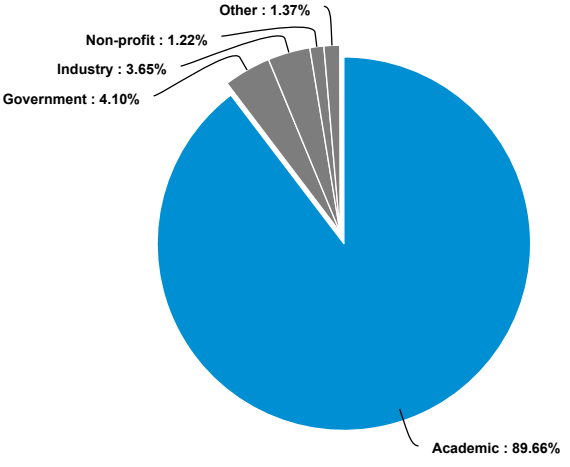
NAMD User Survey - Dashboard

VIEWED	STARTED	COMPLETED	COMPLETION RATE	DROP OUTS	TIME TO COMPLETE
1530	1117	673	60.25%	444	6 mins

Email Address

Email Address

What is your affiliation?



Answer	Count	Percent
Academic	590	89.67%
Government	27	4.1%
Industry	24	3.65%
Non-profit	8	1.22%
Other	9	1.37%
Total	**658**	**100 %**

What is your affiliation? - Text Data for Other

03/17/2016	49250624	private
03/16/2016	49238734	computer manufacturer
03/16/2016	49224752	comp oem
03/16/2016	49184750	Industry & Academic
03/16/2016	49179315	lay person
03/15/2016	49167901	HPC Solutions, inc.

03/15/2016	49154187	student
03/15/2016	49151939	Reutovskiy patsan
03/15/2016	49147107	Academic HPC Centre support staff

What is your area of study?

What is your area of study?		
04/06/2016	50238244	Biochemistry
04/05/2016	50152363	Biomedical Engineering
04/04/2016	50133124	Soft Matter
04/04/2016	50120427	biomedical engineering
04/01/2016	50017212	chemistry
04/01/2016	49986939	protein engineering
04/01/2016	49982422	Computational Chemistry / Computational Biophysics
03/31/2016	49970099	Biotechnology
03/31/2016	49962657	biomolecular kinetics and thermodynamics
03/31/2016	49952789	photosynthesis
03/29/2016	49817766	Chemistry
03/26/2016	49670038	Activ laser media
03/24/2016	49581588	Biophysics
03/24/2016	49564109	chemistry, biology
03/23/2016	49547891	Computational Biology
03/23/2016	49546663	DNA Nanotechnology
03/23/2016	49533042	Software Engineering
03/23/2016	49529792	chemical engineering
03/23/2016	49528191	Quantum chemical and spectral study
03/23/2016	49526597	Biochemistry and molecular biology
03/23/2016	49514885	enzymes
03/22/2016	49511665	computational biophysics
03/22/2016	49505218	Cancer research
03/22/2016	49504163	Structural biology
03/22/2016	49502338	Virology
03/22/2016	49500643	Chemistry - bacterial membranes
03/22/2016	49473036	physics
03/22/2016	49468724	linux admin
03/22/2016	49467437	Computer Science
03/21/2016	49458465	biophysics
03/21/2016	49451834	Biomolecular Simulation
03/21/2016	49446863	GPCR and Cannabinoids
03/21/2016	49440970	Bioinformatics and Computational Biology
03/21/2016	49438333	protein dynamics
03/21/2016	49436779	Polymorphisms and tunnel analysis
03/21/2016	49431208	Protein interactions / Extracellular matrix
03/21/2016	49427529	Computational Biology
03/21/2016	49425830	Theoretical Chemistry
03/21/2016	49423440	Computational Biochemistry
03/21/2016	49420451	Molecular study
03/20/2016	49415317	molecular modelling applied to cellulose
03/20/2016	49414349	rheology
03/20/2016	49409962	Chemistry
03/20/2016	49401700	Pharmacy

03/20/2016	49399568	visual molecular dynamics
03/20/2016	49391650	Computational Molecular Biology
03/19/2016	49387530	Biotechnology
03/19/2016	49386876	quantum chemistry
03/19/2016	49384908	chemistry
03/19/2016	49383805	Computer aided drug design
03/19/2016	49375381	molecular structural biology
03/19/2016	49372080	chemistry
03/19/2016	49371406	Computational biophysics
03/19/2016	49370820	Computational Chemistry
03/19/2016	49364561	Chemical - physical theory
03/19/2016	49361957	Chemistry
03/18/2016	49351270	protein crystal structure and function
03/18/2016	49349594	Protein Dynamics and resistance mutations
03/18/2016	49348261	
03/18/2016	49346768	Biochemistry
03/18/2016	49339790	computer-aided drug discovery
03/18/2016	49338443	Protein-protein interactions
03/18/2016	49334524	Accelerated Dynamics
03/18/2016	49334107	Computational Chemistry
03/18/2016	49324207	Biochemistry
03/18/2016	49320297	polymers
03/18/2016	49319847	drug engineering
03/18/2016	49318038	High Performance Computing
03/18/2016	49313281	Biomolecular Physics
03/18/2016	49311077	
03/18/2016	49308347	
03/17/2016	49305335	biophysical chemistry, MD simulatoin of proteins
03/17/2016	49304680	biophysics, molecular biology
03/17/2016	49304100	Computational Biology
03/17/2016	49298331	Biophysics
03/17/2016	49297814	Biophysics
03/17/2016	49292910	Nanotecnology
03/17/2016	49284809	Natural product chemistry
03/17/2016	49280558	bioconformation
03/17/2016	49280408	
03/17/2016	49274496	drug target, molecular modeling, protein structure
03/17/2016	49274001	carbon nanotubes, soft matter, biopolymers
03/17/2016	49274737	Chemistry
03/17/2016	49273575	Structure-function relationships in viruses
03/17/2016	49269781	Structural biology of DNA binding proteins
03/17/2016	49273170	Drug Vectors for Alzheimer's Disease
03/17/2016	49271223	membrane proteins and cancer biology
03/17/2016	49268017	Materials Chemistry
03/17/2016	49267767	Computational chemistry
03/17/2016	49267843	Drug Design / Protein-Ligand-Interactions
03/17/2016	49262479	Structural biology/NMR
03/17/2016	49262323	ligand gated ion channels
03/17/2016	49260940	structure biology
03/17/2016	49259611	peptide
03/17/2016	49256222	Biochemical and Molecular Pharmacology

03/17/2016	49257499	numerical computing
03/17/2016	49256383	Computational Chemistry and Biology
03/17/2016	49254725	Computational chemistry
03/17/2016	49253580	Biophysics
03/17/2016	49252386	Lipid membranes.
03/17/2016	49251541	Biochemistry
03/17/2016	49250624	Chemistry
03/17/2016	49250181	Computational Biophysics
03/17/2016	49249962	Mechanical engineering
03/17/2016	49247146	molecular biology
03/17/2016	49247349	computer simulation of organic materials and supramolecular systems
03/17/2016	49246812	biomass conversion
03/17/2016	49245968	
03/17/2016	49245226	Biophysics
03/17/2016	49244715	THz spectroscopy of biomolecules
03/17/2016	49244660	Computational chemistry
03/17/2016	49244323	
03/17/2016	49242397	computational biology, computational protein design
03/16/2016	49241367	medicinal chemistry
03/16/2016	49240796	Molecular dynamics and simulations
03/16/2016	49238734	software performance and benchmarking
03/16/2016	49238042	Antimicrobial resistsnce
03/16/2016	49237667	biophysics
03/16/2016	49231816	mechanical engineering
03/16/2016	49230444	Computational chemistry
03/16/2016	49228123	Biophysics
03/16/2016	49227310	Bichemistry/Structural biology
03/16/2016	49227244	Computational Molecular Biophysics
03/16/2016	49225359	bioinformatics - structural biology
03/16/2016	49224752	Theo Chem
03/16/2016	49222061	Life Sciences
03/16/2016	49220190	Physcis
03/16/2016	49219500	Biochem
03/16/2016	49219338	Biophysics
03/16/2016	49219042	Computational chemistry
03/16/2016	49218526	biocolloidal system (proteins, polymers)
03/16/2016	49216635	
03/16/2016	49216706	
03/16/2016	49215048	Structural biology
03/16/2016	49214265	ion channels, proteins,
03/16/2016	49214006	Molecular dynamics of stimuli-responsive polymer
03/16/2016	49213486	physics
03/16/2016	49212083	Biophysics
03/16/2016	49212556	Undergraduate Chemistry
03/16/2016	49211137	Systems Biology
03/16/2016	49211283	Bioinformatics
03/16/2016	49207737	homology modeling, molecular dynamics, virtual Screening, molecular docking, molecular biology.
03/16/2016	49209693	Physics
03/16/2016	49208902	MD simulation, mutations, stabilization, temperature, dockimg, layers
03/16/2016	49209601	Biophysics
03/16/2016	49208995	Biotech

03/16/2016	49206049	Medical parsitology-drug design-Biochemistry-biophysics,thermodynamics-Host-parasite interaction
03/16/2016	49207148	Computational math
03/16/2016	49206999	QM & relativity, electronic structure, MD sims., essentially anything
03/16/2016	49204826	Neurochemistry. protein structure and phramacology
03/16/2016	49204669	Food Science
03/16/2016	49204531	chemistry
03/16/2016	49202055	
03/16/2016	49201782	Cancer
03/16/2016	49199276	Synthesis and conformational analysis of biomolecules
03/16/2016	49199507	Computational chemistry
03/16/2016	49199894	physical chemistry
03/16/2016	49199059	Biophysics
03/16/2016	49198519	Chemistry
03/16/2016	49198832	Protein Folding
03/16/2016	49197768	Biomedical
03/16/2016	49197118	Theoretical and Computational Chemistry
03/16/2016	49196030	Basic Medical Research
03/16/2016	49196413	biology and physics
03/16/2016	49196131	Soft matter physics
03/16/2016	49195977	structure biology
03/16/2016	49195392	Molecular Dynamics Simulations, nanoparticles, water-protein dynamics
03/16/2016	49193466	Drug Discovery, Virology, HIV, HCV, HBV, immuno-oncology
03/16/2016	49194555	molecular interaction prediction
03/16/2016	49194157	chemistry
03/16/2016	49194525	Computer Science
03/16/2016	49193240	
03/16/2016	49193858	food engineering
03/16/2016	49193353	proteins
03/16/2016	49193002	Milecular biophysics
03/16/2016	49193273	Computational Bioelectromagnetics
03/16/2016	49193263	Biomembrane structure and interactions
03/16/2016	49192944	Biochemistry
03/16/2016	49192277	Bioinformatics, Molecular Modelling
03/16/2016	49189917	IT
03/16/2016	49189930	Biophysics
03/16/2016	49189318	HPC
03/16/2016	49188694	Biochemistry
03/16/2016	49188356	computational chemistry, drug discovery
03/16/2016	49188209	Extracellular matrix proteins/peptides
03/16/2016	49187552	Membrane Proteins
03/16/2016	49187632	
03/16/2016	49185823	Chemistry
03/16/2016	49187151	peptide-lipid interactions
03/16/2016	49186580	Chemistry
03/16/2016	49185588	macromolecules
03/16/2016	49185731	Bio and nano photonics
03/16/2016	49183836	Computational Materials Science
03/16/2016	49185400	Biophysics of membrane proteins
03/16/2016	49184750	
03/16/2016	49184937	Structural bioinformatics

03/16/2016	49184846	Colloids and Interfaces (interaction of ions with proteins, polymers, surfaces...)
03/16/2016	49184939	Computational Chemistry
03/16/2016	49184550	computational chemistry
03/16/2016	49184186	Protein structure
03/16/2016	49184237	Computational Chemistry
03/16/2016	49184158	Computing and Molecular Simulation in Membranes
03/16/2016	49183460	pharmarcutical science
03/16/2016	49181902	High Performance Computing
03/16/2016	49183247	theoretical and computational chemistry
03/16/2016	49182412	biomechanics
03/16/2016	49182434	PAH extraction from napha
03/16/2016	49182551	Chemistry
03/16/2016	49182399	Structural Biology
03/16/2016	49181879	Biophysical Chemistry
03/16/2016	49180654	Computational Structural Biology
03/16/2016	49181400	chemistry
03/16/2016	49181353	Protein crystallography
03/16/2016	49181413	Molecular dynamics of proteins
03/16/2016	49180746	Computational Biophysics
03/16/2016	49181166	Biochemistry
03/16/2016	49181054	Biophysics
03/16/2016	49180534	Biophysics
03/16/2016	49180335	Biomolecular Simulation
03/16/2016	49180400	drug design
03/16/2016	49180200	NAMD performance on Intel architecture
03/16/2016	49180144	kinetics
03/16/2016	49179947	Drug Design
03/16/2016	49179730	molecular modeling and numerical simulation of protein-ligand interactions
03/16/2016	49179392	Structure Based Drug Design
03/16/2016	49179315	i'm learning how our body works in nano-scale.
03/16/2016	49179363	computational biophysics, computational chemistry
03/16/2016	49179373	Biochemistry - biophysics
03/16/2016	49179291	protein molecular dynamics
03/16/2016	49179050	chemistry
03/16/2016	49178756	Biosimulation
03/16/2016	49178582	structural bioinformatics
03/16/2016	49179086	Structural biology
03/16/2016	49179017	Quantum Chemistry and Molecular modelling of biological system
03/16/2016	49178964	Structural biology
03/16/2016	49178721	lipids
03/16/2016	49178170	biophysics
03/16/2016	49178277	Physical chemistry, molecular recognition
03/16/2016	49178173	Physical Chemistry
03/16/2016	49177998	Physical Chemistry of Materials and Biochemicals
03/16/2016	49177887	Theoretical Biophysics
03/16/2016	49177810	G protein-coupled receptor modeling and simulation
03/16/2016	49177724	computational structural biology
03/16/2016	49177633	Membrane biophysics
03/16/2016	49177711	Structural Biology
03/16/2016	49177523	
03/16/2016	49177466	drug design

03/16/2016	49177548	Structural Biology
03/16/2016	49177382	computational chemistry
03/16/2016	49177364	
03/16/2016	49177282	biomolecules
03/16/2016	49177036	Biophysics, Membranes, Membrane Proteins
03/16/2016	49176398	biological macromolecules modelling
03/16/2016	49176768	GPCR - ligand interactions in explicit membrane system
03/16/2016	49176652	interaction protein-ligand
03/16/2016	49176775	Drug discovery
03/16/2016	49176365	Drug Design, Selectivity, Protein flexibility
03/16/2016	49176330	Structural biology
03/16/2016	49176231	protein crystallography
03/16/2016	49175197	Computational biophysics
03/15/2016	49175627	enzymology
03/15/2016	49175565	protein lipase
03/15/2016	49175409	Supporting science done via modelling
03/15/2016	49175583	structural biology
03/15/2016	49175533	Studying membrane proteins
03/15/2016	49175395	biochemistry
03/15/2016	49175193	biochemistry
03/15/2016	49174847	biomedical, nanotechnology
03/15/2016	49174859	adsorption, heterogeneous catalysis
03/15/2016	49174506	
03/15/2016	49174881	Computational biochemistry
03/15/2016	49174725	Chromatine structure
03/15/2016	49174633	Biochemistry - Biophysics
03/15/2016	49174553	medicinal chemistry and Molecular modeling
03/15/2016	49174386	
03/15/2016	49174151	Protein and peptide Self-assembly
03/15/2016	49174266	computaional biology
03/15/2016	49174053	Adsorbtion on activated carbons
03/15/2016	49173992	First principle study on Proteins and their interaction mechanism
03/15/2016	49173925	
03/15/2016	49173581	Molecular Dynamics
03/15/2016	49173785	laser media
03/15/2016	49173534	biochemistry
03/15/2016	49173719	molecular modeling and drug designing
03/15/2016	49173438	Computational biology
03/15/2016	49173327	Chemistry
03/15/2016	49173041	drug discovery and proteomics
03/15/2016	49173019	structural biology
03/15/2016	49172735	SAR and drug design
03/15/2016	49172715	Structural biology, especially of membrane proteins
03/15/2016	49172511	nano-mechanics
03/15/2016	49172449	pharmacology
03/15/2016	49172375	Bioinformatics
03/15/2016	49172198	Computational structural biology
03/15/2016	49172212	Biophysics
03/15/2016	49171774	Computational Biophysics
03/15/2016	49171895	Plant Biology
03/15/2016	49171694	Molecular modeling in computer aided drug discovery

03/15/2016	49171835	soft matter physics
03/15/2016	49171803	structural biology
03/15/2016	49171534	Chemistry
03/15/2016	49171445	metallo enzyme
03/15/2016	49171410	Biotechnology
03/15/2016	49171084	Chemoinformatics
03/15/2016	49171049	Molecular Biology
03/15/2016	49170915	materials modeling
03/15/2016	49170663	Nanobiotechnology
03/15/2016	49170497	molecular modelling
03/15/2016	49169581	Molecular Biology
03/15/2016	49170022	computer modeling
03/15/2016	49169878	colloid systems
03/15/2016	49170043	Medical Science - Virology
03/15/2016	49168646	Bioinformatics
03/15/2016	49169441	Mechanical Engineering
03/15/2016	49169289	high performance computing
03/15/2016	49169407	
03/15/2016	49169273	Biochemistry
03/15/2016	49169082	Biochemistry
03/15/2016	49169366	MD
03/15/2016	49167901	benchmarking for sales
03/15/2016	49169214	Molecular Biology
03/15/2016	49169000	Desalination
03/15/2016	49168968	
03/15/2016	49168679	Computational science
03/15/2016	49169013	Biochemistry
03/15/2016	49168534	Plant Protein Structure and Biochemistry
03/15/2016	49168864	nanopore
03/15/2016	49168522	ion transport
03/15/2016	49168525	
03/15/2016	49168621	Biophysics
03/15/2016	49168411	structural bioinformatics
03/15/2016	49168474	Computational Biophysics
03/15/2016	49168400	Chemistry
03/15/2016	49168373	nanofluidics
03/15/2016	49168384	chemistry
03/15/2016	49168273	Membrane Biophysics / Protein Design
03/15/2016	49168150	Biochemistry
03/15/2016	49168095	
03/15/2016	49166964	biophysicalchemistry, ionic hydration
03/15/2016	49167903	Ion channels, GABAA receptors
03/15/2016	49168043	structural biology
03/15/2016	49167716	Biophysics & Chemistry
03/15/2016	49167735	biophysics
03/15/2016	49167696	Quantum chemistry, theoretical chemistry
03/15/2016	49167410	Chemistry
03/15/2016	49166850	Ab Initio Molecular Dynamics
03/15/2016	49166864	MD simulation, QM/MM, Free Energy
03/15/2016	49166591	Enzymology

03/15/2016	49166672	Computer Science
03/15/2016	49166481	biophysics
03/15/2016	49166417	
03/15/2016	49166390	Serine proteases involved in coagulation
03/15/2016	49166208	Biophysics
03/15/2016	49166257	Natural Products Chemistry
03/15/2016	49165926	Nuclear Engineering
03/15/2016	49165578	LGICs
03/15/2016	49164417	Thermodynamic properties of proteins
03/15/2016	49165324	
03/15/2016	49165286	Protein modelling ater experimental data
03/15/2016	49165188	drug development
03/15/2016	49165303	QM/MM
03/15/2016	49164420	peptide adsorption
03/15/2016	49164384	biochemistry
03/15/2016	49164278	Biophysics
03/15/2016	49164467	Mathematics
03/15/2016	49164348	MD simulations of biomolecules
03/15/2016	49164006	Biotecnology
03/15/2016	49163943	Biophysics of transporter proteins
03/15/2016	49163754	biochemistry
03/15/2016	49163190	
03/15/2016	49163610	Cryo electron microscopy
03/15/2016	49163573	Biochemistry
03/15/2016	49162586	Chemistry
03/15/2016	49163198	Medicinal Chemistry
03/15/2016	49163269	molecular dynamics simulation
03/15/2016	49163185	Computational Biophysics
03/15/2016	49162870	membrane biophysics
03/15/2016	49160674	Ligand-Protein interactions
03/15/2016	49161545	Computational chemistry, polymer science, structural biology
03/15/2016	49162201	molecular dynamic of polymers
03/15/2016	49162490	molecular modelling
03/15/2016	49161930	Drugdesign
03/15/2016	49162388	Computational Biology
03/15/2016	49161948	
03/15/2016	49161951	Membranes
03/15/2016	49161485	computational biology
03/15/2016	49161310	Biomolecular Modeling
03/15/2016	49159897	Chemistry
03/15/2016	49160382	NeuroPhysics.
03/15/2016	49160218	materials
03/15/2016	49160480	Computational Biology
03/15/2016	49160024	Pharmaceutical chemistry
03/15/2016	49159883	Enzymatic reactions
03/15/2016	49159494	Physical chemistry
03/15/2016	49159801	biochemistry
03/15/2016	49159422	Biophysics
03/15/2016	49159253	Theoretical biophysics
03/15/2016	49159416	Protein Design
03/15/2016	49159047	Medicinal Chemistry

