Automated Convergence: Find Converged VASP Settings Automatically

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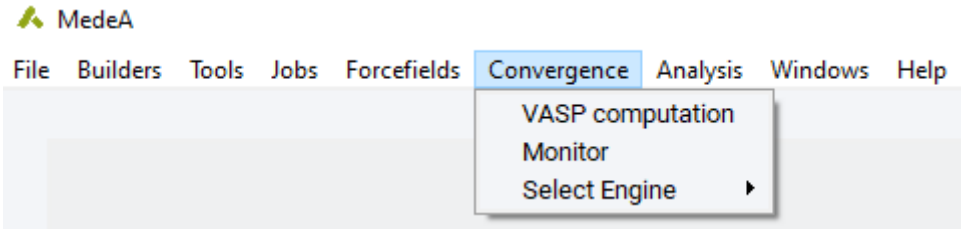
The accuracy of computed materials properties such as equilibrium lattice parameters, binding energies, and elastic moduli depend on a variety of computational parameters, most notably the quality of the plane wave basis sets and the density of k-meshes for integrations in reciprocal space.

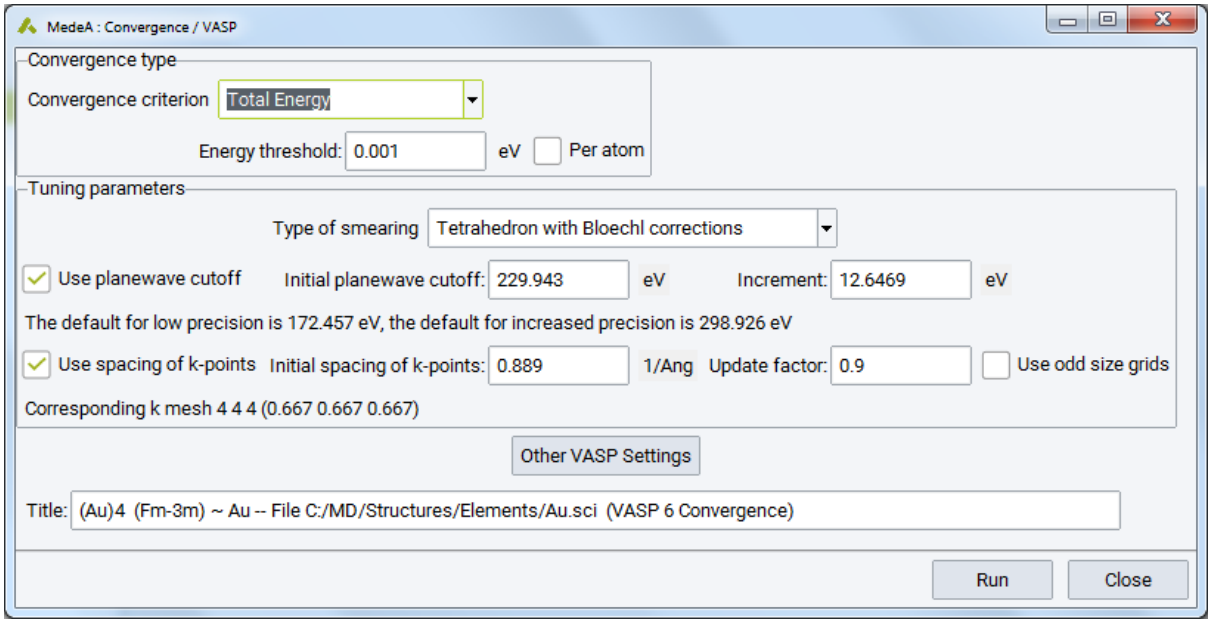
The optimal choice of these parameters depends both on the material under investigation and on the properties of interest. For example, metallic aluminum requires very fine k-meshes to achieve convergence of the total energy while semiconductors are well described by a rather coarse k-mesh. Finding the most appropriate parameter setting is important, but tedious to do by hand. The *Automated Convergence* Module automates the process of determining optimal parameter settings in VASP for achieving the desired level of accuracy in calculations of materials properties.

