Project: Actin

Job Information

Jobs Page

Select job:

➢Kill this job

➢Forget this job

Page refresh rate: 20 sec.

Last page update at:
1:47:43 p.m.
06/12/01

Refresh now

Molecule Viewer (JMV)

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Standard job information for NAMD job: Equil applet view

Running on account:	SGI-DQS
Processors requested:	4
Work directory:	/home/brunner/strun
DQS job id:	11812
Timestep:	On step 20 of 1000
Input files:	**equil.namd**, bpti.min, bpti.psf, param19.pro
Output files:	equil.out, bpti_equil.coord, bpti_equil.rel, bpti_equil.dcd
Futher info.:	Click here for NAMD Energy Table

Notes:

Save Notes changes

Monitoring Graph Production for NAMD job: Equil applet view

Step 1: Set graph options

Select y-axis:

☐BOND ☐ANGLE ☐DIHED ☐IMPRP ☐ELECT ☐VDW
☐BOUND ☐MISC ☐KINET ☒TOTAL ☐TEMP ☐SMD Force
☐SMD Dist ☐Periodic Box (X, Y, Z) Other vars

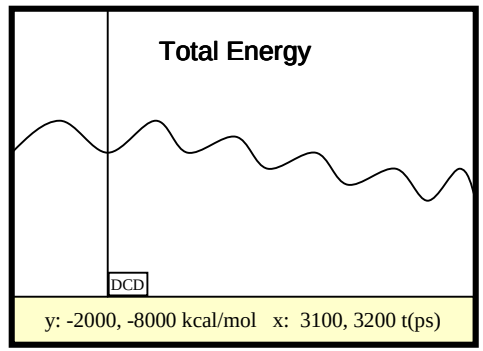
Select x-axis: Show me Time (ps) on x-axis

Set y-axis: ◉Fit all y ○Min: Max:

Set x-axis: ◉Fit all x ○Min: Max:

Data manipulation:
☐Change from initial value
☐Running backward difference
☐Smoothing: MA window size # samples

Graph:



