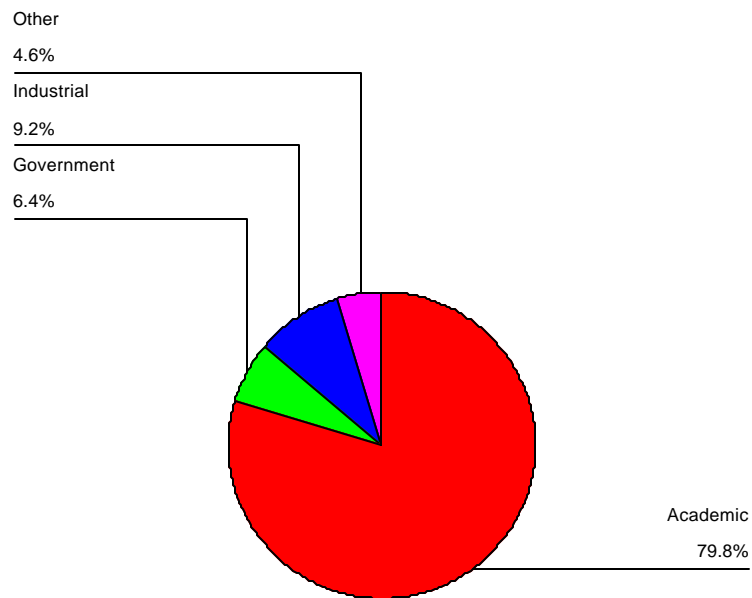


# NAMD User Survey 2000

Item-by-item responses for each question asked in the survey.

# Q. 2: Affiliation



**Affiliation**

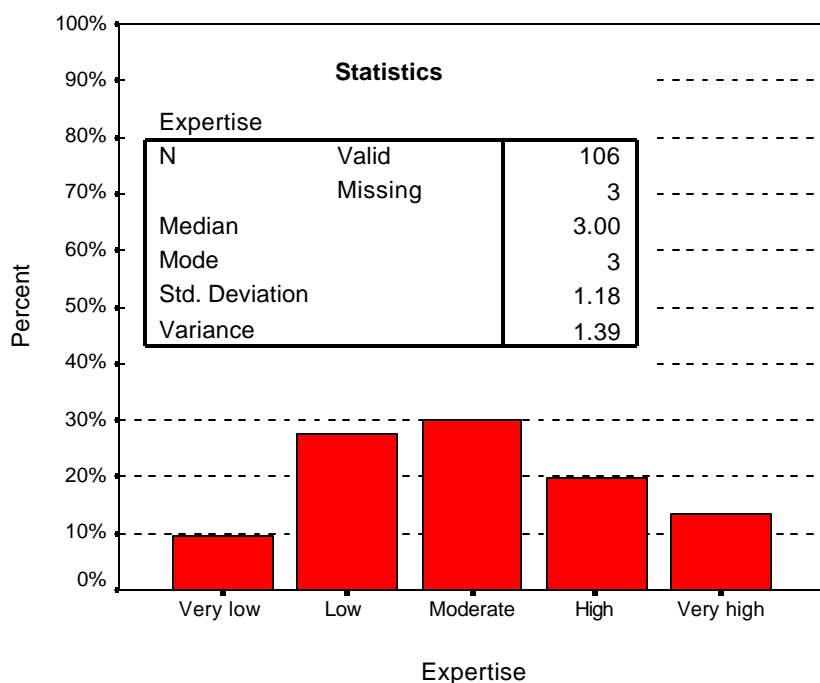
	Frequency	Percent	Valid Percent	Cumulative Percent
Valid academic	87	79.8	79.8	79.8
government	7	6.4	6.4	86.2
industrial	10	9.2	9.2	95.4
other	5	4.6	4.6	100.0
Total	109	100.0	100.0	

•Answer options: Academic, government, industrial, other

### Statistics

Affiliation		
N	Valid	109
	Missing	0

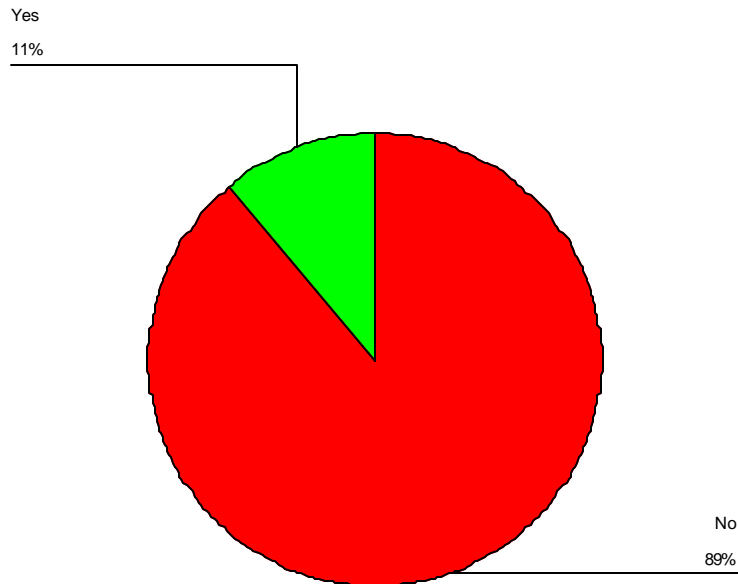
# Q. 3: My level of expertise with molecular modeling is . . .



		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Very low	10	9.2	9.4	9.4
	Low	29	26.6	27.4	36.8
	Moderate	32	29.4	30.2	67.0
	High	21	19.3	19.8	86.8
	Very high	14	12.8	13.2	100.0
	Total	106	97.2	100.0	
Missing	System	3	2.8		
Total		109	100.0		

Coding: Very low=1, low=2, moderate=3, high=4, very high=5

# Q. 4: The work I do is funded (at least partially) by NIH



NIH Funded

	Frequency	Percent	Valid Percent	Cumulative Percent
Valid No	97	89.0	89.0	89.0
Valid Yes	12	11.0	11.0	100.0
Total	109	100.0	100.0	

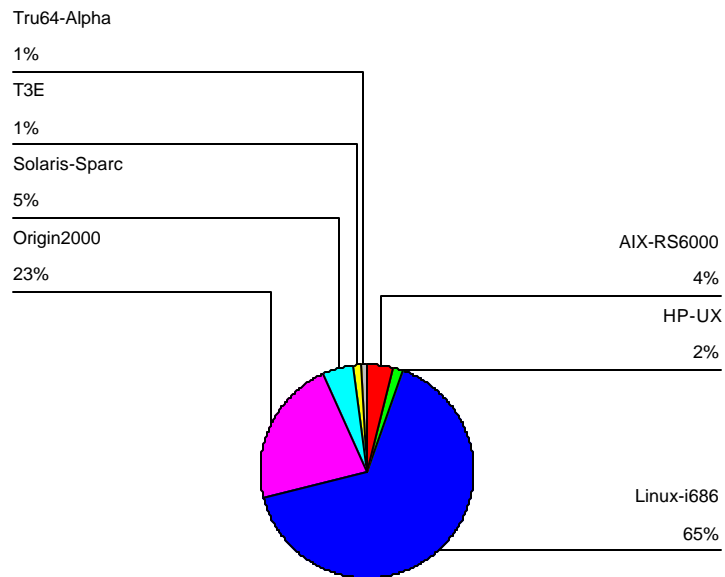
Answer options: Yes, no

## Statistics

NIH Funded

N	Valid	109
	Missing	0

# Q. 5: I primarily use NAMD on . . .



		Platform			
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	AIX-RS6000	4	3.7	3.8	3.8
	HP-UX	2	1.8	1.9	5.7
	Linux-i686	69	63.3	65.1	70.8
	Origin2000	24	22.0	22.6	93.4
	Solaris-Sparc	5	4.6	4.7	98.1
	T3E	1	.9	.9	99.1
	Tru64-Alpha	1	.9	.9	100.0
	Total	106	97.2	100.0	
Missing	1	3	2.8		
Total		109	100.0		

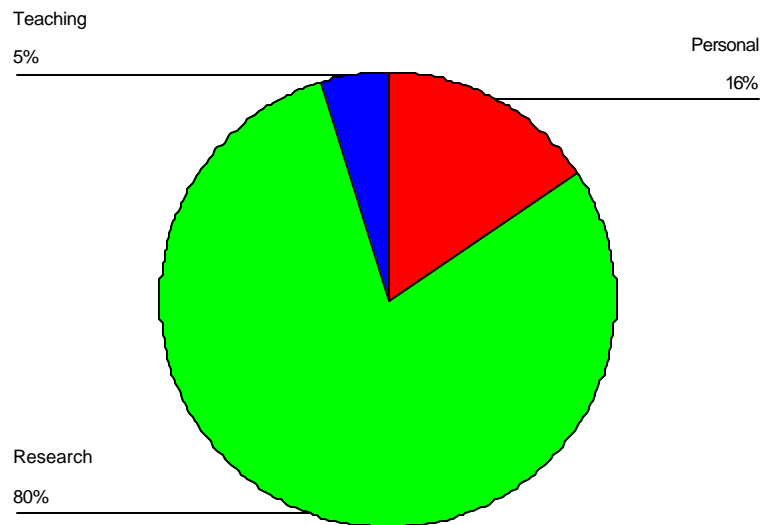
Answer options: AIX-RS6000, AIX-SP, HP-UX, Linux-i686, Origin2000, Solaris-Sparc, T3E, Tru64-Alpha

## Statistics

Platform

N	Valid	106
	Missing	3

# Q. 6: I use NAMD primarily for . . .



**Primary Use**

	Frequency	Percent	Valid Percent	Cumulative Percent
Valid personal	17	15.6	15.6	15.6
research	87	79.8	79.8	95.4
teaching	5	4.6	4.6	100.0
Total	109	100.0	100.0	

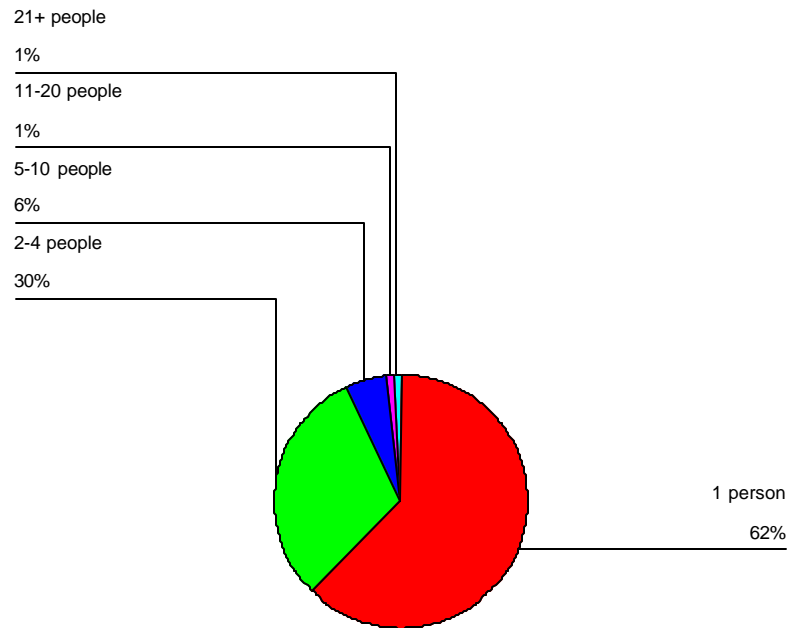
Answer options: Research, teaching, commerce, personal

