THEORETICAL AND COMPUTATIONAL BIOPHYSICS GROUP

VMD 2003 SURVEY REPORT

D. BRANDON, J. STONE, & G. BUDESCU

Theoretical and Computational Biophysics Group
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign
www.ks.uiuc.edu

EXECUTIVE SUMMARY

The VMD 2003 User Survey was announced on April 14, 2003 to 14,158 users of VMD (versions 1.7 through 1.8) and ran through May 12 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 few demographic questions were asked as well.

- A total of 2,146 usable responses were returned by the survey, yielding a response rate of 15.2%.

- Survey results indicate that the majority of VMD users are affiliated with academic institutions (84.0%) and use VMD for research purposes (81.1%), with some of this research funded at least in part by NIH (19.8%). Nearly half of users (48.8%) are the sole users of VMD at their site, a similar proportion considers themselves moderate-expert users of VMD (46.1%), and just over half of VMD users are repeat users of the program (51.8%). While VMD is used on several different computer platforms, the most popular is Windows (40.1%), followed by Linux (36.8%).

- The majority of users are satisfied with VMD – 77.3% agree or strongly agree with the statement "I am satisfied with VMD". Most users feel that using VMD has a positive impact on their work quality – 63.3% agreed or strongly agreed with the statement "VMD has improved the quality of my work".

- Repeat users of VMD were significantly more satisfied with VMD than non-repeat users, and also indicated a greater impact of VMD on their work quality.

- The greater the level of respondent expertise (low, moderate, or high) in using VMD, the greater the rating of satisfaction and the greater the rating of a positive impact of VMD on work quality. High expertise ratings for both satisfaction and work quality were significantly higher than the other expertise group ratings.

- While a slightly greater proportion of NIH-funded users expressed satisfaction with VMD and its positive impact on their work quality, no significant differences by funding source (NIH, other) were found.

- Academically affiliated users indicated significantly greater satisfaction with VMD and a greater impact of VMD on their work quality than the other users.

OVERVIEW

VMD (Visual Molecular Dynamics) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS-X, Unix, or Windows, is distributed free of charge, and includes source code. More about VMD is available at its TCBG home page, http://www.ks.uiuc.edu/Research/vmd/. The VMD 2003 Survey is part of an ongoing effort (similar surveys were conducted in 1999 and 2000) to ensure that VMD is up to date, relevant, and of high quality by collecting and analyzing user opinion about the application. VMD users were identified via registration records, and contacted via e-mail with a request that they complete an on-line survey about VMD (see locations below for a copy of the survey) during April-May of 2003. The following report details the results and administration of the survey.

VMD 2003 Survey (complete copy)

A link to the survey forms the users completed is available here. Note that for analysis, interpretation and review purposes that all references to the items within the report are based on the numbering of the items as was used in the original survey.

The VMD 2003 Survey
http://www.ks.uiuc.edu/Research/biocore/evaluation/vmd2003survey/VMD2003Survey.pdf

Table of Contents

*Features planned for future versions of VMD

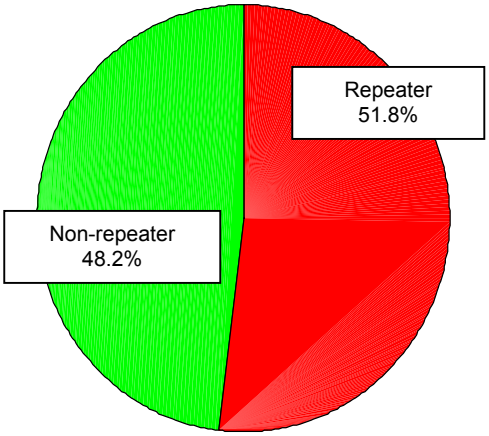
VMD USER PROFILE

The user profile characteristics are illustrated below.

- 51.8% are repeat users of VMD
- 84.0% have academic affiliations
- 19.8% are funded at least partially by NIH
- 81.1% use VMD for research purposes
- 11.7% consider themselves expert users of VMD
- 48.8% are the sole users of VMD at their site
- 36.8% use VMD on a Linux platform

