Concentration region input file (Default: crange.in)
 -he=[real]     Highest predicted energy, above ground state hull, allowed when generating
                     structures (default: no limit)
 -mv=[int]      Maximum volume (number of atom per unit cell) allowed when generating structures
                     (default: no limit)
 -mw=[real]     Maximum weight allowed when try to match ground states (Default: 16)
 -2d            Find supercells along a and b axes only (Default: Off)
  -p=[string]   Predictor plugins to use (examples: -p=es or -p=es_cs) (Default: )
 -ks=[string]   same as -p (Default: )
 -fa=[string]   Select fitting algorithm (default: built-in)
-crf=[string]   Select correlation functions (default: trigo)
 -pn=[string]   Property to cluster expand (default: energy)
 -ig            Ignore whether cluster expansion predicts correct ground states (Default: Off)
 -pa            Quantity to expand is already per atom (Default: Off)
  -q            Quiet mode (do not print status to stderr) (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
  -d            Use all default values (Default: Off)
```

7.2.25 nnshell

```
Nearest Neighbor Shell 3.41, by Axel van de Walle and Paul Dalach
```

```
  -l=[string]   Input file defining the lattice (default: lat.in)
 -lb            List bond types in given structures (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 5)
  -r=[real]     Define a max radius for neighbor search (Default: 0)
  -d            Use all default values (Default: On)
```

7.2.26 nntouch

```
nntouch 3.41, by Axel van de Walle
 Scales a lattice so that nearest neighbor atom just touch.
  -l=[string]   Input file defining the lattice (default: lat.in) Use filename - to specify stdin
  -r=[string]   Input file defining the atomic radii (default: rad.in)
  -s=[real]     Multiplicative scaling factor (Default: 1)
-sig=[int]      Number of significant digits to print in output files (Default: 6)
  -d            Use all default values (Default: Off)
```

7.2.27 pdef

```
Point DEFect generator 3.41, by Axel van de Walle
  -l=[string]   Input file defining the lattice (default: lat.in)
  -s=[string]   Input file defining the lattice (default: str.out)
  -p=[string]   Prefix of the directories that will contain the defected structures (Default pdef)
 -er=[real]     Minimum distance between point defects (Default: 0.00000)
-sig=[int]      Number of significant digits printed (default: 5)
  -h            Display more help (Default: Off)
```

7.2.28 phb

```
PHase Boundary 3.41, by Axel van de Walle
     -h            Help (Default: Off)
    -mu=[real]     initial chemical potential (Default: Off)
     -T=[real]     initial temperature (Default: Off)
   -dmu=[real]     chemical potential adjustment step (Default: Off)
    -dT=[real]     temperature step (Default: Off)
   -mug=[real]     Gap between the mu in phase 1 and mu in phase 2 (default: 0)
  -ltep=[real]     threshold free energy precision to use MC instead of LTE (in units of T)
                     (default: always MC)
    -er=[real]     enclosed radius (Default: 0)
   -gs1=[int]      ground state for phase #1 (Default: -2)
   -gs2=[int]      ground state for phase #2 (Default: -2)
   -is1=[string]   File name containing a user-specified initial configuration (replaces -gs1)
                     (Default: )
   -is2=[string]   File name containing a user-specified initial configuration (replaces -gs2)
                     (Default: )
    -d1=[string]   directory for phase #1 (default: current dir)
    -d2=[string]   directory for phase #2 (default: current dir)
   -lro            print long range order parameter (Default: Off)
 -tstat=[real]     Critical value of the test for discontinuity (Default: 3)
  -smax=[real]     Maximum step (experimental feature) (Default: 1e+50)
-sigdig=[int]      Number of significant digits printed (Default: 6)
     -q            Quiet (do not write to stdout) (Default: Off)
     -o=[string]   Output file (default: mc.out)
     -k=[real]     Boltzman's constant (conversion factor from T to energy) (Default: 1)
   -keV            Set Boltzman's constant to 8.617e-5 so that temperature is in K when energy is in
                     eV (Default: Off)
    -sd=[int]      Seed for random number generation (default: use clock)
    -dn            Go down in temperature (Default: Off)
    -dx=[real]     Concentration Precision (Default: 0)
    -ks=[string]   Specify how k space ECI are calculated (e.g. -ks=cs). (Default: )
```

7.2.29 simplexize

```
Simplexize 3.41, by Axel van de Walle
   -t=[string]   Input table file (Default: tab.in)
 -col=[real]     Color (Default: 0)
 -rgb=[real],... RGB Color (Default: )
-rmax=[real]     Maximum radius of curvature (Default: 0.1)
```

```
-rmin=[real]     Minimum distance between points kept (Default: 0.001)
   -l            Plot lines (Default: Off)
 -sig=[int]      Number of significant digits printed (default: 5)
  -ef=[string]   Export format (default: vtk)
  -cs            Cross-Section (Default: Off)
  -cf=[string]   Cross section input File (Default: cut.in)
   -h            Display more help (Default: Off)
   -d            Use all default values (Default: Off)
```

7.2.30 strpath

```
STRucture PATH generator 3.41, by Axel van de Walle
 -s1=[string]   Input file defining structure 1 (default: str1.out)
 -s2=[string]   Input file defining structure 2 (default: str2.out)
 -ni=[int]      Number of images (Default: 0)
  -f=[real]     Interpolation fraction in [0,1] (Default: 0.5)
 -df=[real]     Dimer distance [0,1] (Default: 0)
 -dp=[string]   Directory name pattern (default 00)
 -ci            Calculate inflection point (Default: Off)
-cil            Calculate inflection point location (Default: Off)
-sig=[int]      Number of significant digits printed (default: 5)
  -h            Display more help (Default: Off)
  -d            Use all default values (Default: Off)
```

7.2.31 svsl