### Statistics

Primary Use

N	Valid	109
	Missing	0

# Q. 7: The number of people using NAMD at my site is . . .



Number Of Users

	Frequency	Percent	Valid Percent	Cumulative Percent
Valid 1	68	62.4	62.4	62.4
2-4	33	30.3	30.3	92.7
5-10	6	5.5	5.5	98.2
11-20	1	.9	.9	99.1
21+	1	.9	.9	100.0
Total	109	100.0	100.0	

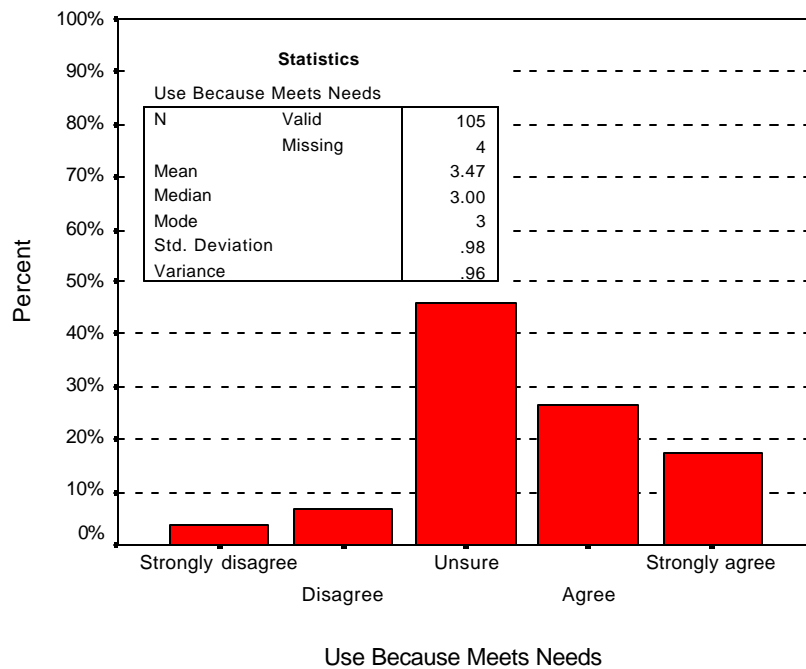
Answer options: 1, 2-4, 5-10, 11-20, 21 or more

## Statistics

Number Of Users

N	Valid	109
	Missing	0

# Q. 8a: Meets my needs



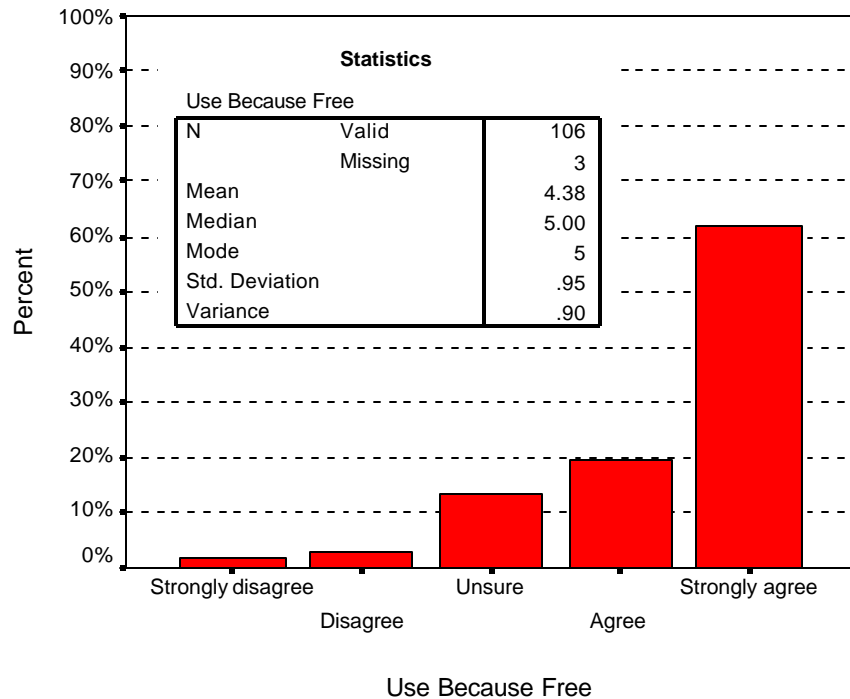
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	4	3.7	3.8	3.8
	Disagree	7	6.4	6.7	10.5
	Unsure	48	44.0	45.7	56.2
	Agree	28	25.7	26.7	82.9
	Strongly agree	18	16.5	17.1	100.0
Total		105	96.3	100.0	
Missing	System	4	3.7		
Total		109	100.0		

Question stem for question 8: I use NAMD because it . . .

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5



# Q. 8b: Is free

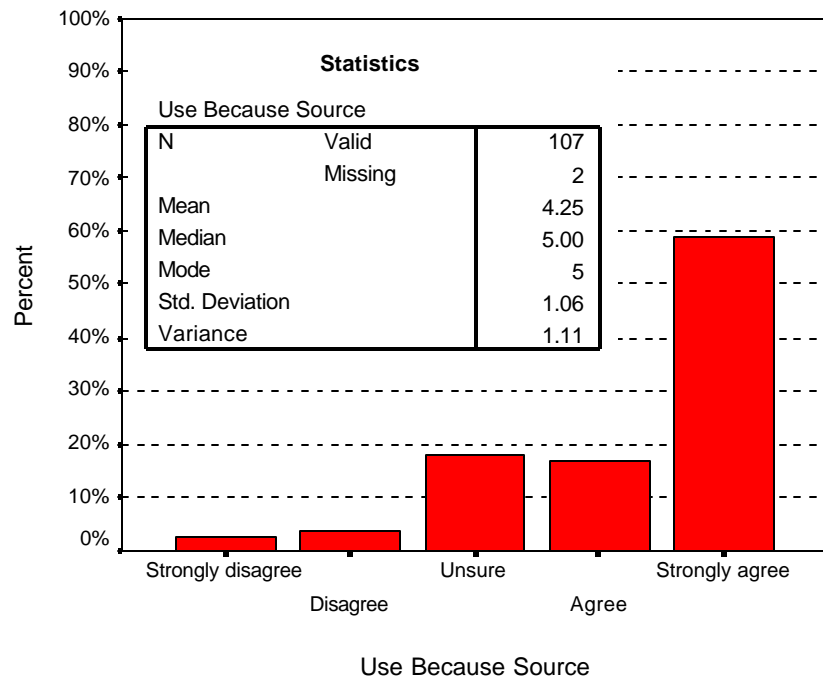


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	1.9	1.9
	Disagree	3	2.8	2.8	4.7
	Unsure	14	12.8	13.2	17.9
	Agree	21	19.3	19.8	37.7
	Strongly agree	66	60.6	62.3	100.0
Total		106	97.2	100.0	
Missing	System	3	2.8		
Total		109	100.0		

Question stem for question 8: I use NAMD because it . . .

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 8c: Includes source code



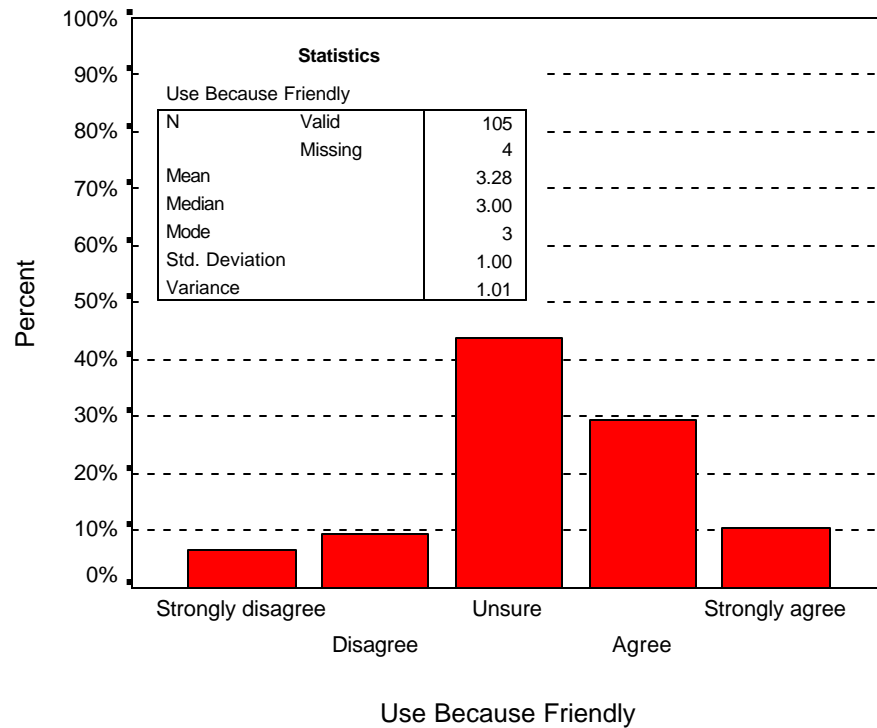
**Use Because Source**

	Frequency	Percent	Valid Percent	Cumulative Percent
Valid Strongly disagree	3	2.8	2.8	2.8
Disagree	4	3.7	3.7	6.5
Unsure	19	17.4	17.8	24.3
Agree	18	16.5	16.8	41.1
Strongly agree	63	57.8	58.9	100.0
Total	107	98.2	100.0	
Missing System	2	1.8		
Total	109	100.0		

Question stem for question 8: I use NAMD because it . . .