03/15/2016	49158789	Chemistry
03/15/2016	49158782	mathematics; parallel and high performance computing
03/15/2016	49158343	bioenergetics
03/15/2016	49158520	Biological Engineering
03/15/2016	49158566	crystallography
03/15/2016	49158281	Chemical Engineering
03/15/2016	49158609	Biochemistry
03/15/2016	49158537	Physics
03/15/2016	49157715	biophysics
03/15/2016	49158086	Biophysical Chemistry
03/15/2016	49152898	Structural Biochemistry
03/15/2016	49156338	Mechanical Engineering
03/15/2016	49157368	Biomedical Engineering
03/15/2016	49157023	esterases
03/15/2016	49156824	sub-THz spectroscopy
03/15/2016	49157177	Physical Chemistry
03/15/2016	49156356	Bioinformatics: docking, molecular dynamics; drug discovery.
03/15/2016	49154187	Biochemistry
03/15/2016	49156239	materials science, physical chemistry
03/15/2016	49156209	Solid state simulations with ab initio gaussian crystalline orbital code (e.g. Crystal14)
03/15/2016	49154456	Biophysics
03/15/2016	49152899	
03/15/2016	49156268	Biophysics
03/15/2016	49153990	biomaterials
03/15/2016	49156710	clinical of biochemistry
03/15/2016	49156429	None, we're a HPC platform provider
03/15/2016	49156275	Biochemistry
03/15/2016	49156285	Application Scientist helping others that use NaMD
03/15/2016	49155997	computational biology
03/15/2016	49155717	drug development, virtual screening methods, protein-ligand interactions
03/15/2016	49156078	Biophysics
03/15/2016	49156195	Polymer
03/15/2016	49155538	Computational chemistry
03/15/2016	49155738	
03/15/2016	49156009	Bioinformatics
03/15/2016	49155877	Allergy & Infectious Diseases
03/15/2016	49156055	engineering
03/15/2016	49151774	Biomolecular Spectroscopy
03/15/2016	49155815	Biophysics and drug design
03/15/2016	49155510	Computational Biophysics
03/15/2016	49155776	Computational Chemistry
03/15/2016	49155544	
03/15/2016	49155499	biomedical
03/15/2016	49155596	Biophysics
03/15/2016	49155164	medicinal chemistry
03/15/2016	49155369	CSE
03/15/2016	49155367	physics
03/15/2016	49153695	theoretical chemistry
03/15/2016	49155209	biochemistry
03/15/2016	49155184	Protein Folding and Classification
03/15/2016	49154795	Serine Proteases/Biochemistry

03/15/2016	49154449	Chemistry
03/15/2016	49155035	protein-ligand binding, DNA simulations, reverse micelle simulations
03/15/2016	49154986	biophysics
03/15/2016	49154914	Bioinformatics
03/15/2016	49154848	lipid membranes
03/15/2016	49154960	Biomaterials
03/15/2016	49154854	
03/15/2016	49154779	Computational chemistry
03/15/2016	49154833	Biophysics
03/15/2016	49154288	biophysics
03/15/2016	49154393	Chemistry
03/15/2016	49153918	Protein science
03/15/2016	49154286	simulation of protein in a membrane environment
03/15/2016	49153816	Physics
03/15/2016	49154216	Computational enzyme design
03/15/2016	49154261	Hydration of Small Peptides
03/15/2016	49153916	Polymers
03/15/2016	49153992	Computational Biophysics
03/15/2016	49153944	Medicinal chemistry; Chemical biology
03/15/2016	49153458	Cyclic peptides
03/15/2016	49153733	Computational Biochemistry
03/15/2016	49153408	computational bioenergetics
03/15/2016	49153683	Molecular dynamics and quantum chemistry
03/15/2016	49153316	biophysics
03/15/2016	49153717	HIV nonnucleoside reverse transcriptase inhibitors
03/15/2016	49153663	Chemistry
03/15/2016	49153686	computational biophysics
03/15/2016	49153615	drug discovery
03/15/2016	49153664	Applied science
03/15/2016	49153374	Biophysics
03/15/2016	49153343	
03/15/2016	49153514	Chemical Engineering
03/15/2016	49153305	molecular dynamics
03/15/2016	49152786	bioinformatics
03/15/2016	49153392	Infectious Diseases
03/15/2016	49153238	Chemistry
03/15/2016	49153203	Computational Biology
03/15/2016	49153209	GPCRs
03/15/2016	49153460	
03/15/2016	49153000	Cell biology
03/15/2016	49153077	Ecology
03/15/2016	49152483	nanomedicine
03/15/2016	49152936	
03/15/2016	49153050	Chemical Engineering
03/15/2016	49152305	protein modelling
03/15/2016	49152816	biochemistry
03/15/2016	49152861	Biophysics
03/15/2016	49152622	nanofluidics, nanopore sensing, protein mechanics
03/15/2016	49152761	
03/15/2016	49152058	Molecular Biology, Biotechnology

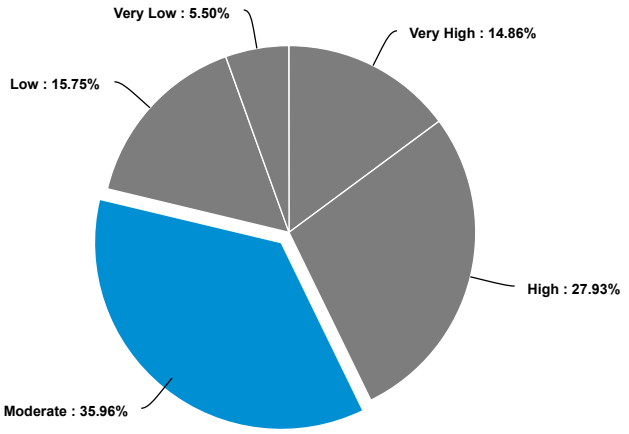
03/15/2016	49152689	Materials science and engineering
03/15/2016	49152287	virus structure and assembly
03/15/2016	49152595	Biophysics
03/15/2016	49152598	HPC
03/15/2016	49152126	High Performance Cluster Benchmarking
03/15/2016	49152312	Molecular Structural Biology
03/15/2016	49152328	
03/15/2016	49152171	membrane biophysics
03/15/2016	49149711	Protein biophysics
03/15/2016	49151691	Molecular modeling, Theoretical chemistry
03/15/2016	49152386	Physics
03/15/2016	49152322	Medicinal Chemistry
03/15/2016	49151938	photochemistry of transition metal complexes
03/15/2016	49152278	
03/15/2016	49152261	Computational Chemistry
03/15/2016	49152373	
03/15/2016	49151391	protein engineering
03/15/2016	49151706	Biophysics
03/15/2016	49151880	
03/15/2016	49151939	Hyu vam
03/15/2016	49151744	Physiology
03/15/2016	49151712	Biophysics
03/15/2016	49151386	theoretical chemistry
03/15/2016	49151698	biological physics
03/15/2016	49151626	Structural bioinformatics
03/15/2016	49148589	Protein-protein interactions
03/15/2016	49151655	Computational Biophysics
03/15/2016	49151605	Bioinformatics
03/15/2016	49151465	Biophysics
03/15/2016	49151566	biophysics
03/15/2016	49151630	QSAR
03/15/2016	49151451	biophysics
03/15/2016	49151297	protein crystallography
03/15/2016	49151535	structural biology
03/15/2016	49151577	Physics
03/15/2016	49151214	enzymology, drug-design, Med chemistry, biochemistry
03/15/2016	49151462	chemistry
03/15/2016	49151134	protein Biophysics
03/15/2016	49150729	IT Industry
03/15/2016	49151069	Bioinformatics
03/15/2016	49148098	replication mechanisms of poliovirus
03/15/2016	49151156	docking
03/15/2016	49148538	Computational Biology
03/15/2016	49151107	Bioinformatics
03/15/2016	49150973	nanoengineering
03/15/2016	49151109	
03/15/2016	49150779	computational biology
03/15/2016	49148971	Biophysics
03/15/2016	49150768	Biotechnology
03/15/2016	49150260	computational biochemistry
03/15/2016	49150824	Quantum chemistry

03/15/2016	49150319	pharmaceutics
03/15/2016	49150751	chemistry
03/15/2016	49150454	Structural biology
03/15/2016	49150219	Physics
03/15/2016	49150231	Statistics/computation
03/15/2016	49150650	computational biology
03/15/2016	49150470	Bioinformatics
03/15/2016	49150214	Chemical engineering, membrane proteins, protein-DNA interactions
03/15/2016	49149984	Structural Computational Biology
03/15/2016	49150385	computer biology
03/15/2016	49150501	drug design
03/15/2016	49149837	Biophysics
03/15/2016	49150356	medicinal chemistry and biophysics
03/15/2016	49150641	Chemistry
03/15/2016	49150125	glycoside hydrolase biophysics
03/15/2016	49150458	Molecular Biophysics
03/15/2016	49150346	Biomolecular Engineering
03/15/2016	49150238	Sysadmin
03/15/2016	49149977	Pharmaceutics
03/15/2016	49149989	Biochemistry
03/15/2016	49149812	Biomaterials, Material science
03/15/2016	49149983	informatics
03/15/2016	49149458	organic chemistry / synthesis of Nitrogen-containing heterocycles
03/15/2016	49150032	Biochemistry
03/15/2016	49149842	protein biophysics
03/15/2016	49149455	Environmental Engineering
03/15/2016	49149318	IRAN
03/15/2016	49149754	Molecular Modelling
03/15/2016	49149577	computational Biophysics
03/15/2016	49149762	Biophysics
03/15/2016	49149438	Mathematical modelling
03/15/2016	49149643	Materials Science and Nanotechnology Engineering
03/15/2016	49149544	Molecular Biomedicine and Biotechnology
03/15/2016	49149285	Biocatalysis
03/15/2016	49149566	Quantum Mechanics
03/15/2016	49149327	Biophysics
03/15/2016	49149449	protein ligand complex
03/15/2016	49149334	physical sciences
03/15/2016	49149276	
03/15/2016	49149232	Electronic and Computer Engineering
03/15/2016	49149182	proteins, DNA
03/15/2016	49149448	Biophysics
03/15/2016	49149370	Chemical Engineering
03/15/2016	49149157	drug design
03/15/2016	49149062	Membrane biophysics
03/15/2016	49148592	Benchmarking quantum mechanics (DFT) and bioinformatics codes
03/15/2016	49148755	molecular dynamic
03/15/2016	49148866	Physical Chemistry
03/15/2016	49146382	Bioinformatics
03/15/2016	49148988	computational biophysics
03/15/2016	49148936	Structural Biology

03/15/2016	49148787	Structural biology
03/15/2016	49148843	biology
03/15/2016	49148953	Catalysis
03/15/2016	49148888	Membrane proteins
03/15/2016	49149089	Chemoinformatics
03/15/2016	49148873	Physics
03/15/2016	49148834	Biophysics
03/15/2016	49148760	Physical Chemistry
03/15/2016	49148465	biophysics
03/15/2016	49148385	Theoretical Chemistry
03/15/2016	49148451	material science
03/15/2016	49148308	Computational Bio-Physics
03/15/2016	49148370	Theoretical and Computational Biophysics
03/15/2016	49148442	nanotech
03/15/2016	49148733	Biophysics
03/15/2016	49148469	Bioinformatics
03/15/2016	49148446	Computational Biology
03/15/2016	49148367	Nuclear
03/15/2016	49148321	Computational Chemistry
03/15/2016	49148637	Chemistry
03/15/2016	49147716	support computational chemistry applications for hardware vendor
03/15/2016	49148383	Software development for simulations
03/15/2016	49148429	
03/15/2016	49148058	biophysics and material science
03/15/2016	49147986	Enzyme design and modelling
03/15/2016	49147979	Molecular Dynamics
03/15/2016	49148243	Chemistry
03/15/2016	49148129	Biochemistry
03/15/2016	49147967	Physical Chemistry
03/15/2016	49147898	Biochemistry bone cartilage
03/15/2016	49147903	electron microscopy of complexes
03/15/2016	49147997	Biophysical Chemistry
03/15/2016	49148027	
03/15/2016	49147822	Biomembranes
03/15/2016	49146020	biosystems engineering
03/15/2016	49147839	
03/15/2016	49147555	Biophysics
03/15/2016	49147459	Ion Channels
03/15/2016	49147189	Engineering Physics
03/15/2016	49146631	Enzymology
03/15/2016	49147107	Theor Chemistry
03/15/2016	49146944	drug discovery
03/15/2016	49147069	Biological fusion
03/15/2016	49146889	Biophysics
03/15/2016	49146903	systems programming
03/15/2016	49146934	Chemistry
03/15/2016	49146826	Membrane and membrane protein biophysics
03/15/2016	49146558	Biophysics
03/15/2016	49145915	Computational biochemistry
03/15/2016	49146378	computational chemistry and biophysics

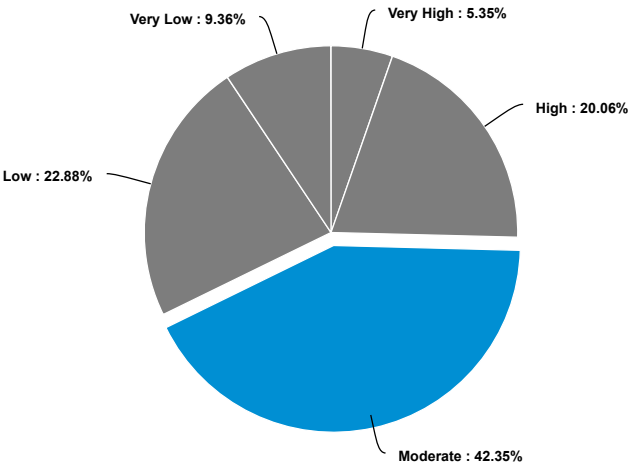
03/15/2016	49146288	Biomolecular dynamics and free energy calculations
03/15/2016	49146106	Medicinal Chemistry
03/15/2016	49145782	biochemistry
03/15/2016	49145975	Computational Chemistry
03/15/2016	49146128	
03/15/2016	49145477	Membrane proteins
03/15/2016	49145396	Bioinformatics
03/13/2016	49060420	biology
03/05/2016	48649707	bioinformatics
02/28/2016	48298462	
02/26/2016	48209932	Medicinal Chemistry
02/26/2016	48209237	biophysics
02/26/2016	48208396	Molecular Biophysics
02/25/2016	48202726	mechanical properties of polypeptides
02/25/2016	48201945	Biophysics
02/25/2016	48201615	Computational drug discovery
02/25/2016	48199362	peptide
02/25/2016	48190063	Protein structure and function
02/25/2016	48190089	Applied Informatics
02/25/2016	48189939	Chemical Engineering
02/25/2016	48189981	QM/MM

My level of expertise in molecular modeling is:



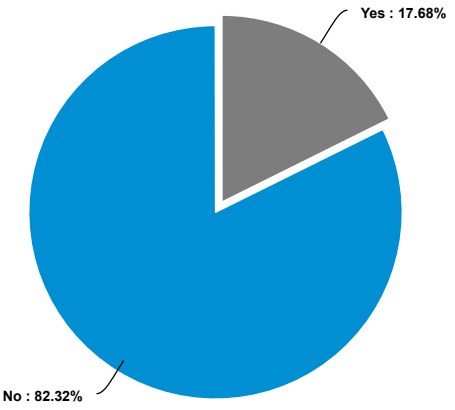
Answer	Count	Percent	20% 40% 60% 80% 100%
Very High	100	14.86%	
High	188	27.93%	
Moderate	242	35.96%	
Low	106	15.75%	
Very Low	37	5.5%	
Total	**673**	**100 %**	

My level of expertise with NAMD is:



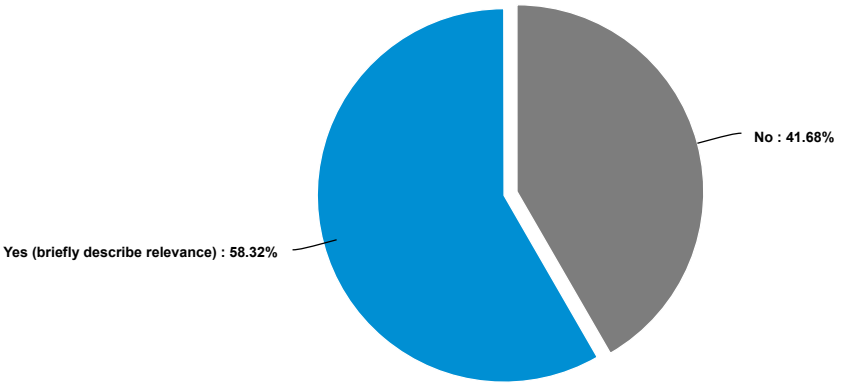
Answer	Count	Percent	20% 40% 60% 80% 100%
Very High	36	5.35%	
High	135	20.06%	
Moderate	285	42.35%	
Low	154	22.88%	
Very Low	63	9.36%	
Total	**673**	**100 %**	

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



Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	119	17.68%	
No	554	82.32%	
Total	**673**	**100 %**	

The work I do with NAMD is biomedically relevant:



Answer	Count	Percent	20% 40% 60% 80% 100%
No	273	41.68%	
Yes (briefly describe relevance)	382	58.32%	
Total	**655**	**100 %**	

The work I do with NAMD is biomedically relevant: - Text Data for Yes (briefly describe relevance)

04/06/2016	50238244	Designing Antimicrobial Peptides
04/01/2016	50017212	for some projects.
04/01/2016	49982422	We use NAMD to simulate different proteins for biomedical applications (i.e. Schistosomiasis venus fly-trap receptors)
03/31/2016	49970099	Antiviral peptides design
03/31/2016	49962657	We study proteins relevant to design of anti-HIV therapeutics
03/23/2016	49547891	Proteins / membrane interactions
03/23/2016	49526597	Ligand binding, alostery
03/23/2016	49514885	enzymatic mechanisms
03/22/2016	49505218	Evaluate the binding affinity of hits from virtual screening
03/22/2016	49504163	Evaluation of point mutations in a protein structure
03/22/2016	49502338	Antivirals
03/22/2016	49500643	Antiobiotics
03/21/2016	49458465	membrane proteins and lipids
03/21/2016	49451834	GPCR modeling and simulations
03/21/2016	49446863	Cannabinoids are drug targets and drugs of abuse.
03/21/2016	49440970	Relevant for simulation of biological molecules
03/21/2016	49438333	sudying HCV protease genotypes
03/21/2016	49423440	Drug design, molecular polymorphism study
03/20/2016	49409962	signalling pathways
03/20/2016	49391650	I studied Chemotaxis which is a major virulence factor in some human pathogens
03/19/2016	49387530	Cancer, Ebola virus
03/19/2016	49386876	fluorescent proteins, LH-RC systems
03/19/2016	49384908	I use NAMD to simulate phospholipid aggregation
03/19/2016	49375381	My work is essentially protein-ligand interaction which is quite relevant in drug design and interaction
03/19/2016	49371406	Studying oncogenic proteins structure and dynamics
03/18/2016	49338443	search for inhibitors for cancer deregulated proteins
03/18/2016	49334524	prions proteins
03/18/2016	49334107	finding binding sites on proteins
03/18/2016	49324207	Anticancer drug discovery
03/18/2016	49319847	drug design
03/18/2016	49318038	Molecular Dynamics Simulations applied to Protein Folding
03/18/2016	49313281	research on skin affection
03/18/2016	49308347	Research of ion selectivity in biological channel systems (ion channels); selectivity in nanopore systems; TI calculations for membranprotein mutants; observation and analysis of correlation phenomena in membrane proteins; Ion behavior on hydrophobic pore systems (tubes, sheets of different materials);

03/17/2016	49304680	bacterial resistance to beta-lactam antibiotics
03/17/2016	49298331	I did with P53 and mutant residues
03/17/2016	49297814	Antimicotic drugs
03/17/2016	49292910	For Cancer.
03/17/2016	49284809	drug delivery systems and cellular barriers
03/17/2016	49274496	in silico search and test active molecules from natural extracts
03/17/2016	49274001	biopolymers for drug delivery
03/17/2016	49273575	If we understood the mechanism of viral assembly, this would offer potential new targets for pharmacological intervention.
03/17/2016	49273170	My work analyzes drug-delivery vectors for Alzheimer's disease.
03/17/2016	49271223	drug discovery for failed chemotherapies
03/17/2016	49268017	RNA loaded nanoparticles; gene therapy
03/17/2016	49267767	Simulation of transmembrane proteins
03/17/2016	49267843	Development of new enzyme inhibitors
03/17/2016	49262479	Characterization of the activation state of the receptor
03/17/2016	49262323	dynamics of GABA receptor (main human inhibitory receptor)
03/17/2016	49259611	peptide recognition
03/17/2016	49256222	Drug development
03/17/2016	49254725	Provide chemical information about a peptide catalyzed asymmetric reaction of a phamaceutical drug candidate.
03/17/2016	49250181	MD simulations of ion channels clarify the mechanism of permeation and selectivity aiding in the design of channel blockers used as anaesthetics
03/17/2016	49245968	GPCRs
03/17/2016	49244715	My work is aimed to developing a phenomenological model for reconstructing the DNA parametrs (such as length and helix structure) in the biological sample by THz spectroscopy methods. For verifying the model, I need to visualise thd DNA molecular dynamics
03/17/2016	49244660	Potential drug carrier
03/17/2016	49242397	we have used NAMD as part of our design of peptide inhibitors towards biomedically relevant targets
03/16/2016	49241367	research about new drugs
03/16/2016	49238734	perhaps improved computing efficiency and increased problem resolution
03/16/2016	49238042	Explained the mechanism for wide range of antibiotic catalysis.
03/16/2016	49230444	lipid remodeling
03/16/2016	49228123	Alzheimer's Disease
03/16/2016	49227244	All systems on which I work have been implicated as potential drug targets.
03/16/2016	49222061	Epigenetics and drug design.
03/16/2016	49219500	protein misfolding diseases
03/16/2016	49218526	protein adsorption on solid suport
03/16/2016	49216706	Symulation of protein ligand complexes
03/16/2016	49214265	modeling ion channel conductance might have some physiological relevance.
03/16/2016	49214006	How do the phisological changes affect the polymeric materials as a drug carrier.
03/16/2016	49211137	Understanding structure/functional relationships in proteins
03/16/2016	49209693	Ageing processes.
03/16/2016	49208902	drugs
03/16/2016	49206049	Host-parasite structural and thermodynamical interactions
03/16/2016	49204826	Biochemistry of nicotinic addiction
03/16/2016	49204531	proteins, drug-targets, disease mechanisms
03/16/2016	49201782	Looking for a cancer profilactic
03/16/2016	49199276	To develop supported biosensors for early detection
03/16/2016	49199507	The three-dimensional structure of carbohydrates is a major challenge in glycobiology. It is essential for a better understanding of their chemistry and in order to develop carbohydrate based drugs.
03/16/2016	49198519	We are simulating lipid-binding of a peptide that is a potential cancer targetting agent
03/16/2016	49197768	I study the interactions of new drugs with proteins
03/16/2016	49197118	molecular dynamics simulations of biomolecular motors
03/16/2016	49196030	collagen
03/16/2016	49196413	protein allostery
03/16/2016	49196131	to investigate the interaction between target proteins and drugs

