Updated comments about the homework and useful information on periodic systems.

The version of G03 that we are using has trouble converging calculations on periodic systems when using methods that include exact exchange. So it is best to adopt functionals such as BLYP that do not use exact exchange.

Using the tutorial for diamond, one can build the primitive cell for bulk Si
See http://www.gaussian.com/g_gv/tutorials.htm

The input file is attached

```
----------------------------------------
%chk=silicon_bulk_gjf.chk
%mem=65MW
%nproc=1
#p lsda/sto-3g pbc=nkpoints=8 scfcyc=6

Title Card Required

0 1
 Si                  0.00000000    0.00000000    0.00000000
 Si                  1.87383297    1.08185797    0.76498911
 Tv                  3.74766594    0.00000000    0.00000000
 Tv                  1.87383297    3.24557391    0.00000000
 Tv                  1.87383297    1.08185797    3.05995643

----------------------------------------------
```

Here are some timings on my not-so-fast PC:

Primitive cell, 1 kpoint	3.7 min
Primitive cell, 8 kpoints	4.3 min
Non-primitive cell, 1 kpoint	8.3 min

So the job runs about 2.25 times faster with the primitive cell than with the 8-atom cell. The difference would probably be much greater with a larger basis set.

Here is an example of a unit cell for studying the silicon dimer on the Si(100) surface.

```
%chk=surface.chk
%mem=6MW
%nproc=1
#p lsda/sto-3g pbc=nkpoints=16

silicon surface

0 1
 Si                  1.64783010    1.31993484    2.49493743
 Si                  3.82783010    1.31993484    2.49493743
 Si                  0.90783010    3.23993484    1.49493743
 Si                  4.56783010    3.23993484    1.49493743
 Si                  2.73783010    3.23993484    0.02493743
 Si                  6.57783010    3.23993484    0.26493743
 Si                  2.73783010    1.31993484   -1.23506257
```

```
Si                  6.57783010    1.31993484   -1.09506257
Si                  0.81783010    1.31993484   -2.49506257
Si                  4.65783010    1.31993484   -2.49506257
H                   4.67879816    2.51848412   -3.34590918
H                   0.61391834    2.53313785   -3.29971061
H                   0.61391834    0.10673183   -3.29971061
H                   4.67879816    0.12138555   -3.34590918
Tv                  7.68000000    0.00000000    0.00000000
Tv                  0.00000000    3.84000000    0.00000000
```

Note that this has five layers of Si atoms, and the bottom layer is terminated with H atoms. This is a reasonable number of layers.

Note also that there is a small symmetry breaking in the bottom layers and in the placement of the H atoms. This must have happened in the building of the structure and should be fixed before doing production runs.

Generally, for such a cell, one would freeze the bottom two layers of silicon at their bulk positions and also freeze the terminating H atoms.

To freeze the bottom two Si layers and the H atoms add after the geometry specification (remembering to skip a line) lines:

9 F
11 F
……
16 F
etc.

and to add opt=modredudant.

If computer time is an issue when you proceed to a more reasonable basis set such a 6-31G(d) , you could drop down to four layers. Another strategy for reducing the computer time would be to use a smaller basis set on say the bottom three layers than employed for the top two.

With split valence or larger basis, you would achieve a large reduction of computer time by adopting a pseudopotential for the Si atoms.

An input file with which an ECP is used for together with a 2s2p1d basis set on Si and the 6-31G basis set on H, is given below. On my PC this took about 40 minutes of CPU time.

Here is an input file for a single-point calculation on the silicon(100) reconstructed surface in which an external ECP and comparable basis set is used for the Si atoms.

```
%mem=30MW
%nproc=1
#p beckelyp pbc=nkpoints=8 gen pseudo=cards

silicon surface with ECP

0 1
 Si                 1.64783010    1.31993484    2.49493743
 Si                 3.82783010    1.31993484    2.49493743
 Si                 0.90783010    3.23993484    1.49493743
 Si                 4.56783010    3.23993484    1.49493743
 Si                 2.73783010    3.23993484    0.02493743
 Si                 6.57783010    3.23993484    0.26493743
 Si                 2.73783010    1.31993484   -1.23506257
 Si                 6.57783010    1.31993484   -1.09506257
 Si                 0.81783010    1.31993484   -2.49506257
 Si                 4.65783010    1.31993484   -2.49506257
 H                  4.67879816    2.51848412   -3.34590918
 H                  0.61391834    2.53313785   -3.29971061
 H                  0.61391834    0.10673183   -3.29971061
 H                  4.67879816    0.12138555   -3.34590918
 Tv                 7.68000000    0.00000000    0.00000000
 Tv                 0.00000000    3.84000000    0.00000000

H 0
6-31G
****
Si 0
S    3 1.00
 4.0143780000  -0.395080000D-01
 1.3937070000   0.296150000
 0.2516580000  -0.599752000
S    1 1.00
 0.1001800000  1.00000000
P    3 1.00
 1.1024810000   0.845830000D-01
 0.5831270000  -0.185748000
 0.2086750000  -0.554852000
P    1 1.00
 0.691470000D-01  1.00000000
D    1 1.00
 0.4500000000D+00  0.1000000000D+01
****

Si 0
SiC 2 10
Vd
 8
 1            4.98133037           4.00000000
 2            0.98224665          -6.14137554
 2           29.93446250          -0.24776129
 3            1.72269991          61.24187288
 3            1.76461698         -41.31655141
 4            2.33760242          47.80111485
 4            1.91627270        -101.90161220
 4            1.60950710          40.65155066
Vs - Vd
```

```
 8
 2            2.00290881           62.05121032
 2            6.28521865          -54.75192064
 3            3.16671223          913.53220367
 3            2.48118773         -731.09591881
 3            5.78720050         -182.43628485
 4            3.37554174        -1729.70440653
 4            2.95864449         1486.21692663
 4           11.19664066           23.64260333
Vp - Vd
 8
 2            3.25133398        20593.52167775
 2            3.23933192       -20589.38501808
 3            2.20625916        -1210.26634336
 3            1.84878145       -19216.44646104
 3            1.87013902        20426.71280440
 4            2.51593801         -314.98851226
 4            1.60800606          149.17941008
 4            3.16968263          426.37381217
```

Another thing of interest is how to go from periodic to cluster models. Once one has built a periodic model and replicated the unit cell, it is pretty easy to cut out cluster models of different sizes. These can then be used with theoretical methods that cannot be used with pbc.