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 8d: Is user friendly

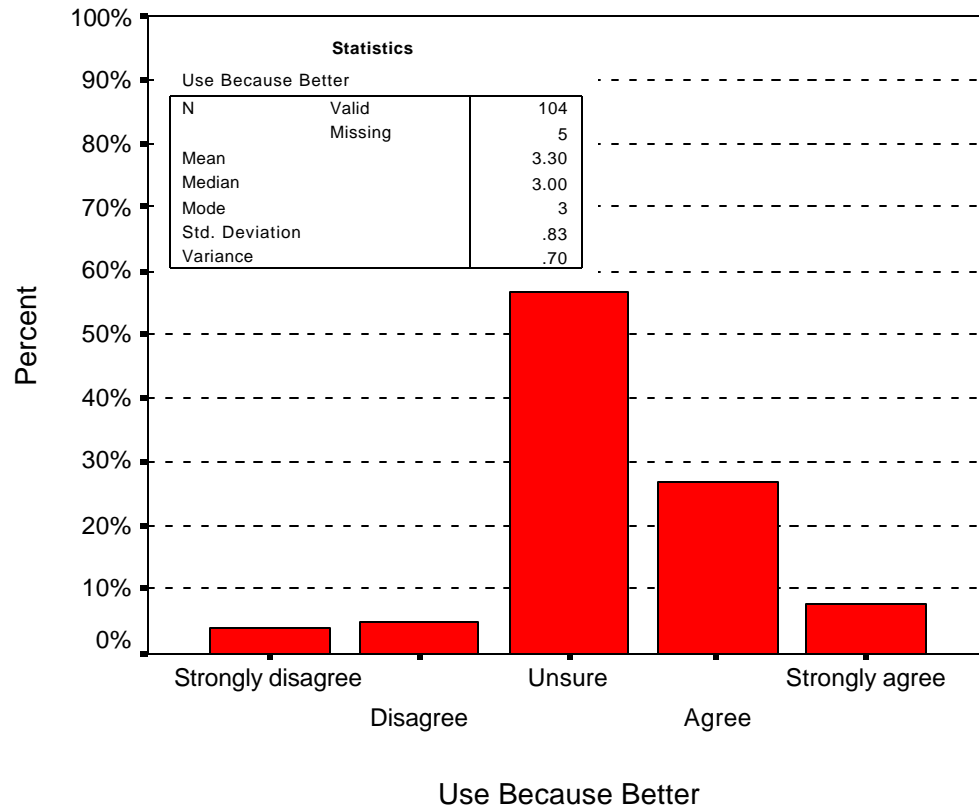


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	7	6.4	6.7	6.7
	Disagree	10	9.2	9.5	16.2
	Unsure	46	42.2	43.8	60.0
	Agree	31	28.4	29.5	89.5
	Strongly agree	11	10.1	10.5	100.0
Total		105	96.3	100.0	
Missing	System	4	3.7		
Total		109	100.0		

Question stem for question 8: I use NAMD because it . . .

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 8e: Is better than other MD programs

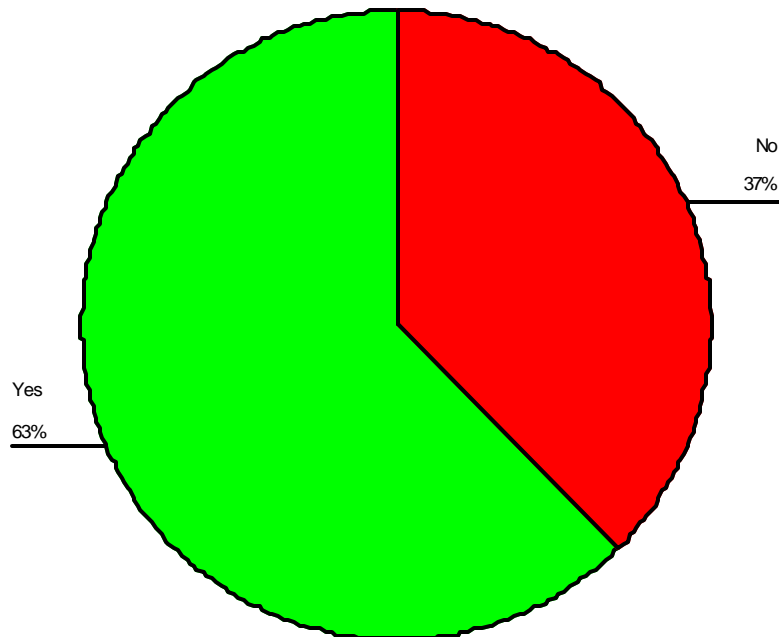


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	4	3.7	3.8	3.8
	Disagree	5	4.6	4.8	8.7
	Unsure	59	54.1	56.7	65.4
	Agree	28	25.7	26.9	92.3
	Strongly agree	8	7.3	7.7	100.0
Total		104	95.4	100.0	
Missing	System	5	4.6		
Total		109	100.0		

Question stem for question 8: I use NAMD because it . . .

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 9a: Examine algorithms



## Statistics

Examine Source Code

N	Valid	99
	Missing	10

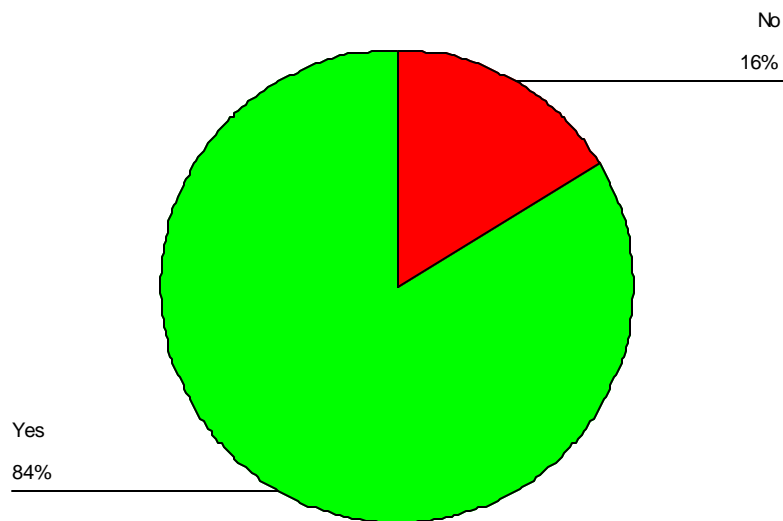
Examine Source Code

		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	No	37	33.9	37.4	37.4
	Yes	62	56.9	62.6	100.0
	Total	99	90.8	100.0	
Missing	System	10	9.2		
Total		109	100.0		

Question stem for question 9: I have downloaded the NAMD source code to . . .

Answer options: Yes, no

# Q. 9b: Compile executables



## Statistics

### Compile Source Code

N	Valid	97
	Missing	12

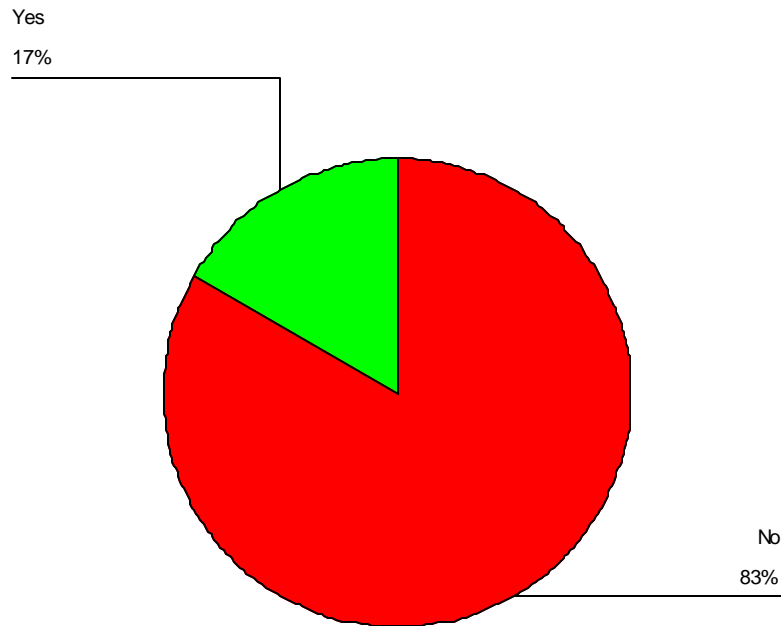
## Compile Source Code

		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	No	16	14.7	16.5	16.5
	Yes	81	74.3	83.5	100.0
	Total	97	89.0	100.0	
Missing	System	12	11.0		
Total		109	100.0		

Question stem for question 9: I have downloaded the NAMD source code to . . .

Answer options: Yes, no

# Q. 9c: Locate bugs



## Statistics

Debug Source Code

N	Valid	90
	Missing	19

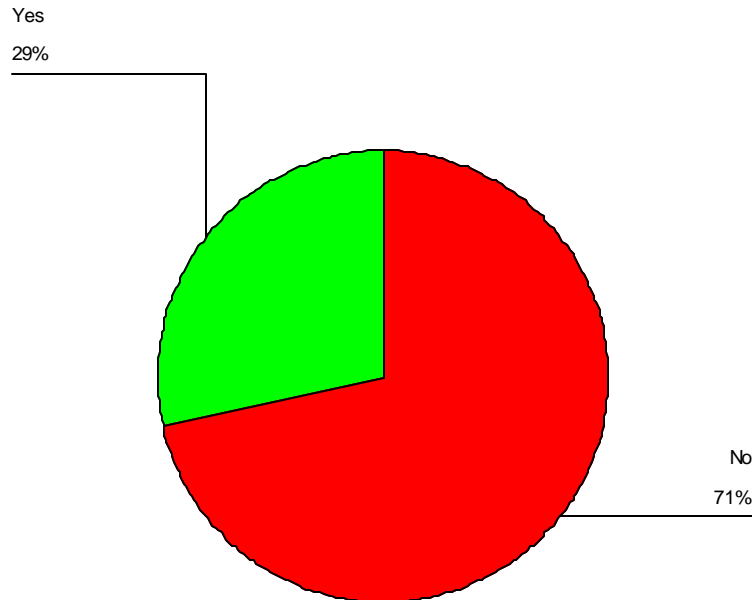
## Debug Source Code

		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	No	75	68.8	83.3	83.3
	Yes	15	13.8	16.7	100.0
	Total	90	82.6	100.0	
Missing	System	19	17.4		
Total		109	100.0		

Question stem for question 9: I have downloaded the NAMD source code to . . .

Answer options: Yes, no

# Q. 9d: Add new features



## Statistics

Extend Source Code

N	Valid	94
	Missing	15

## Extend Source Code

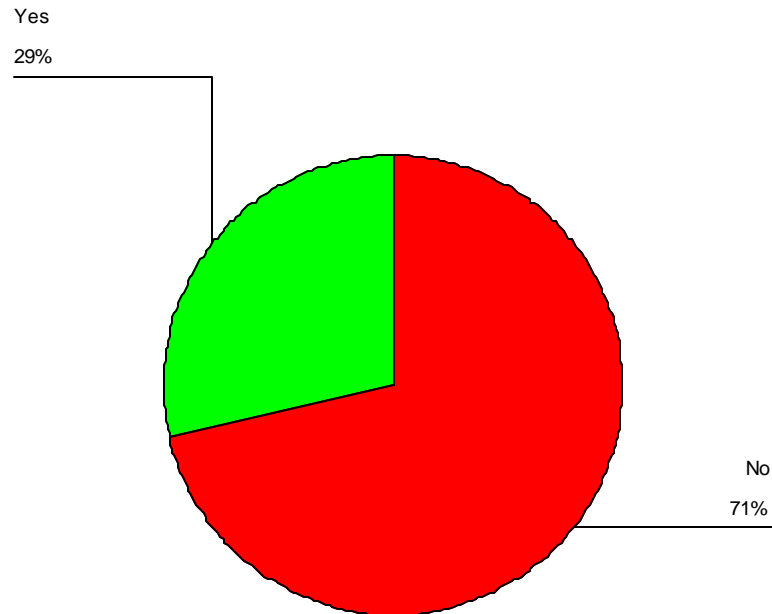
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	No	67	61.5	71.3	71.3
	Yes	27	24.8	28.7	100.0
	Total	94	86.2	100.0	
Missing	System	15	13.8		
Total		109	100.0		

Question stem for question 9: I have downloaded the NAMD source code to . . .

