Molpro:

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Step 1. Login to your local linux system
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Step 2. For knowing the local_system_ip_no, give the command at the prompt. \$\sifconfig -a\$

Step 3. Give the following commands at the prompt

\$telnet 10.2.1.53

or

\$ssh user_id@10.2.1.53

\$xhost +

Step 4. Login to the system {169.254.0.110}

\$telnet 169.254.0.110

Step 5. Set the Display settings

\$export DISPLAY= {local_system_ip_no}:0.0

Step 6. Edit the existing .bashrc file

\$vi .bashrc

Step 7. Add the path {/usr/local/bin/} to the line "set path ="

Step 8. Save the file by pressing Esc key and :wq

Step 9. Logout from the system {169.254.0.110}

\$exit

or

\$logout

Step 10. To Run the software follow the Step 1 to Step 5 and give the command \$ molpro [-rc rcfile] [-o outputfile] [-x execfile] [-vsef] [+vsef] [-I intdir] [-W wfdir] datafile

Note:

- 1. You should have local linux system.
- 2. For user_id on 10.2.1.53 and 169.254.0.110 Contact System Administrator, CMSD.