

Center for Macromolecular Modeling and Bioinformatics

NAMD 2011 User Survey Report

Administration and Results

D. Brandon, J. Phillips, J. Strümpfer
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NAMD 2011 USER SURVEY REPORT

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Executive Summary

The 2011 NAMD User Survey was announced to 7,008 users of NAMD (versions 2.7b4 through 2.8) on July 19, 2011 and ran until July 26 of that year. Survey questions examined user satisfaction, the impact of the program on work quality, and user ratings of existing and planned features.

- A total of 436 usable responses were returned for the survey, a sample which provides a confidence level of 95% and a confidence interval of +/-4% (i.e., one is 95% confident that an answer from the sample represents the population value at plus or minus 4%)
- 93% of respondents use NAMD for research
- 56% of respondents reported that they do biomedically relevant work with NAMD
- 20% of all respondents reported at least partial NIH funding
- 94% of respondents are satisfied with NAMD
- 86% feel that NAMD has improved the quality of their work
- 60% of respondents use NAMD for all or most of their MD simulations
- 60% of users indicate that NAMD is critical for their work
- 80% of users report that not having NAMD available would negatively impact their scientific productivity
- The top 3 future developments, rated by respondents, are: Trajectory analysis tools, improved GPU acceleration and mixed quantum/classical simulation methods

Overview

NAMD (Nanoscale Molecular Dynamics) is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large, biomolecular systems; more information on NAMD is available via its webpage (www.ks.uiuc.edu/Research/namd). The 2011 NAMD user survey is part of an ongoing effort (similar surveys were conducted in 2005, 2003 and 2000) to ensure that NAMD is up-to-date, relevant and of high quality. NAMD users were identified via registration records and contacted via e-mail with a request that they complete an online survey during July 2011 (see appendix for survey questions; the form completed by participants is available here: www.ks.uiuc.edu/Research/namd/survey/survey2011.html). The following report details the administration and results of the survey.

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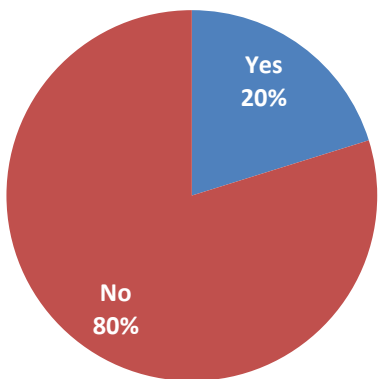
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2011 NAMD Survey Results

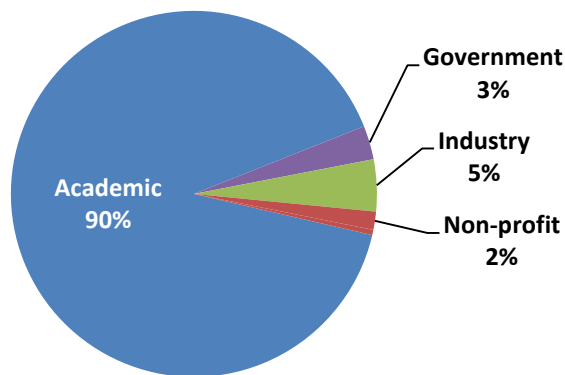
NAMD USER PROFILE

- 90% of user have academic affiliations, and 93% use NAMD for research
- 56% of users use NAMD for biomedically relevant work, and 20% are NIH funded
- 73% of users rate their NAMD expertise as moderate or higher, and 82% rate their molecular modeling expertise as moderate or higher