Answer options: Yes, no



# Q. 9e: Reuse in my own programs



Reuse Source Code

		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	No	67	61.5	71.3	71.3
	Yes	27	24.8	28.7	100.0
	Total	94	86.2	100.0	
Missing	System	15	13.8		
Total		109	100.0		

Question stem for question 9: I have downloaded the NAMD source code to . . .

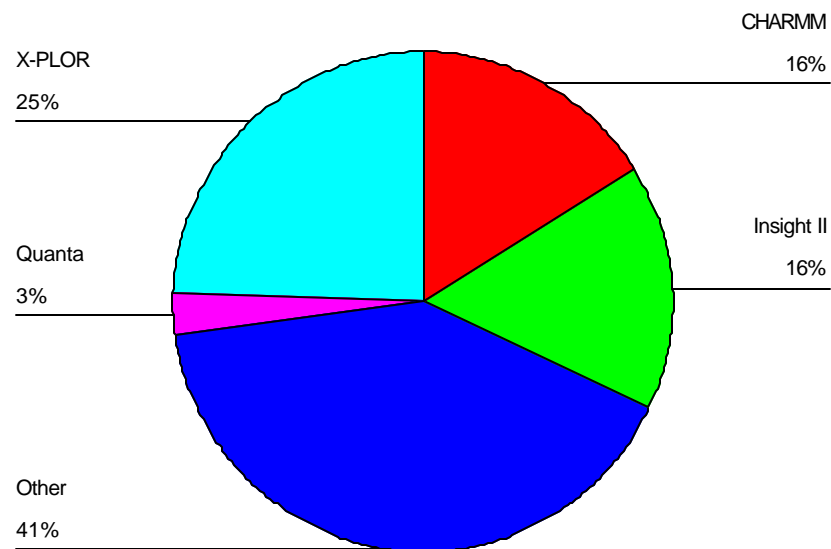
Answer options: Yes, no

## Statistics

Reuse Source Code

N	Valid	94
	Missing	15

# Q. 10: I generate input files for NAMMD with . . .



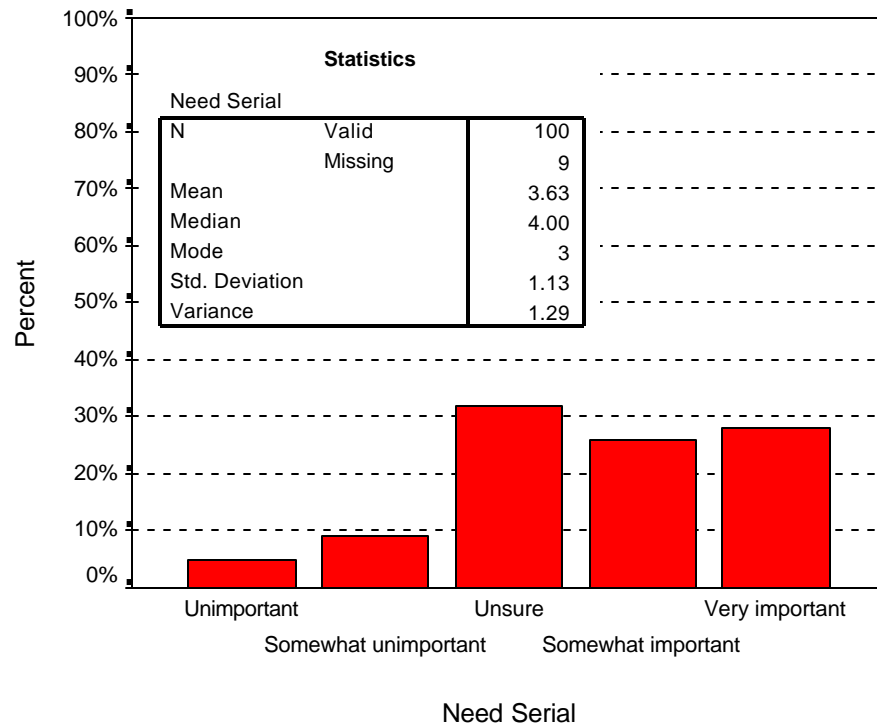
	Frequency	Percent	Valid Percent	Cumulative Percent
Valid				
charmm	17	15.6	16.0	16.0
insight	17	15.6	16.0	32.1
other	43	39.4	40.6	72.6
quanta	3	2.8	2.8	75.5
xplor	26	23.9	24.5	100.0
Total	106	97.2	100.0	
Missing	1	3	2.8	
Total	109	100.0		

Answer options: X-PLOR, CHARMM, Quanta, Insight II, Other

## Statistics

N	Valid	Missing
	106	3

# Q. 11a: Tuned serial performance

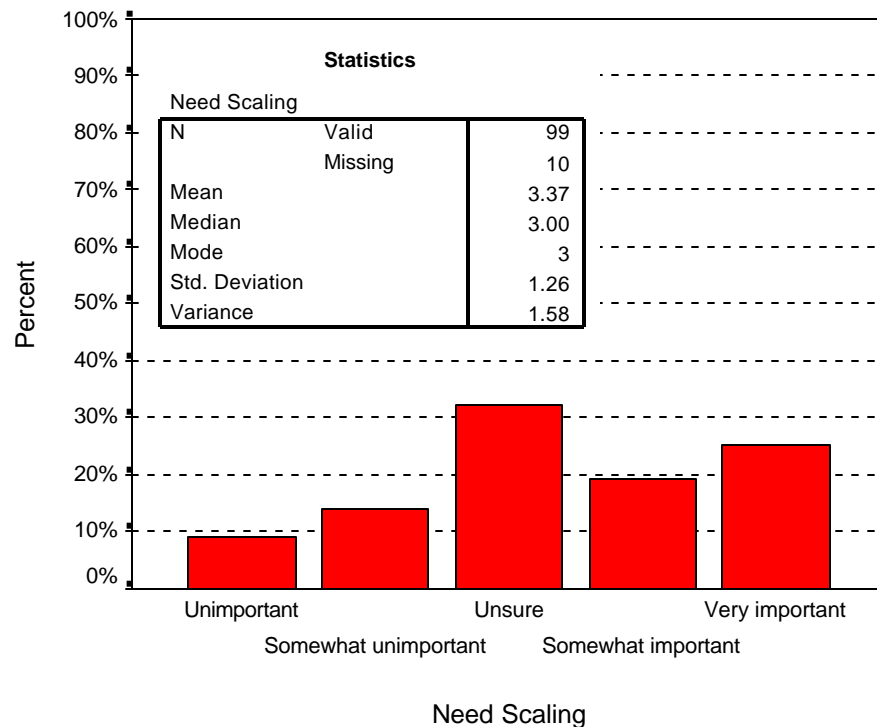


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	5	4.6	5.0	5.0
	Somewhat unimportant	9	8.3	9.0	14.0
	Unsure	32	29.4	32.0	46.0
	Somewhat important	26	23.9	26.0	72.0
	Very important	28	25.7	28.0	100.0
Total		100	91.7	100.0	
Missing	System	9	8.3		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11b: Scaling on 100's of CPUs

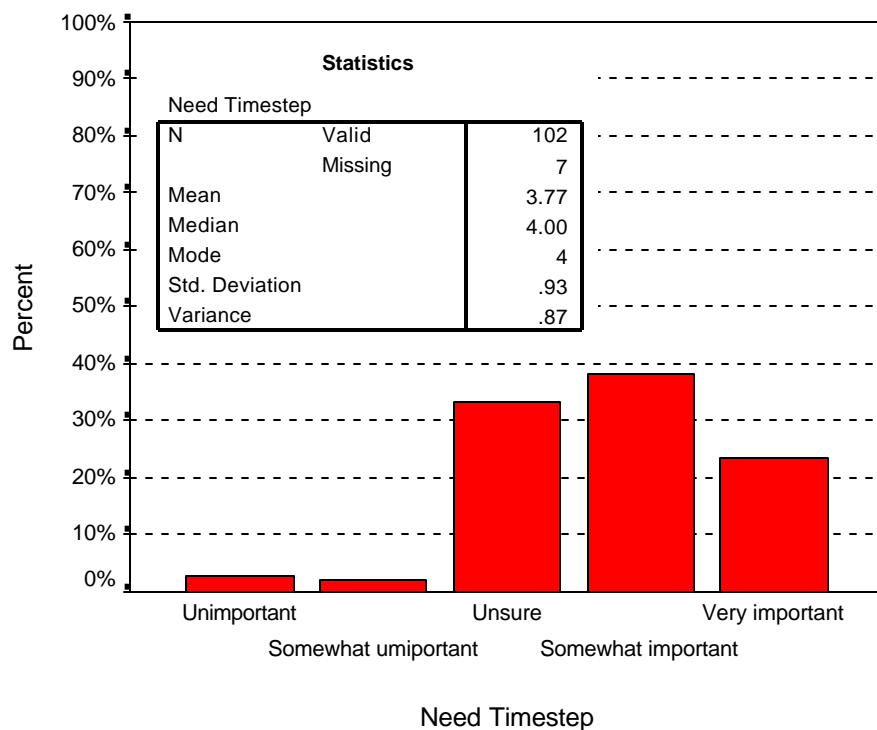


Need Scaling					
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	9	8.3	9.1	9.1
	Somewhat unimportant	14	12.8	14.1	23.2
	Unsure	32	29.4	32.3	55.6
	Somewhat important	19	17.4	19.2	74.7
	Very important	25	22.9	25.3	100.0
Missing	Total	99	90.8	100.0	
	System	10	9.2		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11c: Longer timesteps

