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Gaussian 16 user manual pdf

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Gaussian 16 is the latest quantum chemistry package, replacing its predecessor Gaussian 09. The current revision is C.01, with older versions B.01 and A.03 still available. The software can be found on all CHPC clusters at /uufs/chpc.utah.edu/sys/installdir/gaussian16/C01. Four executable directories exist due to the presence of SSE4, AVX, or AVX2 instruction sets: legacy for nodes without these features, SSE4 for lonepeak and 12 core ash nodes, AVX for tangent nodes with 16 or 20 cores on kingspeak and ash, and AVX2 for notchpeak, kingspeak, and ash nodes with 24 or 28 cores. The newer processors' compatibility ensures that the older instruction sets can run on all nodes, but performance is affected, making it optimal to use the correct version. This is addressed in the provided slurm batch script. For queries regarding Gaussian, visit or contact the developers directly. An important note: the licensing agreement restricts usage to academic research purposes and only for research associated with the University of Utah. Commercial development and application are not permitted, nor using the program to compare performance with competitors' products. To use gaussian16, one must be part of the gaussian users group and load the module by running "module load gaussian16". The SSE4 version is set as default but can be changed by specifying a different version, such as "module load gaussian16/SSE4.C01" for SSE4 or "module load gaussian16/AVX2.C01" for AVX2. Once loaded, start Gaussview with "gv &". Additionally, the new B01 version introduces a "gaussian" family in the module that prevents multiple gaussian modules from being loaded simultaneously. If you load a module with one version and then try loading another module with a different version, you'll see a message saying that the new version replaces the original one. For example, there's a provided script called `rng16` in `/uufs/chpc.utah.edu/sys/installdir/gaussian16/etc/` that queries the cluster and chooses which module to load based on the core count if needed. Note that for using it on notchpeak AMD nodes, you need to add `setenv PGI_FASTMATH_CPU sandybridge`. In this script, make sure to set your partition, account, wall time, and constraints as necessary, especially when dealing with partitions that have multiple choices for cores. You'll also need to set four environment variables: `WORKDIR`, `FILENAME`, `SCRFLAG`, and `NODES`, taking into consideration the comments in the batch script and the considerations on this page. When submitting a run, ensure the number of processors (nprocs) matches the value specified in the Gaussian input file. If running in node-sharing mode, remember to also allocate sufficient memory for each node. Refer to the Node Sharing page for further details on this process.