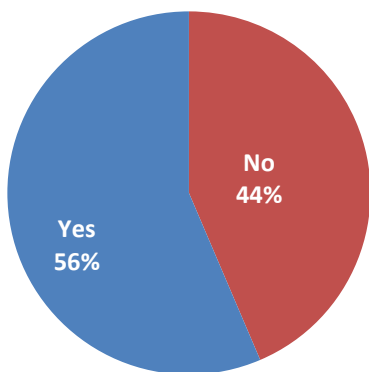
NIH Funded



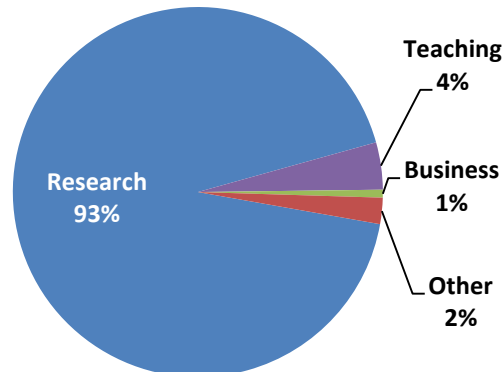
Affiliation



Biomedically Relevant Work



Primary use of NAMD



Molecular Modeling Expertise

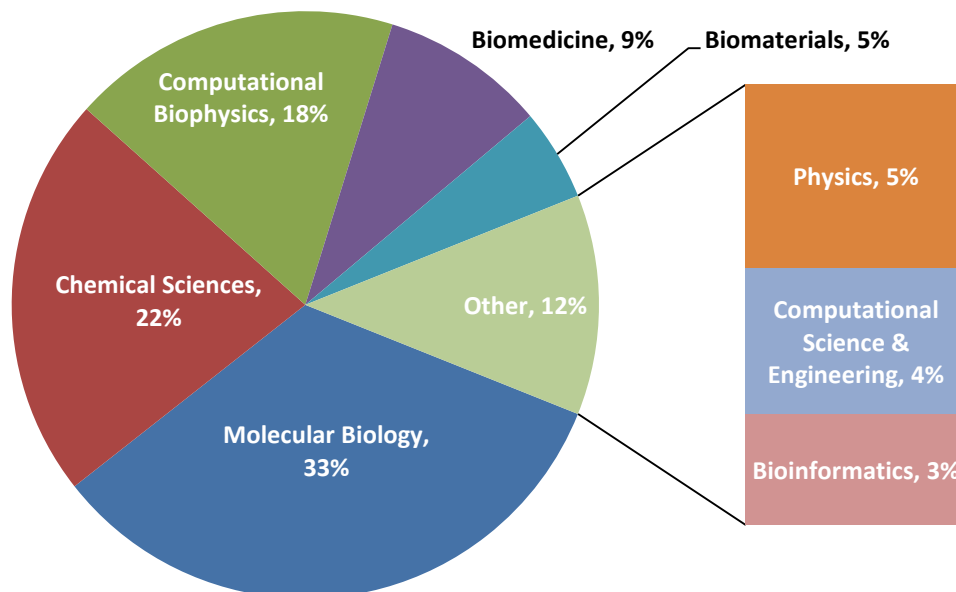


NAMD Expertise



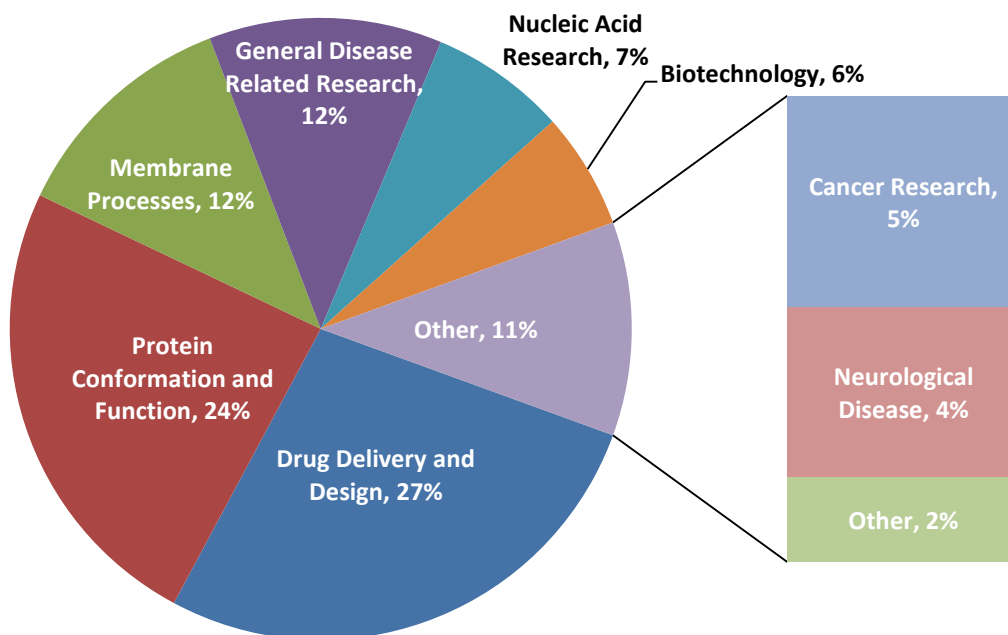
RESEARCH INTEREST / AREA OF STUDY

- Molecular Biology, Chemical Sciences, and Computational Biophysics describe the areas of study of 73% of NAMD users



RESEARCH INTEREST / BIOMEDICALLY RELEVANT WORK

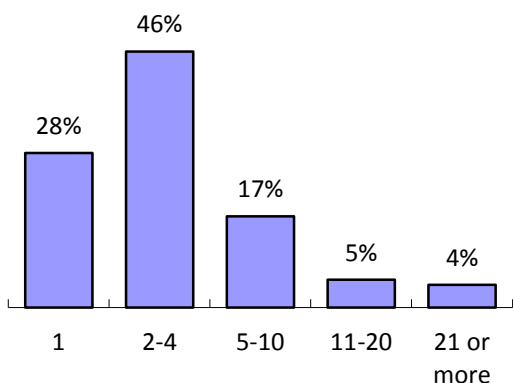
- Drug delivery and design, and protein conformation and function, are popular areas of study for the 56% of users who indicate using NAMD for biomedically relevant work