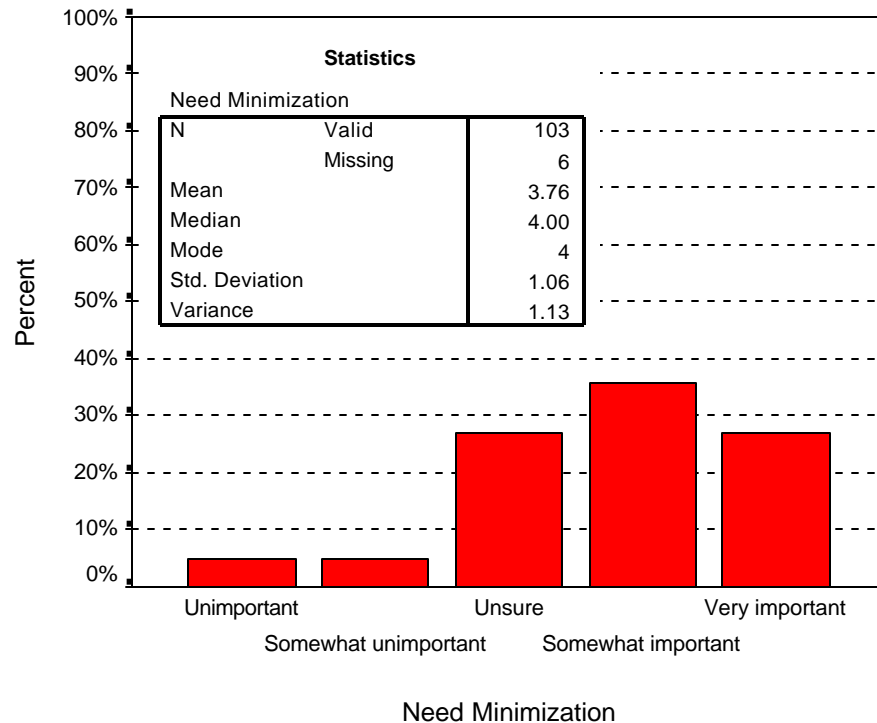


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	3	2.8	2.9	2.9
	Somewhat unimportant	2	1.8	2.0	4.9
	Unsure	34	31.2	33.3	38.2
	Somewhat important	39	35.8	38.2	76.5
	Very important	24	22.0	23.5	100.0
Total		102	93.6	100.0	
Missing	System	7	6.4		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11d: Faster minimization

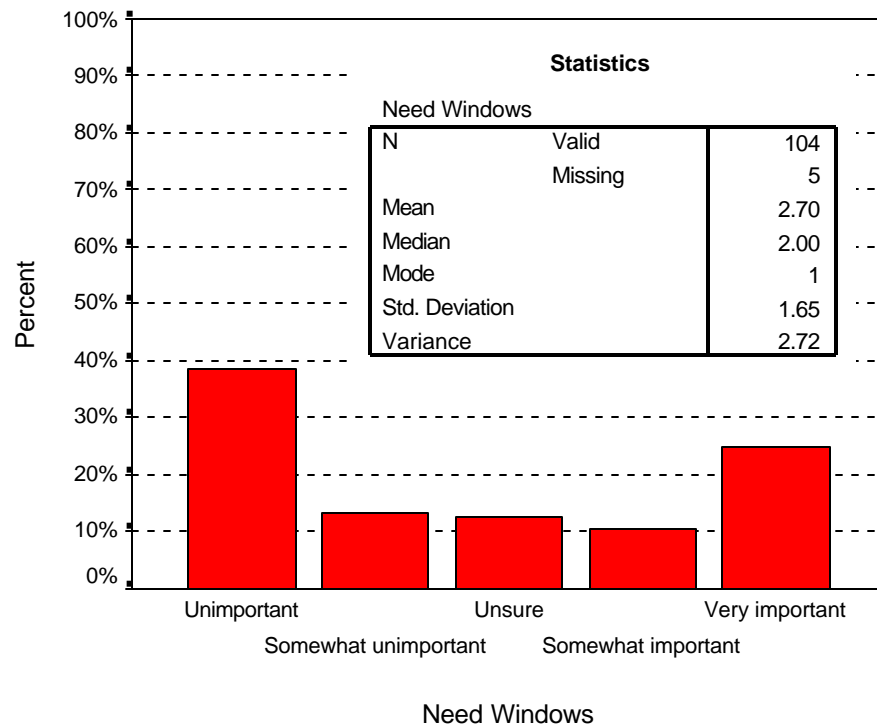


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	5	4.6	4.9	4.9
	Somewhat unimportant	5	4.6	4.9	9.7
	Unsure	28	25.7	27.2	36.9
	Somewhat important	37	33.9	35.9	72.8
	Very important	28	25.7	27.2	100.0
Total		103	94.5	100.0	
Missing	System	6	5.5		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11e: Support for Windows NT

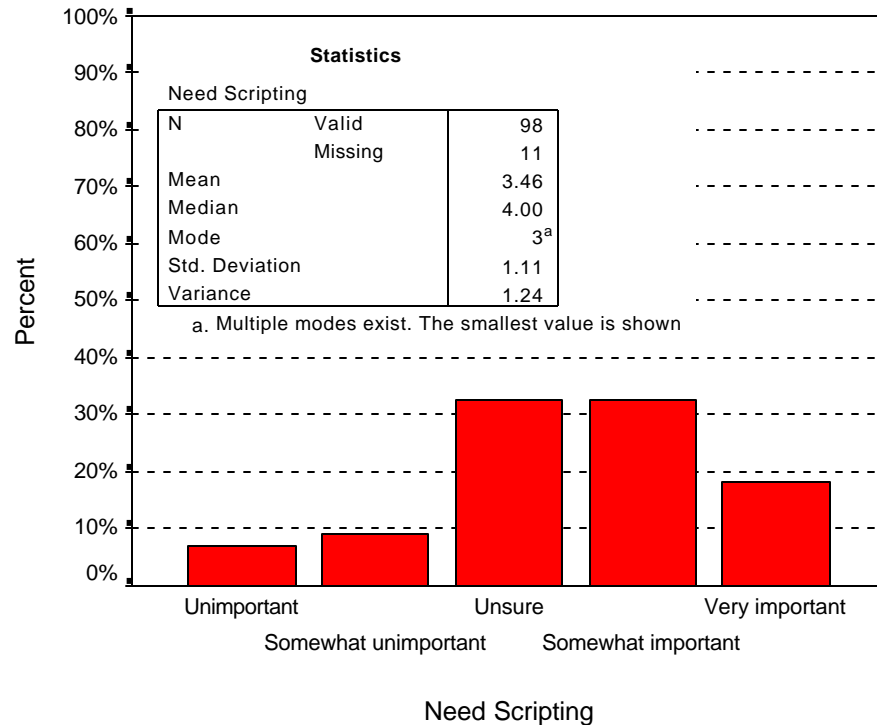


Need Windows					
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	40	36.7	38.5	38.5
	Somewhat unimportant	14	12.8	13.5	51.9
	Unsure	13	11.9	12.5	64.4
	Somewhat important	11	10.1	10.6	75.0
	Very important	26	23.9	25.0	100.0
Total		104	95.4	100.0	
Missing	System	5	4.6		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11f: Extended Tcl scripting



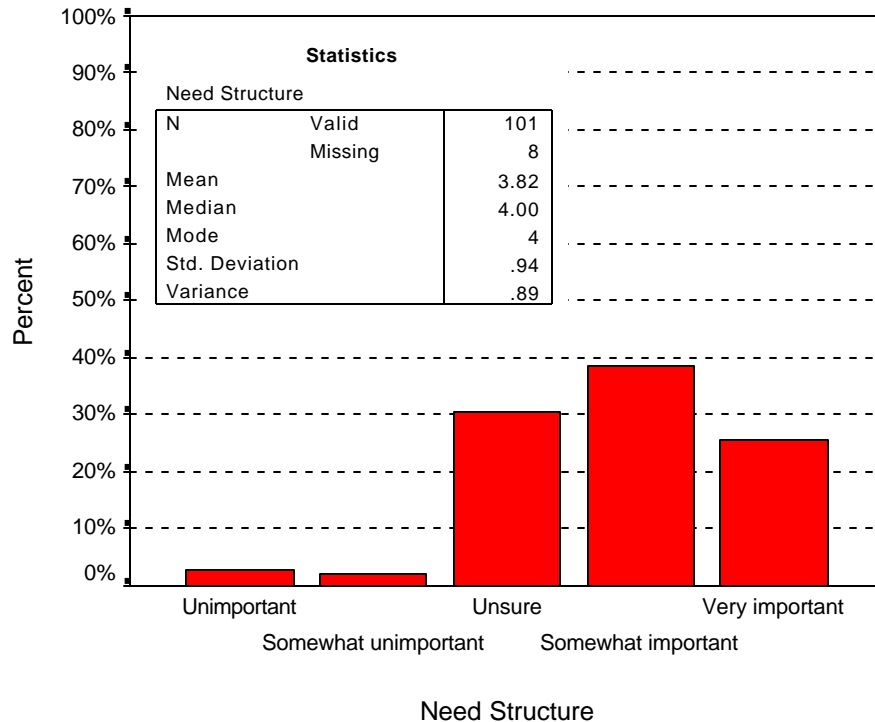
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	7	6.4	7.1	7.1
	Somewhat unimportant	9	8.3	9.2	16.3
	Unsure	32	29.4	32.7	49.0
	Somewhat important	32	29.4	32.7	81.6
	Very important	18	16.5	18.4	100.0
Total		98	89.9	100.0	
Missing	System	11	10.1		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5



# Q. 11g: Structure (PSF) file generation

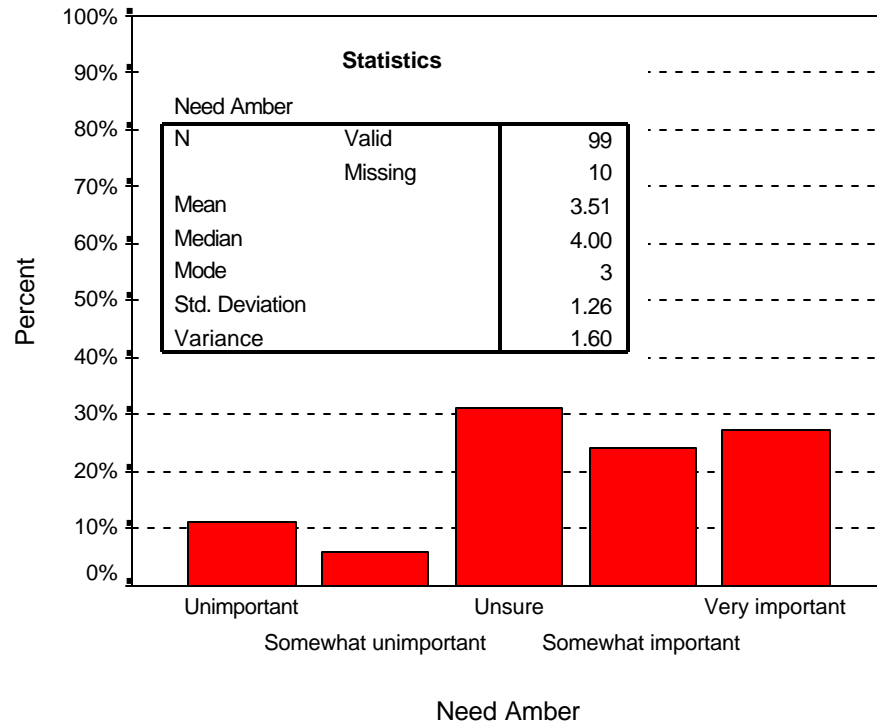


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	3	2.8	3.0	3.0
	Somewhat unimportant	2	1.8	2.0	5.0
	Unsure	31	28.4	30.7	35.6
	Somewhat important	39	35.8	38.6	74.3
	Very important	26	23.9	25.7	100.0
Total		101	92.7	100.0	
Missing	System	8	7.3		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11h: Interoperability with Amber