Activate the Convergence menu entry in *MedeA* by clicking Tools >> Automated Convergence. Next select Convergence >> VASP computation to start a Convergence job or Convergence >> Monitor to analyze results.



1 Submitting VASP Convergence Jobs

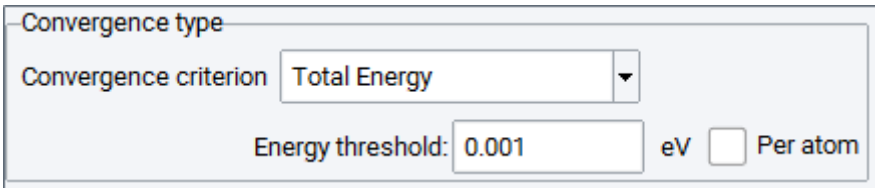
Convergence >> VASP computation launches the Convergence interface to run the VASP computations:



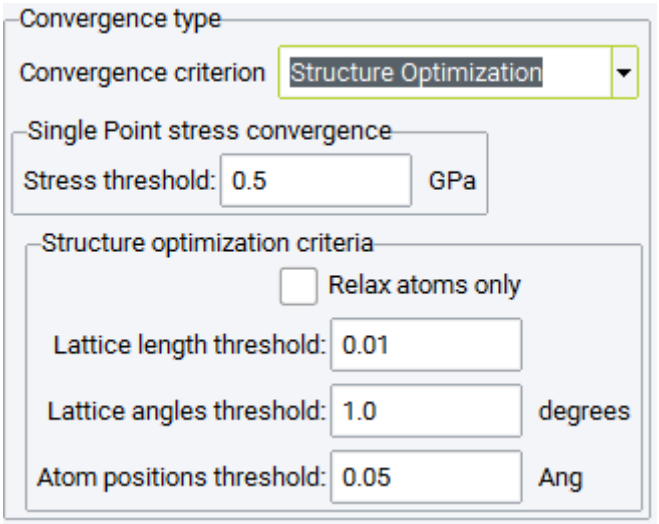
Convergence type

You can use the following criteria for Convergence:

Total Energy : Converges the VASP total energy, where you can select a value for the Energy threshold , either for the whole system or Per atom .



Structure Optimization : Converges both, the Single Point stress, as well as the lattice parameters and atom positions. You can select to Relax atoms only .



The convergence will be studied as follows:

- Single Point stress convergence calculations with the stress tensor (Stress threshold in GPa) as the convergence criterion
- Using results from a Structure Optimization with convergence based on the relative change of the cell

length, angles, and atom positions. To keep the cell fixed, select Relax atoms only.

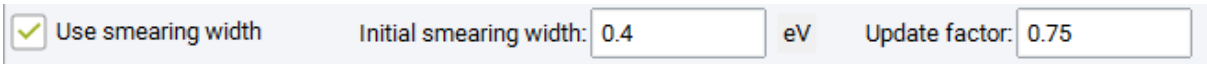
2 Tuning Parameters

Using the above convergence criteria the module will optimize the following parameters:

Use planewave cutoff (PWC, energy cutoff): Starting from the Initial planewave cutoff the module will increase the cutoff by Increment until convergence is reached. VASP potentials provide two cutoff energies for each atom, *ENMIN* for low precision and *ENMAX* otherwise. The default value for Initial planewave cutoff is set to the maximum *ENMAX* value of all potentials used for the atoms present in the system. The default Increment is 1/10 of the difference between the maximum *ENMAX* value increased by 30 % (corresponding to the Increase planewave cutoff (cell optimizations) setting in the VASP GUI) and the maximum *ENMIN* value for all potentials used for the atoms.

Use spacing of k-points: The value for the Initial spacing of k-points is set such that the resulting k-mesh is 3x3x3 to allow using the tetrahedron method. For subsequent refinement of the k-mesh, the initial spacing of k-points is progressively multiplied by the Update factor until the actual number in the k-mesh increases for the next computation step.