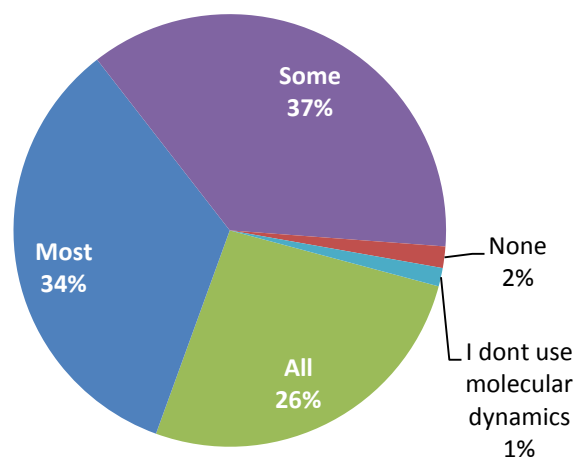
NAMD USAGE PROFILE

- 72% of respondents have multiple users of NAMD at their site
- 60% of respondents use NAMD for most or all of their simulations
- 62% of respondents use NAMD on Linux, while 25% use it on Windows
- For parallel computing, respondents typically run on small clusters.

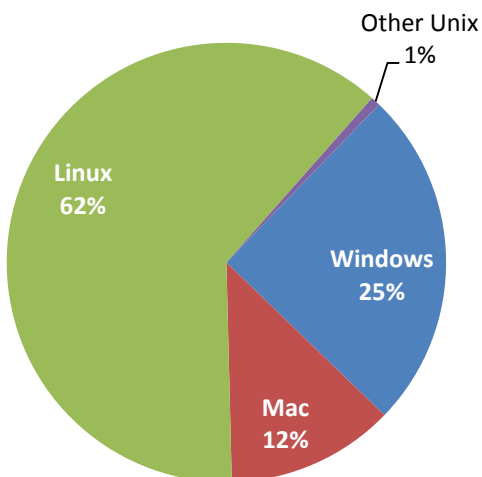
The number of people using NAMD at my site is:



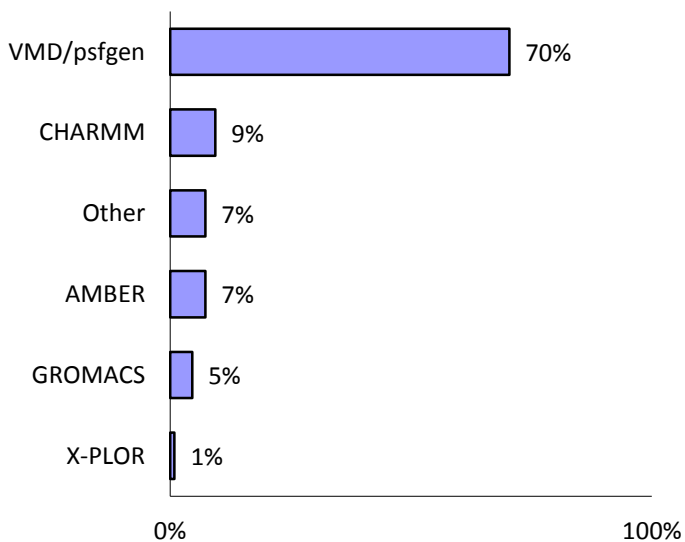
I use NAMD for _____ of my molecular dynamics simulations:



On my desktop/laptop I primarily use NAMD on



I generate NAMD input files with:

