

Basic requirements:

A UNIX or LINUX system.

The GAUSSIAN03/09 package (source code).

A FORTRAN90 compiler.

Installation:

Before installing **ANT.G**, the GAUSSIAN03/09 package must have been compiled using the standard procedure as described in its installation instructions. Once the installation log file *make.log* has been generated in the GAUSSIAN03/09 installation directory, the installation script *install.g03/g09* can read the preprocessor (PFLAGS) and compilation flags (CFLAGS) GAUSSIAN03/09 has been compiled with. If you don't have the *make.log* file available or the automatic installation does not work for some reason, you have to find out the flags yourself and edit the installation script *install.g03/g09* accordingly, i.e., you have to edit the variables *PFLAGS*, *CFLAGS*, *EXTRALIBS*, *LFLAGS* (see below for further explanations). Now follow these steps to install **ANT.G** on your computer:

Untar the **ANT.G** package in a directory of your choice:

```
> tar -xvf ANT.G-x.x.x.tar
```

This creates a directory *ANT.G-x.x.x* with the directory tree containing all files necessary for the installation of **ANT.G**. Change to the installation directory:

```
> cd ANT.G-x.x.x/install
```

Edit the installation script *install.g03/g09* (choose the appropriate one according the version of GAUSSIAN you are using). This script automatically reads the GAUSSIAN03/09 source files *l101.F*, *l503*, and *l502.F* and creates modified versions. The subroutine *caldsu.f* is also extracted from the file *utilam.F* and a modified version is generated which does not abort when the charge density does not integrate exactly to the number of electrons of the cluster. You must change the system dependent variables *g03root/g09root* and *F90* which hold information on the path of the GAUSSIAN03/09 package and the path of the FORTRAN90 compiler. Now run the script:

```
> ./install.g03
```

or

```
> ./install.g09
```

This creates two new links: *l101.exe*, which reads the string `<job_name>`

from the title line in the GAUSSIAN input file to be used to name all files, and *l103.exe*, which stops a geometry optimization even if the forces are not converged (and this is always the case when a selfenergy is added to the Fock matrix). It also creates the library *l502.a*. Do not worry about the error messages towards the end as long as the library *l502.a* has been created in the directory *lib*. The include file *make.in* is also created and moved to the *src* directory. The file *make.in* holds the preprocessor (*PREPROC*), compilation (*CFLAGS*), and linking flags (*LFLAGS*), and the library paths (*GAUSSLIBS*) that are necessary to compile **ANT.G** and link it with GAUSSIAN03/09. Change now to the *src* directory:

```
> cd ../src
```

Compile and link **ANT.G** by executing the make file:

```
> make -f Makefile.g03/g09
```

This creates the main new link *l502.exe* which calls **ANT.G** for the calculation of the density matrix in the NEGF formalism during the self-consistency and evaluates the transmission function, DOS, etc. after convergence.

If some error occurs during compilation or linking or if the program does not work properly, edit the include file *make.in*: You might need to get rid of some compilation flags (*CFLAGS*). Taking away almost all the compilation flags normally solves the problem. But don't take away the target processor flag (e.g., *-tp* for Portland compiler). You should also check that the preprocessor flags (*PFLAGS*) are the ones needed. You can check all this in the *make.log* file generated in the GAUSSIAN compiler. Then try to compile and link again by executing:

```
> make -f Makefile.g03/g09 clean
```

If the installation was successful the modified links *l101.exe*, *l103.exe*, and *l502.exe* should have been generated in the directory *ANT.G-x.x.x/bin*. You might have to change permissions.

After the installation is completed set an environment variable *ALACANT* in your shell script (*.bashrc* *.tcshrc*, etc.) which holds the directory path where **ANT.G** has been installed as, e.g., for bash:

```
> export ALACANT=$HOME/.../ANT.G-x.x.x.
```

And you are all set.