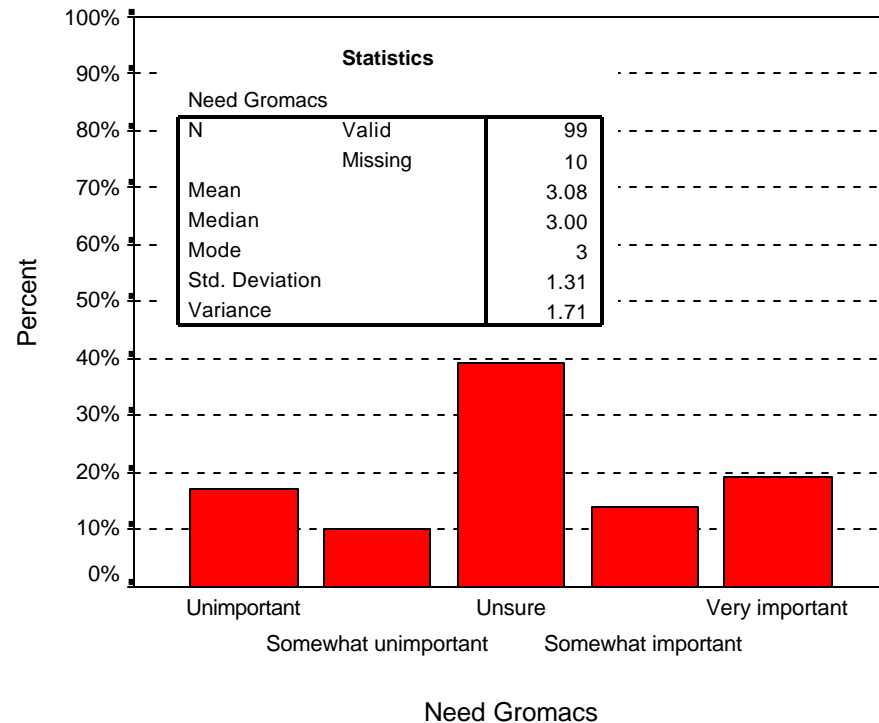


		Need Amber			
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	11	10.1	11.1	11.1
	Somewhat unimportant	6	5.5	6.1	17.2
	Unsure	31	28.4	31.3	48.5
	Somewhat important	24	22.0	24.2	72.7
	Very important	27	24.8	27.3	100.0
Total		99	90.8	100.0	
Missing	System	10	9.2		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11i: Interoperability with GROMACS

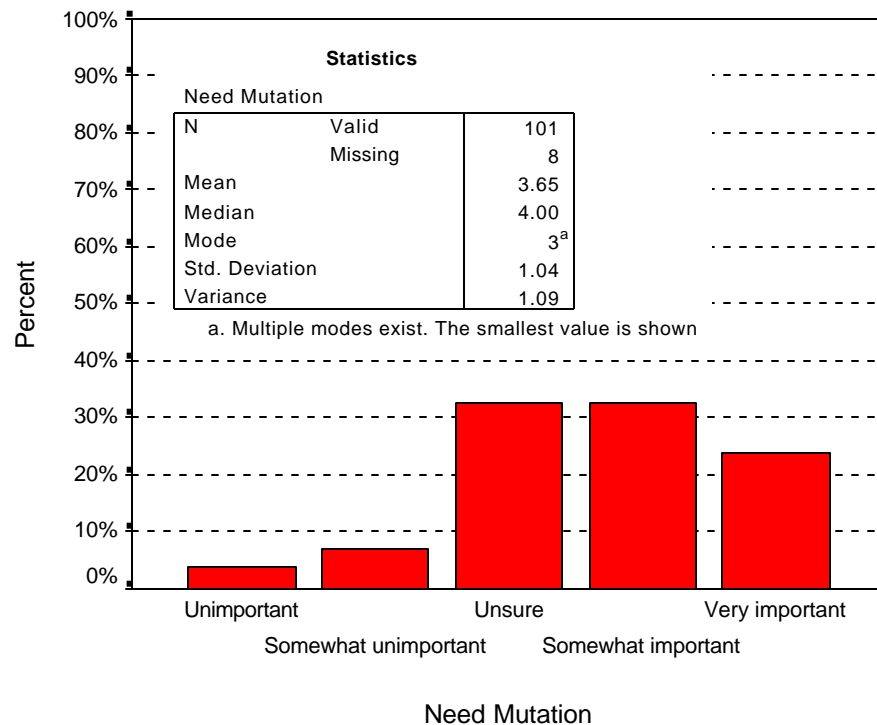


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	17	15.6	17.2	17.2
	Somewhat unimportant	10	9.2	10.1	27.3
	Unsure	39	35.8	39.4	66.7
	Somewhat important	14	12.8	14.1	80.8
	Very important	19	17.4	19.2	100.0
Total		99	90.8	100.0	
Missing	System	10	9.2		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11j: Free energy of mutation

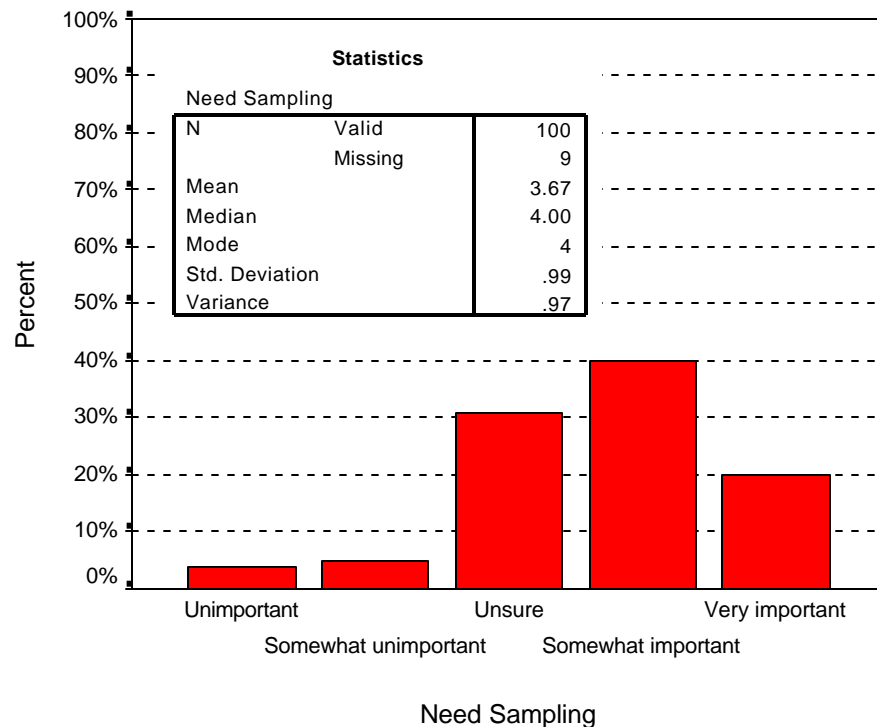


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	4	3.7	4.0	4.0
	Somewhat unimportant	7	6.4	6.9	10.9
	Unsure	33	30.3	32.7	43.6
	Somewhat important	33	30.3	32.7	76.2
	Very important	24	22.0	23.8	100.0
Total		101	92.7	100.0	
Missing	System	8	7.3		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 11k: Locally enhanced sampling

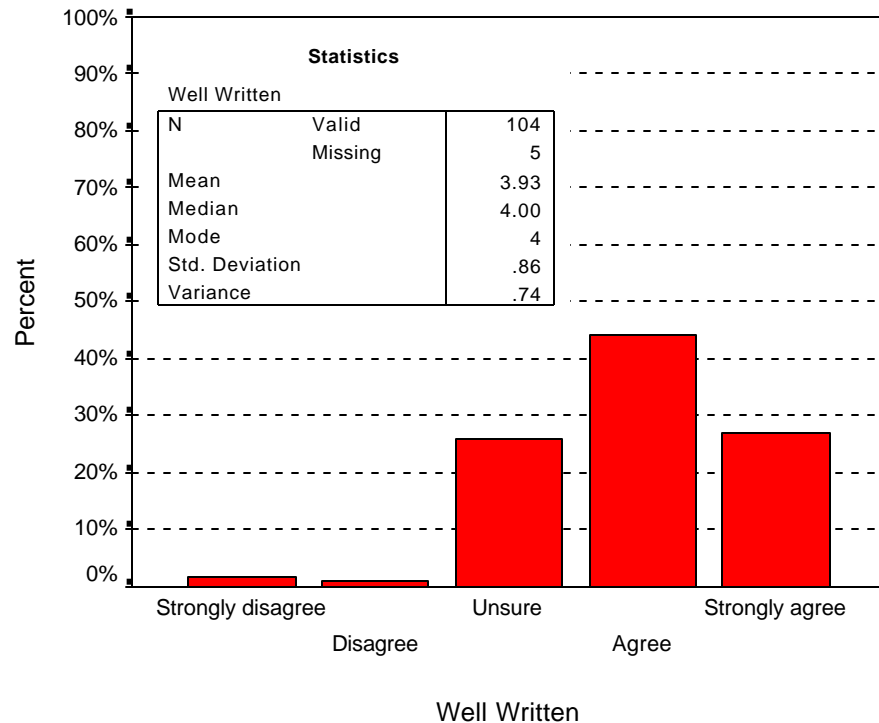


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Unimportant	4	3.7	4.0	4.0
	Somewhat unimportant	5	4.6	5.0	9.0
	Unsure	31	28.4	31.0	40.0
	Somewhat important	40	36.7	40.0	80.0
	Very important	20	18.3	20.0	100.0
Total		100	91.7	100.0	
Missing	System	9	8.3		
Total		109	100.0		

Question stem for question 11: Rate the usefulness of these PLANNED features to your work . . .

