

Tutorial Application Input Files and Parameters

All the input files for applications in PGA are available in <https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7>

Folder by the application name exists with input files.

For your ease of use few are existing here.

1. Gaussian Application Input Files

a. Gaussian Input 1

[Gaussian.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

b. Gaussian Input 2

[caco3wat2.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

c. Gaussian Input 3

[si3s3h3.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

d. Gaussian Input 4

[ptc2h3.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

e. Gaussian Input 5

[pxylene.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

f. Gaussian Input 6

[ch5n2o.com](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

2. Espresso Application Input Files

a. AI_Pseudopotential_File

[Al.pz-vbc.UPF](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

b. AI_Primitive_Cell

[Al.sample.in](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

3. NWChem Application Input File

a. Water_Molecule_Input

[water.nw](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

4. WRF Input Files

a. Namelist File - [namelist.input](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

b. WRF Boundary File - [wrfbdy_d01](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)

c. WRF Initialization File - [wrfinput_d01](https://iu.box.com/s/9ztdby709kso8siachz16svn2y511nn7)