Step 2: Click to create graph

Step 3: Click to float graph off page

Refresh at: Off, 5s, 10s, 20s, 1min, 5min

Project: Actin, Job: Equil_app view

File Edit View Go Communicator Help

NAMD Energy Table

Go to:
- ➢Top
- ➢Bottom

Page refresh rate:
20 sec. ▽

Last refresh at:
1:47:43 p.m.
06/12/01

On refresh go to:
- ○ Top
- ◉ Bottom

Refresh now

Shade by:
- ☐ Row
- ☒ Column

Save to file

Close window

Help

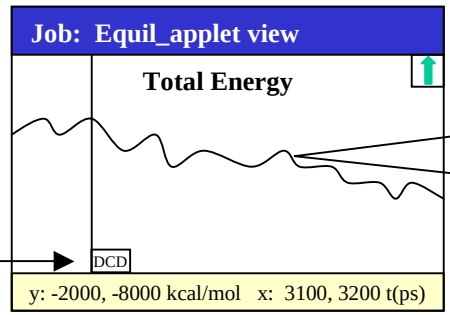
FAQ

Feedback

BioCoRE

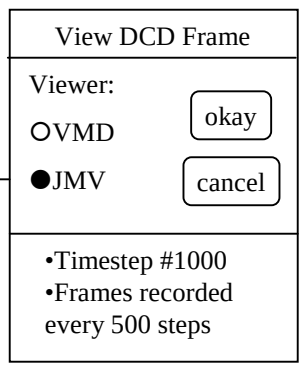
TS	BOND	ANGLE	DIHED	IMPRP	ELECT	VDW	BOUNDARY	MISC	KINETIC	TOTAL	TEMP
0	10.3058	87.6035	101.2983	20.1708	-1873.3578	-313.5594	0	0	37.7643	-1929.7745	24.4266
10	12.0122	84.6578	99.6367	21.8241	-1876.9889	-315.9842	0	0	45.2846	-1929.5577	29.2908
20	13.6227	81.3557	99.5802	22.3084	-1880.0624	-322.9192	0	0	56.6232	-1929.4914	36.6248
30	15.6707	86.3242	97.2439	23.8654	-1884.222	-330.5497	0	0	62.1892	-1929.4784	40.2249
40	15.5296	87.9488	94.1463	21.52	-1887.0433	-336.5971	0	0	75.0596	-1929.4362	48.5498
50	18.0272	82.2548	92.0441	22.0772	-1891.0666	-334.954	0	0	82.2369	-1929.3802	53.1922
60	15.1575	80.9596	90.3743	21.5342	-1897.8004	-332.9857	0	0	93.3124	-1929.4481	60.3559
70	16.4619	80.8108	89.7558	22.6956	-1913.4014	-333.8417	0	0	108.1332	-1929.3857	69.9423
80	16.591	84.2664	90.2361	21.2635	-1924.7481	-336.2416	0	0	119.347	-1929.2858	77.1956
90	17.7302	85.5607	91.9936	20.6645	-1942.5297	-333.3969	0	0	130.6521	-1929.3256	84.5079
100	17.0008	86.2295	92.2133	20.6125	-1963.544	-327.3133	0	0	145.4153	-1929.3858	94.057
110	24.5562	87.511	92.6792	23.081	-1983.1848	-307.965	0	0	133.9623	-1929.36	86.649
60	15.1575	80.9596	90.3743	21.5342	-1897.8004	-332.9857	0	0	93.3124	-1929.4481	60.3559
70	16.4619	80.8108	89.7558	22.6956	-1913.4014	-333.8417	0	0	108.1332	-1929.3857	69.9423
80	16.591	84.2664	90.2361	21.2635	-1924.7481	-336.2416	0	0	119.347	-1929.2858	77.1956
90	17.7302	85.5607	91.9936	20.6645	-1942.5297	-333.3969	0	0	130.6521	-1929.3256	84.5079
100	17.0008	86.2295	92.2133	20.6125	-1963.544	-327.3133	0	0	145.4153	-1929.3858	94.057
110	24.5562	87.511	92.6792	23.081	-1983.1848	-307.965	0	0	133.9623	-1929.36	86.649
110	24.5562	87.511	92.6792	23.081	-1983.1848	-307.965	0	0	133.9623	-1929.36	86.649
60	15.1575	80.9596	90.3743	21.5342	-1897.8004	-332.9857	0	0	93.3124	-1929.4481	60.3559
70	16.4619	80.8108	89.7558	22.6956	-1913.4014	-333.8417	0	0	108.1332	-1929.3857	69.9423
80	16.591	84.2664	90.2361	21.2635	-1924.7481	-336.2416	0	0	119.347	-1929.2858	77.1956
90	17.7302	85.5607	91.9936	20.6645	-1942.5297	-333.3969	0	0	130.6521	-1929.3256	84.5079
100	17.0008	86.2295	92.2133	20.6125	-1963.544	-327.3133	0	0	145.4153	-1929.3858	94.057
110	24.5562	87.511	92.6792	23.081	-1983.1848	-307.965	0	0	133.9623	-1929.36	86.649
60	15.1575	80.9596	90.3743	21.5342	-1897.8004	-332.9857	0	0	93.3124	-1929.4481	60.3559
70	16.4619	80.8108	89.7558	22.6956	-1913.4014	-333.8417	0	0	108.1332	-1929.3857	69.9423
80	16.591	84.2664	90.2361	21.2635	-1924.7481	-336.2416	0	0	119.347	-1929.2858	77.1956
90	17.7302	85.5607	91.9936	20.6645	-1942.5297	-333.3969	0	0	130.6521	-1929.3256	84.5079

Small, floating graph view of data



New window appears when click on graph:
- Timestep or time
- For each y (e.g. total energy):
  - Moving average
  - Min & Max values
- Text for y-value in same color as trace
- Close box, scroll bar included in window

Click on DCD flag to activate dialog box. Flags appear based on frame recording settings. Shows most recent DCD frame, not whole trajectory.



