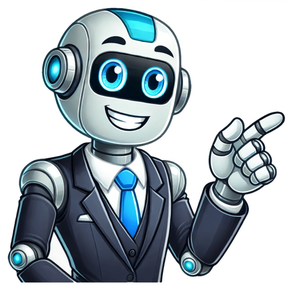
I'm human



Gaussian is a renowned computational quantum chemistry program that offers cutting-edge capabilities for modeling electronic structures and predicting molecular properties. Developed by the J. A. Pople group, Gaussian has been widely used in the field of quantum chemistry since its inception. The software is continuously updated to provide state-of-the-art features and capabilities. The latest version, Gaussian 16 Rev. C, is available now, offering enhanced functionality for electronic structure modeling. This release includes new features, improved performance, and bug fixes. Users can access more information on the Gaussian Inc. website or contact HPC SYSTEMS for technical details and manuals. Gaussian 16 provides an array of tools for predicting molecular energies, structures, vibrational frequencies, and properties in various chemical environments. The program's versatility makes it suitable for a wide range of applications, from small molecules to complex systems. To use Gaussian 16, users can load the module using the command `module load gaussian/g16c01` and specify the required resources based on their system size and calculation type. Key considerations include memory, processor count, and scratch space, which can be adjusted as needed. The program's user guide provides detailed information on efficiency considerations and resource allocation. For more information, please visit the Gaussian Inc. website or contact HPC SYSTEMS for support and updates on this powerful computational tool. #!/bin/bash #PBS -P your_project_code #PBS -l walltime=24:00:00 #PBS -l ncpus=12 #PBS -l mem=24GB #PBS -l jobfs=200GB #PBS -l software=g16 #PBS -l wd module load gaussian/g16c01 cpulist=`grep Cpus_allowed_list: /proc/self/status | awk '{print $2}'` export GAUSS_CDEF="$cpulist" g16 < inputdeck > outputfile 2>&1 %nproc must be taken out of the Gaussian input file, and for the case above, correspond to: %mem=(24-overhead for your method)Gb %chk=checkpoint.chk Maxdisk=200Gb PBS requires additional memory for system libraries and other overheads. For post-SCF methods, this can be considerably more depending on the size of the system. Scratch disk usage is also important; in this case, the route card uses the Maxdisk keyword, which should match the value set in the GAUSS_SCRDIR environment variable.

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