Evaluation of the NAMD Workshop, April 17 - 19, 2002

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Analysis: Mary Ellen Michael, NCSA, UIUC

Background of the NAMD Workshop

The UIUC's Theoretical Biophysics (TB) Group, an NIH Resource for Macromolecular Modeling and Bioinformatics is headed by Klaus Schulten, and CO-PIs L. Kale, R. Skeel, T. Martinez, G. Budescu. As part of their outreach, the Resource offers workshops to introduce and transfer its programs and technological solutions to the biomedical community. Jim Phillips is the lead developer of NAMD, the molecular dynamics program created and distributed by the Resource, and has organized the workshop together with the NCSA EOT division. NCSA has provided a computer training lab, food, and supercomputing access and time to all participants. During the event on April 17 and 18, NCSA also offered a back channel long distance telephone line in case there was a loss of audio.

In the past NAMD workshops and tutorials have been offered at single locations, such as at Pittsburgh Supercomputing in August, 2001. Presentations and hands-on sessions at the Pittsburgh workshop were arranged so that each morning or afternoon would provide a mix of theoretical, technical, applied (case studies) and hands-on sessions. This was done to provide a balanced learning experience for the twenty highly dedicated participants. At the NCSA workshop, the first day was dedicated to applications, case studies, and information applicable to molecular modeling in general. Day two sessions centered around specific technical information on using NAMD. This breakdown allowed modularity and participants could easily skip a day if they desired. The distance between the Access Grid node and the computer lab forced the hands-on session to be held on a separate day.

NCSA has worked with the Resource to sponsor the April, 2002 NAMD workshop at more than one location, reaching remote sites across the U.S via the Access Grid (AG) and the use of the Resource's online collaborative environment BioCoRE (lead programmers R. Brunner and K. Vandivort) and of VMD, the Resource's visualization package (lead programmer John Stone). Participating sites were Boston University, North Dakota State University, Ohio Supercomputing, Pittsburgh Supercomputing, and Purdue University. Each site coordinator advertised the workshop, reserved the AG site, provided food and snacks for participants, all at their own expense.

The workshop participants concluded the workshop with an optional hands-on session on Friday, April 19 from 8:30 to noon. There were 16 computers in the lab for the on-site 32 participants who took turns watching and working with the BioCoRE software application. Remote users at the other five sites also received a training signon but worked at their own desktops. Questions and answers during the half-day tutorial were processed within BioCoRE.

At the end of each day, participants, on and off site completed an evaluation questionnaire. Section 1 covered the presentations; section 2 covered their experience with the Access Grid. The workshop originated solely from UIUC (32 people) with 4 AG nodes participating – Boston University (7 people), North Dakota State University (17 people), Ohio Supercomputing (12 people), Pittsburgh Computing (6 people), and Purdue University 18 people). Evaluation forms on the hands-on session were given only to on-site participants.

The evaluation is divided into the UIUC participants and the AG site participants who saw the workshop remotely.

Breakdown of Participants

According to the EXCEL registration, attendance is broken down by Access Grid node:

AG Location	Grad. Student	Post-Doc	Faculty	Staff	Gov.
Boston Univ.	4	1	0	2	0
UIUC	17	4	5	1	1
North Dakota S.U.	8	3	5	1	0
Ohio Supercomp.	4	3	5	0	0
Pittsburgh Supercom	2	2	1	1	0
Purdue	5	2	4	7	0
TOTAL	**92**				

Of the 92 participants, 43.4% were graduate students, 16.3% were postdoctoral fellows, 21.7% were faculty, and 13% were staff. One participant came from a government institution.