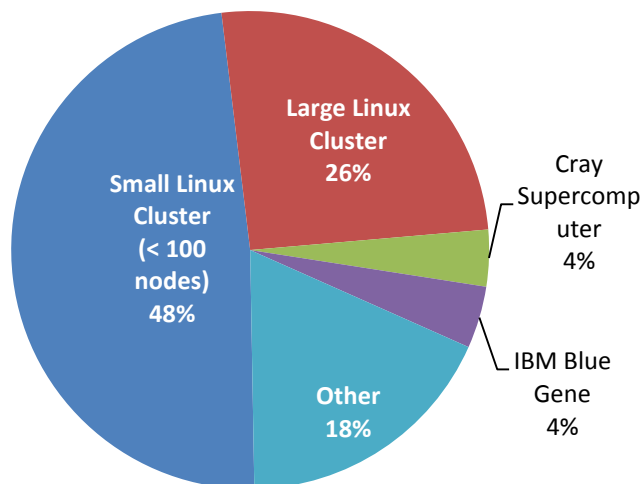


NAMD USAGE PROFILE, continued

I have used the NAMD tutorial



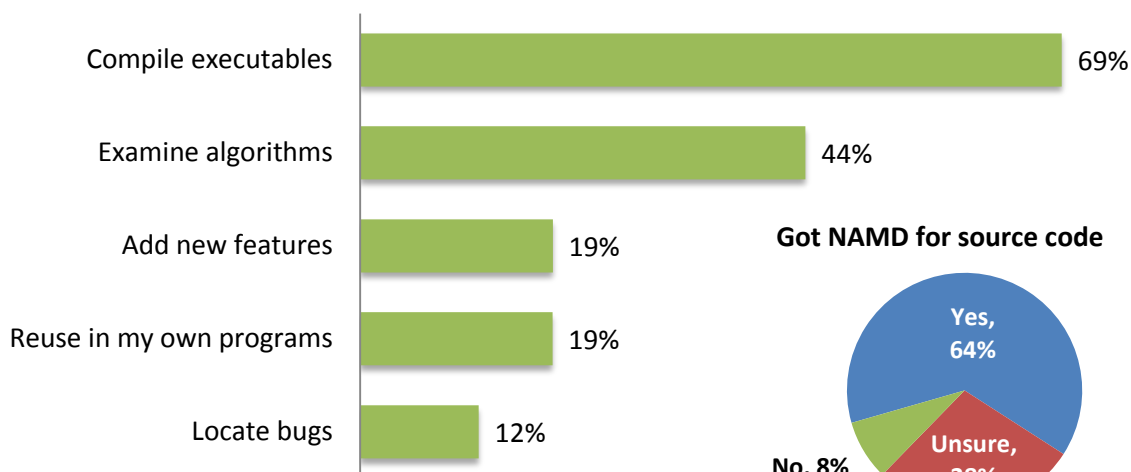
For parallel computing I use NAMD on



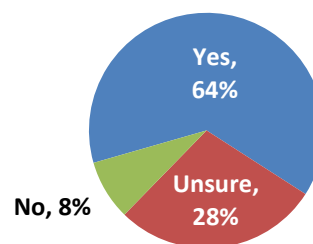
NAMD SOURCE CODE

- Over 60% of respondents downloaded NAMD to get its source code
- Of those who downloaded the NAMD source code, most did so to compile their own executables and to examine algorithms