```
Vibrational free energy calculator using the Stiffness VS Length method 3.41, by Axel van de Walle
  -l=[string]   Input file defining the lattice (defaults: lat.in, ../lat.in, str.out)
 -us=[string]   Input file defining the unrelaxed structure (default: str.out)
 -rs=[string]   Input file defining the   relaxed structure (default: str_relax.out)
 -sp=[string]   Input file defining the springs (default: slspring.out)
  -m=[string]   Input file defining the atomic masses (default: ${atatdir}/data/masses.in)
  -b=[real]     Bulk modulus (Default: 0)
 -bf=[string]   Bulk modulus file (Default: )
 -ms=[real]     Maximum stretching of the lattice parameter (default: 0.05)
 -ns=[int]      Number of lattice parameter stretching step (default: 1 => harmonic approximation)
 -T0=[real]     Minimum temperature (default: 0)
 -T1=[real]     Maximum temperature (default: 2000)
 -dT=[real]     Temperature step (default: 100)
 -kp=[real]     Number of k-points per reciprocal atom (default: 1000)
 -s0            Use a gamma-centered k-point mesh (default shift: 1/2 1/2 1/2) (Default: Off)
 -sx=[real]     k-point shift (along 1st recip lat. vect.) (Default: 0.5)
 -sy=[real]     k-point shift (along 2nd recip lat. vect.) (Default: 0.5)
 -sz=[real]     k-point shift (along 3rd recip lat. vect.) (Default: 0.5)
 -hp=[real]     Planck's constant (default in (eV s))
 -kb=[real]     Boltzman's constant (default in eV/K)
-cfk=[real]     Conversion factor for force constants into energy/dist^2 (default: converts eV/A^2
                    into J/m^2)
 -mu=[real]     Mass units (default: converts a.u. mass into kg)
 -rl=[real]     Robust Length algorithm parameter for soft modes (beta) (Default: 0)
 -pa            Output free energy per atom instead of per unit cell (Default: Off)
 -sc=[real]     Correction factor if spectator ion are present (default: 1)
 -fn            Force continuation of calculations even if unstable (Default: Off)
 -df=[string]   Phonon dispersion curve calculation input file. (Default: )
 -sf=[string]   Extra strain file (Default: )
-msl=[real]     Maximum spring length (Default: Off)
-sig=[int]      Number of significant digits to print in output files (Default: 5)
 -up=[string]   User-specified Potential Plug-in (optional) (Default: )
  -d            Use all default values (Default: Off)
  -h            Display more help (Default: Off)
```

7.2.32 triph

```
TRIangulate PHase 3.41, by Axel van de Walle
  -t=[string]   Input table file (Default: tab.in)
 -sc=[real]     Scale for the unique axis (1st) (Default: 1000)
-col=[int]      Color (Default: 0)
```

```
-nfn            do Not fix Normal vector (Default: Off)
 -bf            generate back face (Default: Off)
-sig=[int]      Number of significant digits printed (default: 5)
 -ef=[string]   Export format (default: vtk)
  -h            Display more help (Default: Off)
  -d            Use all default values (Default: Off)
```

7.2.33 getclus

```
Syntax: getclus [-e] [ecifile]
extracts, from clusters.out, the cluster sizes, lengths and multiplicities
if ecifile is given, it also prints the eci therein
if -e is specified, it prints eci from eci.out
```

7.2.34 mapsrep

```
Display the output of maps in graphical form.
Syntax: mapsrep [-e]
the optional switch -e tells the code to plot structures flagged with error too.
Thanks to Ruoshi Sun and Mike Widom for updating the script for recent versions of gnuplot.
```

7.2.35 mmapsrep

```
Display the output of mmaps in graphical form.
Syntax: mmapsrep [-e] c1 c2 c3
where c1,c2,c3 are the column numbers of the compositions to plot
the optional switch -e tells the code to plot structures flagged with error too.
```

7.2.36 str2xyz

```
Utility to convert structure files into xyz files suitable for viewing with rasmol
Syntax: str2xyz [-v] na nb nc [scale] infile
-v (optional) calls rasmol (otherwise, xyz file is written to stdout
na nb nc define the number of periodic repetition to plot
scale (optional) scales the structure to adjust which bonds are plotted
```

7.2.37 makelat

```
MAKE LATtice, by Axel van de Walle
Utility setting up directories with maps input files for a given alloy system
and for one or multiple lattices.

Syntax: makelat [-o] [-s=scale] atom1,atom2,... lattice1,lattice2,...

Make sure that there are commas but no spaces between atoms and similarly between the lattices.

Examples:
  makelat Al,Ni bcc,fcc
  makelat Ca,Mg:O rocksalt

  (note the : to separate sublattices)
  The default scale is 1. It can be changed to allow for units other than angstroms.
  The -o option outputs to strout.

