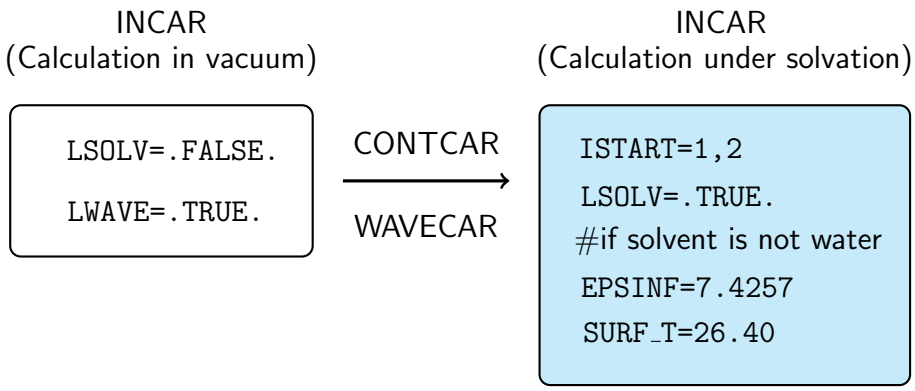
VASP-MultiGrid Continuum Model (VASP-MGCM) Quick Guide

1 Running a VASP-MGCM Calculation

- Set `LSOLV=.TRUE.` in the INCAR file to perform a calculation under solvation. This tag is set to `FALSE` by default (calculation in vacuum).
- Water is the solvent by default. In this case, the user only needs to set `LSOLV=.TRUE.` If another solvent is to be considered, the user should specify the value for the dielectric permittivity of the bulk (`EPSINF`) and its surface tension in units of dyne/cm (`SURF_T`). For instance, for the case of tetrahydrofurane (THF): `EPSINF=7.4257`, `SURF_T=26.40`.
- In order to run a calculation under solvation, one needs first to perform a calculation in vacuum for the same system to generate the WAVECAR file. As VASP-MGCM uses a slightly different grid than that used by VASP, the calculation in vacuum should be done with the VASP-MGCM executable but with `LSOLV=.FALSE.` Once the WAVECAR file is generated, copy it to the folder where the calculation under solvation is to be launched together with the CONTCAR file (that will be the new POSCAR file), and set `ISTART=1` or `2` and `LSOLV=.TRUE.` A general scheme that describes how to launch a calculation with VASP-MGCM using THF as solvent is shown below in Scheme 1.



Scheme 1: Tags to be specified in the INCAR file to launch a calculation under solvation using VASP-MGCM (THF as solvent). Both calculations (in vacuum and in solution) should be performed with the same VASP-MGCM executable.

2 Known Issues

When running VASP-MGCM some issues can appear. These problems are related to (i) the lack of the appropriate input files, (ii) some tags in the INCAR file, (iii) memory requirements. Before running a calculation using VASP-MGCM please **READ CAREFULLY** this section.

2.1 The calculation diverges after few electronic steps

When this occurs, the calculated system energy, which is displayed in the OUTCAR and OSZICAR files, is too large and the following line appears at the end of the OUTCAR file: `WARNING in EDDRMM: call to ZHEGV failed, returncode = 3 2 1.`

- Check that the WAVECAR file (generated from the vacuum calculation) is in the same folder with the rest of input files (INCAR, POSCAR, KPOINTS, ...) and that the CONTCAR file was renamed as POSCAR.
- Divergence after few electronic cycles has been observed for the case of some molecules isolated in the center of the simulation cell. In these cases, the issue is solved by modifying slightly the box side-length. That is, if a water molecule is simulated in a cubic cell of 20 Å side-length, one just needs to reduce it to e.g: 15 Å.

2.2 Intramolecular adsorbate bonds rotate too much when IBRION=2

In the case of adsorbed molecules on surfaces it has been observed that, for `IBRION=2`, the adsorbate atoms tend to move too much due to the interaction with the solvent. Set `IBRION=1`.

2.3 Insufficient virtual memory

In the VASP-MGCM the Generalized Poisson Equation (GPE) is discretized on a fine tridimensional grid. This fact results in the allocation of several big matrices. If the system to simulate is too big, or the energy cutoff (`ENCUT`) is too high, then the simulation grid will be too fine and the calculation will stop (due to the limited memory available on the nodes of tekla2). The finest grid that VASP-MGCM can simulate on tekla2 nodes is $N_{\max}$ =`NGXF`×`NGYF`×`NGZF`= 7077888. VASP-MGCM has been programmed then in such a way that if the chosen grid is larger than $N_{\max}$, then the grid is reduced automatically. However, the resulting grid can be too small if we aim at having an accurate value for the energy of the system. If one wants to know if the box partition is ok, check the fort.71 file. If the resulting partition in any of the three space directions is smaller than that suggested by VASP, the following line will appear "`NGX(YF)F lower than the minimum VASP grid size`".

There exist different ways to overcome this problem:

- Make the system smaller. For the case of isolated molecules on a box, reduce slightly the side-length. For periodic systems, the user should construct a smaller surface.
- Reduce `ENCUT`. To do so, take a look to the POTCAR file and check the largest value of `ENMAX` for the different species.
- Modify the `PREC` tag.

3 Charged Systems

Although the VASP-MGCM parametrization set included some charged species, the set contained mainly neutral molecules (some hundreds). If one needs to simulate charged periodic slabs, it is important to take into account that, in VASP, the total energy for such systems can not be corrected (see the section in the VASP manual where the `NELECT` tag is described). Then, the user should place a countercharge, if possible, far away from the region of interest.

For the case of isolated charged molecules, if the energy of the system needs to be considered to compute adsorption or replacement energies, it is always preferred that the user designs the systems in such a way that the total system charge is equal to 0. If this can not be done, the simulation cell should be big enough to avoid undesired interactions between the implicit solvent and the periodic images of the charged isolated species.