Reasons for downloading source code



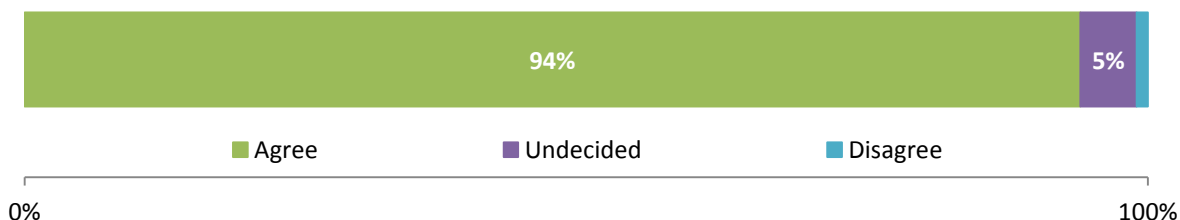
Got NAMD for source code



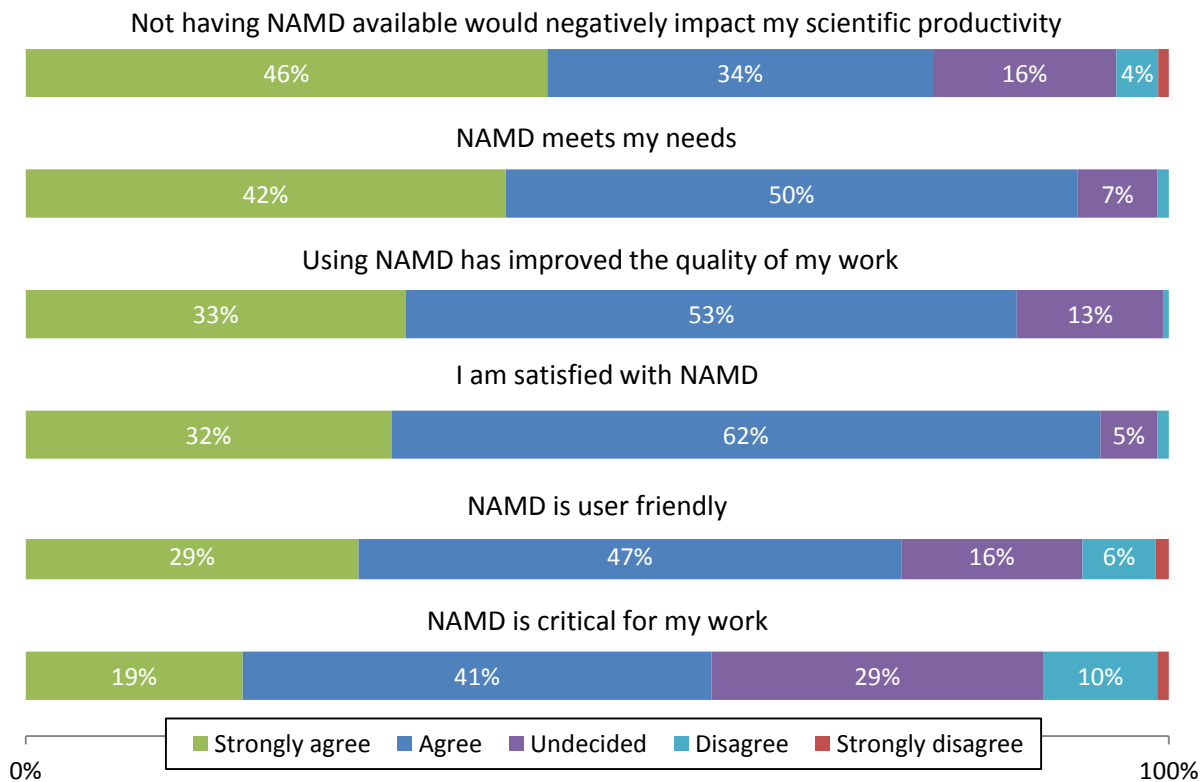
SATISFACTION RATINGS

- 94% of respondents are satisfied with NAMD
- NAMD meets 92% of respondents needs and 86% consider NAMD to have improved the quality of their work
- 60% of respondents consider NAMD critical for their work and 80% indicate that not having NAMD available would negatively impact their scientific productivity.
- 77% of respondents consider NAMD user-friendly

Percentage agreement with the statement "I am satisfied with NAMD"