Wednesday Session –UIUC/NCSA Site

1. Please rate the following presentations:

		Not Useful	Somewhat Useful	Unsure	Useful	Very Useful
a.	NCSA Resources	0	0	3	9	9
b.	Intro to Molecular Dynamics Simulations	0	1	2	6	15
c.	What Can We Learn from MD Simulations	1	0	3	12	11
d.	Case Study: Unfolding the Muscle Protein Titin	0	2	1	15	7
e.	Case Study: Aquaporin Membrane Channels	0	3	1	7	14
f.	Case Study: ATP Synthase Stalk Rotation	0	2	3	15	4
g.	Overview of Hardware/Software	1	0	0	13	12
h.	Questions & Answers	1	1	2	6	8
i.	The workshop overall	0	0	0	8	14

N = 32 participants

Items a through h refer to presentations throughout Wednesday. Not all people responded to each item; in some cases, they were late for a presentation or simply gave no opinion. Of those responding, most people (86%) found the presentation by Bruce Loftis on NCSA resources very helpful. Prof. Klaus Schulten led the next two presentations (b and c). Of the 24 respondents, 88% found item b useful or very useful. Of the 27 respondents for his second lecture, 85% found it useful or very useful. The three case studies (d, e, and f, by Mu Gao, Emad Tajkhorshid, and Barry Isralewitz) also faired well with 84%, 84%, and 79%, respectively, finding the information useful or very useful. Similarly for the Question and Answer session at the end of the day, 77% found it useful or very useful. The presentation on hardware and software (g) by Jim Phillips was found useful or very useful by 96% of respondents. For the workshop overall, one third (36%) found it useful while two thirds (63%) found the workshop very useful.

2. Please rate the following:

		Strongly Disagree	Disagree	Unsure	Agree	Strongly Agree
a.	Presenter was clearly visible.	0	0	1	4	27
b.	Materials were clearly visible.	0	2	1	5	15
c.	Participants at other sites were clearly visible.	0	3	2	11	8
d.	Quality of audio was satisfactory.	0	4	3	8	10
e.	Quality of video was satisfactory.	0	1	2	9	12
f.	Use of technology (i.e., participation from multiple sites) enhanced the workshop experience.	1	1	2	13	7

Question 2 focused on participants' experience in having the Access Grid as a component of the live, in-person workshop. While a brief explanation was given to participants that the AG allowed many more people to attend the workshop, one person found the AG intrusive. 97% found the presenter to be clearly visible; 87% found the materials clearly visible; 79% said participants were clearly visible. They also agreed that the audio and video were satisfactory (75% and 87%, respectively).

Please provide any comments or suggestions about the workshop content, presentation, or experience so far.

1. Well organized, very helpful to me
2. Handouts were incomplete, missing pages; additionally, a few audience members tended to repeatedly interrupt presenters, interrupting flow of ideas
3. Some slides missing in handout (overview of hardware/software, NCSA resources).
4. I think it would be interesting to hear from the visitors about why they are here. That way during breaks, we know who might be in interested in the same investigations.
5. The lights need to be turned down in the front so we can read the slides better! Many appear unclear! Speakers must have laser pointers!!
6. Provide speakers with laser pointers.
7. It would be nice if presenter could point out by some means (laserpointer, for example) what he is talking about on the slide (screen).
8. The information was very informative but the support staff and the workshop's overall environment were outstanding! Thank you.
9. You need to organize the Q & A time. But totally, it's very good, interesting time.
10. A better order of events would be [order of events in question 1] a, g, b, c, h, then hands-on (let us play with it), followed by case studies d, e, f so we have a framework for our questions based on (limited) personal experience.

Each one of the comments is a unique observation. Two participants requested laser pointers to use with the complex slides (laser pointers were then used in the Thursday session). Comment 10 suggested a different order of presentation of interspersing hands-on experience with BioCoRE before introducing the three case studies.

Thursday Session, April 18, UIUC/NCSA Site

1. Please rate the following presentations:

	Not Useful	Somewhat Useful	Unsure	Useful	Very Useful
a. Configuring & Running NAMD Simulations	0	1	1	10	18
b. Building Molecular Structures	0	0	1	11	19
c. Assembling Molecular Systems	0	0	1	9	20
d. Integrating Equations of Motion	0	2	4	10	19
e. Accelerating Processes via Steered MD	1	1	2	10	18
f. Analysis of MD Trajectories	0	1	4	13	18
g. Efficient Evaluation of Forces	0	2	7	10	16
h. NAMD Serial & Parallel Performance	0	2	7	10	16
h Discussion, Questions & Answers	0	2	3	9	18
i. The workshop overall	0	0	0	10	20

Jim Phillips presented topics a, d, g and h. Justin Gullingsrud presented topics b, c, and f. Klaus Schulten presented topic e. Participants found the first three lectures useful or very useful (93%, 97% and 97%, respectively). Participants were positive about the remaining presentations, although the more technical presentations g and h were only found useful or very useful by 74% of respondents, with 20% unsure. For the workshop overall, one third found it very useful and the other two thirds found it very useful.

