HOW TO RUN GOLD JOBS ON THE CLUSTER
An Alternative to Using gold_parallel_auto

1. Bring up the Gold GUI by typing **gold** at the ddfe console or in an X-window remotely.

2. Set up your Gold job and save your configuration file as gold.conf.

3. You will now exit gold. Type the following to submit multiple jobs to the queuing system:

$GOLD_DIR/gold_scan *first last slice ligand_database_filename*

where *first* is the index of the ligand in your database to start with (usually 1; the first ligand of the database has index 1),
last is the index of the ligand in the database to end with (usually the same as the number of compounds in the file),
slice is the number of compounds to be docked by a single process (should be 1000 or more; it is required that *slice* * *n* = *last* – *first* + 1, where *n* is an integer),
ligand_database_filename is the name of the sdf or mol2 file containing ligand compounds to be docked in your run.

Ex. $GOLD_DIR/gold_scan 1 12300 3075 /home/databases/KINASet.sdf will start 4 jobs (processes on the cluster) screening 3075 ligands each using parameters found in gold.conf.

The jobs are submitted through the SGE queuing system installed on the cluster. The queuing system will choose to which nodes to submit your jobs based on current usage. The jobs' cpu usage will show up with the **ganglia cpu_user**.

6. To monitor your jobs from a computer within the X-ray VLAN in Welch, point your browser to the following:

https://ddfe.cm.utexas.edu/wordpress

Click on **Cluster Status** in the panel at the top. While your jobs are running, they will show up in the list presented after clicking **Job Queue** or **Cluster Top**.

Alternatively, to monitor your jobs, on the ddfe console or in an X-window while logged onto the ddfe, type:

qmon &

Click on the **Job Control** icon. While your jobs are running, they will show up under the **Running Jobs** tab. As they finish, they'll move under **Finished Jobs**.

7. When all jobs are done, you'll want to examine your results. Output from each process will be written in a separate sub-directory under the directory from which you initiated the jobs. These directories will have the names *output_* followed by the indices of the first and last compounds docked by the process. (e.g. output_1_3075, output_3076_6150, etc.)

Type the following to concatenate files of the same name written in each of the output directories:

$GOLD_DIR/gold_cat *first last slice outfile*

where *first*, *last*, and *slice* are the same values you used with the **gold_scan** command to start your Gold jobs.

Ex. To concatenate the bestranking.lst files generated from the example **gold_scan** jobs above, you would type:

$GOLD_DIR/gold_cat 1 12300 3075 bestranking.lst

Your working directory would need to be same one you were in to start the gold_scan jobs.