What is the optimal amount of memory for Gaussian jobs?

Since Gaussian performance is often limited by memory, it is important to set memory limits correctly. The Gaussian directive *Mem* and the SLURM options *--mem* shouldn't be confused:

- --mem: Is the total amount of memory requested per node that SLURM needs to allocate. The default value depends on the partition, and goes from 3900 MB to 24180 MB per core requested.
- *Mem:* Limits the total amount of dynamic memory (in words or mega-words) that Gaussian will use during the calculation. Gaussian may implement some methods differently depending on this memory limit. You can use the Gaussian utility *freqmem_ext-link* to estimate how much memory a Gaussian calculation needs. It is recommended to assign an amount ~75% of the SLURM requested memory.

The default memory allocation in Gaussian 16 is 100MW (800MB).