

Automated Convergence

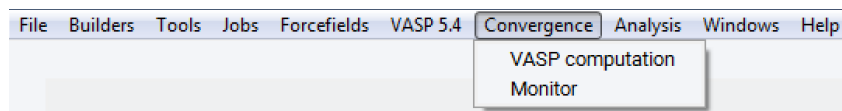
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The accuracy of computed materials properties such as equilibrium lattice parameters, binding energies, and elastic moduli depends on a variety of computational parameters, most notably the quality of plane wave basis sets and the density of k-meshes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

The Convergence run interface looks like this:

Convergence type

Convergence criterion: Total Energy ▼

Energy Threshold: 0.001 eV Per Atom

Tuning parameters

Type of smearing: Tetrahedron with Bloechl corrections ▼

Use energy cutoff Initial energy cutoff: 229.943 eV Increment: 12.6469 eV

The default for low precision is 172.457 eV, the default for increased precision is 298.926 eV

Use k spacing Initial k spacing: 0.889 Update factor: 0.9 Use odd size grids

Corresponding k mesh 4 4 4 (0.667 0.667 0.667)

Other VASP Settings

Title: (Au)4 (Fm-3m) ~ Au (VASP 5.4 Convergence)

Run
Close

Convergence type

You can use the following criteria with Convergence:

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

Convergence type

Convergence criterion: Total Energy ▼

Energy Threshold: 0.001 eV Per Atom

Structure Optimization : Converges both the single-point stress and the lattice parameters and atomic positions. You can select to **Relax atoms** only.

Convergence type

Convergence criterion: Structure Optimization ▼

Single Point Stress Convergence

Stress Threshold: 0.5 GPa

Structure optimization criteria

Relax atoms only

Lattice length Threshold: 0.01

Lattice angles Threshold: 1.0 degrees

Atoms Positions Threshold: 0.05 Ang

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 atomic 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:

Energy cutoff (Plane wave cutoff, PWC): Starting from the initial energy cutoff the module will increase the cutoff by Increment until convergence is reached. VASP potentials provide a range of cutoff energies for each atom, defined by the limits *EMIN* and *EMAX*. The default value is the average between *EMIN* and *EMAX*. For systems with more than one type of atoms, the average between the highest *EMIN* and the highest *EMAX* is taken. The default increment is 1/10 of the difference between these two values.

K spacing (k-point spacing, KPS): The initial value of the KPS is set by the parameter **k-spacing** in such a way that the resulting k-mesh is at least 3x3x3 to allow using the tetrahedron method. In the refinement of the k-mesh, the initial k-spacing is multiplied by the **Update factor** until the actual number in the k-mesh increases.

Smearing width: You can optimize this parameter only when Methfessel-Paxton k-integration is chosen. The default is to use the tetrahedron method with Blöchl corrections, 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.

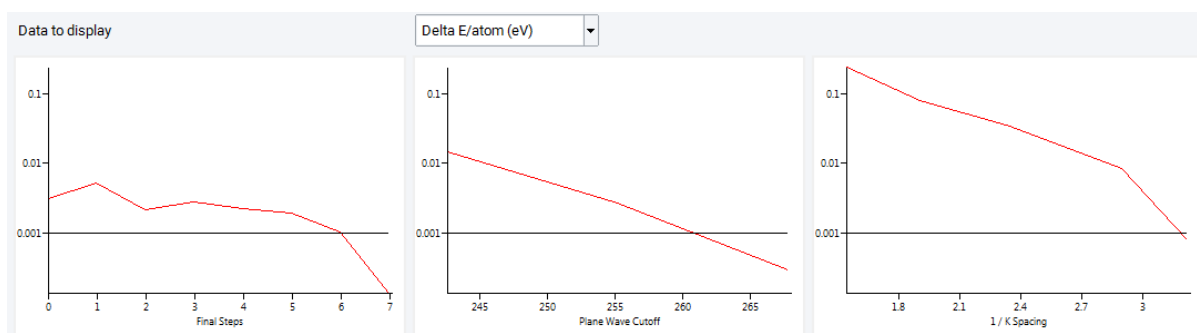
Monitor window.

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

Step	Parameter indices	Convergence phase	Plane Wave Cutoff (eV)	K Spacing (1/Ang)	Actual Mesh	Computation time	Total energy (eV)
0	0 0	Initial	229.943	0.889	4 4 4	1.527 s	-3.00882
1	1 0	PWC only	242.59	0.889	4 4 4	1.51 s	-3.023
2	0 1	K-mesh only	229.943	0.648081	5 5 5	1.709 s	-3.24373
3	2 0	PWC only	255.237	0.889	4 4 4	1.538 s	-3.02566
4	0 2	K-mesh only	229.943	0.524946	6 6 6	2.031 s	-3.16557
5	3 0	PWC only	267.884	0.889	4 4 4	1.527 s	-3.02596
6	0 3	K-mesh only	229.943	0.425206	7 7 7	2.296 s	-3.199
7	0 4	K-mesh only	229.943	0.344417	8 8 8	2.85 s	-3.19078
8	0 5	K-mesh only	229.943	0.309975	9 9 9	3.129 s	-3.19157
9	2 4	Final	255.237	0.344417	8 8 8	2.78 s	-3.2052
10	3 5	Final	267.884	0.309975	9 9 9	3.183 s	-3.20829
11	4 6	Final	280.531	0.278977	10 10 10	3.891 s	-3.20317
12	5 7	Final	293.178	0.251079	11 11 11	4.409 s	-3.20101
13	6 8	Final	305.825	0.225971	12 12 12	5.412 s	-3.19822
14	7 9	Final	318.472	0.203374	14 14 14	7.768 s	-3.19601
15	8 10	Final	331.119	0.183037	15 15 15	8.841 s	-3.19407
16	9 11	Final	343.766	0.164733	17 17 17	11.804 s	-3.19304
17	10 12	Final	356.413	0.14826	18 18 18	13.895 s	-3.19318

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

- Parameter indices
- Convergence phase
- Plane Wave Cutoff (eV)
- K Spacing (1/Ang)
- Actual K Spacing (1/Ang)
- Actual Mesh
- Computation time
- Total energy (eV)
- Delta E (eV)
- Total energy/atom (eV)
- Delta E/atom (eV)



The selection of columns can be adjusted via **Column Display** : **Parameter indices** , **Convergence phase** , **K Spacing** , **Actual K Spacing** , **Actual mesh** , **Computation time** , and **Total energy** and differences per atom and cell.

When the monitored job is running, some of the computed values are still missing and are indicated by a - symbol.

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.

Basic features of the **Automatic Convergence** module are also found in **Point Defect Analysis** tool.