2. Please rate the following:

	Strongly Disagree	Disagree	Unsure	Agree	Strongly Agree
a. Quality of audio is satisfactory	0	2	1	12	15
b. Presenter was clearly visible.	0	0	1	9	20
c. Access Grid materials were clearly visible.	0	1	3	11	13
d. Participants at other sites were clearly visible.	0	1	4	13	14
e. Quality of video is satisfactory.	0	0	3	14	13
f. Use of technology (i.e., participation from multiple sites) enhanced workshop experience.	0	3	2	11	13

Participants reported similar agreement to the AG setup and live presentation format as they did on the Wednesday session. For all the items they gave a rating of 82% or higher in terms of their satisfaction. A smaller percentage overall were unsure.

3. Please rate the workshop:

	Strongly Disagree	Disagree	Unsure	Agree	Strongly Agree
a. The workshop is well organized.	0	0	0	13	15
b. Satisfied my research needs	0	0	2	12	19
c. Addressed expected research needs	0	0	1	11	15
d. Web-based NAMD materials met my needs	0	0	4	9	13

All the respondents were positive and reported that the workshop was well organized. 94% felt the workshop satisfied their research needs and 96% said it addressed their expected research needs. Finally, they felt the NAMD materials met their needs (85%). These were the readings placed on the NAMD website before the workshop began. 15% were unsure, possibly because they had not gone to the website to see these readings.

Comments
1. Great job
2. Very well presented
3. A lot of overlap
4. Maybe two hands-on sessions
5. Regarding the presentation on Accelerating Processes via Steered MD, would be more useful if a small bit of the SMD script on how these were done.
6. Second day more informative than first.
7. The workshop was truly well organized and thought out. I am not certain what improvements could be made from my perspective except for the possible addition of animation scripts and expanding the material to include an extra day. Thank you for a JOB WELL DONE.
8. This is a very useful workshop.
9. Really excellent overall.
10. Fantastic – details were all great!! Excellent Q & A forums, A+
11. Regarding Accelerating Processes Via Steered MD presentation, OKAY, but how do you do this? Also, I was a little bit put off by the many comments, "If you do some creative programming, you could do this." OKAY, but how?
12. Very good!
13. May be useful to have a web-based step-by-step demo

Six of the 13 comments were general positive statements about their satisfaction with the workshop overall. Some people made comments for improving the workshop. One person (no. 13) suggested that the BioCoRE program include a step-by-demo for new users. Another individual would have preferred two hands-on sessions instead of the one (no. 4). Another person would have liked another day (no. 7). One person thought there was too much overlap of content while another thought the information given on the second day was more helpful than the first day (no. 6). Finally, two people made comments on the presentation, Accelerating Processes via Steered MD, wanting to know more detail about the actual script that would be used (no. 5 and no. 11).

What suggestions do you have for improving the workshop?

1. More hands-on time
2. Maybe next time you could provide enough computers to let everyone work on.
3. More practice hands-on will help get familiar with this software
4. A bit less science in favor of more explicit treatment of techniques and scripting, not to take away from the science, it's great!
5. More hands-on lectures in morning, hands-on in afternoon.
6. Application of NAMD to non-biological system
7. Dim lights in front during presentations, provide laser pointer, maybe next time include a more theoretical discussion.
8. Please add the possibility for a speaker to use a pointing device (mouse) that can be also observed from the remote sites.
9. Audio [access grid] must be improved.