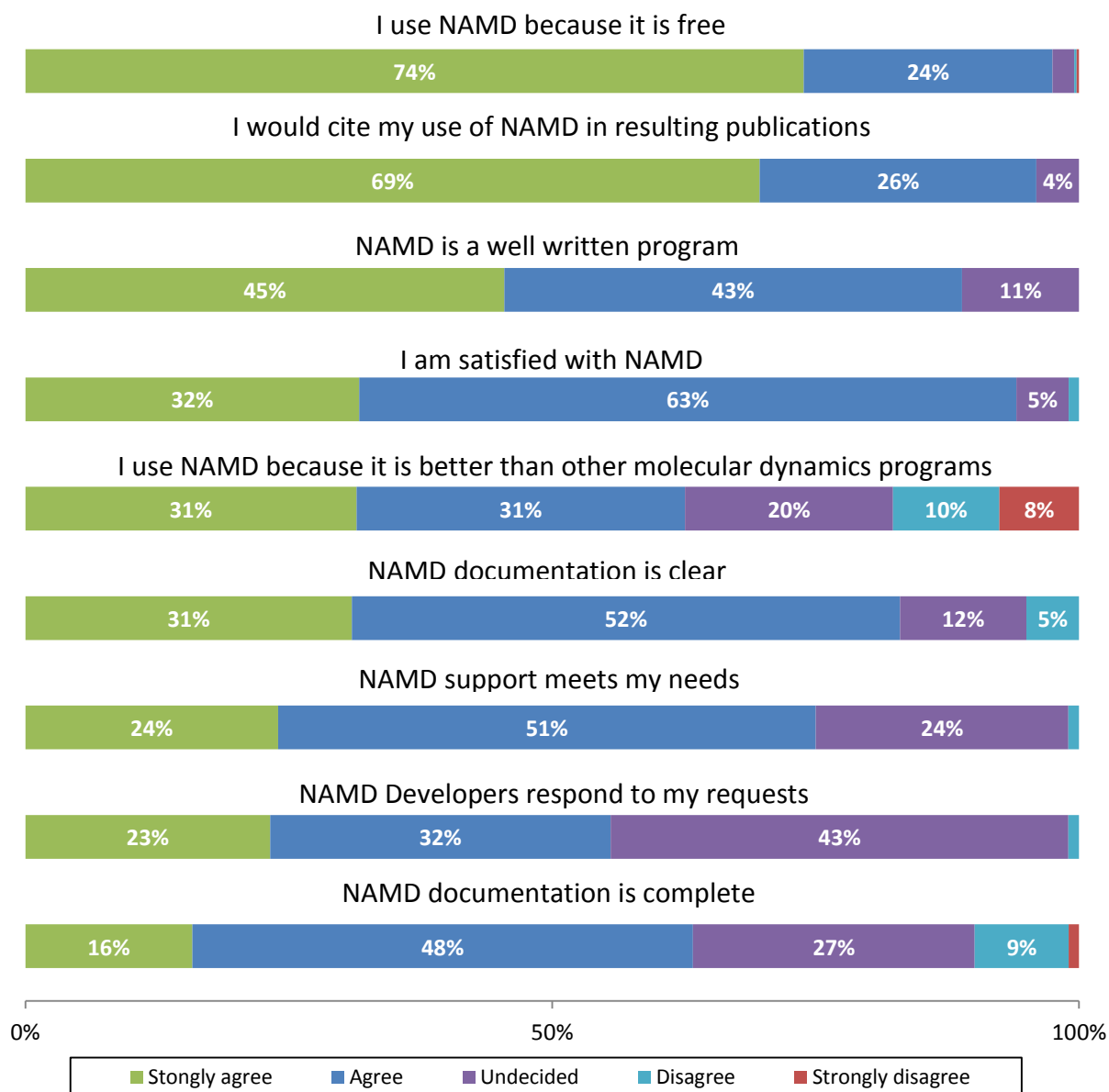


Satisfaction Items



RATINGS OF SUPPORT, DOCUMENTATION AND OVERALL USABILITY

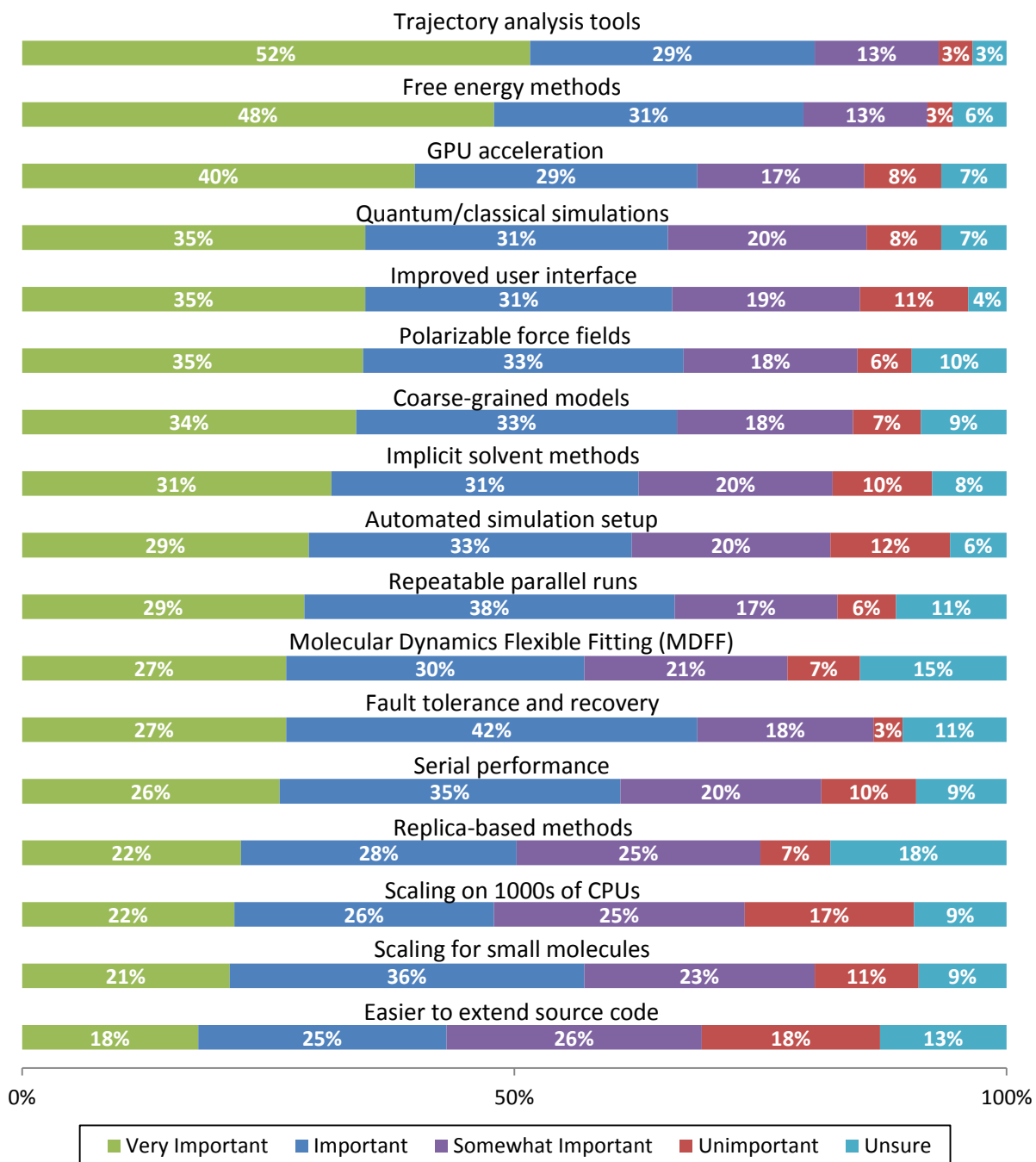
- Having NAMD freely available is important to 98% of users
- Nearly 90% agree that NAMD is a well written program
- A high percentage of respondents, 83%, agree that NAMD documentation is clear, and 64% indicate documentation is complete
- Over 60% of respondents agree that NAMD is better than other molecular dynamics programs
- More than 50% of respondents think that NAMD developers respond to requests and 75% find that NAMD support meets their needs



FUTURE NAMD DEVELOPMENT

- Trajectory analysis tools are rated as the most important planned enhancement
- More than 50% of respondents consider all identified NAMD development avenues of importance, with the exception of easily extending the source code and parallel performance past 1000s of CPUs