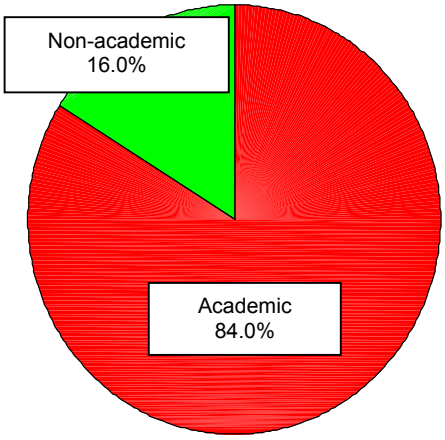
Figure 1: VMD User Characteristics

REPEAT USER STATUS



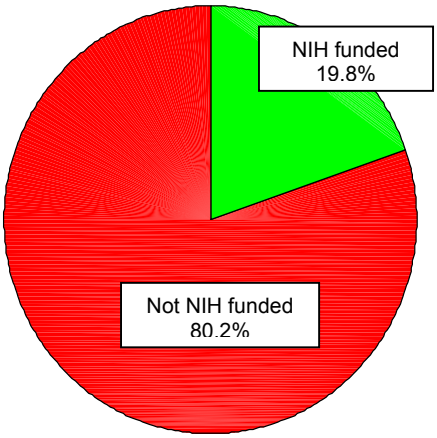
N= 1,112 repeaters, 1,034 non-repeaters

AFFILIATION



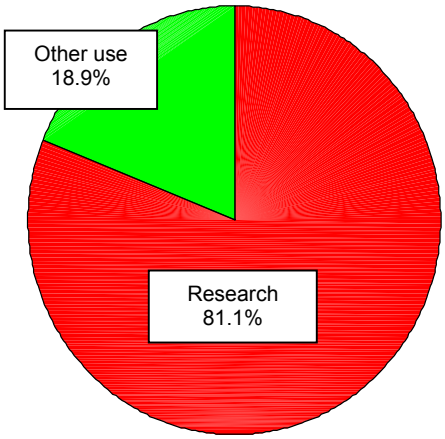
N= 1,800 academic, 343 non-academic

NIH FUNDING STATUS



N= 422 NIH funded, 1,709 not NIH funded

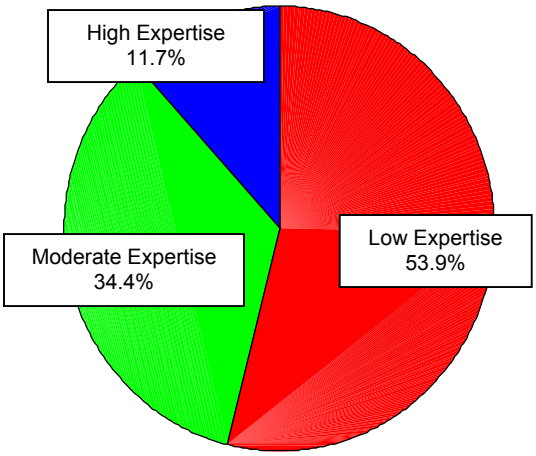
PRIMARY USE OF VMD



N= 1,740 research, 406 other use

Figure 1: VMD User Characteristics, continued

VMD EXPERTISE



Q. 4: My level of expertise in using VMD is . . .

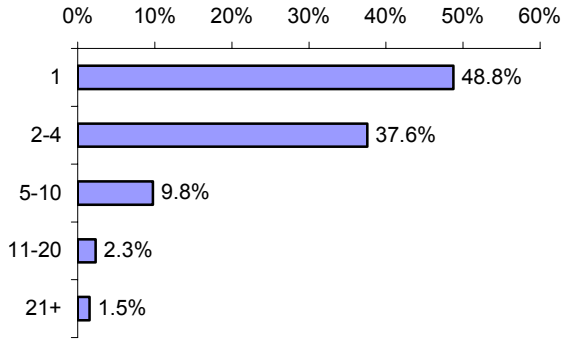
Expertise Level	N
Low	1,115
Moderate	738
High	250

Mean expertise: 2.34 on a 5-point scale, very low=1, very high=5 (scale collapsed to provide low, moderate, high categories used here)

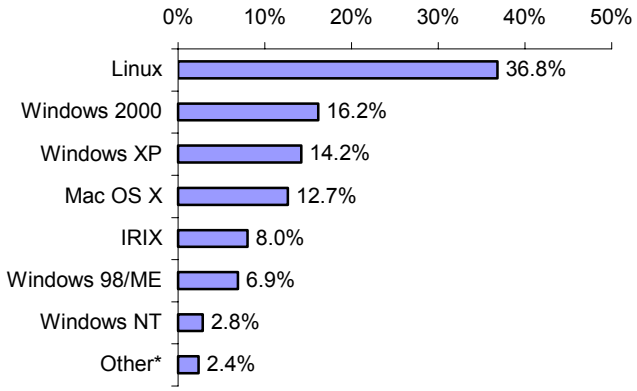
NUMBER USING VMD PER SITE

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

# at Site	N
1	1,043
2-4	804
5-10	209
11-20	50
21+	33



PLATFORM USED



Q. 5: I primarily use VMD on . . .

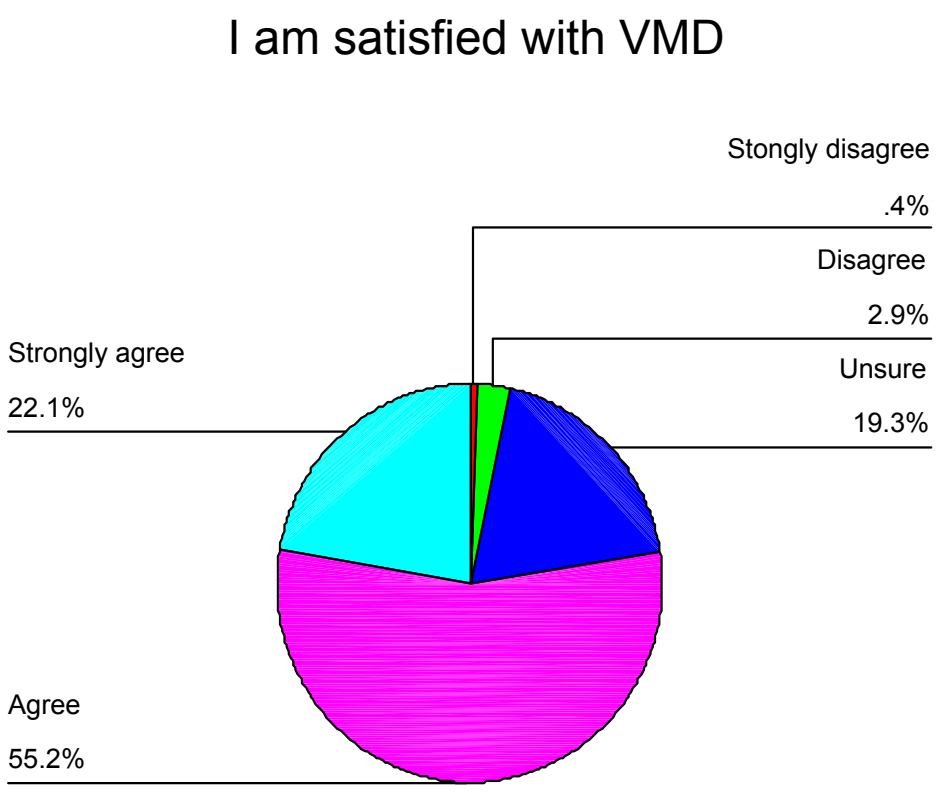
Platform	N
Linux	790
Windows 2000	347
Windows XP	305
Mac OS X	272
IRIX	172
Windows 98/ME	148
Windows NT	61
Other*	51

*Other (>26/1.5%): Solaris, Tru64 Unix , AIX , HP-UX, Other

RATINGS OF SATISFACTION

- A majority of users are satisfied with VMD – 77.3% agreed or strongly agreed with the statement "I am satisfied with VMD" (Q12). See Fig. 2.
- Mean satisfaction was 3.96 on a 5-point scale (1=strongly disagree, 5=strongly agree). See Fig. 2.
- While no significant difference was found it is worth noting that the mean satisfaction has increased since the prior VMD 2000 user survey, where mean satisfaction was 3.84.

Figure 2: Satisfaction with VMD



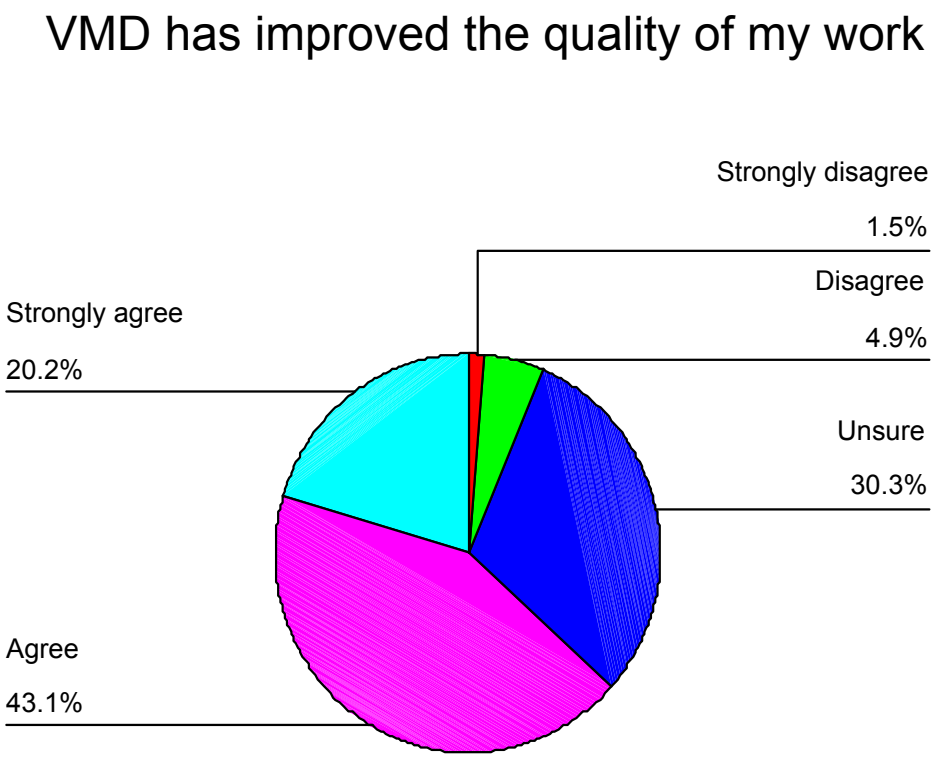
Value	Scale Item	Frequency		Distribution Statistics
1	Strongly disagree	9		Mean: 3.96
2	Disagree	61		Median: 4.00
3	Unsure	414		Mode: 4.00
4	Agree	1,182		Std Deviation: .75
5	Strongly agree	474		Total N= 2,140