Lattices available:
B2 bcc bcc-oct bcc-tet diamond fcc fcc-oct fcc-octtet fcc-tet hcp hcp-oct hcp-tet L11 rocksalt sc
                     wurtzite zincblende

Other lattices can be added in the /home/avdw/avdw/atat/data/ directory or
new atomic radius can be added in the /home/avdw/avdw/atat/data/radii.in file.
```

7.2.38 clusterexpand

```
Syntax: clusterexpand [-e] [-pa] [-s "1,0,1, ..."] filename
Cluster expands the quantity stored in */filename
```

```
Uses the clusters in clusters.out
Outputs to filename.eci filename.ecimult
ecimult contains the eci multiplied by multiplicity
the option -e causes the structures flagged with an error file to be ignored
the option -pa indicates that the quantity is per atom already
   so that the code must NOT divide it by the number of atoms
the option -s lets you select which cluster to include (1) or exclude (0)
the option -g selects a generalized (tensor) cluster expansion
the -cv option prints the cv score.
```

7.2.39 mkteci

```
Syntax: mkteci file1.eci ...
 where file1.eci etc. is a list of T-dependent eci files obtained with
 the clusterexpand command, e.g.
 clusterexpand fvib    in the case of vibrational free energy or
 clusterexpand felec   in the case of electronic free energy.
Usually the file list is: fvib.eci felec.eci
                          ^vibrational ^electronic free energy
```

7.2.40 clusterpredict

```
Syntax: clusterpredict [-pa] file
see clusterexpand for more info.
This command is to be run from within a specific structure directory containing a str.out file.
```

7.2.41 checkrelax

```
Prints the amount of relaxation each structure in */str_relax.out has
undergone, relative to */str.out (or */str_sup.out if it exists)
Typically, values above 0.1 are considered too much for the
cluster expansion to be applicable and the offending structures
should be disabled using the command:
 touch structure_number/error
where structure_number is the appropriate directory name.
The option -1 checks relaxations for one structure only in the current directory.

This command measures the magnitude of the strain that need to be applied
to the unit cell of str.cell to get the unit cell of str_relax.out,
neglecting (i) isotropic scaling and (ii) rigid rotation.
The numbers reported are the sqrt of the sum of each element of the strain tensor squared.
```

7.2.42 calcbulk

```
Calculates bulk modulus.
Syntax: calcbulk mins maxs ds runcommand
where mins and maxs are the minimum and maximum strains (e.g. 0.00 0.01)
ds is the step size (e.g. 0.005)
runcommand is the command to run the ab initio code (e.g. runstruct_vasp)
```

7.2.43 mcdroplast

```
This script reads the output file of a mc run and deletes
the last data point of each inner loop.
(The point after a phase transition occured.)
Same effect as the -dl option of emc2.
```

7.2.44 str2cif

```
Converts an ATAT structure file (from stdin) to the CIF format (stdout).
```

7.2.45 wycked

```
WYCKoff position EDitor, by Axel van de Walle
Syntax:
  wycked [spcgrp] [list_of_wyckoff_position_letter_without_seperators]
The output is meant to first be edited to set the free parameters a,b,c,alpha,beta,gamma,x,y,z,etc
in each of the lines starting with #const
and processed by sspp to create a valid ATAT structure file.

ACKNOWLEDGEMENTS
This code makes use of a Wyckoff position database downloaded from the Bilbao Crystallographic
                    Server
at http://www.cryst.ehu.es/
Accordingly, if you use this code, you should cite, in addition to the usual ATAT citations,
the following papers:
  M. I. Aroyo, J. M. Perez-Mato, D. Orobengoa, E. Tasci, G. de la Flor, A. Kirov
      "Crystallography online: Bilbao Crystallographic Server"
      Bulg. Chem. Commun. 43(2) 183-197 (2011).
  M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga,
  A. Kirov and H. Wondratschek,
      "Bilbao Crystallographic Server I: Databases and crystallographic computing programs"
      Z. Krist. 221, 1, 15-27 (2006). doi:10.1524/zkri.2006.221.1.15
  M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato and H. Wondratschek
      "Bilbao Crystallographic Server II: Representations of crystallographic point groups and
      space groups", Acta Cryst. A62, 115-128 (2006). doi:10.1107/S0108767305040286
```

7.2.46 getproto

```
GET PROTOtypes from database, by Axel van de Walle
Syntax:
  getproto [string]
Returns all structure prototypes matching [string] in ATAT's prototype database.
[string] can be a regular expression, e.g. ^A3
The last 2 columns of the output can be used as arguments to the wycked code
to generate the structure (up to some adjustable parameters not constrained by symmetry).

ACKNOWLEDGEMENTS
 This file contains processed data from the index of the Landolt-Bornstein database available at
 http://www.springermaterials.com/
 If using this data, please cite:
 Villars, P., Cenzual, K., Daams, J., Gladyshevskii, R., Shcherban, O., Dubenskyy,
 V., Melnichenko-Koblyuk, N., Pavlyuk, O., Stoiko, S., Sysa, L.
 "Landolt-Bornstein - Group III Condensed Matter: Numerical Data and Functional Relationships
 in Science and Technology",
 Villars, P., Cenzual, K. (ed.).
 SpringerMaterials - The Landolt-Bornstein Database (http://www.springermaterials.com)
 Volume 43A1-43A10
 2013
```

7.2.47 sqs2tdb

```
sqs2tdb version 3.41 by Axel van de Walle and with contributions to the SQS database
        from Ruoshi Sun, Qijun Hong and Sara Kadkhodaei.