Use smearing width: You can optimize the smearing width, in addition, when the Methfessel-Paxton method is chosen for the Type of smearing instead of the default Tetrahedron with Bloechl corrections method, which has no smearing parameter. The Update factor decreases the smearing width during the convergence process.



3 Monitoring VASP Convergence Jobs

Choosing a job

The Monitor menu queries the selected JobServer for a list of Convergence jobs. Select a job to retrieve and display the results from an ongoing or finished job.

Multi-parameter convergence

Before detailing the content of the monitor window, let us explain the progress of a Convergence job.

As long as only one parameter is used for tuning, the convergence process simply consists in updating the parameter until convergence is reached. If, however, several parameters are used simultaneously, the parameter space is multi-dimensional and there might be several paths that lead to different points, where convergence is reached.

The strategy used for our problem is intended to limit the overall cost as follows. For the sake of simplicity, let us consider 2 tuning parameters p_1 and p_2, but this might be extended directly to any number of parameters. Two series of independent tasks are started with the following settings: in the first series, p_2 is set to its initial value and p_1 is tuned until convergence is reached after n_1 steps; in the second series, p_2 is converged in n_2 steps while p_1 is unchanged. Finally, two tasks are launched with the two last values of both parameters: (p_1 (n_1-1), p_2 (n_2-1)) and (p_1 (n_1), p_2 (n_2)) and the convergence is tested again with the results of these two tasks. This strategy allows running at least as many tasks in parallel as there are tuning parameters, and even more during the early stage of the job.

Monitor window

This window presents a report table and a set of graphics. The table contains a row for each step (VASP task), displaying the parameter values and the computed properties.

Convergence Job 69664 (finished) on server DevCluster_MR

Title : (Au)4 (Fm-3m) ~ Au -- File C:/MD/Structures/Elements/Au.sci (VASP 6 Convergence)

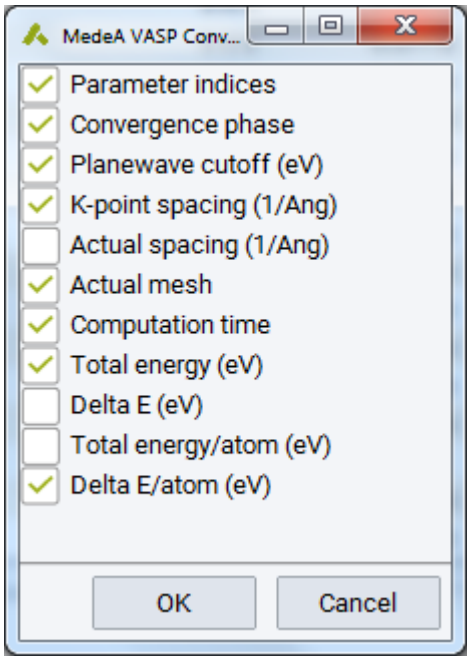
Performing convergence on 'Total Energy' with threshold 0.001 eV