03/16/2016	49195392	nanoparticles as drug carriers
03/16/2016	49193466	Drug Discovery, Virology, HIV, HCV, HBV, immuno-oncology
03/16/2016	49194555	proteomics
03/16/2016	49193002	Drug discovery
03/16/2016	49193273	Because using computational electromagnetics is possible known more about the physical biomedical problems
03/16/2016	49193263	Antimicrobial engineering
03/16/2016	49189930	Bacterial membrane proteins
03/16/2016	49188694	Disease related (TB, Staph, Malaria, neurotransmission)
03/16/2016	49188356	THE EFFECT OF MECHANICAL FORCES ON THE STRUCTURE AND FUNCTION OF BIOPOLIMERS
03/16/2016	49187552	Solute Transporter in Red Blood Cell Membrane
03/16/2016	49187151	design of better cel penetrating peptides for microbial control
03/16/2016	49186580	I study novel anticancer drug
03/16/2016	49185731	I work on experimental studies of conformational dynamics of biomolecules
03/16/2016	49185400	study of proteins involved in disease
03/16/2016	49184937	GPCRs in double layer
03/16/2016	49184186	Development of novel immunoglobulin reagents
03/16/2016	49184237	Investigation of protein involved in cardiovascular diseases
03/16/2016	49182551	Formulation of protein drugs
03/16/2016	49181879	Implants, Biocompatibility
03/16/2016	49181353	understanding the effect of pathogenic mutations
03/16/2016	49181413	immune system complexes
03/16/2016	49181054	bacterial membranes
03/16/2016	49180400	Study of mechanism of action of small molecules targeting relevant proteins (CDK2 and P-glycoprotein) involved in neoplastic and neurodegenerative diseases
03/16/2016	49179392	Calculation of binding energy for docking validation; conformational sampling for ensemble docking; mutagenesis studies to predict in vitro activity changes.
03/16/2016	49179363	cancer signaling, cardiovascular diseases
03/16/2016	49178756	Understanding of partitioning, folding and aggregatio properties of cell penetrating peptides
03/16/2016	49178582	genotype - protein - phenotype correlation in a genetic disease (BMD)
03/16/2016	49178170	MD simulations are an important ingredient of drug design
03/16/2016	49178277	Cyclodextrins, relevant in drug formulations
03/16/2016	49177998	My present interst is about the effects of ions on biomolecules such as proteins. These effects are relavant to most diseases and their diagnosis, drug design and therapy development. MD plays an important role in building a microscopic picture of ion-water and ion-biomolecule interactions.
03/16/2016	49177810	I simulate interactions between drugs and their targets (GPCRs)
03/16/2016	49177633	antivirals, bioactive molecules
03/16/2016	49177711	drug design and disease related protein structures
03/16/2016	49177466	design of dopamine transporter inhibitors
03/16/2016	49177548	structural studies of tumor marker molecules
03/16/2016	49177282	we work on disease realted intrinsically disordered proteins, their self assembly, and mofulation therein wih external entties.
03/16/2016	49177036	fundamental research on potential drug targets
03/16/2016	49176398	antigen-antibody interaction
03/16/2016	49176365	Selective inhibitors despite conserved binding site
03/16/2016	49176231	structural flexibility of bromodomains
03/15/2016	49175409	Well, I don't do the research, just set NAMD up for it
03/15/2016	49174847	molecular dynamics
03/15/2016	49174633	Fracture of microtubule related to brain truma.
03/15/2016	49174553	Drug design and discovery
03/15/2016	49174386	Bio-molecular simulations of DNA, protein etc..
03/15/2016	49174151	protein and peptide are biomedically relevant
03/15/2016	49173534	doing protein simultion for drug design using enzyme inhibition
03/15/2016	49173041	Calculation of binding free energies
03/15/2016	49173019	multi-drug resistance
03/15/2016	49172735	I use NAMD: to refine hits from virtual screening/docking or to validate design of potential new drugs; to identify/validate SARs of biomedically-relevant systems

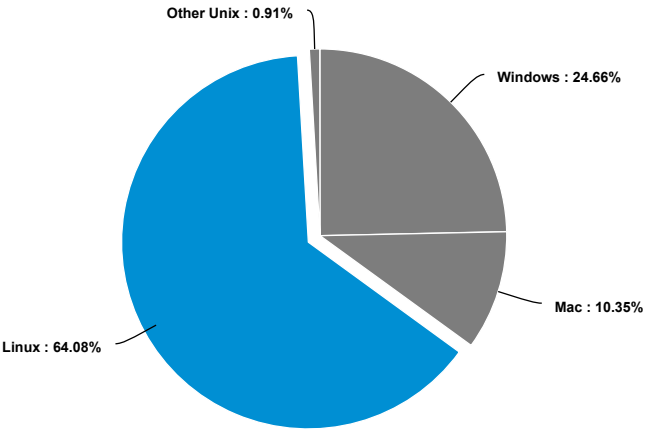
03/15/2016	49172715	I work on membrane proteins including drug targets
03/15/2016	49172449	protein with chemical small molecular
03/15/2016	49172375	drug discovery
03/15/2016	49172212	I work with systems that relate with proteins and membrane systems ans their interactions with potentially pharmacophores
03/15/2016	49171694	We perform parametrization and simulations to obtain binding free energy of synthetic molecules for biologically relevant protein targets.
03/15/2016	49171835	drug delivery
03/15/2016	49171803	understanding the structural conformation of IR can help aid further research
03/15/2016	49171084	Protein
03/15/2016	49170663	Simulating membrane-nanoparticle interaction
03/15/2016	49170497	membrane protein, RNA
03/15/2016	49169581	the protein i am working on are from parasites but has homoloues from human and i want to show how the active site can be targeted by drugs without affecting the human.
03/15/2016	49170043	Public Health applications, WHO polio laboratory. Virus reconstructions, antiviral resistance.
03/15/2016	49168646	structure modeling
03/15/2016	49169273	Protein allostery
03/15/2016	49169082	structural immunology
03/15/2016	49169366	SMD
03/15/2016	49169013	studying base-stacking
03/15/2016	49168525	hit and lead
03/15/2016	49168411	Our research is centered in Drug design for neglected diseases and bioactive compounds for neurodegenerative diseases
03/15/2016	49168400	drug-protein interaction
03/15/2016	49168273	We are interested in the permeation of small molecules into various lipid structures.
03/15/2016	49168150	Protein biophysics class
03/15/2016	49167903	Mechanisms of epilepsy, drug development
03/15/2016	49166864	RNA, Kinases
03/15/2016	49166591	modelling drugs to biomedical targets
03/15/2016	49166481	drug design
03/15/2016	49166208	My research is partially based on how my current research sheds light on the dynamics of beta amyloid.
03/15/2016	49166257	GBLs receptor
03/15/2016	49165578	theory of alcohol action in the nervous system
03/15/2016	49164417	I work with the Alzheimer's disease Ab peptide
03/15/2016	49165286	Qqer study cancer related proteins
03/15/2016	49165188	guide nano-drug design and delivery
03/15/2016	49164420	immune response to medical implants; tissue engineering
03/15/2016	49164348	MD simulations for biomolecules
03/15/2016	49163943	Work on amino acid transporters directly involved in T2D and cancer metabolism
03/15/2016	49163190	3D structures of biological molecules
03/15/2016	49163610	using MDFF for cryoEM model fitting
03/15/2016	49163185	Have published basic research in structural biology related to infectious diseases.
03/15/2016	49162870	ion channels and other proteins participating in mechano-, thermo-, nocio-, and chemical reception, hearing, blood pressure regulation; asparaginase enzymes used in cancer therapy
03/15/2016	49161545	Structural biology application with biomedical or medicinal chemistry interest
03/15/2016	49161930	Molecular dinamics improves the study of new pharmacological leads.
03/15/2016	49162388	Molecular dynamics simulations of ion channels
03/15/2016	49161485	studying the binding affinity of ligands to acetylcholinesterase
03/15/2016	49159897	The work is directed to understand molecular mechanisms underlaying several diseases
03/15/2016	49160480	Investigating anesthesia
03/15/2016	49160024	Study of skin permeation by chemicals
03/15/2016	49159883	thermal equilibration of the crystal structures of the enzymes
03/15/2016	49159801	plasmid partition & microbial antibiotic resistance
03/15/2016	49159422	Drug delivery
03/15/2016	49159253	I am modelling a cytokine that is associated wirh autoimmune diseases

03/15/2016	49159416	Designing scaffolds for vaccines
03/15/2016	49159047	Drug resistence
03/15/2016	49158789	enzyme reactivity
03/15/2016	49158520	protein ligandability
03/15/2016	49158609	Involved rna polymerase. Currently not using
03/15/2016	49157715	fep calculations
03/15/2016	49157368	Preservative formulations for long term storage of biomaterials
03/15/2016	49156824	There is a potental to use nucleic acid spectra as indicators
03/15/2016	49157177	could help designing fluorescent probes
03/15/2016	49156356	Optimization of PDB structures of COX enzyme for accurate drug discovery
03/15/2016	49156239	part of my work is related to drug and gene deivery
03/15/2016	49154456	Possibly, we investigate gating of ion channels
03/15/2016	49155997	drug delivery
03/15/2016	49155717	We use NAMD to examine interactions of drugs with druggable targets. We have used it in past to examine solvation water dynamics at solute/solvent interfaces to predict druggable sites. We will use MD to generate protein conformations for ensemble docking approaches to virtual screening for drugs.
03/15/2016	49156078	artificial water filtration membranes and sequence-selective DNA detection seem medically relevant.
03/15/2016	49155538	Antibiotic resistance mechanisms
03/15/2016	49155877	Vaccines
03/15/2016	49151774	Interaction studies of ligands to their pain receptors / modification of ligands
03/15/2016	49155510	Study conformational dynamics and kinetics of enzymes and transporter proteins
03/15/2016	49155164	main goal is developing enzyme/protein inhibitors
03/15/2016	49155367	chemotaxis in pathogenesis
03/15/2016	49153695	fundamental research
03/15/2016	49154795	We are modeling serine protease inhibition by canonical inhibitors to understand why structurally similar inhibitors are cleaved at different rates. We want to use this knowledge to engineer inhibitors for therapeutic use
03/15/2016	49155035	informs drug discovery
03/15/2016	49154833	Simulation of drug/protein and drug/membrane interactions
03/15/2016	49154288	aquaporin inhibitors
03/15/2016	49154393	modeling virus particles as nanodelivery vehicles
03/15/2016	49153918	Structure Based drug design
03/15/2016	49154286	understanding voltage gated channels important to understnading nerve function
03/15/2016	49153992	Enzyme optimization for cancer treatment
03/15/2016	49153733	Most systems we work on are disease related: A-beta, autophagy related proteins, interleukin, etc.
03/15/2016	49153408	I work with enzymes in respiratory chain (Eg: CcO)
03/15/2016	49153717	I run MD and perform FEP calculations to assess potential drug candidates
03/15/2016	49153663	Molecules I'm working on applications in tissue engineering, muscle growth, drug delivery etc
03/15/2016	49153686	some work related to anti-cancer drug discovery
03/15/2016	49153615	drug discovery
03/15/2016	49153343	modelling of hdac enzyme behaviour on ligand binding
03/15/2016	49153514	antimicrobial peptides
03/15/2016	49152786	Public Health
03/15/2016	49153203	Scientific support for NIH Biowulf cluster
03/15/2016	49153209	GPCR
03/15/2016	49152483	application of polymers in drug delivery
03/15/2016	49152936	Drug-protein interactions
03/15/2016	49152058	drug design
03/15/2016	49152287	may help design antivirals
03/15/2016	49152328	drug kinetics
03/15/2016	49152171	Evaluation of protein-membrane interactions for a Pseudomonas aeruginosa phospholipase.
03/15/2016	49149711	Working on protein modelling and studying effects of flexibility on allostery
03/15/2016	49151691	Molecular dynamic of large biomolecules
03/15/2016	49152386	Studying Alzheimer's related proteins

03/15/2016	49152322	Drug Discovery
03/15/2016	49152261	Drug discovery
03/15/2016	49151391	protein engineering
03/15/2016	49151939	Absolutly relevant
03/15/2016	49151744	Ion channels
03/15/2016	49151712	I study proteins that bind methylated DNA as potential drug targets.
03/15/2016	49151386	we try to find mutants of peptides with potential use in biomedicine
03/15/2016	49151626	Tamiflu resistance
03/15/2016	49151566	effects of mutagenesis on domain folding
03/15/2016	49151451	human protein modeling
03/15/2016	49151297	G protein
03/15/2016	49151214	we develop drugs and study pathogenesis with QMMD methods
03/15/2016	49151069	protein interaction
03/15/2016	49148098	if we'll figure out the mechanisms of interaction between protein 3CD and viral RNA we could be able to construct an inhibitor which would prevent the interaction
03/15/2016	49151156	docking with toxin
03/15/2016	49148971	My groups current projects include understanding iodide transport in the thyroid, deactivation of K+ channels, and drug delivery.
03/15/2016	49150768	nucleic acid structure and function
03/15/2016	49150260	cytochromes P450
03/15/2016	49150319	study of polymer-drug interactions
03/15/2016	49150751	Drug Design Efforts
03/15/2016	49150454	I study G protein-coupled receptors, and we have several collaborations with pharmaceutical industries / biotechs
03/15/2016	49150219	Model DNA and protein structures
03/15/2016	49150231	Simulation of protein structure and dynamics that may lead to useful medical technologies
03/15/2016	49150470	in animal species (salmon)
03/15/2016	49150214	Membrane proteins related to brain injury
03/15/2016	49150501	protein simulation
03/15/2016	49149837	physiologically important enzyme study
03/15/2016	49150356	i study kinases and protein-DNA systems to provide insights for drug design
03/15/2016	49150458	Force field development and evaluation
03/15/2016	49149977	I run simulations with active pharmaceutical ingredients
03/15/2016	49149812	Nanoparticle absorption by cells for imaging and drug delivery
03/15/2016	49149983	receptors
03/15/2016	49149842	electric field effect on protein for therapy
03/15/2016	49149318	Ion channels
03/15/2016	49149577	protein ligand binding
03/15/2016	49149762	Studying membrane transporters
03/15/2016	49149438	potential drug design
03/15/2016	49149643	it's about proteins
03/15/2016	49149327	Drug-protein interactions
03/15/2016	49149182	drugs clinically relevant
03/15/2016	49149448	Cardiac thin filament studies
03/15/2016	49149370	HIV inhibition
03/15/2016	49149157	drug discovery
03/15/2016	49149062	Human membrane proteins
03/15/2016	49148592	Cray customers are regularly using NAMD
03/15/2016	49148988	All of my research subjects are at least loosely related to some kind of medical issue.
03/15/2016	49148787	simulating protein flexibility
03/15/2016	49148936	Surface protein of pathogen
03/15/2016	49148873	Gram negative bacteria outer membrane permeation & nutrient uptake
03/15/2016	49148834	Studies of the structure/function/dynamics relationship in biomolecules.

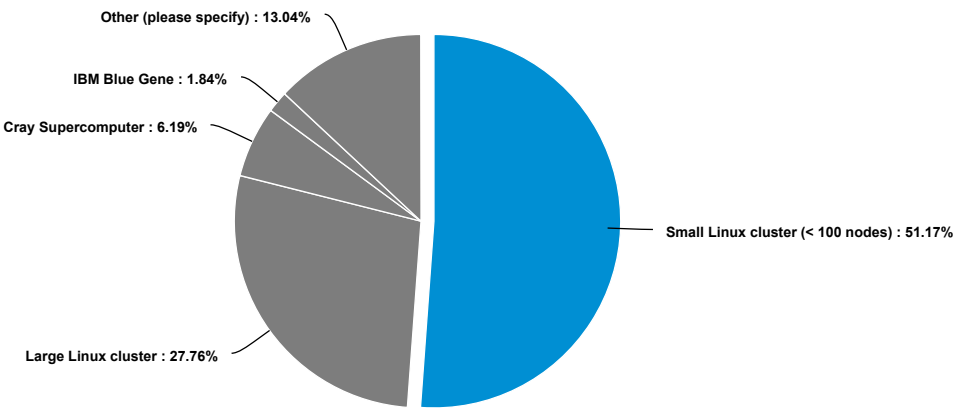
03/15/2016	49148760	--
03/15/2016	49148465	ion channels, related to drug delivery
03/15/2016	49148370	Simulations and tools for range of NIH funded projects, including chromatophore .
03/15/2016	49148469	Antimicrobial peptides membrane interactions and peptide self assembly
03/15/2016	49148446	These are studies of protein motions.
03/15/2016	49147986	Enzyme design and modelling
03/15/2016	49148129	Drug design
03/15/2016	49147898	Simulate first atomic steps in biomineralization
03/15/2016	49147903	virus maturation
03/15/2016	49146020	working on a project related to antibiotic resistance
03/15/2016	49146631	Understanding drug resistivity in hepatitis C
03/15/2016	49146944	drug discovery of Kras inhibitors
03/15/2016	49147069	Find pathway of cell fusion
03/15/2016	49146889	Exploring novel drug targets
03/15/2016	49146934	DNA binding to protein
03/15/2016	49146826	disease related
03/15/2016	49146558	Simulating variants used in membrane protein folding studies.
03/15/2016	49145915	Simulation of proteins that play a role in certain diseases
03/15/2016	49146378	biomembrane permeation and protein pKa, thermal stability...
03/15/2016	49146288	Drug design
03/15/2016	49146106	protein-protein interface prediction
03/15/2016	49145477	Study gpcrs and antimicrobial lipopeptides
03/15/2016	49145396	Drug unbinding pathway and smd
03/05/2016	48649707	The cutting mechanism of enzyme
02/26/2016	48209932	Protein interaction
02/26/2016	48208396	comparison effect of drugs on a protein active site inhibation
02/25/2016	48201615	Computational drug discovery
02/25/2016	48190063	understanding the function of medically important proteins, e.g. ApoD
02/25/2016	48190089	ex. HIV protease deactivation

On my desktop/laptop I primarily use NAMD on:



Answer	Count	Percent	20% 40% 60% 80% 100%
Windows	162	24.66%	
Mac	68	10.35%	
Linux	421	64.08%	
Other Unix	6	0.91%	
Total	**657**	**100 %**	

For parallel computing I use NAMD on:



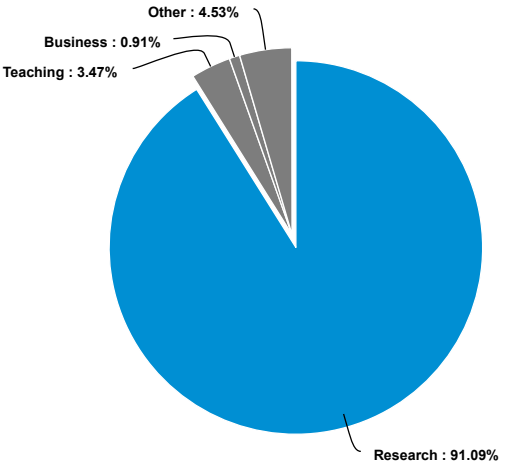
Answer	Count	Percent	20% 40% 60% 80% 100%
Small Linux cluster (< 100 nodes)	306	51.17%	
Large Linux cluster	166	27.76%	
Cray Supercomputer	37	6.19%	
IBM Blue Gene	11	1.84%	
Other (please specify)	78	13.04%	
Total	**598**	**100 %**	

For parallel computing I use NAMD on: - Text Data for Other (please specify)