Usage: sqs2tdb [options]    where the available options are:
-h   : More help.
-cp  : Copy SQS from the database to the current directory. Must specify:
       -lv=[level]
           level indicates how fine of composition mesh to use (0: only end members, 1: mid points,
                    etc.)
       -l=[lattice]
          Available lattices
           AUCD_B19
           AUCD_B19.tar
           AUCU_L10
           BCC_A2
           BETASN_A5
           CDI2_C6
```

```
           CHI_A12
           CR3SI_A15
           CSCL_B2
           CUPRITE_C3
           CUPT_B22
           CUPT_L11
           DIAMOND_A4
           FCC_A1
           FE3AL_D03
           FLUORITE_C1
           GA3PT5
           GAMMA_L12
           HCP_A3
           HEUSLER_D022
           HEUSLER_L21
           hidden
           LIQUID
           MGCU2_C15
           MGZN2_C14
           NI3SN_D019
           NIAS_D81
           OMEGA_C32
           PEROVSKITE_E21
           PYRITE_C2
           REO3_D09
           ROCKSALT_B1
           RUTILE_C4
           SIGMA_D8B
           WURTZITE_B4
           ZINCBLENDE_B3
           ZINTL_B32
           ZIRCONIA_TET

        Optional: -sp=Element,Element,...  to indicate which elements to consider
                     (otherwise read from species.in if it exists).
-fit : Fit solution model from SQS energies (to be run within the desired lattice directory).
-tdb : Combine solution models from one or multiple lattices into a single .tdb file.
       add the -oc (Open Calphad) option to generate a more portable tdb file.
-mk  : Generate input file for SQS generation with mcsqs. (Usually not needed - only for experts.)
       To be run in the SQS database directory:
       /home/avdw/avdw/atat/data/sqsdb/[lattice name]
Note that -h,-mk,-cp,-fit,-tdb are mutually exclusive.


For more information see user guide published in:
  A. van de Walle, R. Sun, Q.-J. Hong, and S. Kadkhodaei.
  Software tools for high-throughput calphad from first-principles data.
  Calphad, 58:70, 2017.
  https://doi.org/10.1016/j.calphad.2017.05.005
(Also, this paper should be cited in any publication resulting from this code's use.)

EXAMPLES

-> A simple session of sqs2tdb could be:

cp ~/atat/example/vasp.wrap .
emacs vasp.wrap   #edit as needed

echo Al,Ni > species.in

sqs2tdb -cp -l=FCC_A1 -lv=1
sqs2tdb -cp -l=FCC_A1 -lv=1

cd FCC_A1
foreachfile wait pwd \; runstruct_vasp

sqs2tdb -fit

Edit the file terms.in to read
```

```
1,0
2,0

sqs2tdb -fit

cd ..

(repeat the above for other lattices if necessary)

sqs2tdb -tdb

The file AL_NI.tdb would contain a valid .tdb file.

-> In a more advanced example, the runstruct_vasp command could be replaced
by a job script submission containing the runstruct_vasp command.

-> When there are lattice instabilities, the runstruct_vasp could be replaced by
robustrelax_vasp -mk  #this is to be run only once (see robustrelax_vasp -h for instructions)
robustrelax_vasp -id

-> If phonons are to be included (for end members) one could do:
foreachfile endmem pwd \; fitfc -si=str_relax.out -ernn=4 -ns=1 -nrr
foreachfile -d 3 wait \; runstruct_vasp -lu -w vaspf.wrap
   where vaspf.wrap contains parameters for a static run to calculate forces.
foreachfile endmem pwd \; fitfc -si=str_relax.out -f -frnn=2
foreachfile endmem pwd \; robustrelax_vasp -vib

sqs2tdb -fit

OPTIONAL input files (to placed in the topmost directory):

    exfromsgte.in : specify which phases should NOT be copied from SGTE database
                    (by default all phases for each relevant element are included,
                    but you may want to use ab initio data for virtual phase)
    subref.sed    : substitution rule (sed command to be applied to final tdb file)

OUTPUT FILES
    In addition to the *.tdb files, there is some diagnostic info available in the files
                    fit_[property].out where property could be
    energy, svib_ht, etc.

ADVANCED FEATURES
    In each sqs subdirectory created, there may be a file called link that contains the path to
    another directory where energy data can be found. This is useful if another structure is
    known be equivalent by symmetry. This file is created by default for equivalence within a
    given structure type can even find symmetries across structure types.
    You can also create the file yourself and the code will follow your link.

    There may also be a file called bump which indicates that a structure must be moved up in energy
                    by the
    amount specified by the -bv option (or 5e-3 by default) to avoid degeneracy with an equivalent
                    higher symmetry structure.
    This file is created by default (during the -cp step) when the code detects higher symmetry
                    (e.g. a GAMMA_L12 phase with all sites occupied
    with the same type of atom is just FCC). You can delete this file if the higher-symmetry
                    structure is not in your
    set of structures. This file is read during the -fit step.

    In summary, if you see a bump file, ask yourself if you have that structure elsewhere and put an
                    appropriate link file.
    If you don't have that structure elsewhere, you can delete the bump file.
    The code will still work and give the right answer if you don't do this, but it will spend  more
                    computer time.

    During the -fit step, one can specify the -sro option to include a low-order CVM approximation
                    to the short range order.

    The default lower and upper temperature limits of 298.15K and 10000K can be changed with the
                    -Tl=... and -Tu=... options, respectively.
```

7.2.48 symbrklib

```
Usage: symbrklib [-s fraction] [element] [initial_structure] [final_structure]
Currently, the initial and final structures can be one of bcc,fcc,hcp.
The -s option (optional) indicates to just generate a small distortion (a given fraction along the
                    instability path).
This command is intended to be run before robustrelax_xxxx
```

7.2.49 ocplotpd

```
A front-end to OpenCalphad for PLOTting Phase Diagrams.
Usage: ocplotpd [-ha] [-nt] [-tlf=fraction] [-1f] [-vtk] [-rmax=r_max] [-rmin=r_min]
                    [-np=nb_of_proc] -tdb=tdbfile -n=nb_of_samples -T0=min_temperature -T1=max_temperature -e=element,element,...