Coding: Unimportant=1, somewhat important=2, unsure=3, somewhat important=4, very important=5

# Q. 12a: NAMD is a well written program

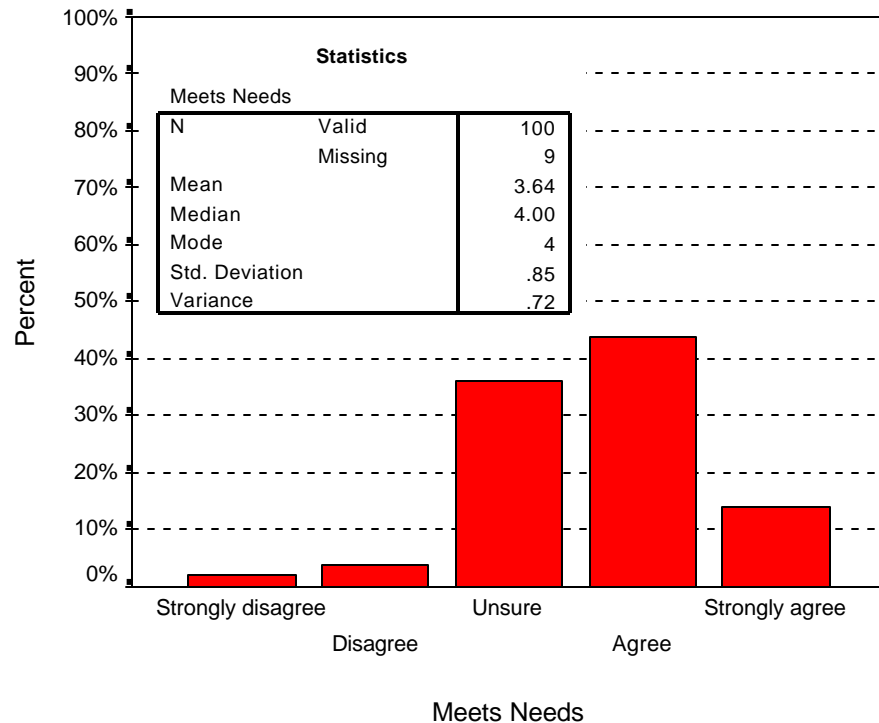


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	1.9	1.9
	Disagree	1	.9	1.0	2.9
	Unsure	27	24.8	26.0	28.8
	Agree	46	42.2	44.2	73.1
	Strongly agree	28	25.7	26.9	100.0
Total		104	95.4	100.0	
Missing	System	5	4.6		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 12b: NAMD meets my needs

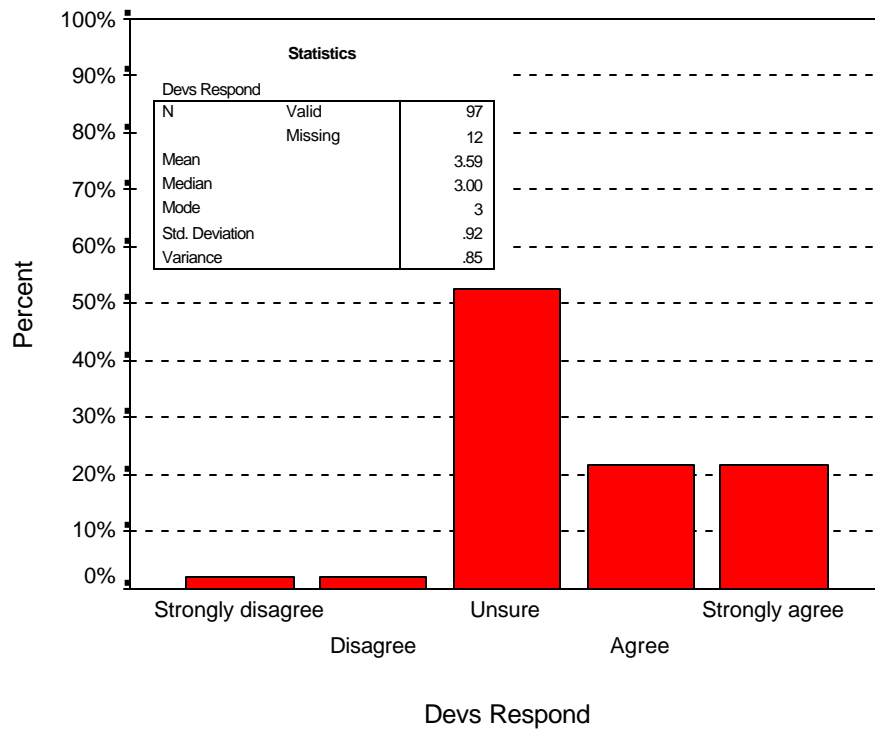


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	2.0	2.0
	Disagree	4	3.7	4.0	6.0
	Unsure	36	33.0	36.0	42.0
	Agree	44	40.4	44.0	86.0
	Strongly agree	14	12.8	14.0	100.0
Total		100	91.7	100.0	
Missing	System	9	8.3		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 12c: NAMD developers respond to my requests



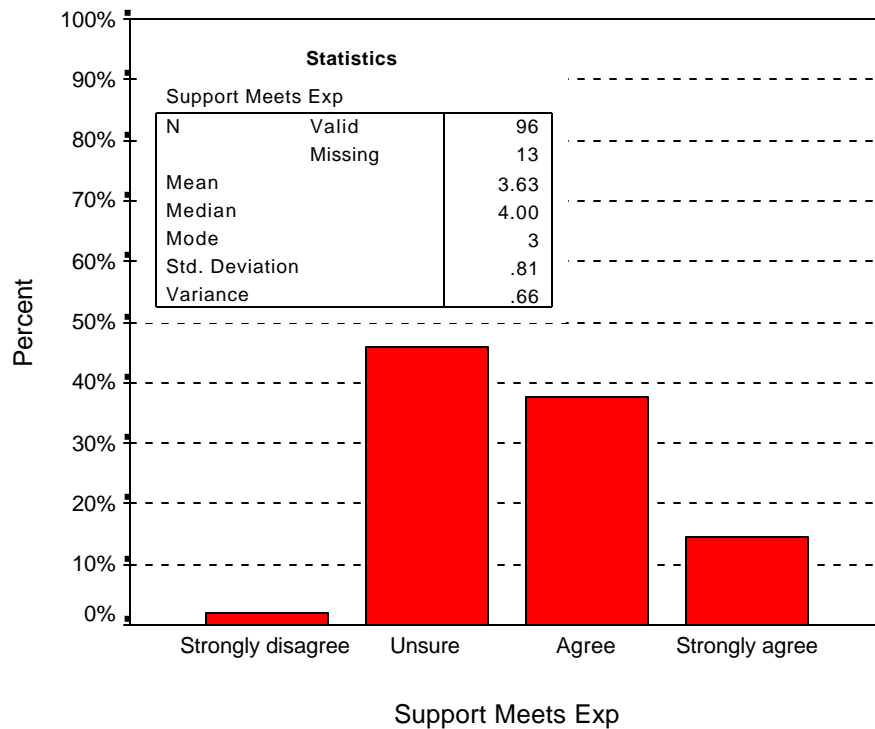
Devs Respond					
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	2.1	2.1
	Disagree	2	1.8	2.1	4.1
	Unsure	51	46.8	52.6	56.7
	Agree	21	19.3	21.6	78.4
	Strongly agree	21	19.3	21.6	100.0
Total		97	89.0	100.0	
Missing	System	12	11.0		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5



# Q. 12d: NAMD support meets my expectations



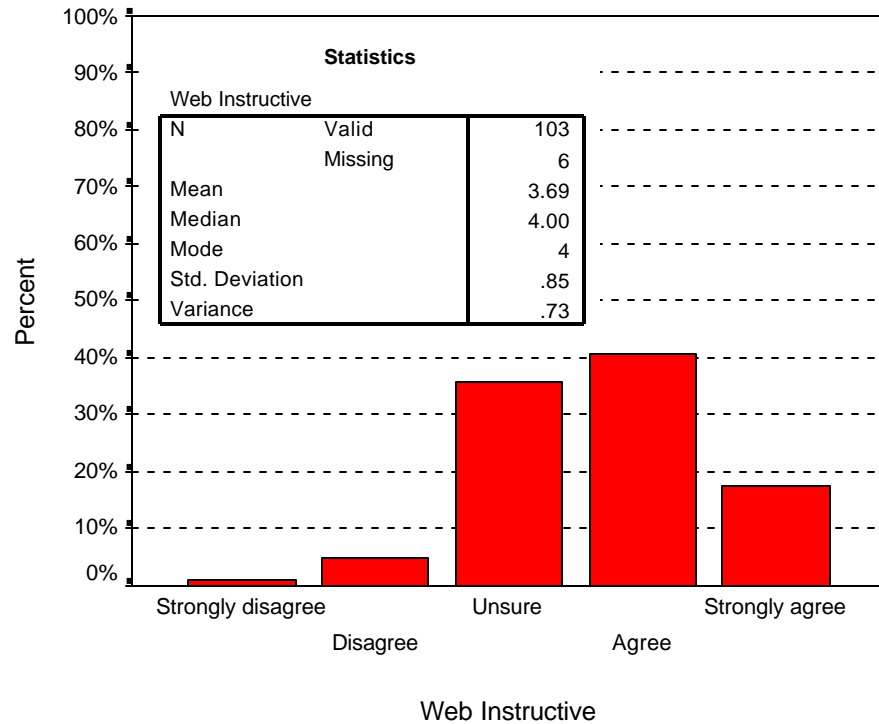
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	2.1	2.1
	Unsure	44	40.4	45.8	47.9
	Agree	36	33.0	37.5	85.4
	Strongly agree	14	12.8	14.6	100.0
Total		96	88.1	100.0	
Missing	System	13	11.9		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Note: No 'Disagree' values selected by respondents.