04/01/2016	50017212	single machine
03/22/2016	49505218	No such resource
03/21/2016	49458465	Fujitsu Primergy
03/19/2016	49375381	Not yet
03/19/2016	49372080	windows
03/19/2016	49371406	Stampede
03/19/2016	49364561	my laptop
03/18/2016	49351270	desktop, 16 nodes
03/18/2016	49348261	Linux cluster each with GPU
03/17/2016	49304680	4 core CPU + 2 GTX670
03/17/2016	49298331	local
03/17/2016	49280558	not sure
03/17/2016	49274496	Small Windows 2012 R2 HPC Cluster
03/17/2016	49251541	None
03/17/2016	49247146	PC
03/17/2016	49244715	no use parallel computing
03/16/2016	49241367	no used
03/16/2016	49224752	SMP + GPU
03/16/2016	49211137	NVIDIA gpu build
03/16/2016	49209601	Linux + GPU
03/16/2016	49204826	NONE
03/16/2016	49199276	Workstation with few cores
03/16/2016	49199894	linux multi-core workstation
03/16/2016	49194157	i don't use
03/16/2016	49193240	not parralleled yet
03/16/2016	49186580	amd
03/16/2016	49184186	CUDA/GPU
03/16/2016	49182434	CUDA GPU
03/16/2016	49181879	Why only one option? I use it on 1. and 3.
03/16/2016	49179392	GPU workstation (1 to 4 gpus per workstation), also CINES occigen cluster (France)

03/16/2016	49179373	Never tried
03/16/2016	49179017	French Supercomputer
03/15/2016	49174053	PC
03/15/2016	49173041	super computer
03/15/2016	49173019	no
03/15/2016	49171694	I am not that lucky to have a Parallel computing facility, we work on small workstations
03/15/2016	49171445	No
03/15/2016	49170663	Using NAMD in cluster giving some trouble for me
03/15/2016	49169581	i dont know
03/15/2016	49169000	I want to use Nvidia Graphics Card
03/15/2016	49168621	none
03/15/2016	49167903	Have not yet used namd on a parallel platform
03/15/2016	49166591	do not use parallel comuting
03/15/2016	49164348	other supercomputers
03/15/2016	49163198	sgi cluster 150 nodes
03/15/2016	49161545	Desktop workstation
03/15/2016	49158537	Discrete workstation with GPUs
03/15/2016	49156824	5000 GPU computer
03/15/2016	49156239	i have used NAMD both, on small clusters and on supercomputing centers
03/15/2016	49156195	Never
03/15/2016	49155815	gpu
03/15/2016	49155510	16-core Intel workstations w/ GTX 980 or GTX 690
03/15/2016	49154833	Everything
03/15/2016	49153000	I don't do parallel computing
03/15/2016	49152816	N/A
03/15/2016	49151134	Desktop 6 cores
03/15/2016	49150729	IBM Power8 clusters
03/15/2016	49148538	workstation
03/15/2016	49150779	Power Linux + GPUs
03/15/2016	49149458	not use
03/15/2016	49149754	No parallel computing
03/15/2016	49149334	OSG
03/15/2016	49149062	Gpu desktop
03/15/2016	49148367	8 Core CPU+ TITAN Z
03/15/2016	49147716	SGI ICE large linux cluster 576 nodes and single OS 1000 core SGI UV
03/15/2016	49147986	Have not used in this method, only on a single machine
03/15/2016	49147979	IBM HPC
03/15/2016	49147898	Teragrid previously
03/15/2016	49147822	All of them
03/15/2016	49147459	GPU workstation
03/15/2016	49146934	desktop computer
03/15/2016	49146288	French national supercomputers

I use NAMD primarily for:

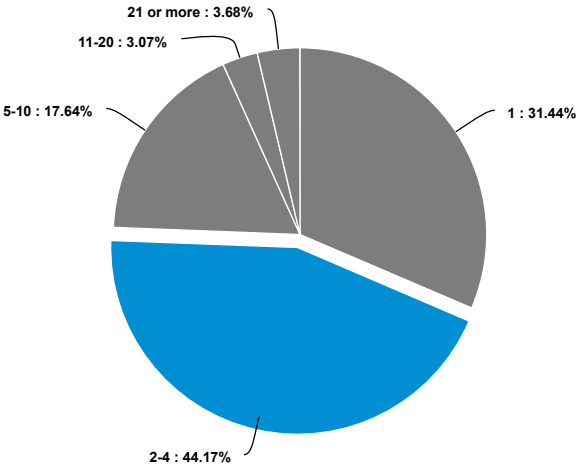


Answer	Count	Percent	20% 40% 60% 80% 100%
Research	603	91.09%	
Teaching	23	3.47%	
Business	6	0.91%	
Other	30	4.53%	
Total	**662**	**100 %**	

I use NAMD primarily for: - Text Data for Other

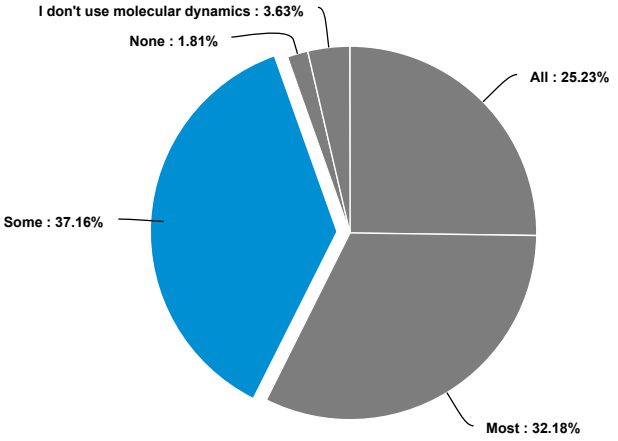
03/23/2016	49546663	Learning/Comparison
03/23/2016	49533042	Performance testing
03/22/2016	49468724	I usually install it at researchers workstations, clusters.
03/21/2016	49440970	Student project
03/17/2016	49257499	competition
03/17/2016	49251541	Fun
03/16/2016	49238734	occasional benchmark requests
03/16/2016	49224752	GPU performance demos
03/16/2016	49194157	personal study
03/16/2016	49185823	I install it, and teach students to use it, but have little use for it myself.
03/16/2016	49184750	Own education/curiosity
03/16/2016	49179315	learning, curiosity for nano-scale dynamics of molecules
03/15/2016	49174506	hardware (Cuda, Phi) benchmark
03/15/2016	49168525	graduation
03/15/2016	49154187	For my own interest
03/15/2016	49155596	Took a class
03/15/2016	49153374	Learning
03/15/2016	49152598	Learning
03/15/2016	49152126	benchmarking
03/15/2016	49151938	hobby
03/15/2016	49150779	Performance measurement
03/15/2016	49149983	check of other programs
03/15/2016	49149276	User Support
03/15/2016	49147716	testing and benchmarking
03/15/2016	49146903	build
02/26/2016	48209932	Learning

The number of people using NAMD at my site is:



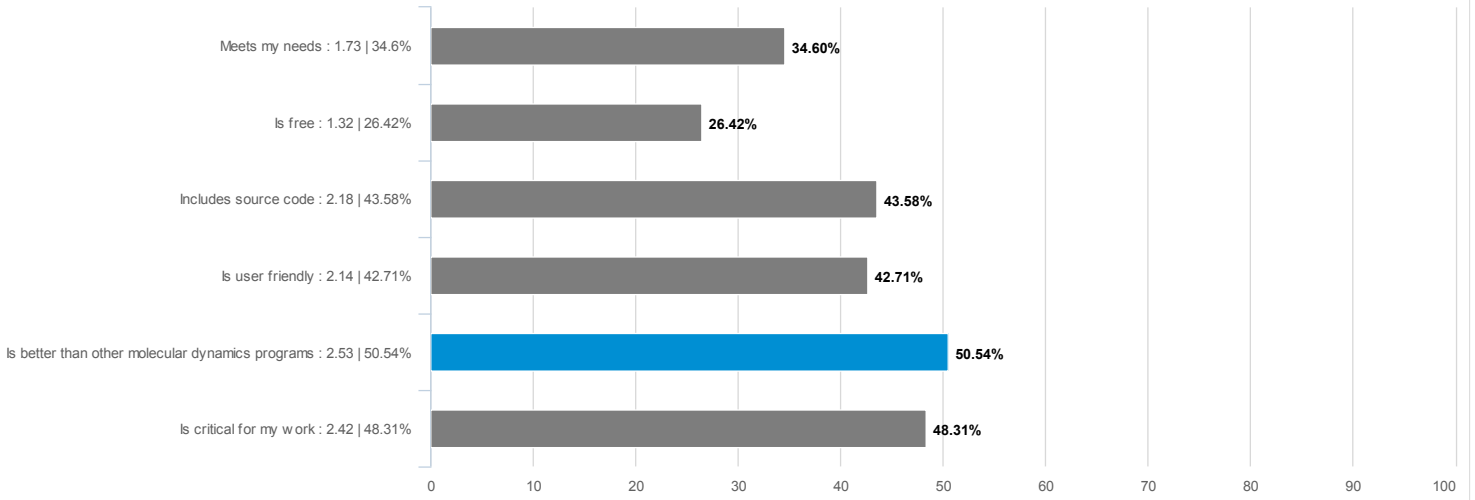
Answer	Count	Percent	20% 40% 60% 80% 100%
1	205	31.44%	
2-4	288	44.17%	
5-10	115	17.64%	
11-20	20	3.07%	
21 or more	24	3.68%	
Total	**652**	**100 %**	

I use NAMD for _____ of my molecular dynamics simulations:



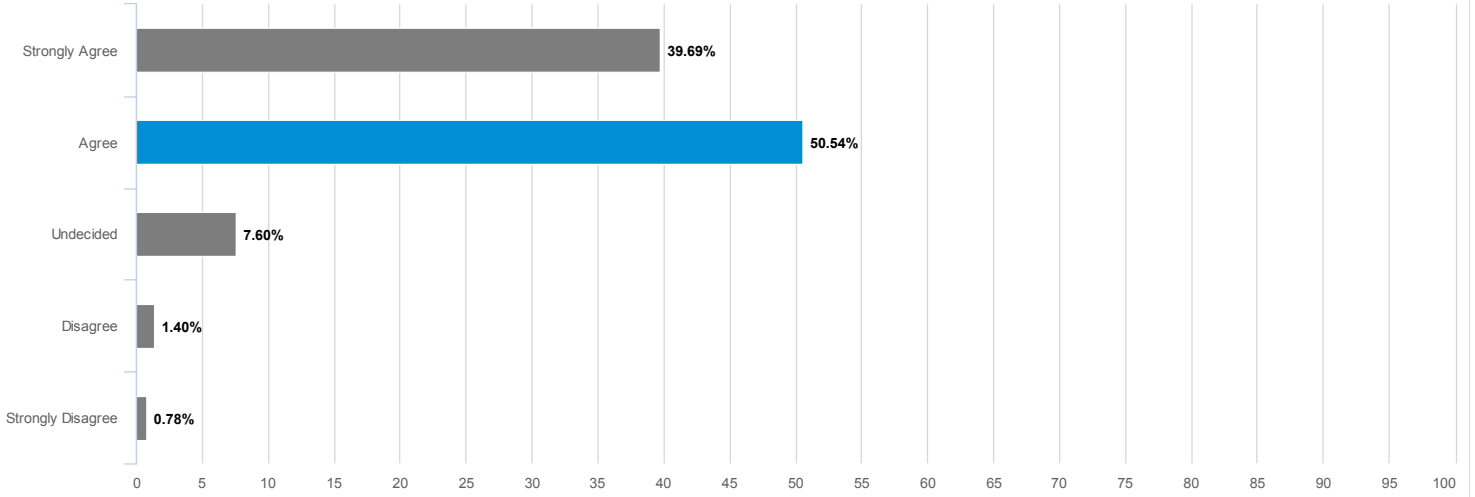
Answer	Count	Percent	20% 40% 60% 80% 100%
All	167	25.23%	
Most	213	32.18%	
Some	246	37.16%	
None	12	1.81%	
I don't use molecular dynamics	24	3.63%	
Total	**662**	**100 %**	

I use NAMD because it:



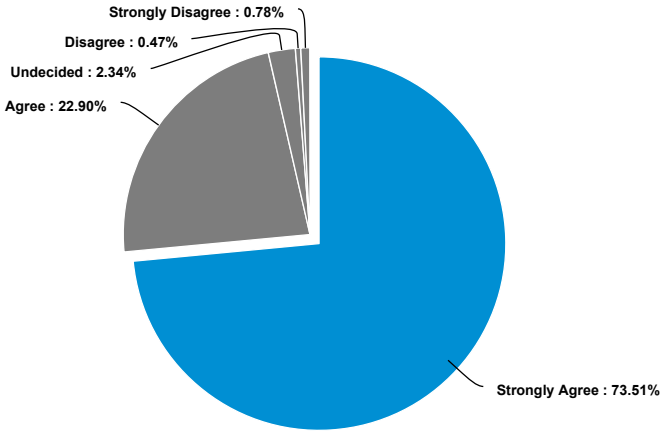
Question	Count	Score	Strongly Agree	Agree	Undecided	Disagree	Strongly Disagree
Meets my needs	645	1.73					
Is free	642	1.32					
Includes source code	636	2.18					
Is user friendly	641	2.14					
Is better than other molecular dynamics programs	649	2.53					
Is critical for my work	640	2.42					
	Average	**2.05**					

Meets my needs



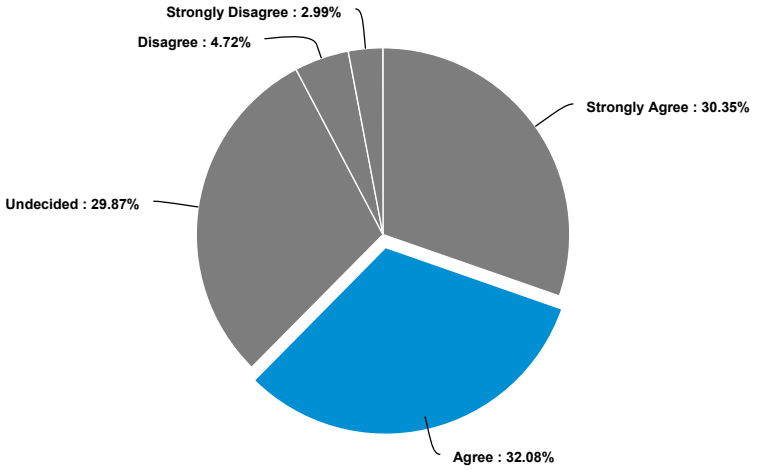
Answer	Count	Percent	20%	40%	60%	80%	100%
Strongly Agree	256	39.69%					
Agree	326	50.54%					
Undecided	49	7.6%					
Disagree	9	1.4%					
Strongly Disagree	5	0.78%					
Total	**645**	**100 %**					

Is free



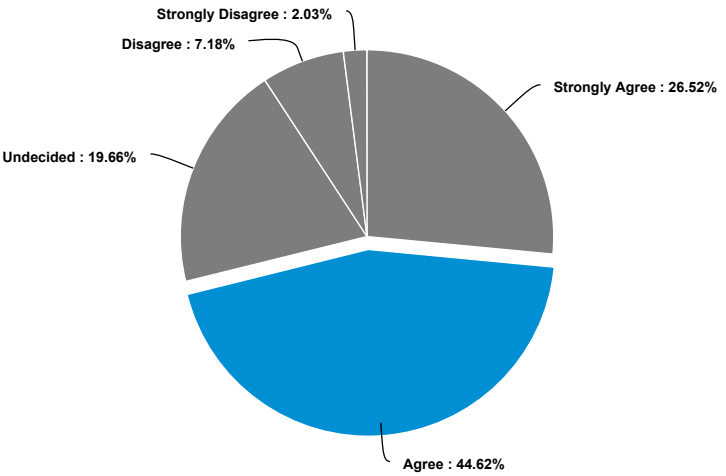
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	472	73.52%	
Agree	147	22.9%	
Undecided	15	2.34%	
Disagree	3	0.47%	
Strongly Disagree	5	0.78%	
Total	**642**	**100 %**	

Includes source code



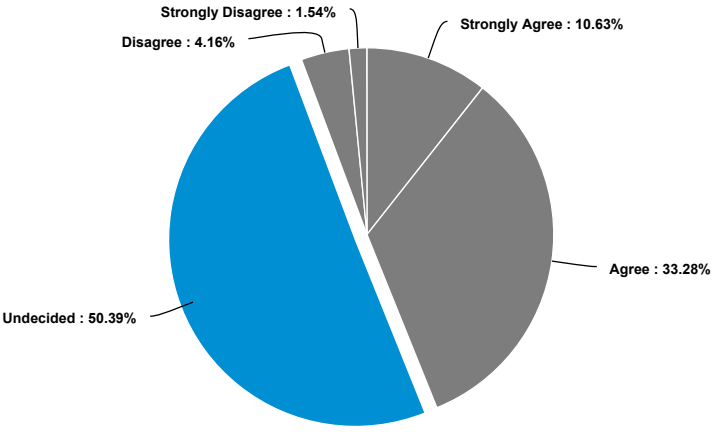
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	193	30.35%	
Agree	204	32.08%	
Undecided	190	29.87%	
Disagree	30	4.72%	
Strongly Disagree	19	2.99%	
Total	**636**	**100 %**	

Is user friendly



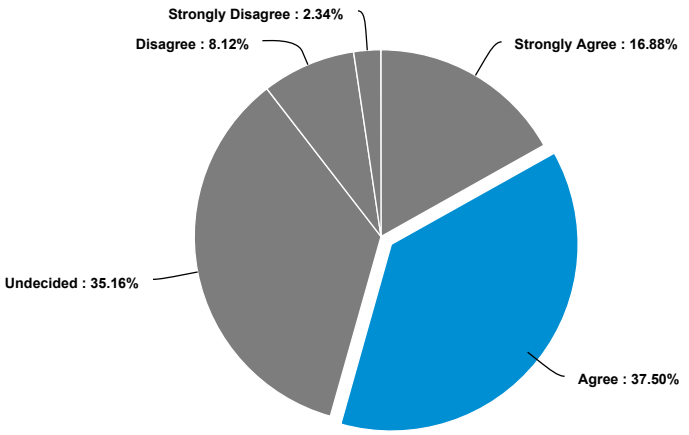
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	170	26.52%	
Agree	286	44.62%	
Undecided	126	19.66%	
Disagree	46	7.18%	
Strongly Disagree	13	2.03%	
Total	**641**	**100 %**	

Is better than other molecular dynamics programs



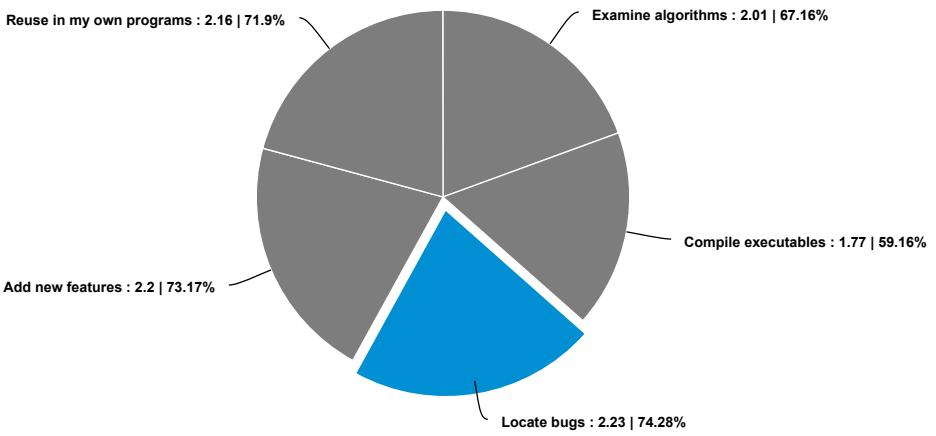
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	69	10.63%	
Agree	216	33.28%	
Undecided	327	50.39%	
Disagree	27	4.16%	
Strongly Disagree	10	1.54%	
Total	**649**	**100 %**	

Is critical for my work



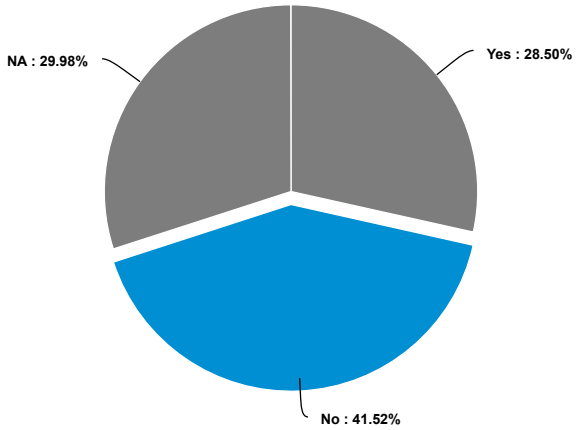
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	108	16.88%	
Agree	240	37.5%	
Undecided	225	35.16%	
Disagree	52	8.12%	
Strongly Disagree	15	2.34%	
Total	**640**	**100 %**	

I have downloaded the NAMD source code to:



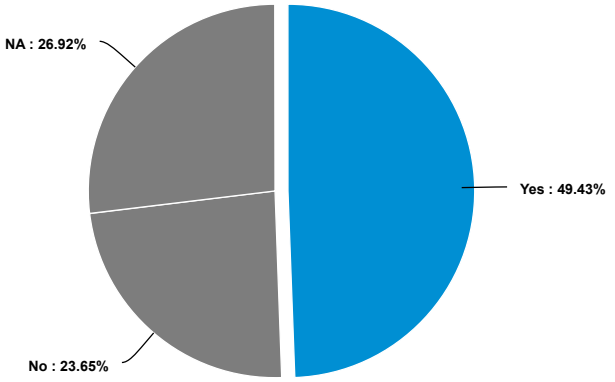
Question	Count	Score	Yes No NA
Examine algorithms	607	2.01	
Compile executables	613	1.77	
Locate bugs	591	2.23	
Add new features	584	2.2	
Reuse in my own programs	599	2.16	
	Average	**2.07**	

Examine algorithms



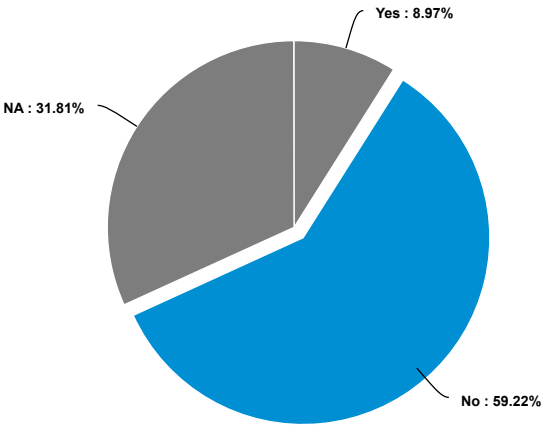
Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	173	28.5%	
No	252	41.52%	
NA	182	29.98%	
Total	**607**	**100 %**	

Compile executables



Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	303	49.43%	
No	145	23.65%	
NA	165	26.92%	
Total	**613**	**100 %**	

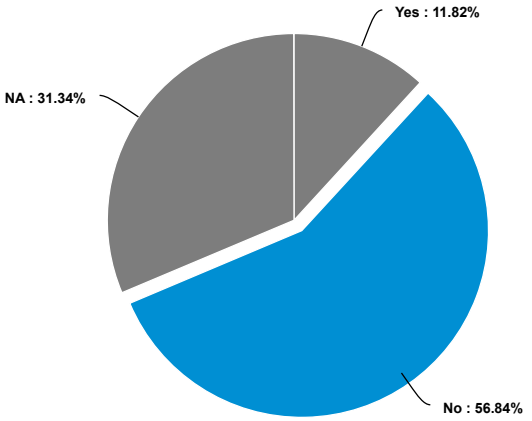
Locate bugs



Answer	Count	Percent	20% 40% 60% 80% 100%

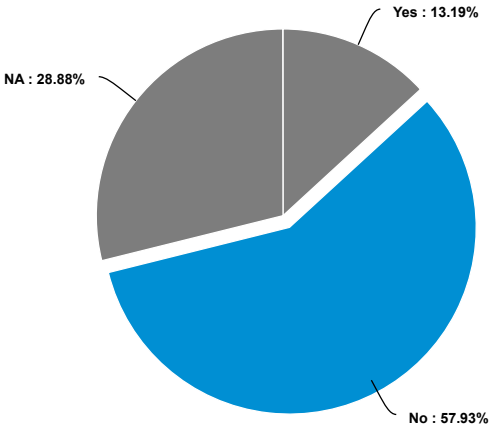
Yes	53	8.97%	
No	350	59.22%	
NA	188	31.81%	
Total	**591**	**100 %**	

Add new features



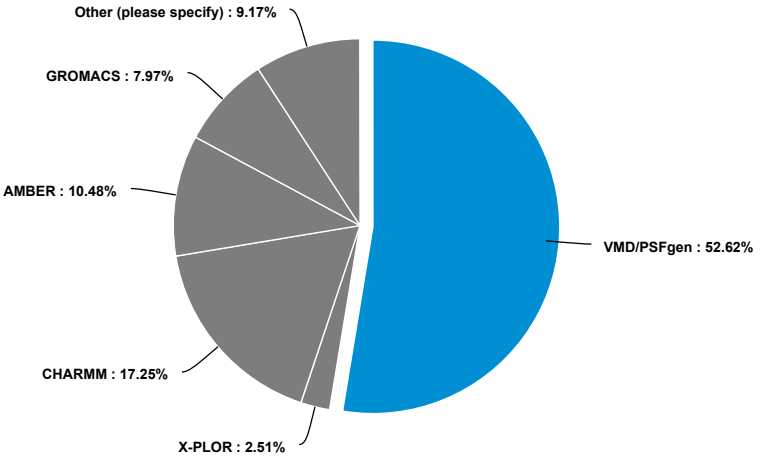
Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	69	11.82%	
No	332	56.85%	
NA	183	31.34%	
Total	**584**	**100 %**	

Reuse in my own programs



Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	79	13.19%	
No	347	57.93%	
NA	173	28.88%	
Total	**599**	**100 %**	

I primarily generate input files for NAMD with:



Answer	Count	Percent	20% 40% 60% 80% 100%
VMD/PSFgen	482	52.62%	
X-PLOR	23	2.51%	
CHARMM	158	17.25%	
AMBER	96	10.48%	
GROMACS	73	7.97%	
Other (please specify)	84	9.17%	
Total	**916**	**100 %**	

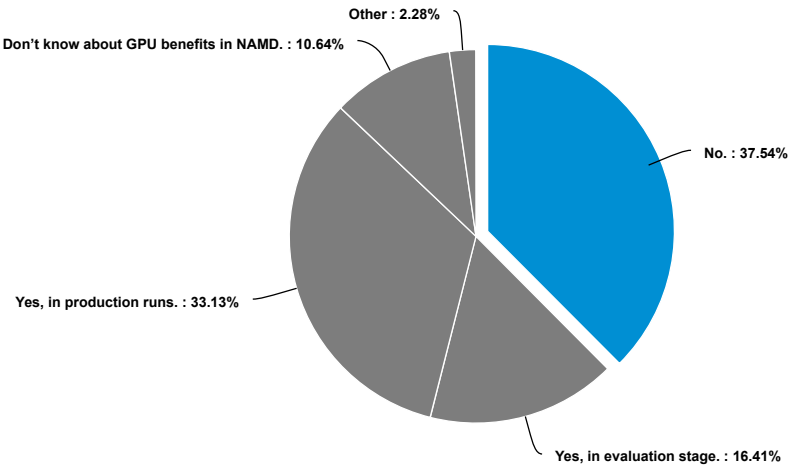
I primarily generate input files for NAMD with: - Text Data for Other (please specify)

03/23/2016	49533042	Use files generated by others
03/20/2016	49415317	cellulose-builder
03/19/2016	49375381	At the exploration stage
03/18/2016	49334107	my own scripts
03/18/2016	49313281	N/A
03/18/2016	49308347	packmole
03/17/2016	49297814	By hand
03/17/2016	49274496	VEGA ZZ
03/17/2016	49274001	self-made scripts
03/17/2016	49268017	python builder
03/17/2016	49254725	OPLS
03/17/2016	49251541	GView
03/17/2016	49244660	VEGA ZZ
03/17/2016	49242397	own scripts
03/16/2016	49238734	provided with benchmarks
03/16/2016	49227244	CHARMM-GUI
03/16/2016	49224752	just common sample jobs
03/16/2016	49207737	vegazz
03/16/2016	49206999	not really
03/16/2016	49204826	VEGA-ZZ
03/16/2016	49193002	SwissParam
03/16/2016	49185823	my own scripts
03/16/2016	49184937	By hand
03/16/2016	49179947	CHARMM-GUI
03/16/2016	49179392	For small ligands parametrization I use Discovery Studio and MOPAC for calculating charges
03/16/2016	49179050	In house programs
03/16/2016	49178756	Charmm-gui
03/16/2016	49178964	MDFF
03/16/2016	49177466	BIOVIA DS 4.5

03/16/2016	49177364	MOE
03/16/2016	49177036	http://www.charmm-gui.org
03/16/2016	49176768	VEGA ZZ
03/16/2016	49176775	VEGA ZZ
03/16/2016	49176330	CHARMM-GUI
03/15/2016	49175533	CHARMM-GUI
03/15/2016	49174847	Materials studio
03/15/2016	49173581	by my hand written code
03/15/2016	49169581	pdb
03/15/2016	49169878	My program on C++
03/15/2016	49167901	prvieded by our customers
03/15/2016	49169000	VMD
03/15/2016	49168679	MOE
03/15/2016	49168522	notepad
03/15/2016	49166850	packmol
03/15/2016	49166257	VegaZZ
03/15/2016	49165578	discovery studio
03/15/2016	49165286	Packmol
03/15/2016	49163754	discoverystudio
03/15/2016	49160674	own suite
03/15/2016	49161545	Ambertool
03/15/2016	49160024	VEGA ZZ
03/15/2016	49159883	Maestro
03/15/2016	49159494	Gaussian
03/15/2016	49158782	so far used only demos
03/15/2016	49156239	own code
03/15/2016	49153990	download
03/15/2016	49155164	VegaZZ
03/15/2016	49153695	vi
03/15/2016	49154779	charmm-gui
03/15/2016	49154216	MOE
03/15/2016	49153944	MOE
03/15/2016	49153615	MOE
03/15/2016	49153305	python
03/15/2016	49153203	I think our users use all of the above
03/15/2016	49152936	CHARMM-GUI
03/15/2016	49152816	N/A
03/15/2016	49152126	download standard benchmark input files
03/15/2016	49151626	charmm-gui
03/15/2016	49151577	in house code
03/15/2016	49148971	CHARMM-GUI
03/15/2016	49150319	VegaZZ (http://www.vegazz.net/)
03/15/2016	49150231	Manual editing/custom scripts
03/15/2016	49150650	charmm-gui
03/15/2016	49149458	vega ZZ
03/15/2016	49149062	Charmm-gui
03/15/2016	49148367	VEGA ZZ
03/15/2016	49147716	I get input from customers and standard benchmarks
03/15/2016	49147555	charmm-gui
03/15/2016	49147189	Matlab, python
03/15/2016	49146631	charm-gui

03/15/2016	49146889	CHARMM-GUI
03/15/2016	49146826	vim
03/15/2016	49145477	Wrote my own membrane builder

Does your group use any of the GPU acceleration capabilities in NAMD?

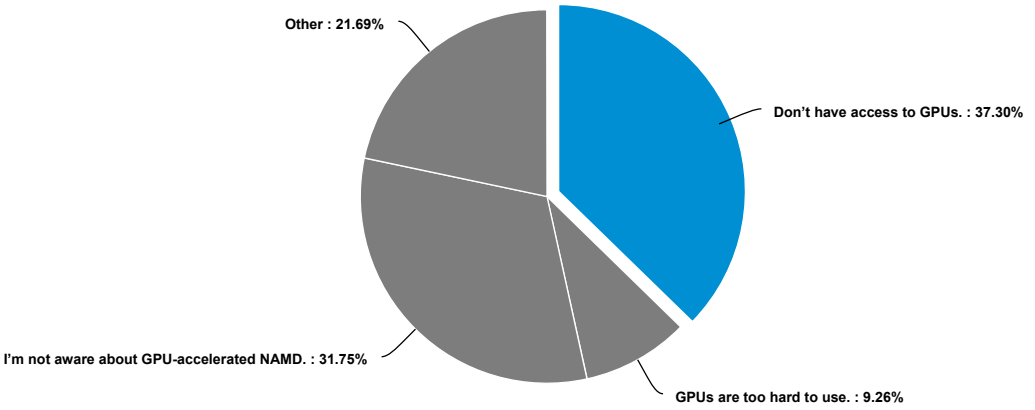


Answer	Count	Percent	20% 40% 60% 80% 100%
No.	247	37.54%	
Yes, in evaluation stage.	108	16.41%	
Yes, in production runs.	218	33.13%	
Don't know about GPU benefits in NAMD.	70	10.64%	
Other	15	2.28%	
Total	**658**	**100 %**	

Does your group use any of the GPU acceleration capabilities in NAMD? - Text Data for Other

03/18/2016	49348261	Doesn't always work. Still in evaluation stages
03/17/2016	49256222	I need this feature very dearly but could not get it to work with AMD R5 M300 graphic card, running on windows
03/16/2016	49224752	Yes, we consider NAMD a "showcase" example of how to do GPU code right!
03/16/2016	49185823	Sometimes, depending on hardware.
03/16/2016	49182551	No, but plan to use it in the near future.
03/16/2016	49178756	Not yet
03/16/2016	49177466	trying to to that
03/16/2016	49177036	not yet but hopefully soon
03/15/2016	49167901	sometimes it's a requirement for the installation
03/15/2016	49153615	could not get it to work with current hardware
03/15/2016	49151744	Interested. Maybe in the future.
03/15/2016	49151577	not yet, but interested
03/15/2016	49149276	Depends on user
03/15/2016	49147898	Working on it
03/15/2016	49145915	Not yet .. But we know NAMD is capable

If you are not using GPU acceleration capabilities in NAMD, why not?



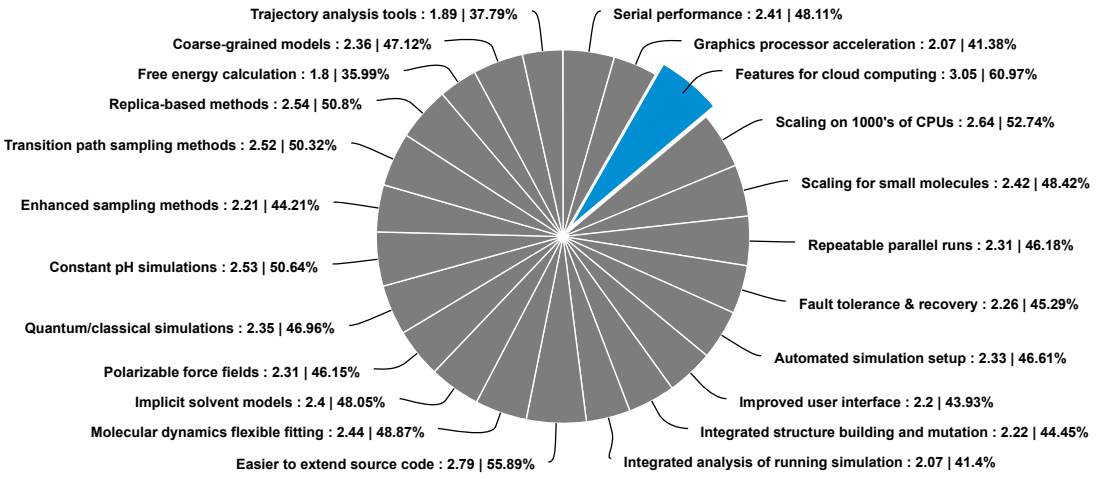
Answer	Count	Percent	20% 40% 60% 80% 100%
Don’t have access to GPUs.	141	37.3%	
GPUs are too hard to use.	35	9.26%	
I'm not aware about GPU-accelerated NAMD.	120	31.75%	
Other	82	21.69%	
Total	**378**	**100 %**	

If you are not using GPU acceleration capabilities in NAMD, why not? - Text Data for Other

04/01/2016	49982422	The cluster we are working with has more requirements for GPU acceleration.
03/23/2016	49514885	errors (bugs or incompatibility issues?)
03/21/2016	49458465	I haven't learnt how to incorporate them yet
03/21/2016	49446863	Lacks performance of AMBER
03/21/2016	49423440	Unstable runs
03/20/2016	49401700	only 10%... means nothing prefer Amber 14
03/19/2016	49364561	I evaluation to use
03/18/2016	49348261	I use GPU acceleration in other software, but the linux namd binaries seem to not work as well as they used to.
03/18/2016	49308347	The benefit of GPU (e.g. 50 cores) acceleration was to small in comparison to the large scaleability on CPUs (which was nearly linear on even > 500 cores)
03/17/2016	49256222	Probably, lack of requisite knownledge
03/17/2016	49252386	I would like to use GPU accelerated NAMD on Cray cluster, but the cluster admin has refused to install it for now. He will review it during the next review cycle. My account space is not enough for local installation.
03/17/2016	49245968	no, I use all time
03/17/2016	49244715	I even haven't hear about this possibility
03/16/2016	49227244	N/A
03/16/2016	49212083	Tabulated potentials are not supported in CUDA version of NAMD
03/16/2016	49199894	I only passively have played with the program. Haven't really dug in yet.
03/16/2016	49197118	have limited access to GPUs
03/16/2016	49196131	NA
03/16/2016	49193353	prefer OpenMM
03/16/2016	49184750	I;m not running NAMD jobs, I just wanted to see your code ;)
03/16/2016	49184937	Will soon get GPUs
03/16/2016	49182399	We did not bother yet
03/16/2016	49179363	no need to
03/16/2016	49178756	Whould be just for local machines right now
03/16/2016	49177466	still figuring out how
03/15/2016	49175409	problems to use many GPU nodes in parallel
03/15/2016	49174506	Xeon Phi
03/15/2016	49174386	Not happy with GPU set up
03/15/2016	49173041	we can use
03/15/2016	49170497	We are not using GPU device now
03/15/2016	49166864	NAMDw/ GPU is slow compared to others.

03/15/2016	49166417	Some bugs with using GPU acceleration of NAMD on my system
03/15/2016	49165303	I did not feel the need to run them over GPUs, because my simulations are usually short, and my primary MD software is GROMACS.
03/15/2016	49164420	I'm not very familiar with GPU. My supervisor used to say that it doesn't behave well with double precision values.
03/15/2016	49163943	Concerns about compatibility with majority of other simulations that were CPU bound
03/15/2016	49161545	Yes, I tried, but two main defect: 1st interesting part of the code does not work on GPU. 2nd graphical driver stability
03/15/2016	49158782	no gpu on our cluster
03/15/2016	49157715	the minimization result from gpu and cpu version of namd already differs. i have no confidence.
03/15/2016	49157368	Current non-GPU computing capability is satisfying
03/15/2016	49156824	i am using
03/15/2016	49156275	GPU is expensive.
03/15/2016	49156285	Tested performance is too poor
03/15/2016	49155369	I use GPU
03/15/2016	49153408	Money
03/15/2016	49153717	Doesn't work for FEP code.
03/15/2016	49152786	We need to buy.
03/15/2016	49153000	I am not doing molecular modeling right now
03/15/2016	49152386	Have other programs already set up for GPU use
03/15/2016	49151698	using other software
03/15/2016	49151655	We are using OpenMM for GPU simulations
03/15/2016	49151462	not needed for now
03/15/2016	49150319	I use NAMD on a Sony VAIO laptop, which is capable of GPU acceleration but I have no idea how to do it, and no time to find out..
03/15/2016	49150125	cannot seem to get my group members to adopt it (likely because they don't understand how the processes are threaded)
03/15/2016	49150458	AMBER is much faster and a better use of GPU resources
03/15/2016	49149989	I currently look at very small systems (fast enough on 1 CPU)
03/15/2016	49149983	-
03/15/2016	49149276	Users are hesitant to switch.
03/15/2016	49148953	Haven't gotten around to configuring for GPU use yet
03/15/2016	49148385	I use other tools for this, specifically OpenMM
03/15/2016	49147716	cross over to faster on Zeon only is about 4 ndoes
03/15/2016	49147898	Tricky so far
03/15/2016	49145915	Previously didn't have access but the next set of simulations will make use of GPUs
03/15/2016	49145477	Primarily run on blue gene
02/25/2016	48190089	I'm using GPU acceleration.