RATINGS OF IMPACT ON WORK QUALITY

- VMD was judged to have a positive impact on work quality – 63.3% of the respondents agreed or strongly agreed with the statement "VMD has improved the quality of my work" (Q13). See Fig. 3.

- The mean response was 3.76 on a 5-point scale (1=strongly disagree, 5=strongly agree. See Fig. 3.

Figure 3: VMD Impact on Work Quality



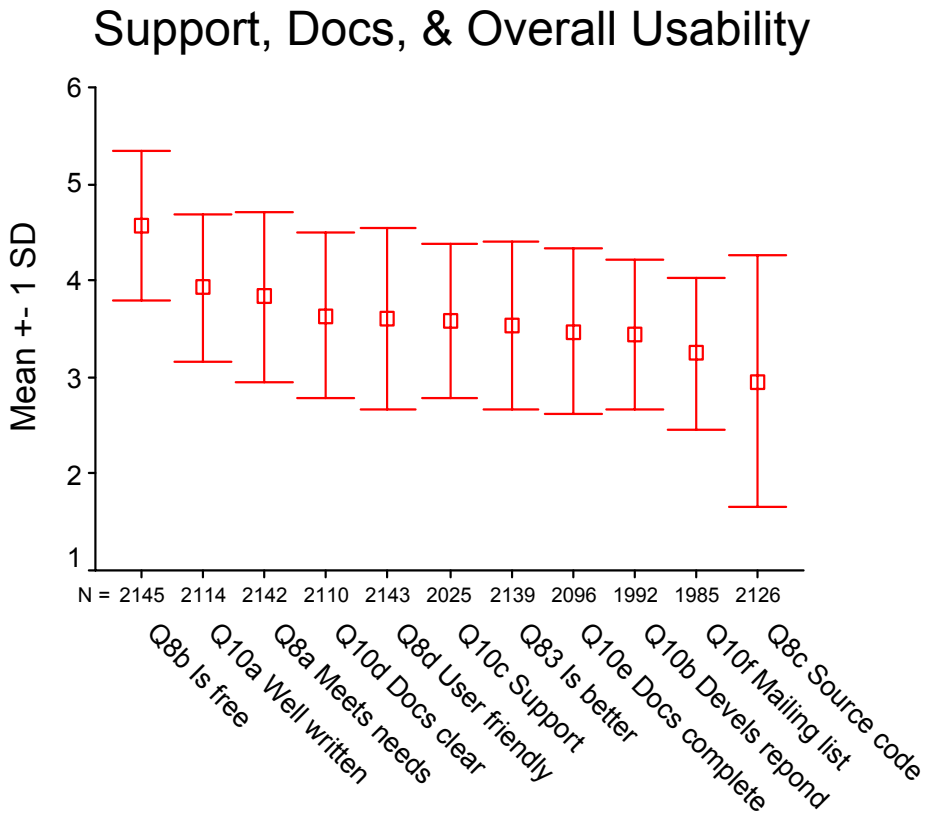
Value	Scale Item	Frequency		Distribution Statistics
1	Strongly disagree	31		Mean: 3.76
2	Disagree	104		Median: 4.00
3	Unsure	645		Mode: 4.00
4	Agree	918		Std Deviation: .88
5	Strongly agree	431		Total N= 2,129

RATINGS OF SUPPORT, DOCUMENTATION AND OVERALL USABILITY

- Responses to usability (Q8), and support and documentation items (Q10) indicated why respondents use VMD, and their agreement with statements about specific aspects of the program.

- The highest rated qualities are: VMD is free (M=4.57), VMD is a well-written program (M=3.93), and VMD meets user needs (M=3.83). A regression analysis found that the following factors explain much of the variation in respondents' overall satisfaction (Q12): VMD meets user needs (Q8a), VMD is well-written (Q10a), VMD is better than other molecular graphics programs (Q8e), documentation is clear (Q10d), support meets expectations (Q10c), and VMD is user friendly (Q8d). It is interesting to note here that the free availability of VMD was not found to be a predicting variable explaining satisfaction. See Figs. 4A, 4B.

Figure 4A: Support, Docs, and Overall Usability



Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree

Figure 4B: Support, Documentation, and Overall Usability		
Question Stem	Mean†	Std Deviation†
Q. 8 I use VMD because it:		
Q. 8b is free	4.57	0.77
Q. 8a meets my needs	3.83	0.89
Q. 8d is user friendly	3.60	0.93
Q. 8e is better than other molecular graphics programs	3.53	0.86
Q. 8c includes source code	2.95	1.31
Q. 10 Indicate your level of agreement with the statements describing VMD:		
Q. 10a VMD is a well written program	3.93	0.76
Q. 10d VMD documentation is clear	3.63	0.86
Q. 10c VMD support meets my expectations	3.58	0.79
Q. 10e VMD documentation is complete	3.47	0.86
Q. 10b VMD developers respond to my requests	3.45	0.78
Q. 10f The VMD-L mailing list is useful	3.25	0.79

