

**Accelrys Suit:****InsightII:**

- Step 1. For user\_id and system\_ip, Contact System Administrator, CMSD.
- Step 2. Login to your local linux system
- Step 3. For knowing the local\_system\_ip\_no, give the command at the prompt.  
\$ifconfig -a
- Step 4. Give the following commands at the prompt  
\$xhost +  
\$ssh user\_id@system\_ip  
\$setenv DISPLAY {local\_system\_ip\_no}:0.0  
\$insightII

**Cerius2:**

- Step 1. For user\_id and system\_ip, Contact System Administrator, CMSD.
- Step 2. Login to your local linux system
- Step 3. For knowing the local\_system\_ip\_no, give the command at the prompt.  
\$ifconfig -a
- Step 4. Give the following commands at the prompt  
\$xhost +  
\$ssh user\_id@system\_ip  
\$setenv DISPLAY {local\_system\_ip\_no}:0.0  
\$cerius2

**Felix:**

- Step 1. For user\_id and system\_ip, Contact System Administrator, CMSD.
- Step 2. Login to your local linux system
- Step 3. For knowing the local\_system\_ip\_no, give the command at the prompt.  
\$ifconfig -a
- Step 4. Give the following commands at the prompt  
\$xhost +  
\$ssh user\_id@system\_ip  
\$setenv DISPLAY {local\_system\_ip\_no}:0.0  
\$felix

**Catalyst:**

- Step 1. For user\_id and system\_ip, Contact System Administrator, CMSD.
- Step 2. Login to your local linux system
- Step 3. For knowing the local\_system\_ip\_no, give the command at the prompt.  
\$ifconfig -a
- Step 4. Give the following commands at the prompt  
\$xhost +  
\$ssh user\_id@system\_ip  
\$setenv DISPLAY {local\_system\_ip\_no}:0.0  
\$catalyst

**GCG:**

- Step 1. For user\_id and system\_ip, Contact System Administrator, CMSD.
- Step 2. Login to your local linux system
- Step 3. For knowing the local\_system\_ip\_no, give the command at the prompt.  
\$ifconfig -a
- Step 4. Give the following commands at the prompt  
\$xhost +  
\$ssh user\_id@system\_ip  
\$setenv DISPLAY {local\_system\_ip\_no}:0.0  
\$gcg

## CHARM:

Step 1. For user\_id, Contact System Administrator, CMSD.

Step 2. Login to your local linux system

Step 3. If it is from Outside the Campus use Public IP (202.41.85.70)  
other wise use Local IP (10.2.1.53)

\$ssh -X [user\\_id@202.41.85.70/10.2.1.53](mailto:user_id@202.41.85.70/10.2.1.53)

Step 4. Connect to the moon system by giving the command

\$rsh [moon](#)

Step 5. Craete a file by name machinefile and add the following 8 entries

\$ vi machinefile

```
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in  
moon.uohyd.ernet.in
```

Step 6. Save the file by pressing Esc key and :wq

Step 7. To run the Software give the following Command.

\$/users/accelrys/Accelrys/CHARMm32b1/bin/charmm -xxlarge -np \* -m  
machinefile <inputfile.inp> <outputfile.log>

Note: 1. Give any name for inputfile and outputfile

2. In Step 7, You can replace \* with no. of required CPU's.