Mandatory parameters:
 tdbfile: name of the Thermodynamic DataBase (TDB) file to use
 element,element,... : a list of the elements (and associated phases) to extract from the TDB file
 nb_of_samples: Number of phase equilibria sampled to generate the phase diagram
 min_temperature: lower bound on the temperature axis
 max_temperature: upper bound on the temperature axis (if min_temperature=max_temperature, a cross
                    section is plotted)

optional parameters:
 -ha:   high accuracy calculations
 -nt:   no tie lines
 -tlf:  fraction of tie lines displayed (between 0.0 and 1.0)
 -1f:   generate a single gnuplot file
 -vtk:  generate vtk files (instead of gnuplot)
 -rmax: max distance between points in triangulation
 -rmin: discard points closer to each other than this cutoff
 -np:   launch nb_of_proc copies of opencalphad
 -noc:  do not run OpenCalphad - just create the graphs from existing phase_*.dat files
```

7.2.50 getvalue

```
Syntax: getvalue [label]
Script that scans standard input for a given label and
write, to standard output, the numerical value following
every occurence of that label.
Any number of : = spaces or tabs can separate the label and the number.
Example: getvalue "Final energy" < gulp.output
```

7.2.51 getlines

```
Syntax: getlines [-h] [ -af | -bf | -bt | -jaf | -jbf | -bt ] string1 string2
Copies selected lines of standard input to standard output.
-h   print this help.
-af  print all lines located *after* a line containing string1
-bf  print all lines located *before* a line containing string1
-bt  print all lines located between a line containing string1 and a line containing string2
     (If there are multiple blocks of lines braketed by [begin string]
      and [end string] they are all copied.)
The prefix j means "just", indicating that the line(s) containing the matching string(s) is (are)
                    ommited.
Don't forget to quote your strings if they contain spaces.
```

7.2.52 nltoblank

```
Converts each newline character to a space.
```

7.2.53 blanktonl

```
Converts each contiguous sequence of blanks to a newline character.
```

7.2.54 foreachfile

```
Syntax: foreachfile [-e] [-n filename_to_skip] [-a and_filename] [-d depth] filename command
Execute the specified command in every first-level subdirectory containing the file filename.
The -e option cause foreachfile to skip directories containing the file "error".
The -n option cause foreachfile to skip directories containing the file filename_to_skip.
The -a option specifies that the file and_filename must also exist.
The -d option specifies to go down to lower level subdirectories as well (the default is 1).
```

7.2.55 calc

```
Syntax: calc "mathematical expression"
```

7.2.56 sspp

```
  Simple symbolic pre-processor
  reads from stdin, writes to stdout (also writes temporary file tmp.awk)
  Interprets simple definitions and evaluates numerical expressions with
  constants definitions.
  invoking sspp -nb produces a output file where all blank
  lines have been removed

  input file syntax:
   understands any C pre-processor commands (see man cpp)
   also understands #const [var1]=[value2]; [var2]=[value2]
   the variables var1 ... can be used later in the file.
   Expression to be evaluated must be enclosed in braces {}
   except when they are in a #const declaration.
   The brace characters are entered as \{ and \}
   Understands c++ comment char //

  Examples:
   #const x=2*3.14
   The value is {1+cos(x)}
   #define PLUS(x,y) ((x)+(y))
   The answer is {PLUS(1,2)}
   Braces are \{ \}

  Implementation details:
   Any line beginning with #const or #awk
   is interpreted as an awk command (see man awk).
   Expression in braces are awk expressions.
   The file tmp.awk is the file sent to awk for interpretation.

  BUGS

   Never start a line with %
   # is not a comment character
```

7.2.57 chl

```
chl [-m alternative_machine_config_file]
Checks the load on the remote machines specified in the ~/.machines.rc file
or as overridden by the -m option
The first column of output is the load and the commands following the + sign
give the command prefix needed to run on that machine
A default ~/.machines.rc is created the first time the command is run.
See comments therein for the format of the file.
```

7.2.58 minload

```
Syntax: minload [-m alternate_machine_config_file] [-w]
Returns the command prefix needed to run a command on the remote
machine having the minimum load, among the
machines listed in the ~/.machines.rc file
(or as specified by the -m option).
```

```
A default ~/.machines.rc file is created the first time
the chl command is run and the file format is described
in the comments therein.
```

7.2.59 node

```
This command is basically like rsh, except that the command
makes sure that the current directory on the remote machine
is the same as on the local machine.
(If the two machines do not share the same disk space, use the -r option.)

Syntax: node [-s] [-r] user@host command
 -s: use ssh instead of rsh
 -r: copy files in current directory to remote host before running command
 if user is the same on remote host, use may use
   node [-s] [-r] host command
```

7.2.60 pollmach

```
Syntax: pollmach [-f] [-e] [-m alternate_machine_configuration_file] [-s] [-w] command_to_run

This command periodically checks the load on various machines
(specified in the file ~/.machines.rc)
and looks for subdirectories containing a file called "wait".
If the load on a machine is sufficiently low, it executes command_to_run
on that machine, in the directory where the oldest wait file lies.
A default ~/.machines.rc file is created the first time the chl command
is run. The format of the file is explained in the comments therein.
If no ~/.machines.rc file exists, command_to_run is run sequentially on
the local computer in each directory containing a "wait" file.
This is the single-machine mode.