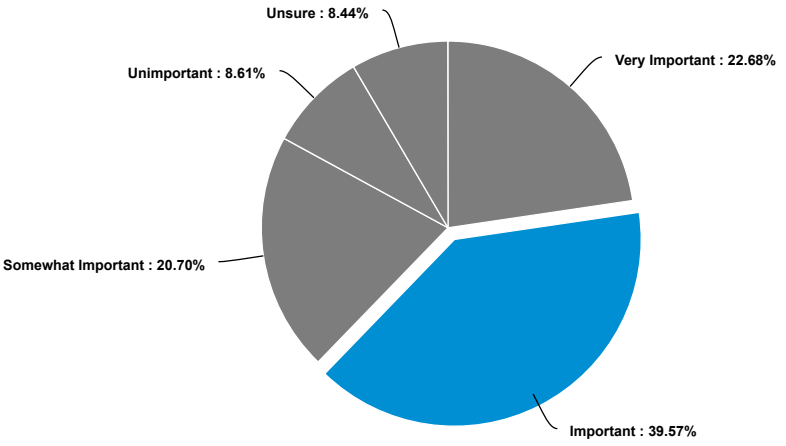
Rate the importance to your work of these PLANNED enhancements:



Question	Count	Score	Very Important	Important	Somewhat Important	Unimportant	Unsure
Serial performance	604	2.41					
Graphics processor acceleration	610	2.07					

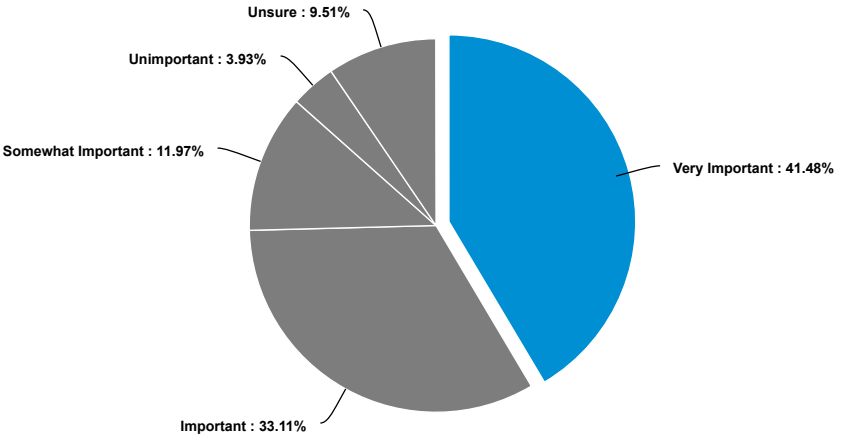
Features for cloud computing	598	3.05	
Scaling on 1000's of CPUs	606	2.64	
Scaling for small molecules	606	2.42	
Repeatable parallel runs	602	2.31	
Fault tolerance & recovery	594	2.26	
Automated simulation setup	605	2.33	
Improved user interface	611	2.2	
Integrated structure building and mutation	602	2.22	
Integrated analysis of running simulation	600	2.07	
Easier to extend source code	594	2.79	
Molecular dynamics flexible fitting	595	2.44	
Implicit solvent models	594	2.4	
Polarizable force fields	602	2.31	
Quantum/classical simulations	598	2.35	
Constant pH simulations	598	2.53	
Enhanced sampling methods	594	2.21	
Transition path sampling methods	597	2.52	
Replica-based methods	589	2.54	
Free energy calculation	609	1.8	
Coarse-grained models	593	2.36	
Trajectory analysis tools	606	1.89	
	Average	**2.35**	

Serial performance



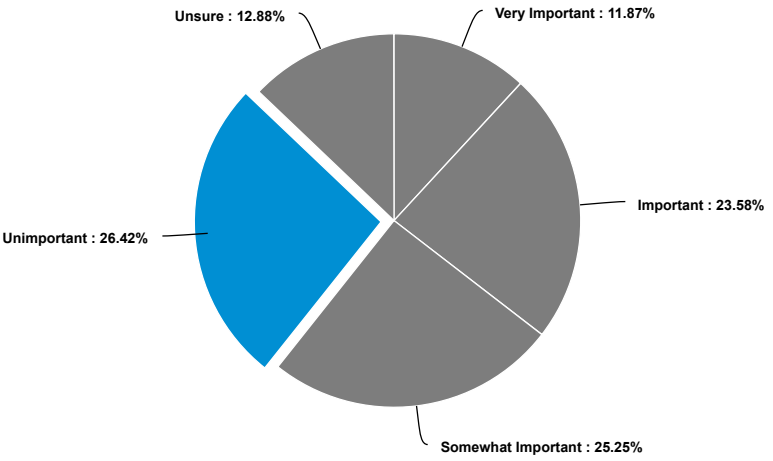
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	137	22.68%	
Important	239	39.57%	
Somewhat Important	125	20.7%	
Unimportant	52	8.61%	
Unsure	51	8.44%	
Total	**604**	**100 %**	

Graphics processor acceleration



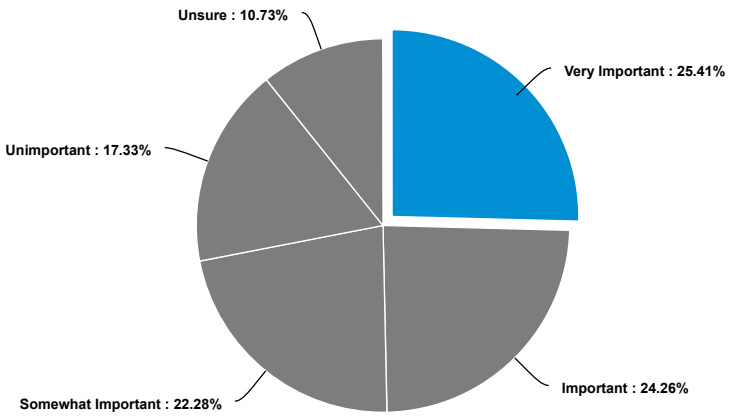
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	253	41.48%	
Important	202	33.11%	
Somewhat Important	73	11.97%	
Unimportant	24	3.93%	
Unsure	58	9.51%	
Total	**610**	**100 %**	

Features for cloud computing



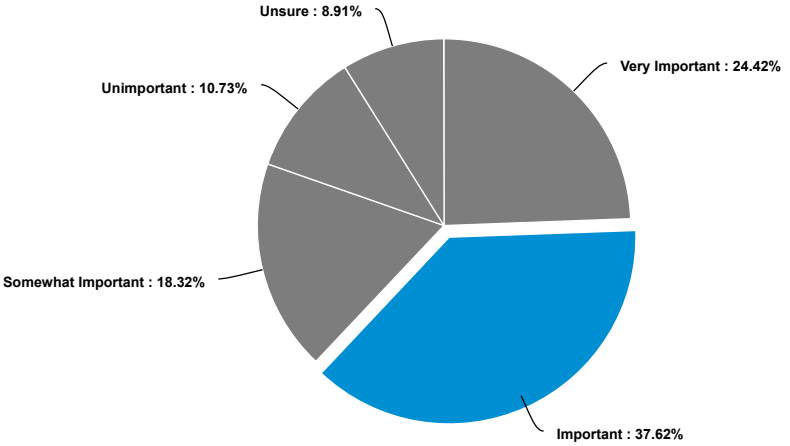
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	71	11.87%	
Important	141	23.58%	
Somewhat Important	151	25.25%	
Unimportant	158	26.42%	
Unsure	77	12.88%	
Total	**598**	**100 %**	

Scaling on 1000's of CPUs



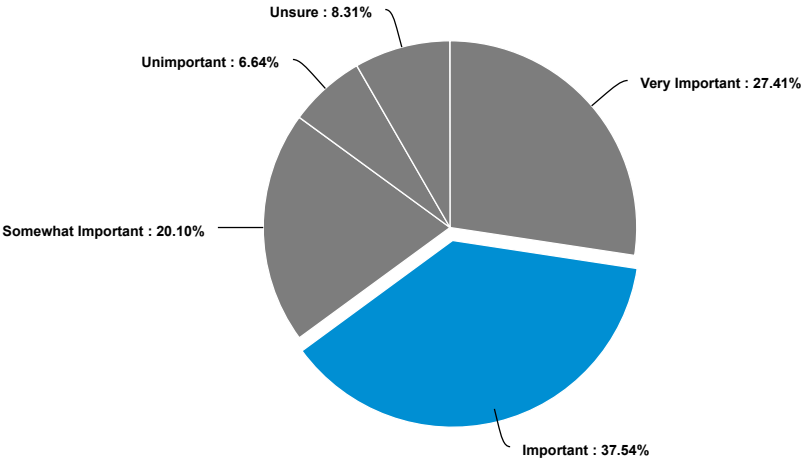
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	154	25.41%	
Important	147	24.26%	
Somewhat Important	135	22.28%	
Unimportant	105	17.33%	
Unsure	65	10.73%	
Total	**606**	**100 %**	

Scaling for small molecules



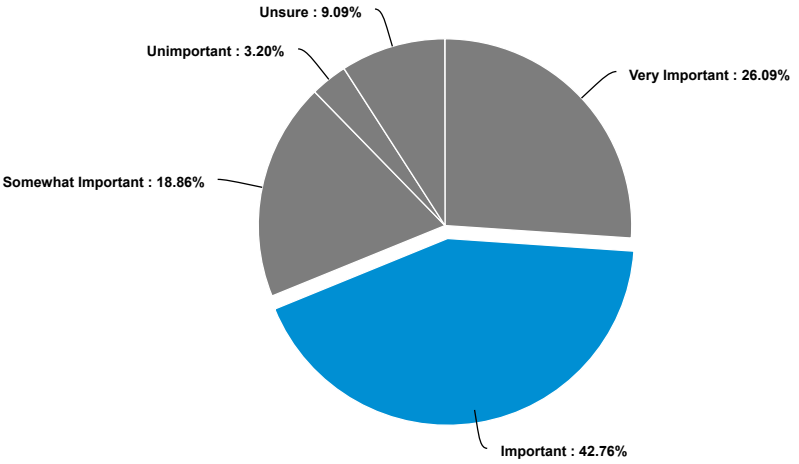
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	148	24.42%	
Important	228	37.62%	
Somewhat Important	111	18.32%	
Unimportant	65	10.73%	
Unsure	54	8.91%	
Total	**606**	**100 %**	

Repeatable parallel runs



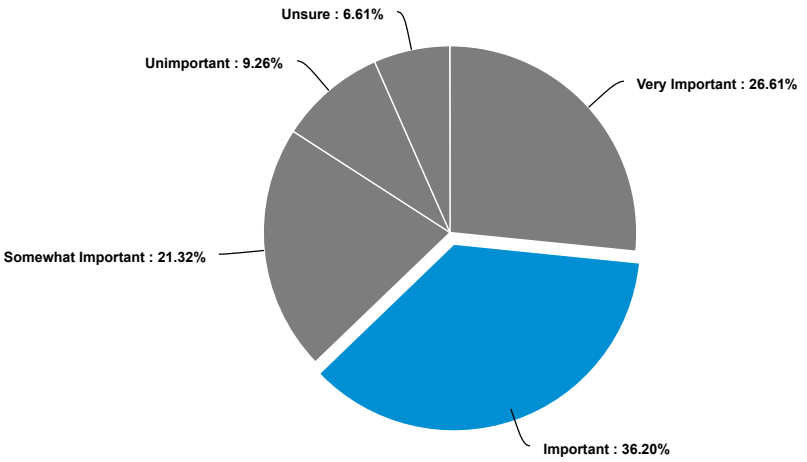
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	165	27.41%	
Important	226	37.54%	
Somewhat Important	121	20.1%	
Unimportant	40	6.64%	
Unsure	50	8.31%	
Total	**602**	**100 %**	

Fault tolerance & recovery



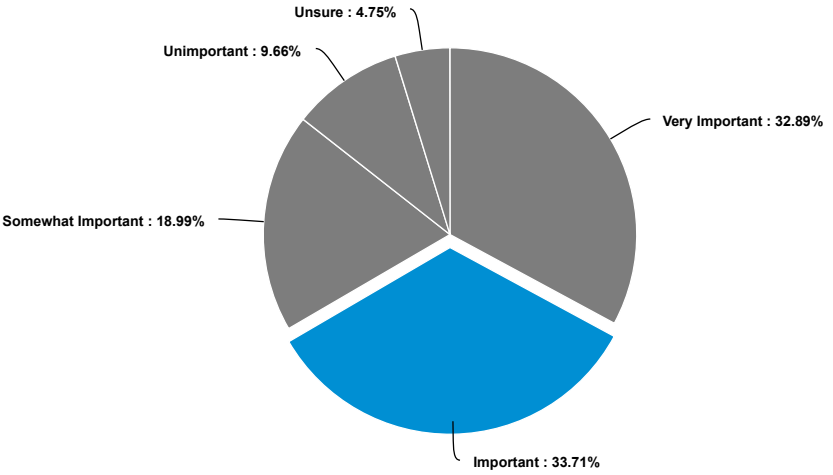
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	155	26.09%	
Important	254	42.76%	
Somewhat Important	112	18.86%	
Unimportant	19	3.2%	
Unsure	54	9.09%	
Total	**594**	**100 %**	

Automated simulation setup



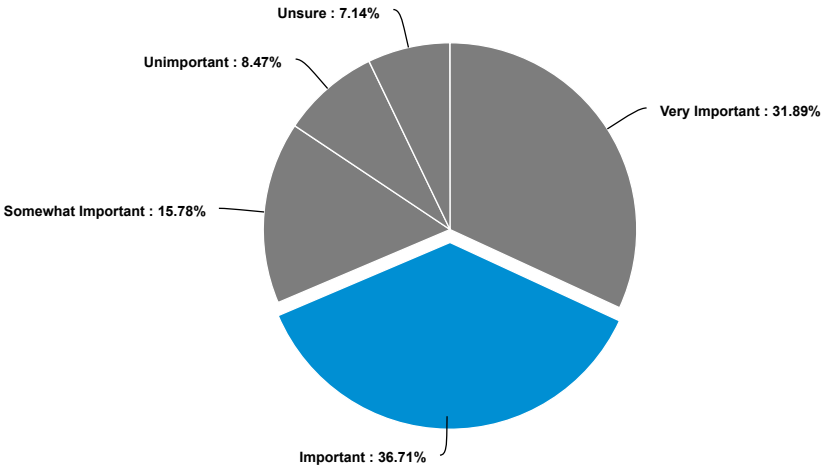
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	161	26.61%	
Important	219	36.2%	
Somewhat Important	129	21.32%	
Unimportant	56	9.26%	
Unsure	40	6.61%	
Total	**605**	**100 %**	

Improved user interface



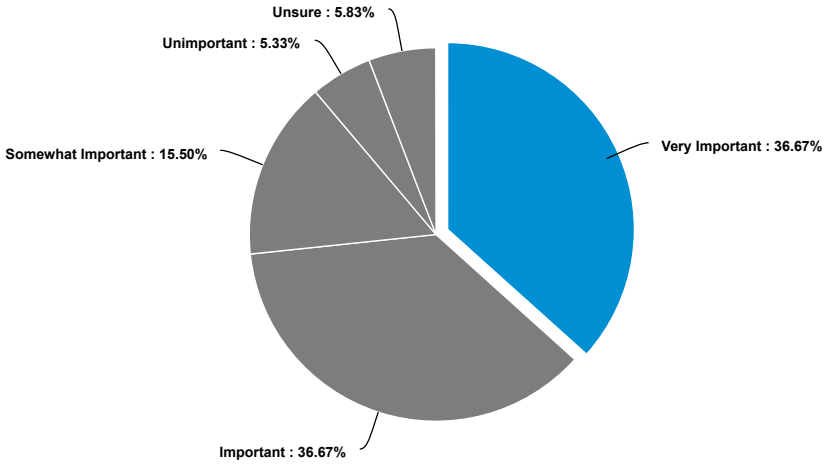
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	201	32.9%	
Important	206	33.72%	
Somewhat Important	116	18.99%	
Unimportant	59	9.66%	
Unsure	29	4.75%	
Total	**611**	**100 %**	

Integrated structure building and mutation



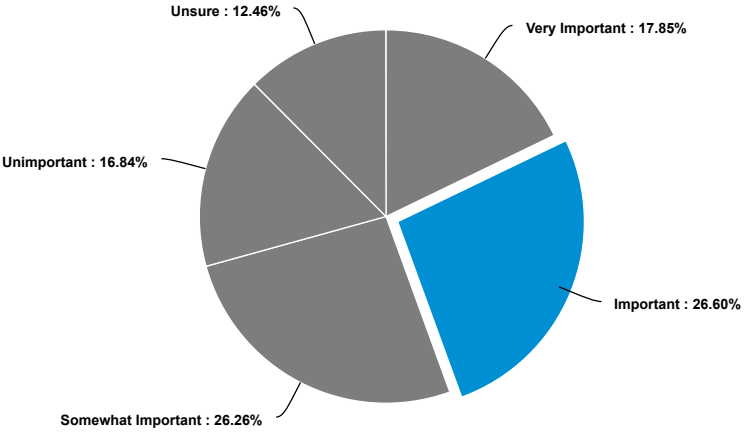
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	192	31.89%	
Important	221	36.71%	
Somewhat Important	95	15.78%	
Unimportant	51	8.47%	
Unsure	43	7.14%	
Total	**602**	**100 %**	

Integrated analysis of running simulation



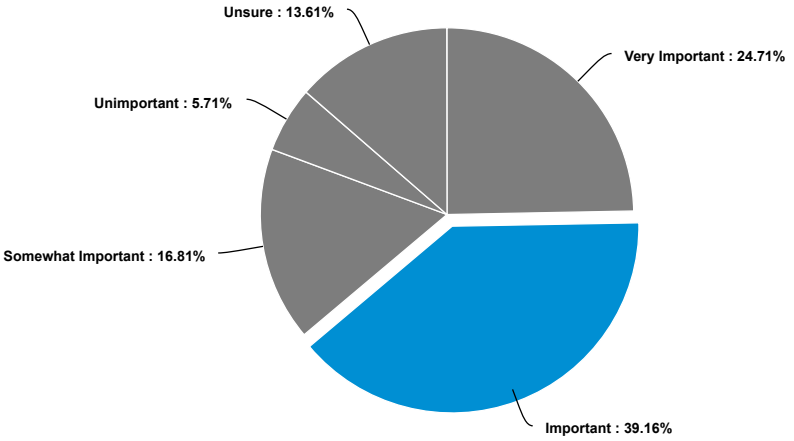
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	220	36.67%	
Important	220	36.67%	
Somewhat Important	93	15.5%	
Unimportant	32	5.33%	
Unsure	35	5.83%	
Total	**600**	**100 %**	

Easier to extend source code



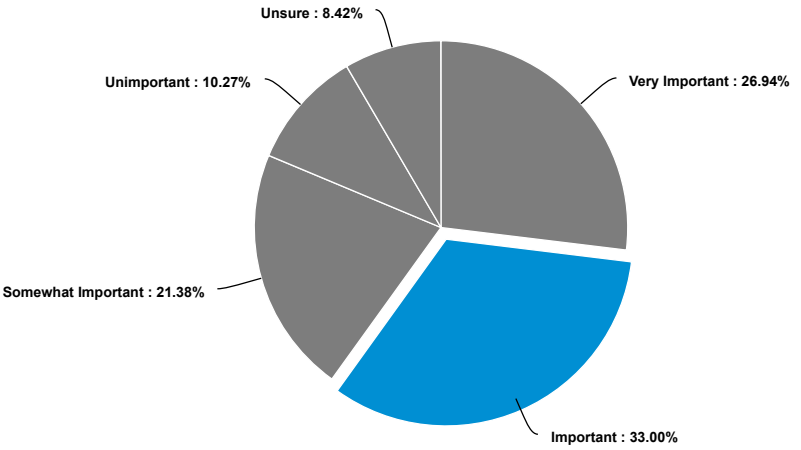
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	106	17.85%	
Important	158	26.6%	
Somewhat Important	156	26.26%	
Unimportant	100	16.84%	
Unsure	74	12.46%	
Total	**594**	**100 %**	

Molecular dynamics flexible fitting



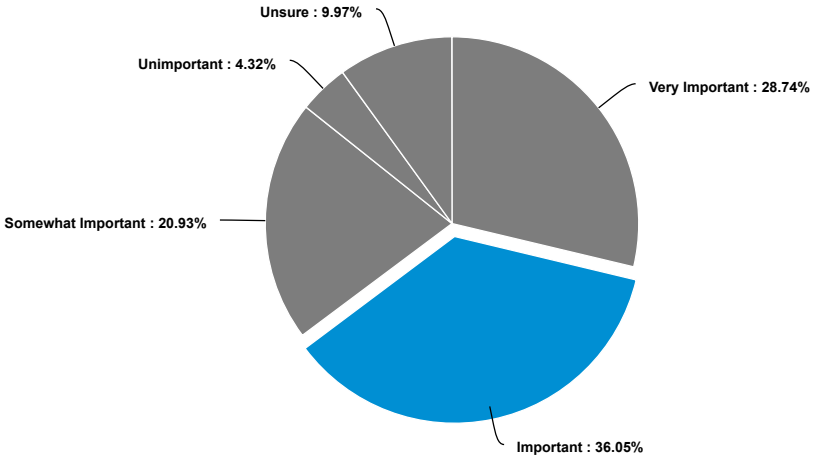
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	147	24.71%	
Important	233	39.16%	
Somewhat Important	100	16.81%	
Unimportant	34	5.71%	
Unsure	81	13.61%	
Total	**595**	**100 %**	

Implicit solvent models



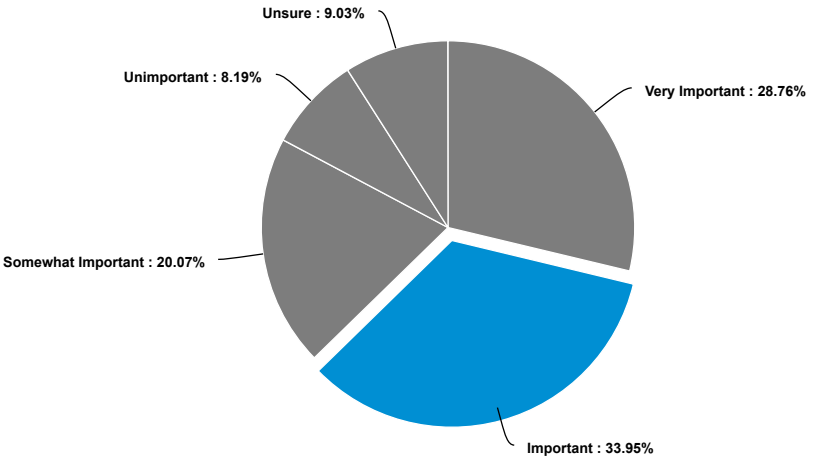
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	160	26.94%	
Important	196	33%	
Somewhat Important	127	21.38%	
Unimportant	61	10.27%	
Unsure	50	8.42%	
Total	**594**	**100 %**	