Nine participants offered suggestions for improving the workshop. Three of them wanted more hands-on time (the hands-on session would be available the next day for 3 hours). Three comments related to the physical setup in the AG room concerning lighting, a laser pointer, and audio). One individual wanted more emphasis on scripting while another wanted to see applications to non-biological systems.

What suggestions do you have for similar workshops?

1. Don't limit food to vegetarian.
2. A pointing device for the Microsoft Powerpoint presentations might be useful.

NAMD Workshop Evaluation by Remote Sites
Day 1, Wednesday, April 17, 2002

Check your location.
___x_ Boston University
___ _ NCSA, Champaign
___x North Dakota State University
____ Purdue University
____ Ohio Supercomputing
__x__ Pittsburgh Supercomputing

Three of the five remote sites forwarded evaluation forms back to NCSA for the Wednesday session.

3. Please rate the following presentations:

		Not Useful	Somewhat Useful	Unsure	Useful	Very Useful
j.	NCSA Resources	0	0	1	5	5
k.	Intro to Molecular Dynamics Simulations	0	1	0	5	7
l.	What Can We Learn from MD Simulations	0	0	0	6	5
m.	Case Study: Unfolding the Muscle Protein Titin	0	0	0	8	2
n.	Case Study: Aquaporin Membrane Channels	0	1	2	7	5
o.	Case Study: ATP Synthase Stalk Rotation	0	1	3	6	3
p.	Overview of Hardware/Software	0	0	0	4	5
q.	Questions & Answers	0	0	1	5	2
r.	The workshop overall	0	0	0	5	6

Similar to the UIUC/NCSA participants, the remote audience found the various presentations useful or very useful (92% or higher). For Case Study 3, only 69% found it useful or very useful with 31% not sure. For the workshop overall, 100% found it useful or very useful.

4. Please rate the following:

		Strongly Disagree	Disagree	Unsure	Agree	Strongly Agree
g.	Presenter was clearly visible.	0	0	0	7	6
h.	Materials were clearly visible.	0	0	0	6	6
i.	Participants at other sites were clearly visible.	0	3	1	4	3
j.	Quality of audio was satisfactory.	0	0	1	4	8
k.	Quality of video was satisfactory.	0	2	2	3	6
l.	Use of technology (i.e., participation from multiple sites) enhanced the workshop experience.	0	1	2	4	6

Unlike the UIUC/NCSA participants who saw the presenters in person, the remote users had to rank their satisfaction based on the AG quality of audio and video at each site. The large majority of respondents were quite satisfied with the quality of the experience. Some were concerned that the participant screens were not large enough or varied in size from node to node. (The size of the image is determined by the AG technician at each site.) They were very positive about the use of the technology (77%).

Please provide any comments or suggestions about the workshop content, presentation, or experience so far.

1. Excellent workshop. Dr. Schulten's presentation was especially useful.
2. Great experience. Participants' voices were not always clear.
3. Questions were sometimes difficult to hear (speaker should repeat question, especially questions from NCSA [host site]. When will we see real-time simulations (e.g., embedded in Powerpoint slides) over the Grid? Why is the window displaying the speaker so small at NCSA (at OSC and Purdue, the speaker window is as large as the slides window)?
4. Pointing to the screen does not work for remote sites. Could we use the pen function in powerpoint or one of the other ways of highlighting or add arrows etc.?
5. It was enriching and would be very use for research.
6. Thanks for making it available on the Access Grid, without this I would never have made this presentation.
7. It was a wonderful experience, very satisfying
8. Great job!
9. I like it very much.
10. I liked the workshop, though I would like it to be more on time.

Six of the 10 comments are general, positive remarks about the workshop overall. One respondent said questions from the NCSA audience were difficult to hear. (UIUC presenters had difficulty coaxing questioners to use the microphone provided.) Other respondents had concerns about knowing where the presenter was pointing to on the Powerpoint slide and that the slides could not show the animations at any of the sites.

Check your location.
____   Boston University
___ _   NCSA, Champaign
___   North Dakota State University
____   Purdue University
____   Ohio Supercomputing
__x__   Pittsburgh Supercomputing

Only Pittsburgh Supercomputing forwarded evaluation forms for the Thursday session.