Larger graph view:

New window appears when click on graph:
- Timestep or time
- For each y (e.g. total energy):
  - Moving average
  - Min & Max values
- Text for y-value in same color as trace
- Close box, scroll bar included in window

Menus

Jobs:
- Lists available jobs, can switch jobs

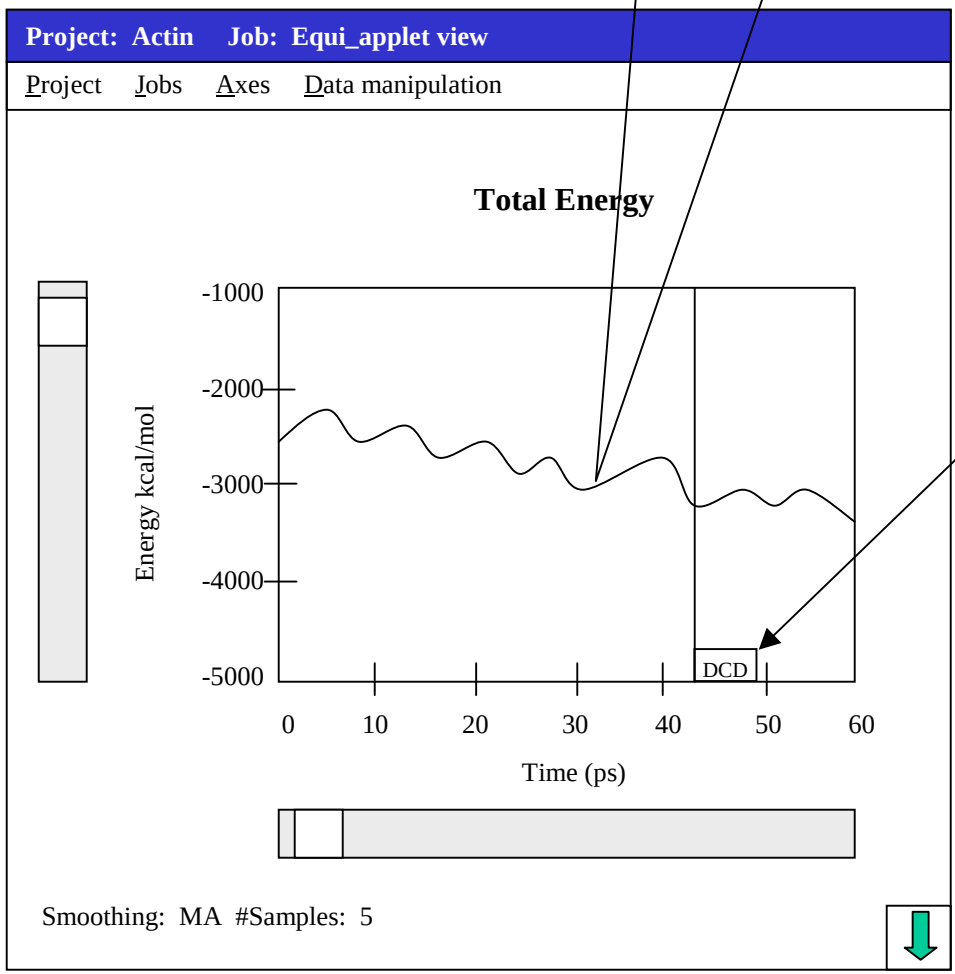
Axes:
- Set x axis min, max*
- Set y axis min, max*
- Show me ___ on x axis*
- Show me ___ on y axis*

Data manipulation
- Change from initial value
- Running backward difference
- Smoothing

Project:
- View main job info page
- Open project summary page

Small view:
- Switches graph back to small view

*New java dialog box opened for data inputs, adjustments



View DCD Frame

Viewer:
- ○ VMD
- ● JMV

okay

cancel

- Timestep #1000
- Frames recorded every 500 steps

Click on DCD flag to activate dialog box. Flags appear based on frame recording settings.

Sample java dialog box, from Axes pull-down menu for Set x axis min, max