Cluster Setup for Schrödinger Jobs

This document summarizes the steps needed to set up a cluster for running Schrödinger jobs via a queueing system and ensuring user access. It is assumed that the manager node (head node) is the node on which the queue commands will be run. For more information, see the appropriate sections of Chapter 7 of the *Installation Guide*.

1. Install the software in a location that is accessible to the manager node and the compute nodes.

   This location will be referred to as *cluster-installation*. Installation on a common file system in the cluster is recommended. The same version of the software must be available to the user's computers (at *user-installation*); it need not be in the same location as the cluster installation.

2. Install and configure a supported queueing system, if not already installed (Section 7.3 of the *Installation Guide*).

3. Edit the file *cluster-installation*`/queues/`*type*`/config` on all queue submission hosts to set the location of the queue binaries (Section 7.3.2 of the *Installation Guide*). Here, *type* is the queueing system type, e.g. `SGE`.

4. Add entries to *user-installation*`/schrodinger.hosts` in the user-accessible software installation for the cluster queues. (Section 7.1 and Section 7.3.1 of the *Installation Guide*).

5. Ensure that the manager node has a static host name that is resolvable from any cluster node and is always associated with the same physical host.

   Communications addressed to that host name must not be redirected to another physical host.

6. Enable the manager node and the compute nodes to open socket connections to the FlexLM license server.

7. Enable the compute nodes and the manager to open socket connections to each other on ports above 1024.

8. Configure passwordless SSH for each user (Section 7.2 of the *Installation Guide*):

   a. between all cluster nodes

   b. between the user's workstation and the manager node

9. Test the installation with the following command (Linux):

   ```
   $SCHRODINGER/run installation_check -testall
   ```

These steps are sufficient for serial jobs and for distributed jobs. If you want to run MPI parallel applications such as Desmond or Jaguar, you should also do the following:

10. Add entries to *user-installation*`/schrodinger.hosts` that are specifically set up for MPI parallel appplications (Section 7.3.3 of the *Installation Guide*).

11. If using the Torque queueing system, install the OpenMPI plugins (Section 7.6.1 of the *Installation Guide*).

You might also want to configure license checking if it is supported by your queueing system (Section 7.3.5 of the *Installation Guide*).