


```

NGsBlkXp= 1          RL      # [Xp] Response block size
% LongDrXp
 1.000000 | 0.000000 | 0.000000 |          # [Xp] [cc] Electric Field
%
PPAPntXp= 27.21138   eV      # [Xp] PPA imaginary energy
% GbndRnge
 1 | 50 |          # [GW] G[W] bands range
%
GDamping= 0.10000    eV      # [GW] G[W] damping
dScStep= 0.10000     eV      # [GW] Energy step to evaluate Z factors
DysSolver= "n"       # [GW] Dyson Equation solver ("n","s","g")
%QPkrange           # [GW] QP generalized Kpoint/Band indices
 1 | 43 | 1 | 50 |
%

```

The default values generated in the input may not be sufficient for your calculations. Convergence tests are required for values of EXXRLvcs, NGsBlkXp, BndsRnXp, GbndRnge, and QPkrange. To keep the calculation simple for the purpose of this tutorial, we simply set them to the values indicated above. Click [here](#) if you would like to explore details about these variables.

The following is a sample job submission file to perform a GW calculation. This will submit your job to the parallel queue by the qsub/sbatch command (this is a long job compared to Quantum Espresso calculations and it will take a while to finish). For details of how to submit jobs in MARCC, please refer to the [running jobs](#) page.

```

#!/bin/bash -l
#SBATCH --job-name=job-gw
#SBATCH --time=06:00:00
#SBATCH --partition=parallel
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=24
mpirun -np 96 ./yambo -F yambo.in > yambo.out

```

After you finish the GW calculation with the above job script, the system will generate an output file “o.qp” with quasiparticle corrections to the band gap.