

Discovery Studio 2.0 Linux Installation for ABCC Users

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The following are some additional information that can help you with the Discovery Studio (DS) installation on Unix/Linux platform.

Please note that Accelrys doesn't provide us with any standard installation/clean-up scripts for Discovery Studio software.

- 1) Discovery Studio software is supported on Windows and Linux. Before you start Discovery Studio Linux installation, please make sure you check the Technical Requirements from Accelrys webpage [Accelrys webpage -> Products -> Discovery Studio -> Technical Requirements for DS).

Here is a minimum requirements list (As of Apr 15,2008):

- * Intel Pentium 4 or compatible processor running at 2 GHz or greater 2 GB RAM
- * (Disk space: Up to 2.6 GB available for installation
- * Graphics card: NVIDIA® Quadro® FX or ATI FireGL™ cards (see Accelrys list for additional Supported Graphics Cards and Drivers)
- * A DVD-ROM drive

x86 (32-bit)

Red Hat Enterprise Linux 3.0, Updates 6-9
Red Hat Enterprise Linux 4.0, Updates 2-5

x86-64 (64-bit):

Red Hat Enterprise Linux 5
SUSE Linux Enterprise 10

Discovery Studio is optimized for the GNOME Desktop. The root password is not necessary for Linux installations. 64-bit support is provided using 32-bit binaries.

- Note: Even though **Red Hat Enterprise Linux** and **SUSE® Linux Enterprise 10** are the recommended software, ABCC have installed DS 2.0 on **Fedora Core 6 and 7** and found the installation to be stable.
- Download the linux Discovery Studio Installation file, tar.gz file from <http://sds.ncifcrf.gov>
 - For example, let us assume the file is DSLinux.tar.gz
- Unzip tar.gz file
 - gunzip DSLinux.tar.gz
- Untar the output file from previous step
 - tar -xvf DSLinux.tar

- Use the following command to find out the DS installation script file
 > **find -type f -name ds_setup_linux.sh**
- Run the **ds_setup_linux.sh** script and follow the instructions.
 - **./ds_setup_linux.sh**
 - You can also use “./ds_setup_linux.sh –console “ for non GUI installation
- After the installation, add the following line in your **/etc/hosts** file (need Admin Privilege)
 - For example, I have added the following line to my **/etc/hosts** file

```
129.43.3.64  ncilm.ncifcrf.gov  vic
```

- Source the **lp_cshrc** file
 Note: **lp_cshrc** can be found under **LicensePack/etc**. For example, in my case it is under, **/home/accelrys/Accelrys/LicensePack/etc**

```
source /home/accelrys/Accelrys/LicensePack/etc/lp_cshrc
```

- Make the connection with the license server
lp_server -c 1715@ncilm.ncifcrf.gov
- Check the license server operation with the following command:

```
lpstat -a
```

The output will show show the license file and other related information etc.

2) During DS installation, Apache/Pipeline Pilot requires the User to assign port numbers (by default, **http:9944, https:9943**). If the default ports (ie 9944, 9943) are in use then the user can select different port numbers (eg. 9988, 9999).

**If the installer says that the default ports are taken, and if the user hasn't assigned them to some software, stop the installation and move on to steps 3 and 4. Make sure that these ports are free before restarting the installation.

Note: By assigning different port numbers, the installation may still be okay.

3) For cleaning up previous installation of DS on Linux platform, Accelrys provides a **uninstaller.sh** script located in **DiscoveryStudio20/Uninstaller** directory. However this uninstaller does not stop or remove SciTegic portion of DS installation. SciTegic installation will have to be manually removed (**rm -fr**), however, prior to removing

SciTegic make sure to stop the 'apache' service via **stopserver** script located in **SciTegic/linux_bin** directory.

Before you do the Steps, make sure you understood point 2

3a) Run **stopserver** located in **SciTegic/linux_bin** to stop the Apache Service

3b) Locate the SciTegic directory and remove the directory by using "rm -fr" command
**** Be careful with **rm -fr** command****

4) To verify things prior to DS installation, use the following commands to check if apache is running and ports are in use:

```
ps -ef |grep SciTegic  
netstat -a |grep 99
```

To free ports that are in use, a reboot should clear the ports.

5) If everything is okay, continue the installation

Related Web links:

ABCC Software Download site (**Accessible only from NCI/NIH domain only**):

<http://sds.ncifcrf.gov/>

or

<http://pcsoftware.abcc.ncifcrf.gov/>

click on **Scientific Applications Accelrys** → **Discovery_Studio** → **Linux**.
Click on **readme.html** for Linux installation instructions.

Please contact me (sravi@ncifcrf.gov) if you have any questions about this document.