How to write the Methods Section?

The methods section for computational research will be quite different from what you write in an experimental lab. Below is an explanation of this section and a few examples from literature to show you what this section should look like for your project.

The methods section is meant to include all the details of the calculations you have done in this work. The *most important requirement* of the methods section is as follows:

You should give enough information such that a competent researcher could replicate the results you achieved in your experiment/calculations.

This is the most important question to ask when evaluating a methods section. However, it may not be clear what is "enough" information for a "competent researcher". To get a sense for how much information to provide, look at similar papers in literature. Below is an explanation of what your methods section should look like and a few example papers from literature:

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1. ***For global optimization projects**:* You should clearly describe the global optimization you have used in your work or if you are modifying a method, describe the original method and the change you have made. I expect everyone on this project to include equations describing how their method works. After reading your methods section, other researchers should be able to implement this method. Here are a few papers to look at as a guide to what your methods section should look like:
    a. A paper called "An investigation of two approaches to basin hopping minimization for atomic and molecular clusters" published in the Chemical Physics Letters by White et. al.
    b. *http://aip.scitation.org/doi/10.1063/1.2900644*

    Here is one suggestions which was a common mistake from last semester:
        a. You do not need to include names of scripts edited or submitted on the cluster (*i.e.* basin_hoping.py, submission scripts, etc.) Only describe the goal of the script. (i.e. The average force calls required to reach the global minimum were calculated to quantify performance.)

2. ***For catalyst/VASP projects**:* This section should include the details of your electronic structure calculations. You may need to look up or remind yourself of electronic structure calculations, Density Functional Theory, and methods for optimization. Include a *brief explanation (a few sentences)* of what these methods are (you may not see this in the literature). Here are a

few papers to look at as a guide to what your methods section should look like:

a. *http://theory.cm.utexas.edu/henkelman/pubs/zhang14_655.pdf*
b. *http://theory.cm.utexas.edu/henkelman/pubs/corona16_244708.pdf*

Here is one suggestions which was a common mistake from last semester:

a. You do not need to include things you do not understand (e.g. Kohn-Sham wave functions, generalized gradient approximation, etc.), but should include information included in this course (e.g. DFT, VASP, convergence criteria, binding energy equations, etc.).
b. You do **NOT** need to include any details of the VASP software or commands you have used (POSCAR, INCAR, outf, oute, etc.).

Here are a few other things to consider when writing your methods section:

- The methods section should let the reader judge the appropriateness of the methods used in the work.
- The methods section should be in the past tense.
- If applicable, put methods used in chronological order