When using this command with maps, command_to_run will typically be runstruct_vasp

The -m option overrides the default ~/.machines.rc (it is optional).

The -e option specifies that the command should terminate when no more
"wait" files are to be found (only works in single-machine (sequential) mode,
when no ~/.machines.rc file is given).

The -f option forces the command to run even if of pollmach_is_running file exists.

The -s option cause pollmach to self-manage the load (it does not poll the nodes for their loads
but instead keeps track of where it sends a job and does not send any other job to that node until
                    it is done.
The first column in the machine_configuration_file is ignored and can be omitted.

The -w option tells pollmach to wait until all sub processes have finished before quitting.

The -il interactive loop option (beta). Here pollmach waits for a file called 'busy' to be created,
        then runs command and then deletes 'busy'.
        This repeats itself until a stop or stoppoll file is created.

The -t "command" option first runs "command" and, only if its return code is 0, runs
                    command_to-run.

To cleanly stop this program, type
        touch stoppoll
```

7.2.61 fixeol

```
converts text files to unix (-u) or to pc (-p) format.
Syntax: fixeol -u|-p [file1, file2 ...]
```

7.2.62 lookup

7.2.63 runstruct-vasp

```
runstruct_vasp [-w file] [-d depth] [-p] [-lu] [-ng] [-nr] [-ex] cmdprefix
  where file is an optional alternate wrap file (default: vasp.wrap)
    If the wrap file is not found in the current directory,
    it searches in the parent directories, up to number specified by depth (default is 5).
    For a description of the syntax of the vasp.wrap file, type
     ezvasp -h
    and look for options under the '[INCAR]' section.

  -p means preserve vasp output file
  -lu means look up one directory for WAVECAR to use as starting point.
  -ng means do not generate a vasp.in file, use the existing one.
  -nr means do not run vasp, just generate input files
  -ex means do not generate vasp.in, do not run vasp, but extract info from vasp output file
  cmdprefix is the prefix needed for vasp to run on a remote machine,
            such as "node -s node2"
```

7.2.64 ezvasp

```
Syntax: ezvasp [-c] [-s] [-n] [-p "..."] input_file

-c: Cell patch. This option will convert the cell you entered into a cell that has the symmetry
                    needed for
    vasp to work properly. The atom positions are altered correspondingly.

-s: Static run. After the relaxations are completed, this option makes vasp start again, turning off
                    relaxations
    and turning on tetrahedron integration with bloech correction. Can acheive the same effect by
    including DOSTATIC in the INCAR portion of the input file.

-n: do Not run vasp. If you want to create the input files now and run them later, perhaps on
                    another machine.

-p: name of the vasp command ("vasp" by default). You can include addition prefix such as:
    ezvasp -p "rsh remote.machine nice +5 /usr/local/bin/vasp" vasp.in

Here is an example of input file:

[INCAR]
SYSTEM = FeNi
ISPIN = 2
PREC = HIGH
ISMEAR = 1
NSW=41
SIGMA = 0.1
IBRION = 2
ISIF = 3
ENMAX = 400
EDIFF = 1e-6
EDIFFG = 1e-4
KPPRA = 1000
USEPOT = PAWGGA
DOSTATIC
SUBATOM = s/Fe$/Fe_h/g
KSCHEME = GAMMA
MAGATOM =

[POSCAR]
 SOME TITLE
 3.55
  -.500000000     -.500000000    -1.000000000
   .500000000    -1.000000000     -.500000000
  -.500000000      .500000000     1.000000000
 1 2
 Direct
  .33333     .33333     .00000     Fe+5
  .00000     .00000     .00000     Vac
  .66667     .66667     .00000     Fe-5
```

```
End of example.

Note that there 6 new tokens in the INCAR section.

1) KPPRA stands for "K-Point Per Reciprocal Atom". This is a way to automatically set the k-point
                    mesh for
   a number of similar systems. Here is how it works. If you know that you need 500 k-points for a
                    2-atom
   structure, then you type in 1000. If you now try a similar structure with 4 atoms, the code
                    automatically
   use 250 k-points. The mesh along the three axes is automatically chosen to make the mesh as
                    uniform as possible.
   (For the algorithm, see atat/src/kmesh.cc).
   You can also specify KPPRA = UPDIR which indicates that the KPOINTS file
   found one directory above should be used.
   (This is useful for cell distorsions used in elastic constant calculations of constituent strain
                    runs).
   If this token is ommited, you need to specify a [KPOINT] section in the input file that contains
                    what
   you want the KPOINT file to be.

2) DOSTATIC indicates that a static run must be done after the relaxation run (NSW tag is removed
                    and the ISIF and IBRION
   token are ajusted accordingly). The output files named *.relax contain the result of the (first)
   relaxation run while the files named *.static contain the results of the (second) static run.
   When DOSTATIC is not specified, all output files are named *.static , whether the VASP input
                    parameters
   allow relaxations or not.

3) KSCHEME specifies the type mesh to use: Gamma shift or Monkorst-Pack. The default is Gamma if
                    KSCHEME is ommited.

4) MAGATOM is similar to the usual token MAGMOM used to specify the moment on each atom. The novelty
                    is that you specify the
   moments in the POSCAR section. (In version 3.15 and above, this token can be ommited. Having
                    spins specified in the POSCAR
   section turns this on automatically. It also set ISPIN=2 automatically.)
   The usual MAGMOM token is still available (but you cannot use both MAGMOM and MAGATOM).