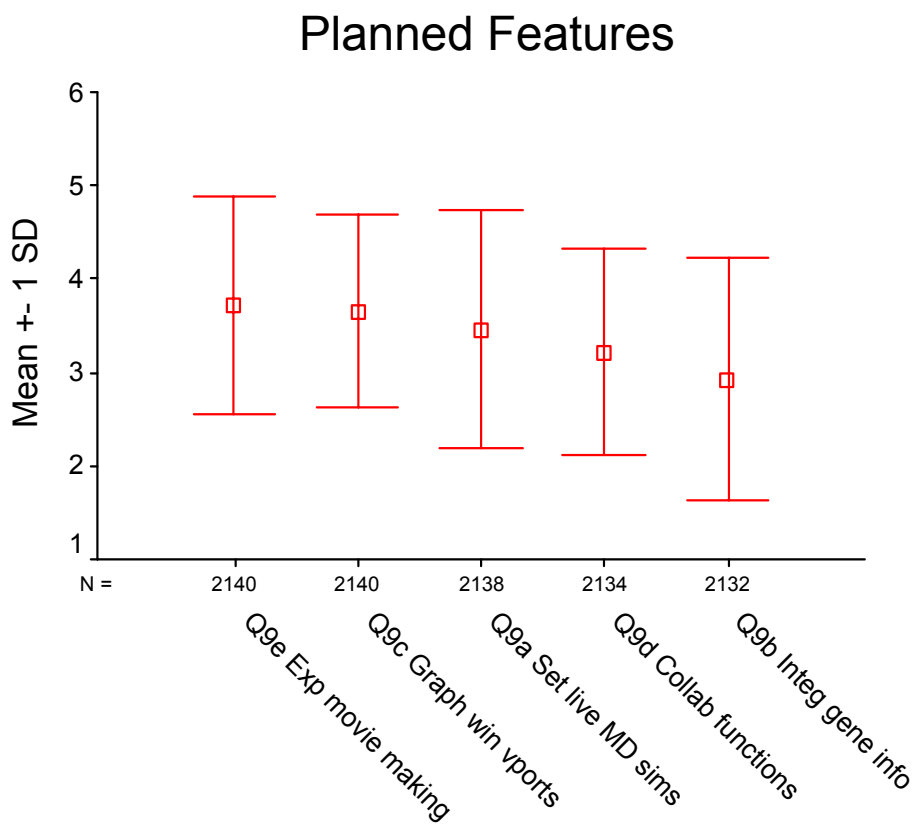
†Figures based on a 5-point scale, with responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.

RATINGS OF PLANNED FEATURES

- Planned features are functionalities being considered for future versions of VMD, e.g. adding a function to integrate genetic information. In Q9 on the survey, users were asked to rate the value of five planned features to their work, using a 5-point importance scale (1-very unimportant, 5-very important).

- Mean results indicated that the most desirable feature is expanded movie making (M=3.72), and the least desirable one is the integration of genetic information (M=2.93). See Figs. 5A, 5B.

Figure 5A: Ratings of Planned Features



Responses: 1-Very unimportant, 2-Unimportant, 3-Unsure, 4-Important, 5-Very important.

Figure 5B: Planned Item Ratings, continued		
Question Stem	Mean†	Std Deviation†
Q. 9e. Expanded movie making	3.72	1.17
Q. 9c. Multiple graphic windows, multiple viewports	3.66	1.03
Q. 9a. Setup and interaction with live MD simulations	3.46	1.28
Q. 9d. Collaborative functions	3.22	1.10
Q. 9b. Integration of genetic information	2.93	1.30

†Figures based on a 5-point scale, with responses: 1-Very unimportant, 2-Unimportant, 3-Unsure, 4-Important, 5-Very important.

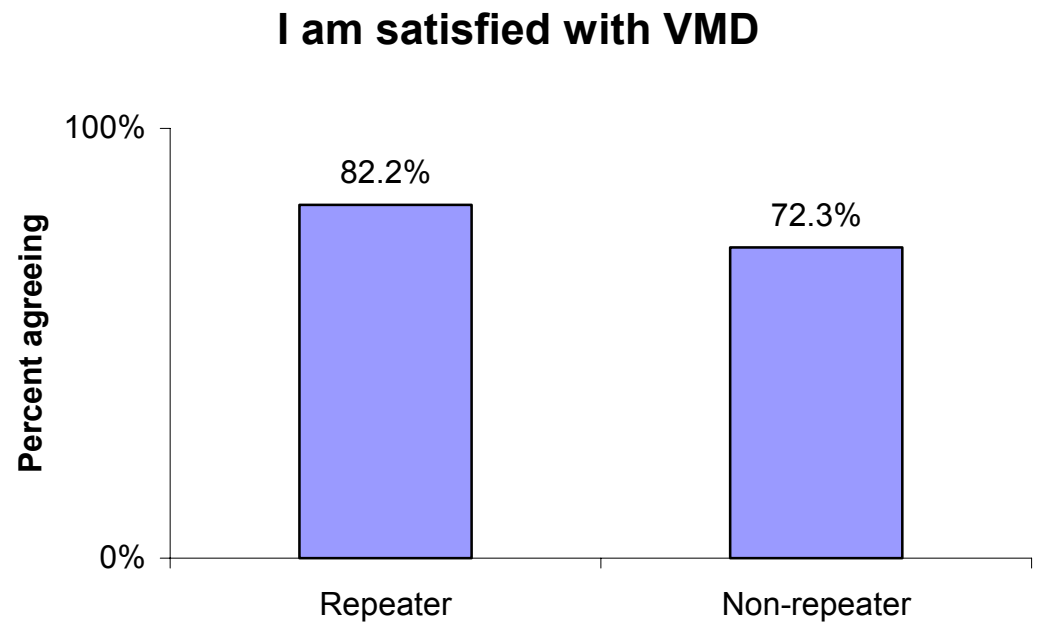
RATINGS BY REPEAT/NONREPEAT USERS

- Repeaters are users who have downloaded more than one version of VMD. Non-repeaters are users who downloaded only one version of VMD by the time they were contacted for the survey.

- A majority of both repeaters (82.2%) and non-repeaters (72.3%) agreed or strongly agreed with the statement "I am satisfied with VMD" (Q12). Mean comparisons indicate repeaters (M=4.05) are significantly more satisfied with VMD than non-repeaters (M=3.86). See Fig. 6A.

- A majority of both repeaters (70.8%) and non-repeaters (55.3%) agree that VMD has improved the quality of their work (Q13). Mean comparisons indicate that repeaters (M=3.90) are significantly more likely to feel VMD has improved their work than non-repeaters (M=3.60). See Fig. 6B.

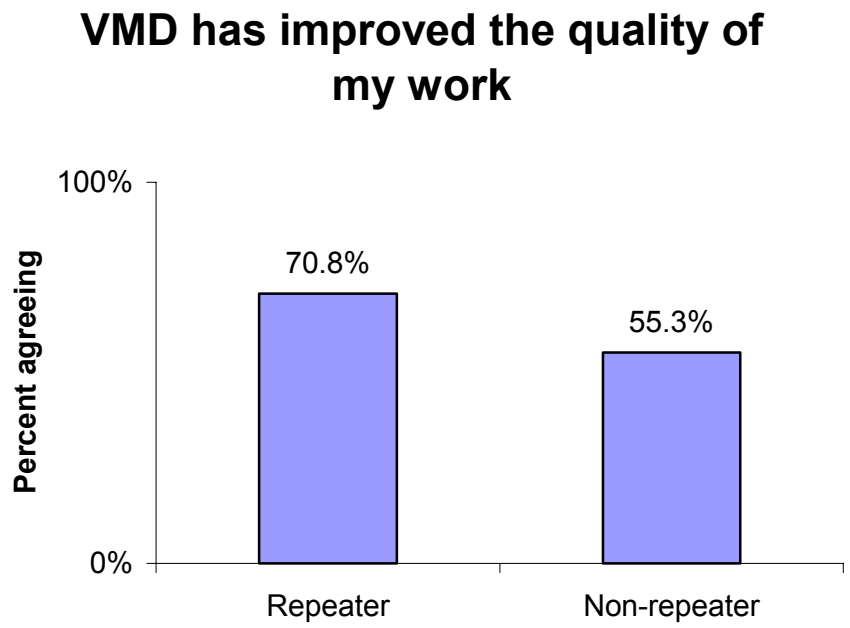
Figure 6A: Satisfaction by Repeat/Non-repeat User Status