1. Please rate the following presentations:

	Not Useful	Somewhat Useful	Unsure	Useful	Very Useful
a. Configuring & Running NAMD Simulations	0	0	0	1	2
b. Building Molecular Structures	0	0	0	1	2
c. Assembling Molecular Systems	0	0	0	1	2
d. Integrating Equations of Motion	0	0	0	2	1
e. Accelerating Processes via Steered MD	1	0	0	1	1
f. Analysis of MD Trajectories	0	0	0	1	1
g. Efficient Evaluation of Forces	0	0	1	1	1
h. NAMD Serial & Parallel Performance	0	0	1	1	1
h Discussion, Questions & Answers	0	0	1	1	1
i. The workshop overall	0	0	0	2	1

The number of people who completed the second day evaluation was small but the handful who did found the presentations useful or very useful.

2. Please rate the following:

	Strongly Disagree	Disagree	Unsure	Agree	Strongly Agree
a. Quality of audio is satisfactory	0	0	0	1	2
b. Presenter was clearly visible.	0	0	1	1	1
c. Access Grid materials were clearly visible.	0	0	1	1	1
d. Participants at other sites were clearly visible.	0	1	1	0	1
e. Quality of video is satisfactory.	0	1	0	1	1
f. Use of technology (i.e., participation from multiple sites) enhanced workshop experience.	0	1	1	1	

The response rate, again, was very low and thus less not of much use.

3. Please rate the workshop:

a. The workshop is well organized.	0	0	0	2	1
b. Satisfied my research needs	0	0	0	2	1
c. Addressed expected research needs	0	0	0	2	1
d. Web-based NAMD materials met my needs	0	1	0	1	1

The response rate, again, was very low and thus less than useful.

Comments

1. Like the workshop very much. Need to provide more descriptive NAMD USER GUIDES online.
2. We could not see the laser pointer so we do not know what is speaker was pointing at.

What suggestions for improving the workshop?

1. Present less amount of examples.
2. If the laser pointer could somehow be seen at remote sites. This is a big problem, since speaker is referring to specifics we couldn't see.
3. I would have preferred more time allotted to talk on "Integrating Efficiency of Motion" so that the speaker can give more details.
4.

What suggestions do you have from similar workshops?

1. Run more of them!

NAMD Workshop Evaluation
Day 3, Friday, April 19, 2002
Hands-on Lab

Summary of Evaluations of Hands-on Lab at REL, Beckman Institute

1. Please rate the following:	**Strongly Disagree**	**Disagree**	**Unsure**	**Agree**	**Strongly Agree**
a. Using BioCoRE is easy.	0	0	1	7	3
b. BioCoRE is a good training platform.	0	0	3	5	3
c. BioCoRE is a good platform for research collaboration	0	0	4	3	3
d. I intend to use BioCoRE in the future.	0	0	2	3	6
e. I am satisfied with the hands-on experience with BioCoRE.	0	0	4	1	4
f. The hands-on session was useful.	0	0	1	1	8
g. The hands-on training was effective.	0	0	2	2	6
h. The three-day workshop overall was useful.	0	0	1	1	9

N = 11 respondents.

Of the 11 people responding, 91% reported that BioCoRE was easy to use; 72% said it was a good training platform. Some people were unsure (40%) how good a platform BioCoRE is for research collaboration. 82% said they intend to use BioCoRE in the future. They were less enthusiastic about the hands-on experience with 44% reporting unsure. However, 90% found the hands-on session useful and 80% found the hands-on training effective. Overall, 82% agreed that the three-day workshop was useful.

Please provide any comments or suggestions about the workshop content, presentation, or experience so far.

1. Have only played a little with BioCoRE. Ran the hands-on without BioCoRE. Will surely use it in the future though.
2. Very nice! Excellent!
3. I don't think I can run VMD or NAMD any better than after I read the user guides. As for the hands-on session, I have had two UNIX machines that failed to work properly so I can only hope to run the tutorial from my home machine at a later date.
4. It would have been nice if the queue on modi4 were open.

One respondent expressed frustration with hardware. Another person found the queue backed up or slow.