Polarizable force fields



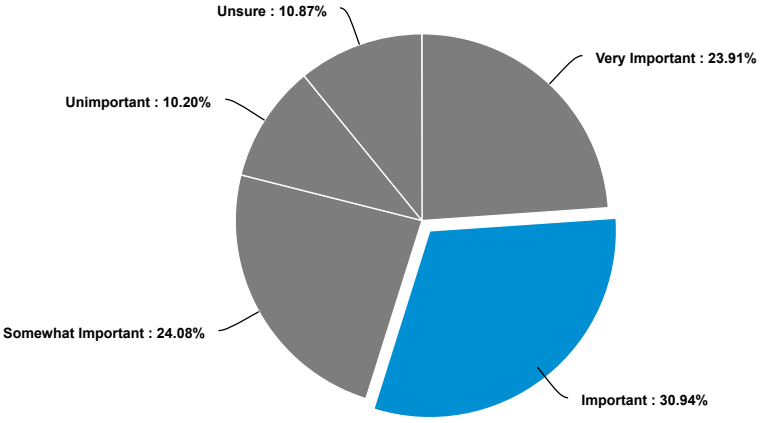
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	173	28.74%	
Important	217	36.05%	
Somewhat Important	126	20.93%	
Unimportant	26	4.32%	
Unsure	60	9.97%	
Total	**602**	**100 %**	

Quantum/classical simulations



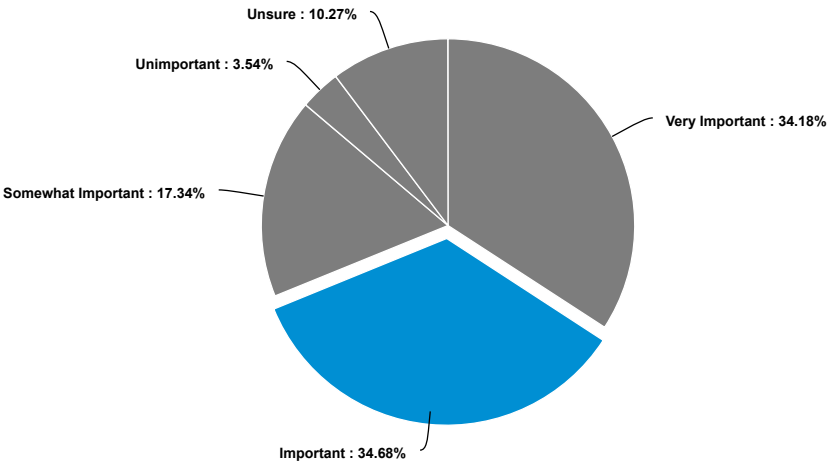
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	172	28.76%	
Important	203	33.95%	
Somewhat Important	120	20.07%	
Unimportant	49	8.19%	
Unsure	54	9.03%	
Total	**598**	**100 %**	

Constant pH simulations



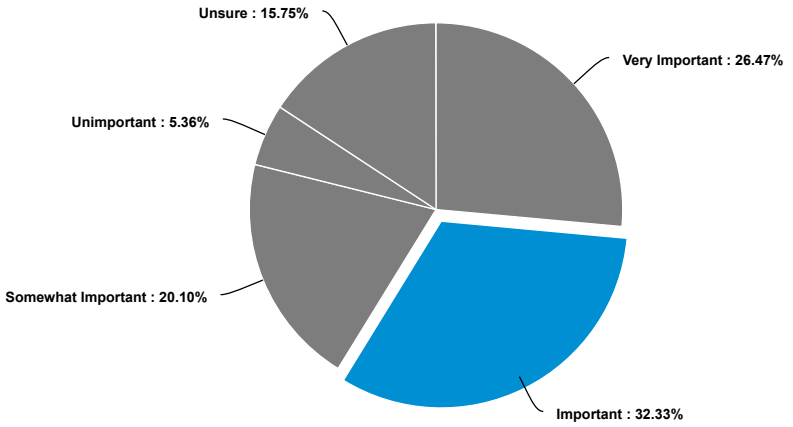
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	143	23.91%	
Important	185	30.94%	
Somewhat Important	144	24.08%	
Unimportant	61	10.2%	
Unsure	65	10.87%	
Total	**598**	**100 %**	

Enhanced sampling methods



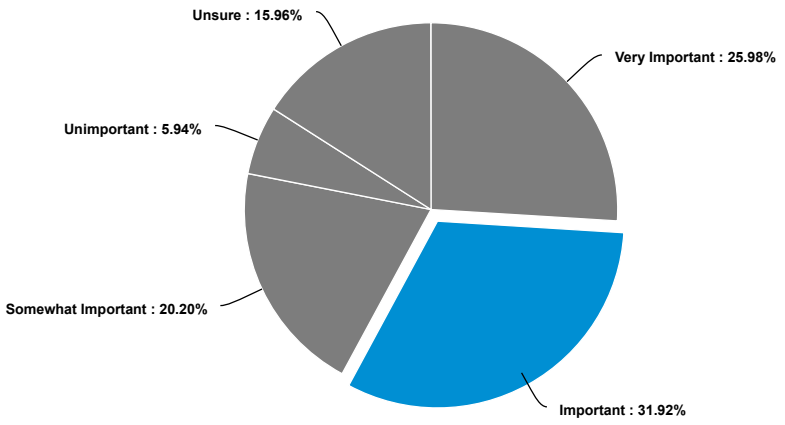
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	203	34.18%	
Important	206	34.68%	
Somewhat Important	103	17.34%	
Unimportant	21	3.54%	
Unsure	61	10.27%	
Total	**594**	**100 %**	

Transition path sampling methods



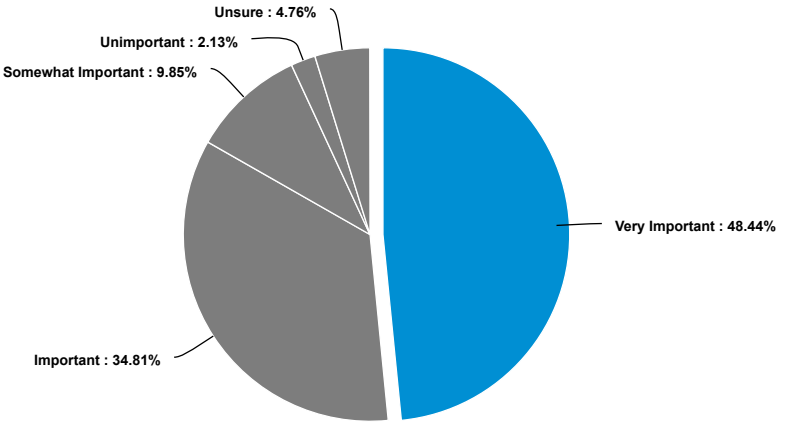
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	158	26.47%	
Important	193	32.33%	
Somewhat Important	120	20.1%	
Unimportant	32	5.36%	
Unsure	94	15.75%	
Total	**597**	**100 %**	

Replica-based methods



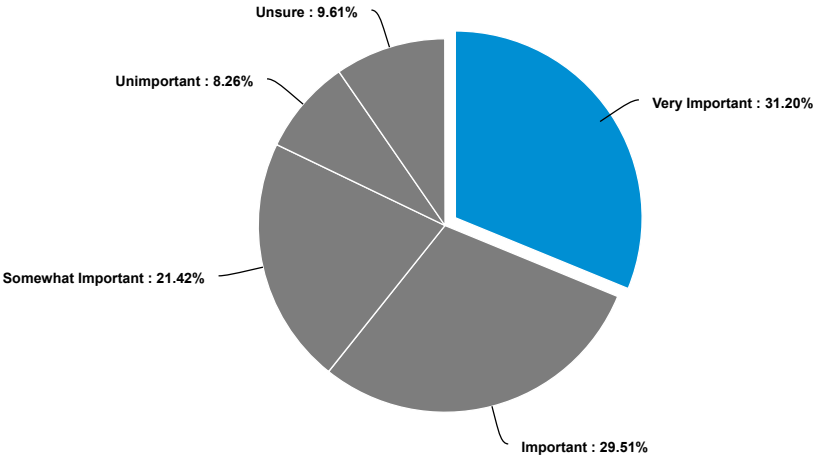
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	153	25.98%	
Important	188	31.92%	
Somewhat Important	119	20.2%	
Unimportant	35	5.94%	
Unsure	94	15.96%	
Total	**589**	**100 %**	

Free energy calculation



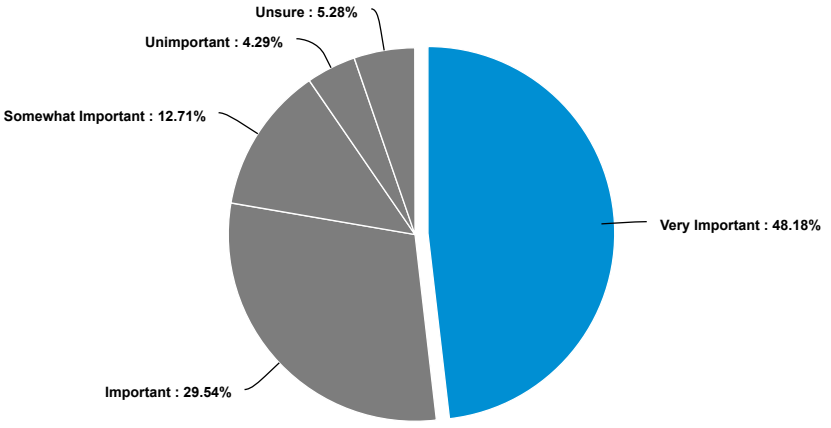
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	295	48.44%	
Important	212	34.81%	
Somewhat Important	60	9.85%	
Unimportant	13	2.13%	
Unsure	29	4.76%	
Total	**609**	**100 %**	

Coarse-grained models



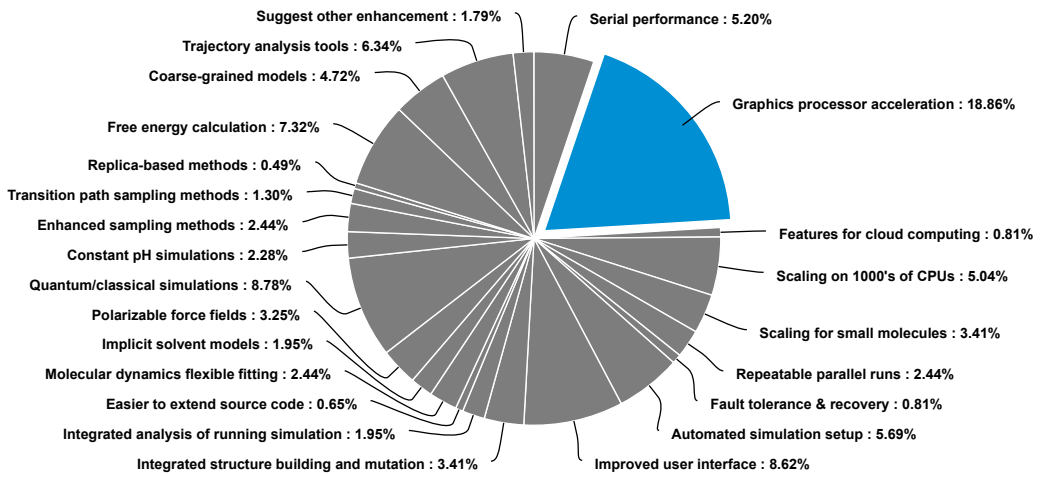
Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	185	31.2%	
Important	175	29.51%	
Somewhat Important	127	21.42%	
Unimportant	49	8.26%	
Unsure	57	9.61%	
Total	**593**	**100 %**	

Trajectory analysis tools



Answer	Count	Percent	20% 40% 60% 80% 100%
Very Important	292	48.18%	
Important	179	29.54%	
Somewhat Important	77	12.71%	
Unimportant	26	4.29%	
Unsure	32	5.28%	
Total	**606**	**100 %**	

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

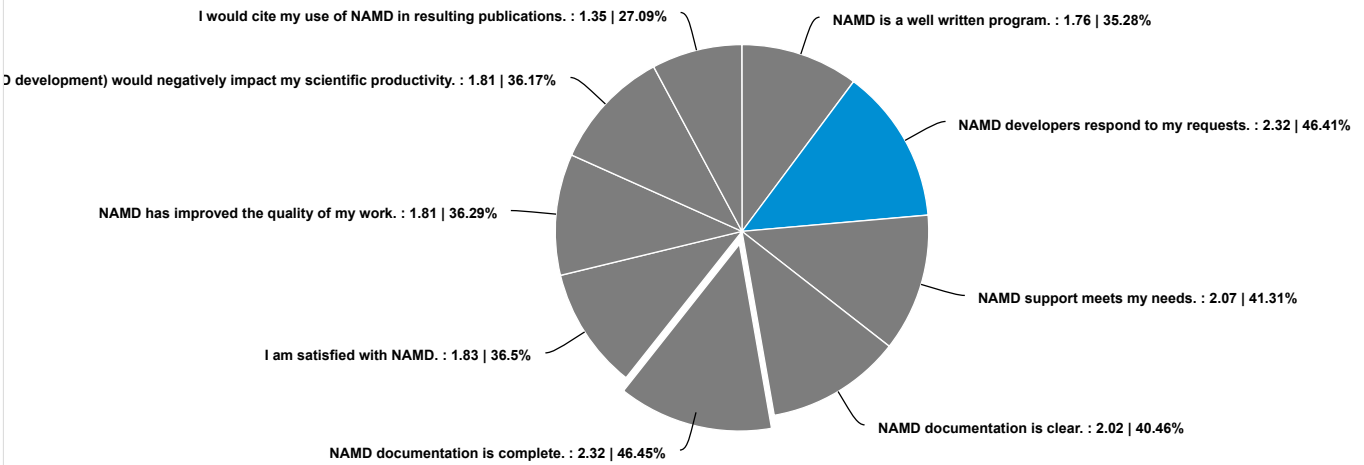


Answer	Count	Percent	20% 40% 60% 80% 100%
Serial performance	32	5.2%	
Graphics processor acceleration	116	18.86%	
Features for cloud computing	5	0.81%	
Scaling on 1000's of CPUs	31	5.04%	
Scaling for small molecules	21	3.41%	
Repeatable parallel runs	15	2.44%	
Fault tolerance & recovery	5	0.81%	
Automated simulation setup	35	5.69%	
Improved user interface	53	8.62%	
Integrated structure building and mutation	21	3.41%	
Integrated analysis of running simulation	12	1.95%	
Easier to extend source code	4	0.65%	
Molecular dynamics flexible fitting	15	2.44%	
Implicit solvent models	12	1.95%	
Polarizable force fields	20	3.25%	
Quantum/classical simulations	54	8.78%	
Constant pH simulations	14	2.28%	
Enhanced sampling methods	15	2.44%	
Transition path sampling methods	8	1.3%	
Replica-based methods	3	0.49%	
Free energy calculation	45	7.32%	
Coarse-grained models	29	4.72%	
Trajectory analysis tools	39	6.34%	
Suggest other enhancement	11	1.79%	
Total	**615**	**100 %**	

Select the PLANNED enhancement that should have highest priority for development: - Text Data for Suggest other enhancement

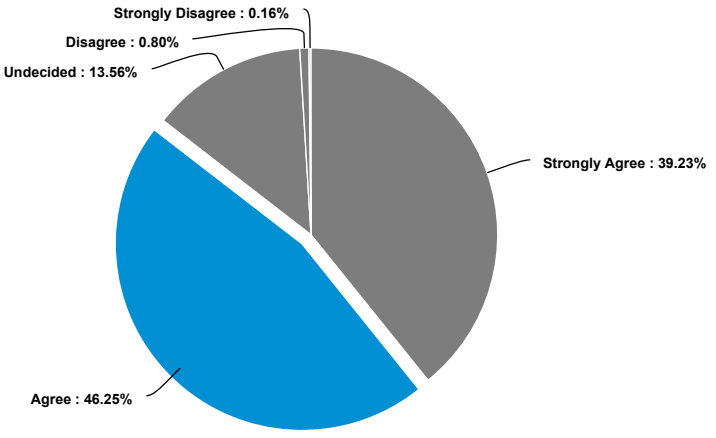
03/20/2016	49414349	Not sure
03/16/2016	49182551	Implementation of SAXS data
03/15/2016	49170663	Capability to build any molecule from the periodic table (like inorganic builder tool [integrated in VMD] which can make a very small number of molecules now)
03/15/2016	49167696	Generation of topology files
03/15/2016	49165188	Easier Force Field generation
03/15/2016	49152171	Not enough experience to say
03/15/2016	49150650	parallel colvar
03/15/2016	49149458	implementation of Universal Force Field
03/15/2016	49149232	FPGAs
03/15/2016	49148383	Move to the OpenCL api to support wider array of hardware
03/15/2016	49146903	intel PHI Knights Landing

Rate your agreement with these statements describing NAMD:



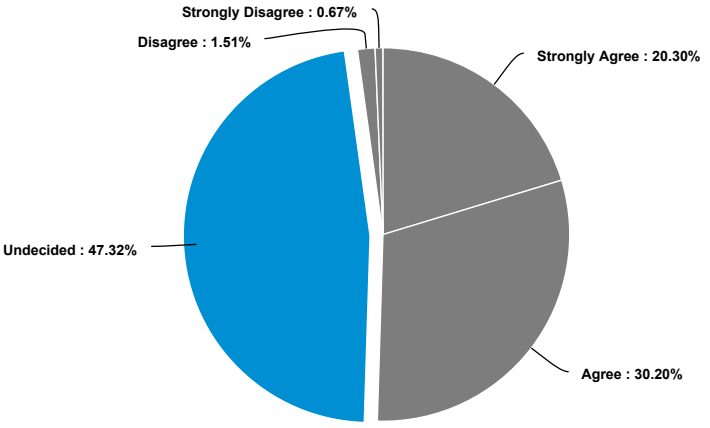
Question	Count	Score	Strongly Agree	Agree	Undecided	Disagree	Strongly Disagree
NAMD is a well written program.	627	1.76					
NAMD developers respond to my requests.	596	2.32					
NAMD support meets my needs.	609	2.07					
NAMD documentation is clear.	610	2.02					
NAMD documentation is complete.	614	2.32					
I am satisfied with NAMD.	612	1.83					
NAMD has improved the quality of my work.	620	1.81					
Not having NAMD available (e.g., in case of discontinued funding of NAMD development) would negatively impact my scientific productivity.	601	1.81					
I would cite my use of NAMD in resulting publications.	615	1.35					
	Average	**1.92**					

NAMD is a well written program.



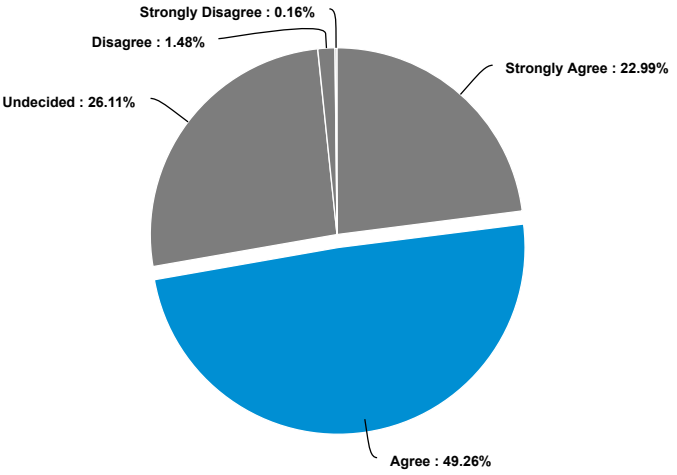
Answer	Count	Percent	20%	40%	60%	80%	100%
Strongly Agree	246	39.23%					
Agree	290	46.25%					
Undecided	85	13.56%					
Disagree	5	0.8%					
Strongly Disagree	1	0.16%					
Total	**627**	**100 %**					

NAMD developers respond to my requests.



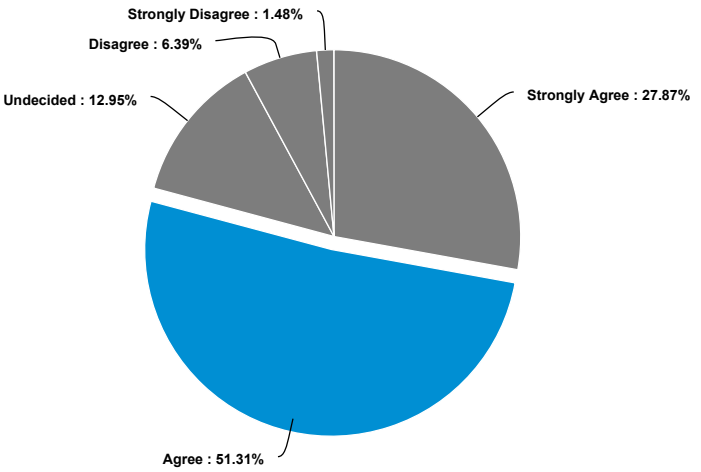
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	121	20.3%	
Agree	180	30.2%	
Undecided	282	47.32%	
Disagree	9	1.51%	
Strongly Disagree	4	0.67%	
Total	**596**	**100 %**	

NAMD support meets my needs.