Display only steps from: Final phase

Refresh | Columns Display | Stop Job

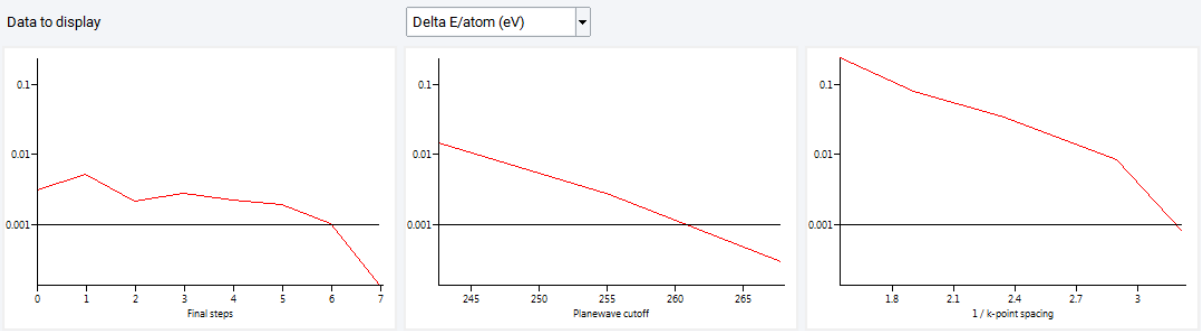
Step	Parameter indices	Convergence phase	Planewave cutoff (eV)	K-point spacing (1/Ang)	Actual mesh	Computation time	Total energy (eV)	Delta E/atom (eV)
0	0 0	Initial	229.943	0.889	4 4 4	0.223 s	-3.00882	-
1	1 0	PWC only	242.59	0.889	4 4 4	0.224 s	-3.023	0.01418
2	0 1	K-mesh only	229.943	0.648081	5 5 5	0.269 s	-3.24373	0.23491
3	2 0	PWC only	255.237	0.889	4 4 4	0.242 s	-3.02566	0.00266
4	0 2	K-mesh only	229.943	0.524946	6 6 6	0.371 s	-3.16557	0.07816
5	3 0	PWC only	267.884	0.889	4 4 4	0.224 s	-3.02596	0.0003
6	0 3	K-mesh only	229.943	0.425206	7 7 7	0.408 s	-3.199	0.03343
7	0 4	K-mesh only	229.943	0.344417	8 8 8	0.561 s	-3.19078	0.00822
8	0 5	K-mesh only	229.943	0.309975	9 9 9	0.617 s	-3.19157	0.00079
9	2 4	Final	255.237	0.344417	8 8 8	0.535 s	-3.2052	-
10	3 5	Final	267.884	0.309975	9 9 9	0.637 s	-3.20829	0.00309
11	4 6	Final	280.531	0.278977	10 10 10	0.798 s	-3.20317	0.00512
12	5 7	Final	293.178	0.251079	11 11 11	0.959 s	-3.20101	0.00216
13	6 8	Final	305.825	0.225971	12 12 12	1.176 s	-3.19822	0.00279
14	7 9	Final	318.472	0.203374	14 14 14	1.827 s	-3.19601	0.00221
15	8 10	Final	331.119	0.183037	15 15 15	2.02 s	-3.19407	0.00194
16	9 11	Final	343.766	0.164733	17 17 17	2.792 s	-3.19304	0.00103
17	10 12	Final	356.413	0.14826	18 18 18	3.366 s	-3.19318	0.00014

The steps can be filtered according to the different phases of the convergence process by checking Display only steps from the selected phase. The selection of columns can be adjusted via the Column Display button: Parameter indices indicating steps for each parameter, Convergence phase discriminating between *PWC only*, *K-mesh only*, *Sigma only* or *Final*, Planewave cutoff (eV), K-point spacing (1/Ang), Actual spacing (1/Ang), Actual mesh, Computation time, and Total energy (eV) and differences in total energy Delta E (eV) per cell or per atom.



The graphics frame contains a graph for each single-parameter convergence axis and one for the final convergence steps (with all parameters):

DOCUMENTATION



When the monitored job is running, some of the computed values are still missing and are indicated by a `-` symbol in the table. The progress of a running calculation can be monitored by updating table and graphs by pushing the `Refresh` button. `Stop Job` allows termination of the entire process.

An estimate of the minimum completion time is calculated by multiplying the time of the longest completed task by the minimum number of remaining tasks.

In addition suggested values for the planewave cutoff energy and the k-point spacing can be found in the **Job.out** file:

```
--------------------------------------------------------------------------------
The final, converged parameters
--------------------------------------------------------------------------------
Planewave cutoff:  488.000 eV
k spacing:    0.601 1/Ang

--------------------------------------------------------------------------------
Results for the minimization using the converged parameters
--------------------------------------------------------------------------------
```

Basic features of the `Automated Convergence` module are also found in `Point Defect Analysis` tool.

DOCUMENTATION