Distribution Statistics					
Mean/Std Deviation	Repeater M=4.05, SD=.74		Non-repeater M=3.86, SD=.76		
Scale Responses†	SD	D	U	A	SA
Repeater (N/%)	4/.4%	27/2.4%	167/15.0%	620/55.9%	292/26.3%
Non-repeater (N/%)	5/.5%	34/3.3%	247/24.0%	562/54.6%	182/17.7%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Repeater, N=1,110; Non-repeater, N=1,030

Figure 6B: Work Quality by Repeat/Non-repeat User Status



Distribution Statistics					
Mean/Std Deviation	Repeater M=3.90, SD=.86		Non-repeater M=3.60, SD=.87		
Scale Responses†	SD	D	U	A	SA
Repeater (N/%)	13/1.2%	40/3.6%	269/24.4%	499/45.2%	283/25.6%
Non-repeater (N/%)	18/1.8%	64/6.2%	376/36.7%	419/40.9%	148/14.4%

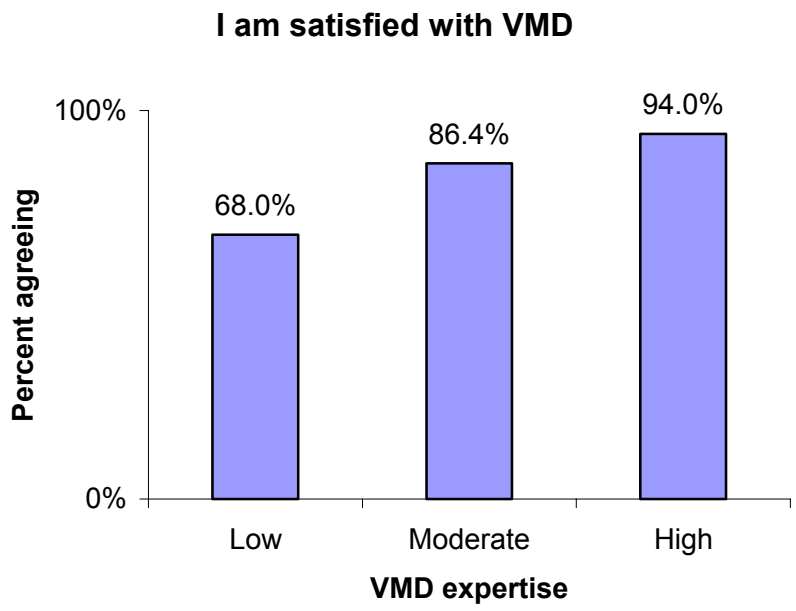
†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Repeater 1,104; Non-repeater 1,025

RATINGS BY LEVEL OF VMD EXPERTISE

- A majority of users across the three expertise levels* agreed or strongly agreed (low-68.0%; moderate-86.4%; high-94.0%) with the statement "I am satisfied with VMD" (Q12). Mean comparisons indicate significant differences among all levels of expertise – high expertise users (M=4.37) are significantly more satisfied than both moderate (M=4.09) and low expertise users (M=3.78); moderate users are significantly more satisfied than low expertise users. See Fig. 7A.

- A majority of moderate (76.6%) and high (83.2%) expertise users agreed or strongly agreed with the statement "VMD has improved the quality of my work" (Q12), while half (50.5%) of low expertise users indicated agreement. As with satisfaction, there were significant mean differences between the high (M=4.21), moderate (M=3.99) and low (M=3.51) expertise users, with high expertise users indicating the strongest agreement with the work quality statement. See Fig. 7B.

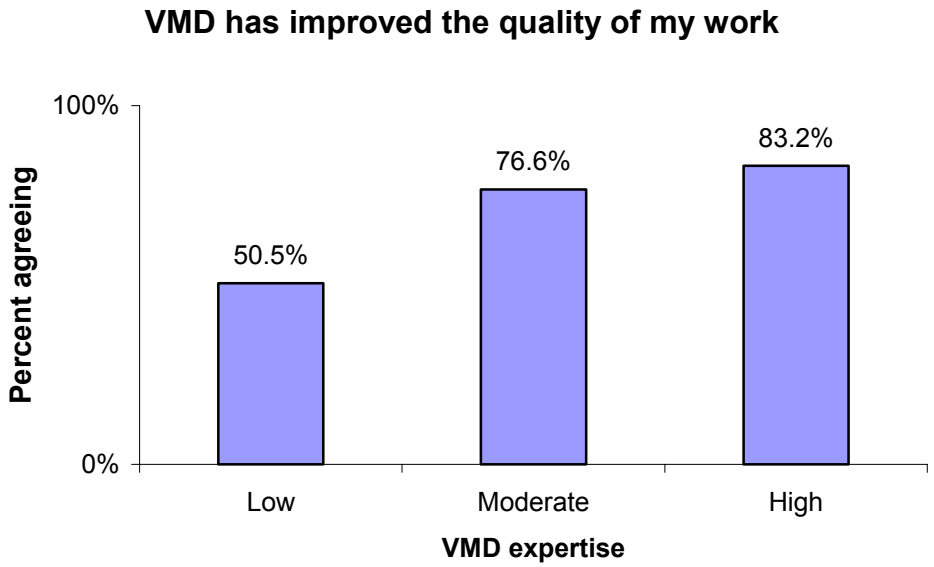
Figure 7A: Satisfaction by Level of VMD Expertise



Distribution Statistics					
Mean/Std Deviation	Low exp.:3.78/.78		Mod exp: 4.09/.65		High exp: 4.37/.65
Scale Responses†	SD	D	U	A	SA
Low expertise (N/%)	6/.5%	52/4.5%	311/27.0%	598/52.0%	184/16.0%
Mod. expertise (N/%)	2/.3%	7/1.0%	91/12.4%	459/62.4%	177/24.0%
High expertise (N/%)	1/.4%	2/.8%	12/4.8%	123/49.2%	112/44.8%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Low expertise 1,151; Moderate expertise 736; High expertise 2,137

Figure 7B: Work Quality by Level of VMD Expertise



Distribution Statistics					
Mean/Std Deviation	Low exp.:3.51/.89		Mod exp: 3.99/.76		High exp: 4.21/.77
Scale Responses†	SD	D	U	A	SA
Low expertise (N/%)	28/2.4%	83/7.3%	455/39.8%	430/37.6%	147/12.9%
Mod. expertise (N/%)	2/.3%	18/2.5%	152/20.7%	378/51.6%	183/25.0%
High expertise (N/%)	1/.4%	3/1.2%	38/15.2%	108/43.2%	100/40.0%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Low expertise 1,143; Moderate expertise 733; High expertise 2,126

- The three expertise groups were significantly different from each other in nearly all their ratings of support, documentation, and overall usability (Q8 & Q10), with the high expertise group always producing the highest means, followed in order by the moderate and low expertise group means. Exceptions are ratings regarding the program being free and providing source code – differences here are between the high and low expertise groups only.