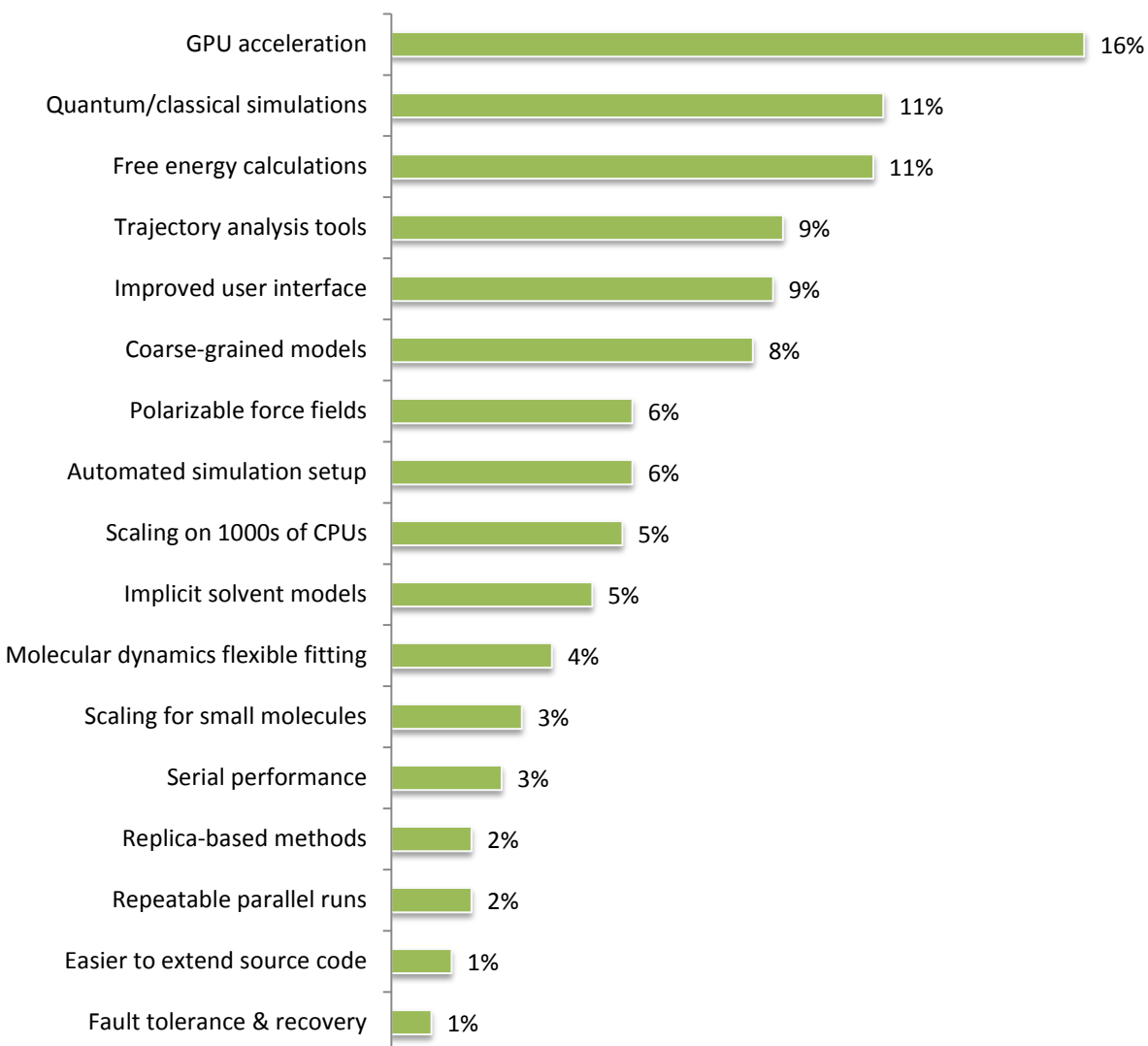
Rate the importance of the following PLANNED enhancement to NAMD



FUTURE NAMD DEVELOPMENT, continued

- GPU acceleration, quantum/classical simulations, and free energy calculations were assigned the top 3 priorities by respondents

Which PLANNED enhancement should have the highest priority?



Survey Methodology

Below are details about the administration of the survey, including survey method, target population, survey schedule and response rates, data editing, and sample validity.

SURVEY METHOD

Population members received an e-mail solicitation asking them to complete an on-line survey, with the link to the survey containing information about the user. Participants were asked to complete all items on the survey form and submit their responses; upon submission, participants were to complete any items they had skipped, with an option to submit without doing so. After submission, users were thanked for their participation.

TARGET POPULATION

Users of NAMD versions 2.7b4 (released September 17, 2010) through NAMD 2.8 (released May 31, 2011), as identified via registration records, constituted the target population of the survey.

