

bash command

```
$ mpirun -np NUM_PROCESSORS MMPBSA.py.MPI -O -i INPUT_FILE.in -o ↵  
↵ gb_results.dat -sp SOLVATED_COMPLEX.parm7 -cp complex.parm7 ↵  
↵ -rp receptor.parm7 -lp ligand.parm7 -y ↵  
↵ PRODUCTION_TRAJECTORY.nc
```