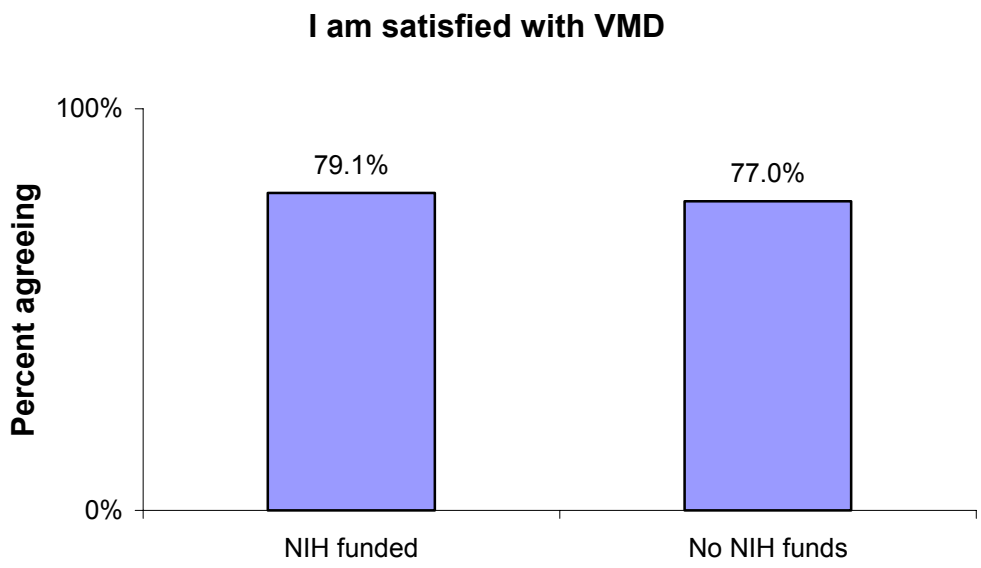
- For planned items (Q9), significant differences by expertise level are limited to the need for multiple windows and viewports (all groups different), collaborative functions, and expanded movie making (low different than moderate and high groups for both). As above, mean ratings increased with level of expertise.

*Level of expertise categories were derived from the survey question "My level of expertise in using VMD is . . ." (Q4) that users answered on a 5-point scale (1-very low, 5-very high). For ease of interpretation, the two lowest expertise values were collapsed together, as were the two highest expertise categories, to produce the low, moderate, high expertise categories used above.

RATINGS BY NIH FUNDING STATUS

- Users were asked to answer 'yes' or 'no' to the question "The work I do with VMD is funded (at least partially) by NIH" (Q3).
- A majority of both NIH funded (79.1%) and those with no NIH funds (77.0%) agreed or strongly agreed with the statement "I am satisfied with VMD" (Q12). Statistical analysis showed no significant difference in mean rankings by NIH funding status for satisfaction (NIH-funded M=3.98 and others M=3.95 respectively). See Fig. 8A.
- A majority of both NIH funded (68.4%) and those with no NIH funds (62.0%) indicated agreement with the statement "VMD has improved the quality of my work" (Q13). A significant difference was found between the means for NIH funded users (M=3.88) and users with no NIH funds (M=3.73). See Fig. 8B

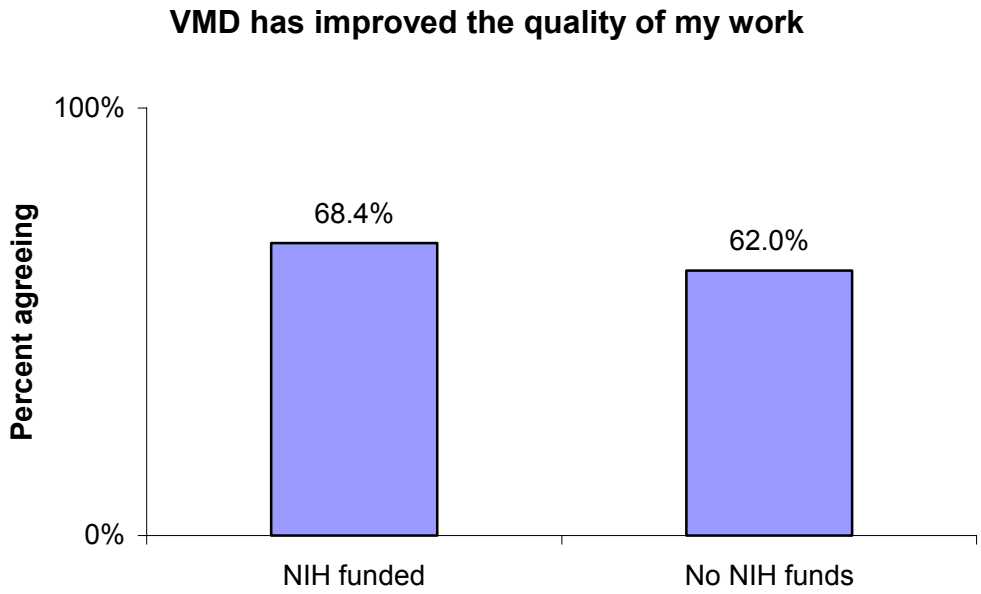
Figure 8A: Satisfaction by NIH Funding Status



Distribution Statistics					
Mean/Std Deviation	NIH funded M=3.98, SD=.77		No NIH funds M=3.95, SD=.75		
Scale Responses†	SD	D	U	A	SA
NIH funded (N/%)	4/1.0%	11/2.6%	73/17.3%	234/55.6%	99/23.5%
No NIH funds (N/%)	5/.3%	50/2.9%	338/19.8%	940/55.2%	371/21.8%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: NIH funded 421, no NIH funds 1,704

Figure 8B: Work Quality by NIH Funding Status



Distribution Statistics					
Mean/Std Deviation	NIH funded M=3.88, SD=.90		No NIH funds M=3.73, SD=.87		
Scale Responses†	SD	D	U	A	SA
NIH funded (N/%)	7/1.7%	16/3.8%	109/26.1%	176/42.1%	110/26.3%
No NIH funds (N/%)	24/1.4%	88/5.2%	533/31.4%	734/43.3%	317/18.7%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: NIH funded 418, no NIH funds 1,696