SURVEY SCHEDULE AND RESPONSE RATE

The initial solicitation email was sent to 7,008 users (including 3,027 that only downloaded a single version of NAMD) on 19 July 2011. The survey was concluded 26 July 2011, by which time 446 responses had been received, corresponding to a 6.4% response rate.

DATA EDITING

Ten records were removed from the dataset due to incomplete submissions, or comments made in the survey itself indicating the respondent had downloaded but not used NAMD.

CONFIDENCE IN SURVEY SAMPLE SIZE

Data editing reduced the sample size to 436 usable records. Consultation of a sample size calculator (www.surveysystem.com/sscalc.htm) indicates that for a population of 7,008, the sample provides a 95% confidence level, with a +/-4.55 confidence interval. The confidence level indicates how certain one can be that the true percentage of the population would pick an answer as represented by the sample, while the confidence interval reflects a margin of error. For example, 90% of respondents in the survey sample indicated they had used the NAMD tutorial. One can be 95% confident that the true percentage of the population lies between 85.45% and 94.55%.

Survey Questions

Following are questions used on the survey, in the order they appeared, and with a description of the scale or response options presented for each item.

1. Email Address:

Response in text box

2. Affiliation:

Response Options: Academic, Government, Industry, Non-profit, Other

3. Area of study:

Response in text box

4. My level of expertise with molecular modeling is:

Scale Options: Very High, High, Moderate, Low, Very Low

5. My level of expertise with NAMD is:

Scale Options: Very High, High, Moderate, Low, Very Low

6. The work I do with NAMD is funded (at least partially) by NIH:

Response Options: Yes, No

7. The work I do with NAMD is biomedically relevant:

Response Options: No, Yes - briefly describe relevance:

8. On my desktop/laptop I primarily use NAMD on:

Response Options: Windows, Mac, Linux, Other Unix

9. For parallel computing I use NAMD on (check all that apply):

Response Options: Small Linux Cluster (< 100 nodes), Large Linux Cluster, Cray Supercomputer, IBM Blue Gene, Other (please specify)

10. I use NAMD primarily for:

Response Options: Research, Teaching, Business, Other

11. The number of people using NAMD at my site is:

Response Options: 1, 2-4, 5-10, 11-20, 21 or more

12. I use NAMD for _____ of my molecular dynamics simulations:

Response Options: All, Most, Some, None, I don't use molecular dynamics

13. I use NAMD because it:

a) Meets my needs

b) Is free

c) Includes source code

d) Is user friendly

e) Is better than other molecular dynamics programs

f) Is critical for my work

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

14. I have downloaded the NAMD source code to:

- a) Examine algorithms
- b) Compile executables
- c) Locate bugs
- d) Add new features
- e) Reuse in my own programs

Response Options: Yes, No, NA

15. I primarily generate input files for NAMD with:

Response Options: VMD/psfgen, X-PLOR, CHARMM, AMBER, GROMACS, Other (please specify)

16. Rate the importance to your work of these PLANNED enhancements:

- a) Serial performance
- b) Graphics processor acceleration
- c) Scaling on 1000s of CPUs
- d) Scaling for small molecules
- e) Repeatable parallel runs
- f) Fault tolerance & recovery
- g) Automated simulation setup
- h) Improved user interface
- i) Easier to extend source code
- j) Molecular dynamics flexible fitting
- k) Implicit solvent models
- l) Polarizable force fields
- m) Quantum/classical simulations
- n) Replica-based methods
- o) Free energy calculation
- p) Coarse-grained models
- q) Trajectory analysis tools

Scale Options: Very Important, Important, Somewhat Important, Unimportant, Unsure

17. Select the PLANNED enhancement that should have the highest priority for development:

- a) Serial performance
- b) Graphics processor acceleration
- c) Scaling on 1000s of CPUs
- d) Scaling for small molecules
- e) Repeatable parallel runs
- f) Fault tolerance & recovery
- g) Automated simulation setup
- h) Improved user interface
- i) Easier to extend source code
- j) Molecular dynamics flexible fitting
- k) Implicit solvent models
- l) Polarizable force fields
- m) Quantum/classical simulations
- n) Replica-based methods
- o) Free energy calculation
- p) Coarse-grained models
- q) Trajectory analysis tools

Response Options: participants selected one item from the above list as their top priority

18. Rate your agreement with these statements describing NAMD:

- a) NAMD is a well written program
- b) NAMD developers respond to my requests
- c) NAMD support meets my needs
- d) NAMD documentation is clear
- e) NAMD documentation is complete

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

19. I am satisfied with NAMD:

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

20. NAMD has improved the quality of my work:

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

21. Not having NAMD available (e.g., in case of discontinued funding of NAMD development) would negatively impact my scientific productivity:

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

22. I would cite my use of NAMD in resulting publications:

Scale Options: Strongly Agree, Agree, Undecided, Disagree, Strongly Disagree

23. I have used the NAMD tutorial:

Response Options: Yes, No

24. What suggestions do you have for improving NAMD and NAMD support?

Response in text box