

To run Gaussian09 on Dextrose:

bsub -n 12 g09 test264.gjf
 The -n flag asks for # of processes (**MUST MATCH %nproc** and be <13)

If you need error files and job labels, try
bsub -n 12 -J test264 -oo test264.stdout -eo test264.stderr g09 test264.gjf
 The -J flag gives the job a jobname so you can find it in queue
 The -oo and -eo are extra files that contain errors reported from the queueing system

Other useful commands: bkill, bjobs, bhist, bqueues
 Learn more about these online at <http://www.lcd.uregina.ca/bsubPrimer.html>

Supercomputer comparison test
 Gaussian03 MP2 OPT, %nproc=2, 1,3-diphenylpropane
Note: Gaussian09 uses a different optimization algorithm that reduces the number of geometry update loops from 16 to 13

Supercomputer	Time (min)	Speed (loops/hour)
Dextrose	53	18.1
Checkers (Westgrid)	66	14.5
Cadmium n027	144	6.7
Cadmium n017	262	3.7

Parallelism tests on Dextrose

BP86 freq, organometallic tungsten complex

%nproc	Trial 1				Trial 2			
	job cpu (s)	walltime (s)	"%cpu"	efficiency	job cpu (s)	walltime (s)	"%cpu"	efficiency
1	6835	6843	99.9	1.00	6832	6839	99.9	1.00
2	6369	3196	99.6	1.07	6370	3195	99.7	1.07
3	6535	2191	99.4	1.04	6531	2188	99.5	1.04
4	7319	1844	99.2	0.93	6671	1680	99.3	1.02
5	7527	1520	99.0	0.90	7517	1515	99.2	0.90
6	7007.5	1182	98.8	0.96	7655	1293	98.7	0.88
7	7883	1134	99.3	0.86				
8	8027	1012	99.1	0.85				

BP86 opt, 1,3-diphenylpropane

%nproc	Trial 1			
	job cpu (s)	walltime (s)	"%cpu"	efficiency
1	6433	6468	99.5	1.00
2	6647	3405	97.6	0.95
3	7520	2607	96.2	0.83
4	7710	2035	94.7	0.79
5	7961	1703	93.5	0.76
6	8193	1480	92.3	0.73
7	7793	1216	91.6	0.76
8	7852	1088	90.2	0.74

MP2 opt, 1,3-diphenylpropane

%nproc	Trial 1				Trial 2			
	job cpu (s)	walltime (s)	"%cpu"	efficiency	job cpu (s)	walltime (s)	"%cpu"	efficiency
1	2651	2684	98.8	1.00	2619	2651	98.8	1.00
2	3204	1669	96.0	0.80	3205	1674	95.7	0.79
3	4331	1534	94.1	0.58	4332	1537	93.9	0.57
4	5322	1434	92.8	0.47	5319	1430	93.0	0.46
5	7572	1625	93.2	0.33	7581	1621	93.5	0.33
6	10400	1844	94.0	0.24	10403	1844	94.0	0.24

Conclusions:

1. DFT (including BP86) parallelizes well, especially the frequency calculations
2. MP2 does NOT parallelize well; use only 3-4 core processors.
3. MP2 is faster than BP86 (surprising; the SCF is 15x faster)
4. "%cpu" is rather meaningless nowadays