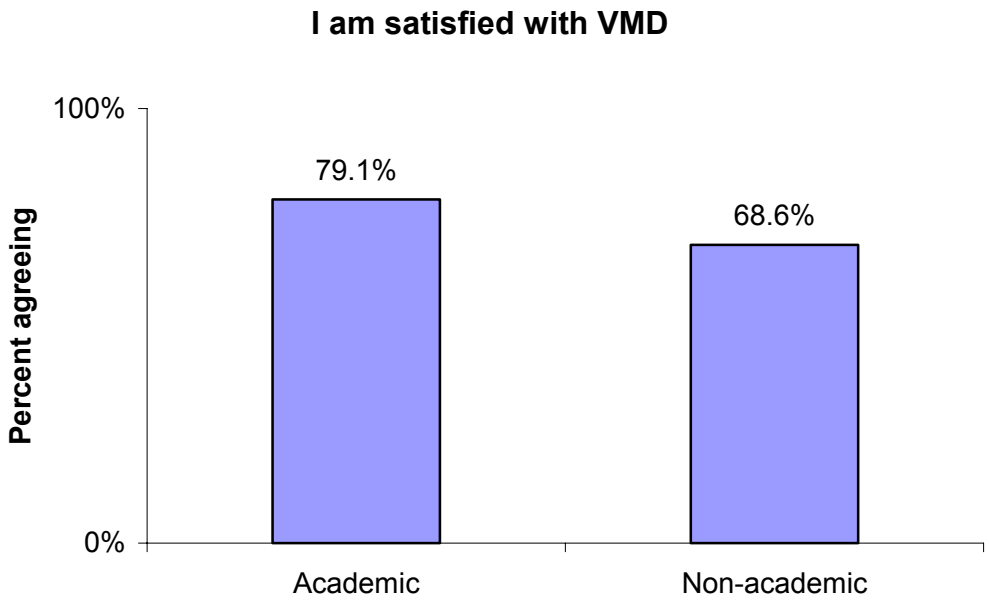
RATINGS BY ACADEMIC/NON-ACADEMIC AFFILIATION

- Survey respondents were asked to identify their affiliation as academic, government, industry, or other (Q2); below are findings by academic/non-academic categories.

- A majority of both academic (79.1%) and non-academic (68.6%) users agreed or strongly agreed with the statement "I am satisfied with VMD" (Q12). A significant difference was found for mean satisfaction by affiliation, with academic users (M=3.98) more satisfied with VMD than non-academic users (M=3.83). See Fig. 9A.

- Ratings of work quality indicate a majority of both academic (65.2%) and non-academic users (53.4%) agreed or strongly agreed with the statement "VMD has improved the quality of my work" (Q13). Our analysis shows that the mean for academic users (M=3.79) is significantly higher than the mean for non-academic users (M=3.61). See Fig. 9B.

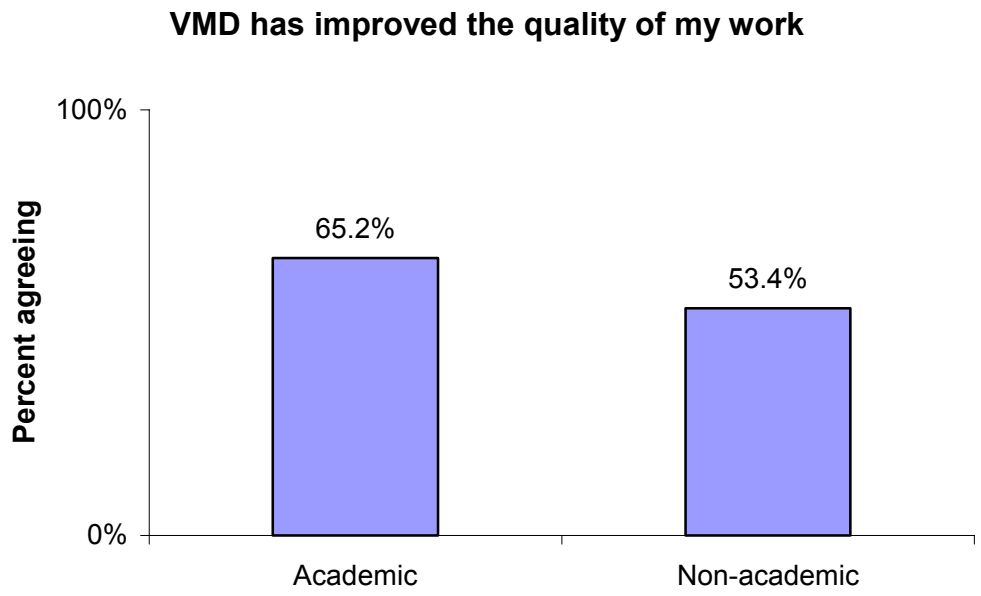
Figure 9A: Satisfaction by Academic Affiliation



Distribution Statistics					
Mean/Std Deviation	Academic M=3.98, SD=.73		Non-academic M=3.83, SD=.86		
Scale Responses†	SD	D	U	A	SA
Academic (N/%)	5/.3%	43/2.4%	328/18.3%	1020/56.8%	400/22.3%
Non-academic (N/%)	4/1.2%	17/5.0%	86/25.2%	160/46.9%	74/21.7%

†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Academic 1,796, Non-academic 341

Figure 9B: Work Quality by Academic Affiliation



Distribution Statistics					
Mean/Std Deviation	Academic M=3.79, SD=.86		Non-academic M=3.61, SD=.96		
Scale Responses†	SD	D	U	A	SA
Academic (N/%)	24/1.3%	76/4.3%	521/29.2%	803/44.9%	363/20.3%
Non-academic (N/%)	7/2.1%	27/8.0%	124/36.6%	113/33.3%	68/20.1%

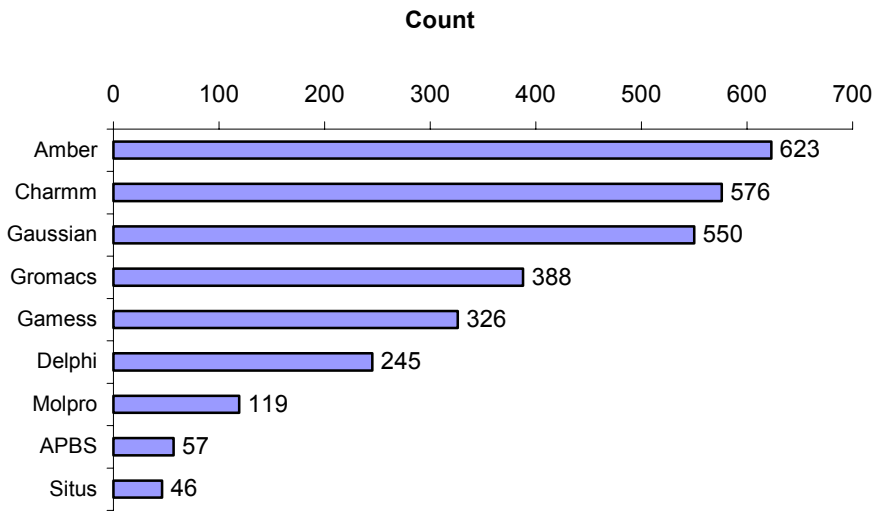
†Responses: 1-Strongly disagree, 2-Disagree, 3-Unsure, 4-Agree, 5-Strongly agree.
Total N: Academic 1,787, Non-academic 339

OTHER SOFTWARE TOOLS USED AND RATINGS OF WILLINGNESS TO CITE VMD

- Two items on the survey asked about other software tools used by respondents, and one item asked about willingness to cite VMD.