5) USEPOT
   selects the potentials used: LDA GGA PAWLDA PAWGGA PAWPBE (or any other potential defined in
                    .ezvasp.rc)
   By default, LDA (without PAW) is used.
   For backward compatibility, you can also use the tag DOGGA instead of USEPOT = GGA

6) The SUBATOM token lets you specify a sed-like substitution command to be
   applied to the name of the atomic species.
   For instance, SUBATOM= s/Fe$/Fe_h/g  will cause ezvasp to use the Fe_h
   pseudopotential instead of the Fe one. Multiple SUBATOM token can be given,
   one for each substitution. Don't forget the s/ and /g and the $ after the first element name
   (to avoid F matching Fe, or Y matching Yb).

There are also familiar VASP tokens that are robustified. For instance ISTART = 2 does not work
                    unless you force
the FFT grid size to match the earlier run.
To help with this, ezvasp fetches the right NGX,NGY,NGZ from the previous run's OUTCAR or CHGCAR in
                    the current directory.

There are new features in the POSCAR section as well.
1) The line that specify the number of atoms (here 1 2) can be ommited (it is ignored).
2) The atomic species are specified to the right of the atom positions.
   The corresponding POTCAR are automatically copied. You can specify pseudopotentials like Li_h or
                    O_s.
3) The number following the species is the magnetic moment on the atom (if MAGMOM is in the INCAR
                    section).
   Identical species with different moments will be considered symmetrically distinct to allow for
   symmetry-breaking relaxations.
4) Do not specify "selective dynamics". It will be written to the INCAR file
```

```
   automatically if you include T's and F's after the atom species, e.g.:
    0.5 0.5 0.5 Al T T F
5) The element "Vac" or "Va" stands for vacancy. It is ignored for everything but
   to compute the k-point mesh with the KPPRA option.
```

7.2.65 robustrelax-vasp

```
This command implements the "inflection-detection" method introduced in
A. van de Walle, Q. Hong, S. Kadkhodaei and R. Sun, "The free energy of mechanically unstable
                    phases"
Nat. Com. 6, 7559 (2015) doi:10.1038/ncomms8559 .
and
A. van de Walle and S. Kadkhodaei and R. Sun and Q.-J. Hong, "Epicycle method for elasticity limit
                    calculations",
Phys. Rev. B 95 144113 (2017) doi:10.1103/PhysRevB.95.144113 .

It calculates the energy of a structure that is potentially mechanically unstable.
In a nutshell: the method finds either a local minimum (for a mechanically stable phase)
or the inflection point on a path joining the unrelaxed and fully relaxed structures
(for a mechanically unstable phase).

Syntax: robustrelax_vasp [options] command_prefix
where options are
  -id             Inflection Detection method
  -idop "options" Options passed to the infdet command.
  -neb            Use the Nudged Elastic Band method to find minimum energy path
                  Otherwise: simply interpolate linearly.
  -ex             Only extract data form VASP files. Do not run anything.
  -c  [real]      Relaxation magnitude cutoff needed to activate robust relax algorithm (default:
                     0).
  -ni [integer]   Number of images in the minimum energy path (default: 6).
  -rc [string]    Command for full relaxation          (Default: runstruct_vasp -w vasp.wrap).
  -vc [string]    Command for volume only relaxation   (Default: runstruct_vasp -w vaspvol.wrap).
  -cc [string]    Command for chain (neb) calculations (Default: runstruct_vasp -w vaspneb.wrap).
  -sc [string]    Command for static runs              (Default: runstruct_vasp -w
                     vaspstatic.wrap).
  -ic [string]    Command for inflection-detection runs (-id option) (Default: runstruct_vasp -p -w
                     vaspid.wrap).
  -idf [real]     Starting point fraction for inflection detection (default: 0.5)
  -ja
  -jc             By how much to jitter atoms (-ja) and cell parameters (-jt) for the initial
                     conditions
                  for inflection-detection method.
  -vib            Update vibrational data in svib_ht file from vol_0/svib_ht file.
  -mk             Make auxiliary vasp input files (vaspvol.wrap, vaspneb.wrap, vaspstatic.wrap,
                     vaspf.wrap) from vasp.wrap.
                  Do not run anything.
  -cln            clean files for a full restart.
  -cip            continue (an prior run) if possible (only implemented for -id algorithm).
  -d              Use all defaults values.
  -h              Display more help.
  command_prefix  Prefix needed for vasp to run on a remote machine or in parallel (e.g. mpirun).

Note: the commands specified by -rc,-vc,-cc,-sc can be set to empty "" to skip the corresponding
  calculation step (useful to restart an aborted run).