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 12e: NAMD web pages are instructive

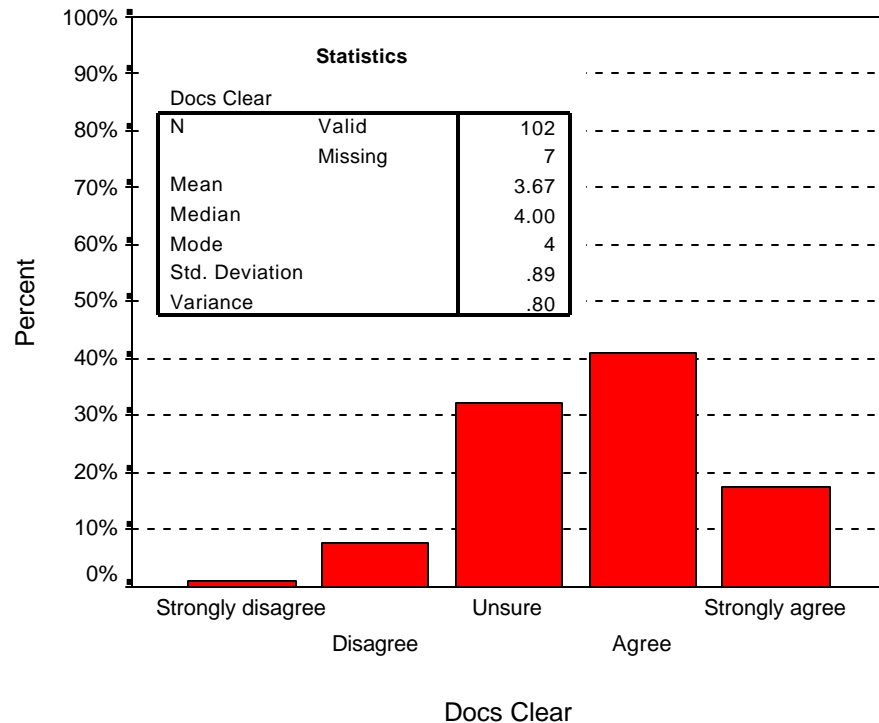


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	1	.9	1.0	1.0
	Disagree	5	4.6	4.9	5.8
	Unsure	37	33.9	35.9	41.7
	Agree	42	38.5	40.8	82.5
	Strongly agree	18	16.5	17.5	100.0
Total		103	94.5	100.0	
Missing	System	6	5.5		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 12f: NAMD documentation is clear

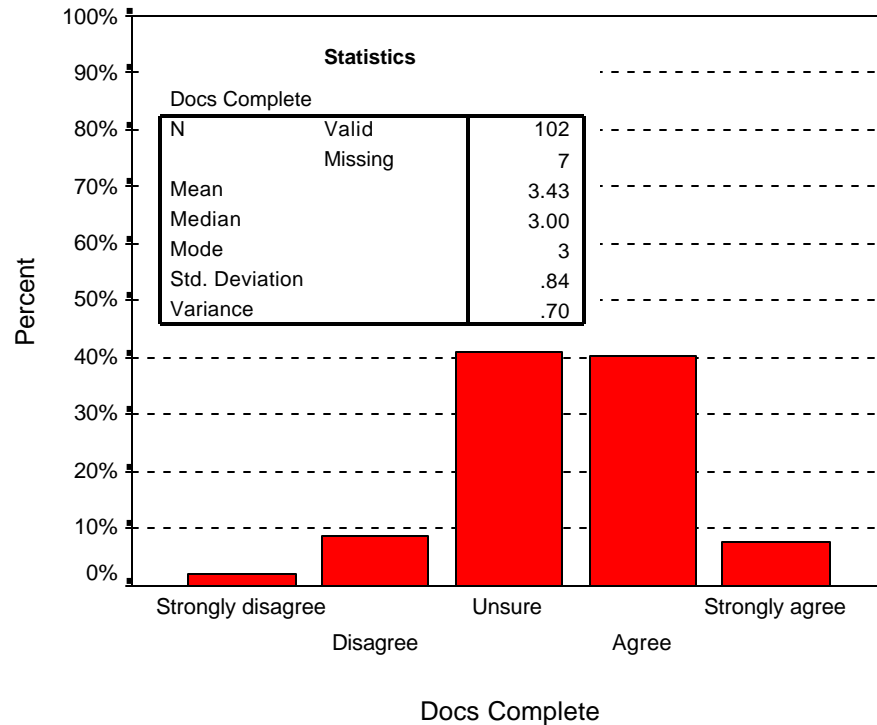


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	1	.9	1.0	1.0
	Disagree	8	7.3	7.8	8.8
	Unsure	33	30.3	32.4	41.2
	Agree	42	38.5	41.2	82.4
	Strongly agree	18	16.5	17.6	100.0
Total		102	93.6	100.0	
Missing	System	7	6.4		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 12g: NAMD documentation is complete

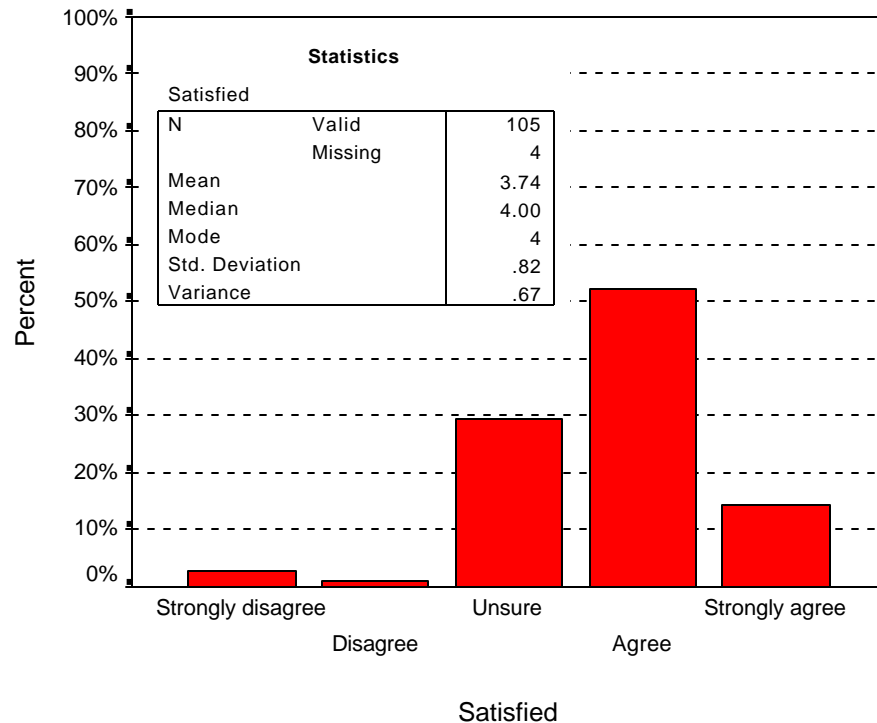


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	2	1.8	2.0	2.0
	Disagree	9	8.3	8.8	10.8
	Unsure	42	38.5	41.2	52.0
	Agree	41	37.6	40.2	92.2
	Strongly agree	8	7.3	7.8	100.0
Total		102	93.6	100.0	
Missing	System	7	6.4		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 13: I am satisfied with NAMD

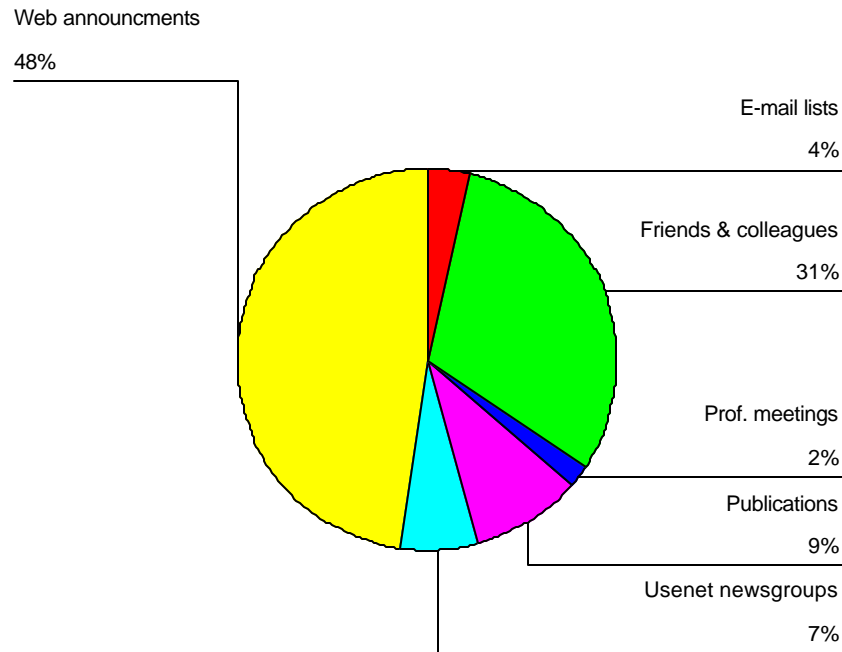


		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	Strongly disagree	3	2.8	2.9	2.9
	Disagree	1	.9	1.0	3.8
	Unsure	31	28.4	29.5	33.3
	Agree	55	50.5	52.4	85.7
	Strongly agree	15	13.8	14.3	100.0
Total		105	96.3	100.0	
Missing	System	4	3.7		
Total		109	100.0		

Question stem for question 12: Rate your agreement with these statements about NAMD

Coding: Strongly disagree=1, disagree=2, unsure=3, agree=4, strongly agree=5

# Q. 14: I first heard of NAMD from . . .



Heard From

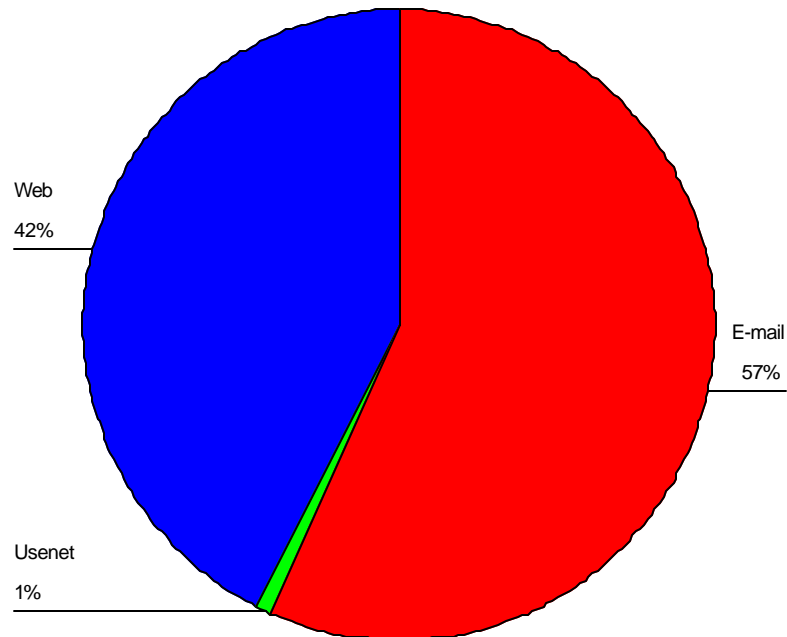
		Frequency	Percent	Valid Percent	Cumulative Percent
Valid	email	4	3.7	3.7	3.7
	friends	33	30.3	30.8	34.6
	meetings	2	1.8	1.9	36.4
	publication	10	9.2	9.3	45.8
	usenet	7	6.4	6.5	52.3
	web	51	46.8	47.7	100.0
	Total	107	98.2	100.0	
Missing	1	2	1.8		
Total		109	100.0		

## Statistics

Heard From

N	Valid	107
	Missing	2

# Q. 15: I would prefer to be informed of NAMD news by . . .



Inform By

	Frequency	Percent	Valid Percent	Cumulative Percent
Valid E-mail lists	60	55.0	56.6	56.6
Usenet newsgroups	1	.9	.9	57.5
Web announcements	45	41.3	42.5	100.0
Total	106	97.2	100.0	
Missing 1	3	2.8		
Total	109	100.0		

**Statistics**

Inform By		
N	Valid	106
	Missing	3