Figure 10: Other Software Tools Used & Ratings of Willingness to Cite VMD

A. APPLICATIONS TO USE WITH VMD



Q. 11: "I would benefit from using VMD with the following tools in my work: (check all that apply)."

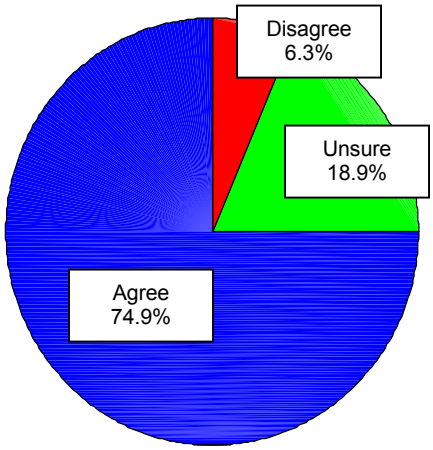
Most popular:
- Amber-623
- Charmm-576
- Gaussian-550

B. OTHER MOLECULAR GRAPHICS PROGRAMS USED

Q14: "In addition to VMD, I often use these other molecular graphics programs in my work."

- Respondents listed about 250 programs.
- Top six programs listed by 5% or more of respondents in this order of popularity: Rasmol, Swiss PDB Viewer, Pymol, Insight II, Molmol, and Molden.

C. WILLINGNESS TO CITE VMD



Q. 15 – "I would cite my use of VMD in resulting publications."

A clear majority, 74.9% agreed or strongly agreed with the above statement. 18.9% were unsure and 6.3% disagreed that they would cite their use of VMD in a publication.

APPENDIX: SURVEY METHODOLOGY

Following are details about the administration of the survey, including survey method, target population, survey schedule and response rates, sample validity, and questions used on the survey.

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 asked 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 VMD versions 1.7 through 1.8 defined the target population of the survey. Versions of VMD included in this set are as follows (versions with 'a' and 'b' in them are alpha or beta test versions):

- 1.7, 1.7.1b1, 1.7.1, 1.7.2, 1.8a10, 1.8a16, 1.8a21, 1.8a29, 1.8b2, 1.8

VMD registration records were accessed to obtain e-mail addresses of users. Of 17,129 survey solicitations sent to the resulting e-mail addresses, 2,971 bounced (e.g. from outdated or false e-mail addresses), producing a final population of 14,158 solicitations received.

Survey Schedule and Response Rates

	Dates/Activities		
	Initial Solicitation	Reminder	Closing/Totals
	April 14	May 5	May 12
Total Population			
Number receiving by date	14,158	13,023	-
Number of responses to next date	1,135	1,011	2,221
Response rate for this population	8.02%	7.14%	15.16%
Repeat User Population			
Number receiving by date	7,334	6,689	-
Number of responses to next date	645	467	1,112
Response rate for this population	8.79%	6.37%	15.16%

Data Editing

Those responses that were considered incomplete were deleted from our dataset. The deletions fell into two categories: Unresponsive and duplicates.

- Unresponsive records were those instances in which respondents did not answer most of the questions in the survey, specifically those cases in which more than 28% of the questions were not answered.

- Duplicates were those instances in which there was more than one response for a person, based on their e-mail address.

Deletions left 2,146 valid records for analyses, as shown in the table below.

Deleted Survey Responses			
Deletions category	Unresponsive	Duplicates	Total
	55	20	75
Number of records in dataset after removing deletions			2,146

- The final response rate, after accounting for deleted records, is 15.2%.

Sample Validity

The validity of a sample size for representing an entire population is always a concern in survey research. Sample size calculators can provide measures of confidence intervals (+/- figures, i.e. 'margin of error') and confidence level measures (how certain you can be that an answer falls within a confidence interval). For a sample of 2,146 and a population of 14,158, using a standard test percentage of 50%, sample size calculations indicate that it can be said with 95% confidence that a given result for a question falls within a +/-2% confidence interval. (Figures were generated using Survey System sample size calculator: http://www.surveysystem.com/sscalc.htm).

Question Sets

To aid in interpreting survey results, it is useful to view the question stems viewed by survey participants. Below are the survey questions, grouped by purpose:

Demographic/User Information Questions:

Q. #	Topic	Question Stem	Scale
1	E-mail address	Auto-completed, but users could change	Text box
2	Affiliation	Academic, Government, Industry, Other (specify)	Select one, Text box (other)
3	Funding	The work I do with VMD is funded (at least partially) by NIH	Select Yes or No
4	VMD expertise	My level of expertise in using VMD is	1-5 scale, very low to very high
5	Platform	I primarily use VMD on: AIX, MacOS X, Windows 98/ME, HP-UX, Solaris, Windows NT, IRIX, Tru64 Unix, Windows 2000, Linux, Other, Windows XP	Select one
6	VMD use	I use VMD primarily for: Research, teaching, business, Personal	Select one
7	Site use	The number of people using VMD at my site is: 1, 2-4, 5-10, 11-20, 20+	Select one
11	Programs used	I would benefit from using VMD with the following tools in my work: APBS, Gamess, Amber, Delphi, Gaussian, Charmm, Situs, Molpro, Gromacs	Check all that apply
14	Programs used	In addition to VMD, I often use these other molecular graphics programs in my work	Three text boxes
15	Citing VMD	I would cite my use of VMD in resulting publications	1-5 scale, strongly disagree to strongly agree

Ratings of Support, Documentation, and Overall Usability: All ratings of existing items used the same 1-5 scale, ranging from strongly disagree to strongly agree.

Q. #	Question Stem
8	I use VMD because it
8a	meets my needs
8b	is free
8c	includes source code
8d	is user friendly
8e	is better than other molecular graphics programs
10	Indicate your level of agreement with the statements describing VMD
10a	VMD is a well written program
10b	VMD developers respond to my requests
10c	VMD support meets my expectations
10d	VMD documentation is clear
10e	VMD documentation is complete
10f	The VMD-L mailing list is useful

Planned Items: All planned items used the same 1-5 scale ranging from very unimportant to very important.

Q. #	Question Stem
9	Rate the importance of these PLANNED features to your work
9a	Setup and interaction with live MD simulations
9b	Integration of genetic information
9c	Multiple graphics windows, multiple viewports
9d	Collaborative functions
9e	Expanded movie making

Evaluation Questions:

Q. #	Question Stem	Scale
12	I am satisfied with VMD	1-5 scale, strongly agree to strongly disagree
13	VMD has improved the quality of my work	
16	What suggestions do you have for improving VMD and VMD support	Text area