This command does the following:
1) Fully relax the structure (in str_hint.out or str.out) to create str_relax.out,
   just like runstruct_vasp.
2) If the relaxation cutoff (-c=...) no exceeded, stop. Typically, should be set to -c=0.05.
3) Relax the volume only of structure in str_sup.out or str.out. Results are in directory 00/
4) Do a neb (-neb) or infection detection (-id) calculation between the two structures obtained in
                    step 1 and 3
   or just a linear interpolation between them (if no -neb or -id). Results are in directories ??/
   Note that you need VTST Tools from http://theory.cm.utexas.edu/vtsttools/ for the neb method
   with variable cell shape.
5) Do static calculations in each directory ??/
6) Find the inflection point on the path optimized in step 4. If it does not exist, find the
   minimum energy along that path.
```

```
7) Report the energy found in 6 in the file energy and the corresponding geometry in str_relax.out

Notes:
1) str_beg.out and str_end.out contain the extremities of the path.
   If you want to restart from scratch, delete these files.
2) For high symmetry phases (e.g. bcc,fcc,hcp) you may need to break the symmetry of the phase for
                    it to relax.
   For that purpose, you can use, e.g.,
      symbrklib W fcc bcc
   or
      cellcvrt -ja=0.01 -jc=0.01 < str.out > str_hint.out .
   Sometimes a supercell is needed (a phonon analysis will tell you that - or symbrklib for
                    bcc,fcc,hcp).
```

Chapter 8

Troubleshooting

8.1 Forum

Please see the new ATAT forum at http://alum.mit.edu/www/avdw/forum for answers to common (and uncommon!) questions.

8.2 FAQ

Q. I can do a least-squares by hand with a much lower mean square error (MSE) than MAPS can. Yet, you claim that MAPS is "optimal". How is this possible?
A. The MSE is not a very good measure of the predictive power of a cluster expansion. It can be made arbitrarily close to zero but merely including enough ECI in the fit! But having a small MSE is no guarantee that the error on the predicted energy of structures not inlcuded in the fit is small. The cross-validation (CV) score, which is used in MAPS, is a better measure of the predictive power of a least-squares fit. The CV score does not systematically decrease as the number of ECI increases and it has been shown that choosing the number of ECI such that the CV score is minimized is an asymptotically optimal strategy. Researchers often have a tendency to use too many ECI because this appears to reduce the error, but this is a illusion. MAPS gives you an unbiased estimaqte of the prediction error, and the magnitude of that number is larger than many would like to believe.
Q. MAPS is frozen. What is going on?
A. MAPS sometimes needs a few minutes to generates new clusters or structures. This is a complex operation, be patient. This generation can occur in the middle of the calculations (finding the best cluster expansion or the best structures) because MAPS only generates these clusters or structures when they are needed.
Q. Where are the results?
A. In a variety of files whose descriptions you can view by typing `maps -h | more`. A utility called `mapsrep` lets you display the most useful output data using `gnuplot`.
Q. What files do I need to get started with MAPS?
A. A `lat.in` files to specify the geometry of the lattice and a "wrapping" file that specifies the parameters of the first-principles code. If you are using vasp, this file is usually called `vasp.wrap`. Examples of those files can be found in the `example` directory.
Q. I already have structures and energies. What if I just want to fit them?
A. You need a `lat.in` files to specify the geometry of the lattice and you need to create one subdirectory for each structure (name them as you which). In each subdirectory, you need a `str.out` file to specify the geometry of the structure and an `energy` file to indicate the energy of that structure. For the format of those files, type `maps -h | more`. Note that the energy must per unit cell of the structure (not the lattice).
Q. When I type `maps` I only get the command line option help. How can I run it?
A. Type `maps -d` to use all the default options. You can also specify any option you want. Either way, the help message will not be displayed and the code will run. If the help is still displayed, it is because there is an error in the options you specified.
Q. When I superimpose the energies of `fit.out` with the energies obtained from the Monte Carlo code, I can see that they don't match. What is happening?

A. The "energies" given by the Monte Carlo code are in fact $E - \mu x$ so you need to add μx to get the true energy. Use the `-g2c` option to tell the Monte Carlo code to output the true energy.
Q. How can I verify that the structures do not relax to a superstructure of a different type of lattice (e.g. fcc becoming bcc)?
A. Run the utility called `checkrelax`. It will give you a list all structures along with a measure of the strain they each experienced during relaxation.
Q. When I look at the calculated and fitted energies in the `fit.out` file there are structures where the difference is very large.
A. Make sure that these structures have properly relaxed. A common problem is to start the first-principles calculations with an unrelaxed geometry where the atoms are too close to one another. Restart the energy calculations of the offending structures by using larger starting volumes.
Q. My input files seem correct but ATAT utilities crash while reading them.
A. Make sure your files have unix-style end-of-lines. The `fixeol -u yourinputfile` command should fix that issue.

8.3 Common mistakes

- Write the energy per atom (or per unit cell of the lattice) in the `*/energy` files. One should write the energy per unit cell of the structure (that is, in the way a first-principles code usually gives it).
- Errors in the `lat.in` file. Use the `corrdump -sym ; more sym.out` command to analyse the symmetry of the lattice and see if it correspond to your expectations. You can also use `corrdump -2=10 -clus ; more clusters.out` to verify the symmetrically distrinct pairs are what you expect them to be.
- When the structures are not generated by MAPS (i.e. you typed them it), beware of typos. MAPS will detect if a structure is incompatible with the lattice but it will not detect another very common mistake: putting the energy and str.out files that correspond to different structures in the same directory. To check for this error, look at the residual plot generated by `mapsrep`.
- When copying the `lat.in` files provided as examples, make sure you make all the required changes. (i) Change the atom names. (ii) Set the lattice parameters (first 3 numbers in the file) to values that are at least as large as the true lattice parameter (otherwise, first-principles code can be unable to properly relax the geometry of the structure is the atoms are too close to one another initially).

Chapter 9

Organization of the Toolkit

- src (source code)
- glue (utilities to interface MAPS with other codes)
- glue/jobctrl (utilities allowing maps to automatically lauch jobs)
- glue/vasp (interface between vasp and maps)
- doc (user guide and documentation regarding the inner workings of the code)