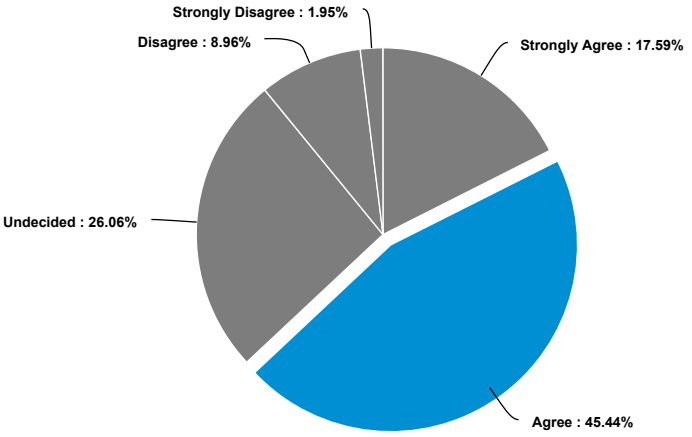
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	140	22.99%	
Agree	300	49.26%	
Undecided	159	26.11%	
Disagree	9	1.48%	
Strongly Disagree	1	0.16%	
Total	**609**	**100 %**	

NAMD documentation is clear.



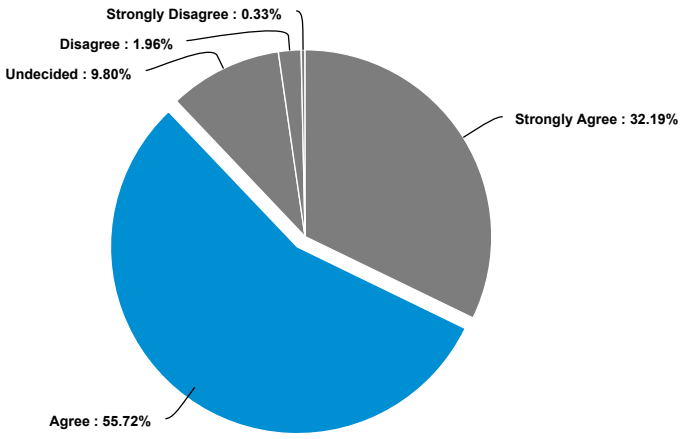
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	170	27.87%	
Agree	313	51.31%	
Undecided	79	12.95%	
Disagree	39	6.39%	
Strongly Disagree	9	1.48%	
Total	**610**	**100 %**	

NAMD documentation is complete.



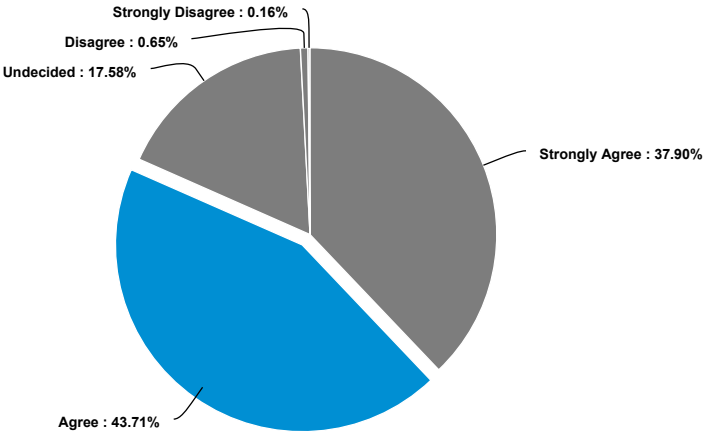
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	108	17.59%	
Agree	279	45.44%	
Undecided	160	26.06%	
Disagree	55	8.96%	
Strongly Disagree	12	1.95%	
Total	**614**	**100 %**	

I am satisfied with NAMD.



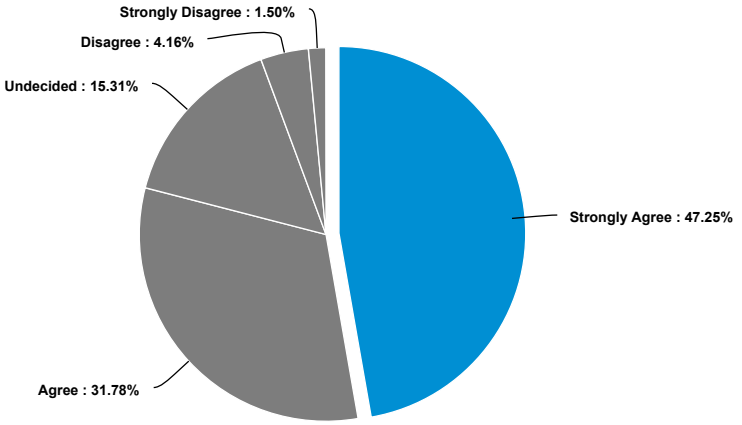
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	197	32.19%	
Agree	341	55.72%	
Undecided	60	9.8%	
Disagree	12	1.96%	
Strongly Disagree	2	0.33%	
Total	**612**	**100 %**	

NAMD has improved the quality of my work.



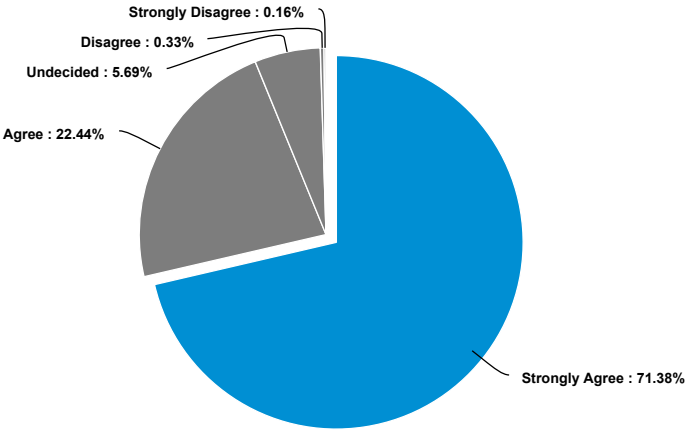
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	235	37.9%	
Agree	271	43.71%	
Undecided	109	17.58%	
Disagree	4	0.65%	
Strongly Disagree	1	0.16%	
Total	**620**	**100 %**	

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



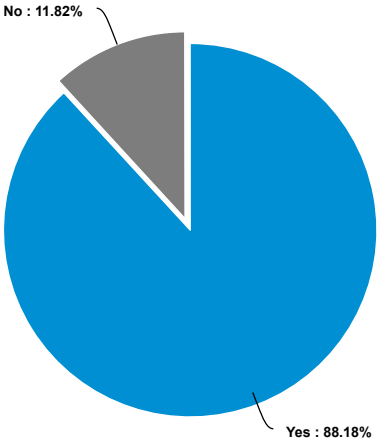
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	284	47.25%	
Agree	191	31.78%	
Undecided	92	15.31%	
Disagree	25	4.16%	
Strongly Disagree	9	1.5%	
Total	**601**	**100 %**	

I would cite my use of NAMD in resulting publications.



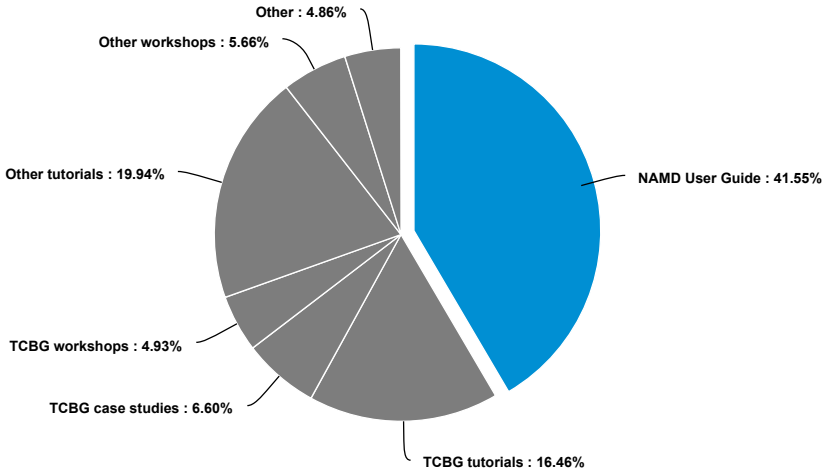
Answer	Count	Percent	20% 40% 60% 80% 100%
Strongly Agree	439	71.38%	
Agree	138	22.44%	
Undecided	35	5.69%	
Disagree	2	0.33%	
Strongly Disagree	1	0.16%	
Total	**615**	**100 %**	

I have used the NAMD tutorial:



Answer	Count	Percent	20% 40% 60% 80% 100%
Yes	567	88.18%	
No	76	11.82%	
Total	**643**	**100 %**	

What resources have you used to learn about molecular dynamics simulations?



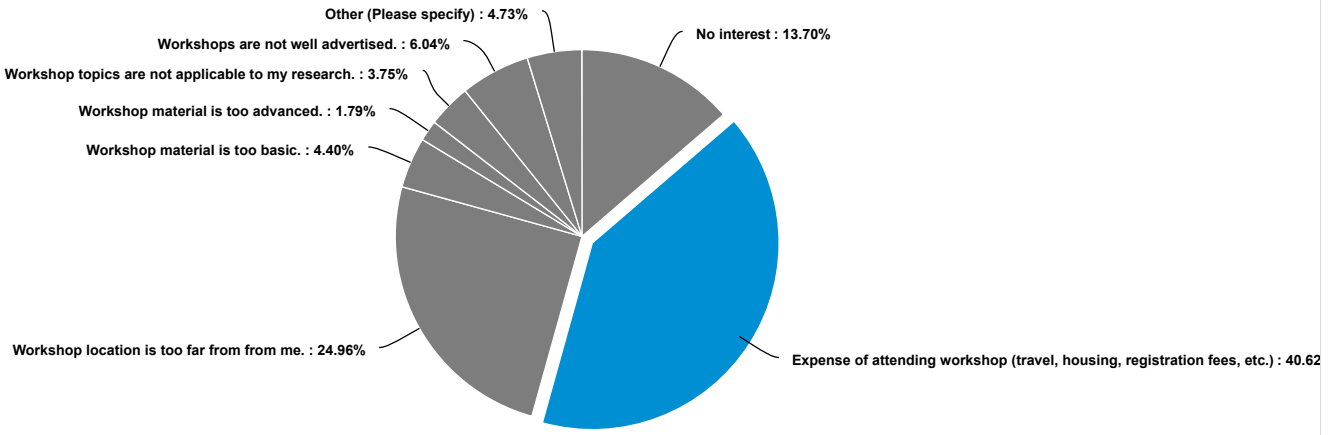
Answer	Count	Percent	20% 40% 60% 80% 100%
NAMD User Guide	573	41.55%	
TCBG tutorials	227	16.46%	
TCBG case studies	91	6.6%	
TCBG workshops	68	4.93%	
Other tutorials	275	19.94%	
Other workshops	78	5.66%	
Other	67	4.86%	
Total	**1379**	**100 %**	

What resources have you used to learn about molecular dynamics simulations? - Text Data for Other

04/01/2016	49982422	Publications and previous works
03/31/2016	49962657	Allen and Tildesley!!!
03/23/2016	49547891	Course work.
03/19/2016	49372080	teacher/university
03/18/2016	49334524	professors
03/18/2016	49324207	What does TCBG stand for? I've used a lot of the tutorial PDFs available on the website
03/17/2016	49242397	literature in general
03/16/2016	49214265	literature and books. We've written MD codes.
03/16/2016	49193466	Ph.D. with David Beveridge
03/16/2016	49194157	gromacs documentation

03/16/2016	49185823	Custom writen documentation that accounts for errors in existing documentation, that no one ever fixes.
03/16/2016	49185731	journals
03/16/2016	49183836	Classic textbooks (Frenkel & Smit, etc)
03/16/2016	49179392	User forums and journal articles (and exchange of information with my collaborators)
03/16/2016	49179315	Google search
03/16/2016	49179373	Youtube
03/16/2016	49178582	Master courses
03/16/2016	49179017	During my post doc
03/16/2016	49178277	Personal help from other users
03/16/2016	49176768	Internet forums
03/15/2016	49174847	professional books
03/15/2016	49174506	Intel tutorials
03/15/2016	49174633	Books
03/15/2016	49173581	From Professor
03/15/2016	49172735	Literature and code (very early versions of GROMOS and AMBER)
03/15/2016	49169082	papers
03/15/2016	49167901	text books in Japanese
03/15/2016	49168679	MOE users guide
03/15/2016	49165578	discovery studio
03/15/2016	49163943	Supervisor support
03/15/2016	49163190	CHARMM, X-PLOR
03/15/2016	49162201	LAMMPS and Material Studio
03/15/2016	49159883	colleagues
03/15/2016	49158537	Tutalage from collegues
03/15/2016	49156356	Google
03/15/2016	49154187	youtube
03/15/2016	49154456	My advisor tought me
03/15/2016	49155510	Papers
03/15/2016	49153695	Supervisor
03/15/2016	49154795	PERL in easy steps
03/15/2016	49154393	Frenkel and Smit book, other books
03/15/2016	49153408	Books, mostly
03/15/2016	49152058	I am just going to learn about MD simulations
03/15/2016	49151880	Various books and wide literature review
03/15/2016	49151712	Through collaboration
03/15/2016	49151465	basic books
03/15/2016	49151535	other web resources/colleagues
03/15/2016	49150454	Colleagues and mentors
03/15/2016	49150231	Research literature
03/15/2016	49150346	Graduate classes at my institution
03/15/2016	49149276	Several texts and monographs
03/15/2016	49148370	Doxygen, source code, documentation
03/15/2016	49148446	Other researchers who are experts in MD
03/15/2016	49148367	VEGA ZZ, CHARMM, AMBER
03/15/2016	49147716	compare scope of use to other molecular modeling codes
03/15/2016	49146631	Non biophysics work
03/15/2016	49146903	build instructions
03/15/2016	49146288	Textbooks, GROMACS tutorials
03/15/2016	49145477	Expertise pre-dates NAMD

What is the most significant limitation for you to attend a NAMD/VMD users workshop?

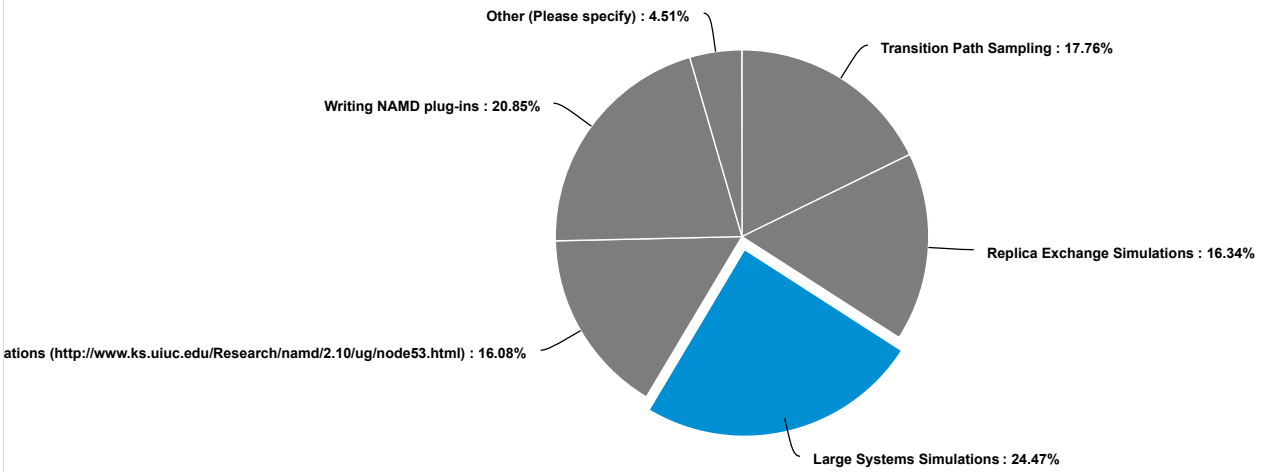


Answer	Count	Percent	20% 40% 60% 80% 100%
No interest	84	13.7%	
Expense of attending workshop (travel, housing, registration fees, etc.)	249	40.62%	
Workshop location is too far from from me.	153	24.96%	
Workshop material is too basic.	27	4.4%	
Workshop material is too advanced.	11	1.79%	
Workshop topics are not applicable to my research.	23	3.75%	
Workshops are not well advertised.	37	6.04%	
Other (Please specify)	29	4.73%	
Total	**613**	**100 %**	

What is the most significant limitation for you to attend a NAMD/VMD users workshop? - Text Data for Other (Please specify)

04/01/2016	49982422	I am not aware of any NAMD workshop in the Philippines.
03/31/2016	49962657	no time; would rather send students (and have)
03/23/2016	49546663	I have attended one. It was great, but due to complexity and scheduling, it was impossible to actually get any of the NAMD portion working during the workshop.
03/18/2016	49348261	I am graduate student, I tried once when an undergraduate, but I didn't get accepted to the workshop.
03/18/2016	49334107	operation was a success, but the patient died
03/16/2016	49212556	I live on another continent
03/16/2016	49206999	time
03/16/2016	49183836	I have already attended VMD/NAMD workshop in 2015
03/16/2016	49182399	Time commitment too high
03/16/2016	49178170	I would like my students to attend, but visas taking too long to issue (in Europe or USA) is an issue. We would like to see more time between acceptance and workshop date to solve this problem.
03/15/2016	49171694	option 1 as well as 2. Expenses and location. I live in India. IT would be a good opportuinity for people like me to have a good hands on experience with NAMD in workshops. There is a huge community using NAMD in India.
03/15/2016	49162870	do not have time
03/15/2016	49154456	No time
03/15/2016	49153408	Visa issues. I am an Indian national
03/15/2016	49153238	I was on one
03/15/2016	49153203	I'm more of a support person than a researcher
03/15/2016	49152287	local workshop too crowded
03/15/2016	49152171	Not applicable
03/15/2016	49151712	Not enought time
03/15/2016	49150219	Timing of workshops
03/15/2016	49150231	Lack of time
03/15/2016	49149812	Not enough time
03/15/2016	49149276	Don't use for active research.
03/15/2016	49148370	Time
03/15/2016	49148058	teaching duties
03/15/2016	49146889	Did not get selected after applying

Which subject(s) would you like be see covered/improved in NAMD tutorials? (Select all that apply)



Answer	Count	Percent	20% 40% 60% 80% 100%
Transition Path Sampling	201	17.76%	
Replica Exchange Simulations	185	16.34%	
Large Systems Simulations	277	24.47%	
Collective Variable-based Calculations (http://www.ks.uiuc.edu/Research/namd/2.10/ug/node53.html)	182	16.08%	
Writing NAMD plug-ins	236	20.85%	
Other (Please specify)	51	4.51%	
Total	**1132**	**100 %**	

Which subject(s) would you like be see covered/improved in NAMD tutorials? (Select all that apply) - Text Data for Other (Please specify)

04/04/2016	50133124	coarse grained models
04/01/2016	49982422	All that can be taught :)
03/20/2016	49414349	Anything other than the big protein molecule which is the only tutorial available
03/19/2016	49375381	Not sure
03/18/2016	49334107	How to use molecules for which there no parameters?
03/17/2016	49256222	GPU acceleration
03/17/2016	49244715	The work of NAMD program is unclear for me. Sometimes I can't even understand, if my processor speed is not enough or there is some problems with code.
03/16/2016	49206999	no idea
03/16/2016	49204826	NA
03/16/2016	49196131	more tutorials needed
03/16/2016	49193466	I am also interested in Cryo-EM and SAXS fitting
03/16/2016	49194157	free energy calculation
03/16/2016	49193240	restarting a simuation from where it stoped
03/16/2016	49185823	integrating NAMD into C/C++ programs. Also I would like to see some of the ancient versions archived, and the overall quality of the tutorials to be improved. I deal with new users, of NAMD, and at this point I no longer point them to the NAMD documentation, as it is too confusing for them.
03/16/2016	49179392	umbrella sampling, extending FEP tutorial for ligand binding ddG analysis
03/16/2016	49179315	Visualization or animation output tips
03/16/2016	49179373	better organisation / more parallels between UI & scripting
03/16/2016	49178277	Basic analysis of trajectories to obtain usefull structural and energetic information
03/16/2016	49177466	SMD
03/16/2016	49177036	Running NAMD in various parallel environments
03/16/2016	49176768	Free energy calculations
03/15/2016	49174633	Coarse Graining
03/15/2016	49174386	Please make available very basic Tutorial which can increase the confidence of new users.
03/15/2016	49172198	Complex configurations may need multiple examples/tutorials
03/15/2016	49170043	Flexible fitting
03/15/2016	49169000	Begginers workshop

03/15/2016	49168384	free energy calculation
03/15/2016	49167410	Free Energy
03/15/2016	49164420	I'm currently interested in QM/MM simulations, so if you implement that feature in the code, it would be nice to have it covered in tutorials, too.
03/15/2016	49162870	constant pH simuations
03/15/2016	49161545	VMD and MD simulation analysis tools
03/15/2016	49158343	membrane and transmembrane proteins calculations
03/15/2016	49158609	Easier startup
03/15/2016	49156239	additional choices for temperature and pressure control (e.g., Nose Hoover)
03/15/2016	49153458	Force field parameterization tutorials
03/15/2016	49153408	QM/MM implementations
03/15/2016	49152171	Not enough experience to say
03/15/2016	49151744	Membrane proteins
03/15/2016	49151535	multiscale simulations
03/15/2016	49150768	Tutorials for nucleic acids and force field modificaiton
03/15/2016	49150319	simulations of organic crystals
03/15/2016	49149842	Coarse grain models
03/15/2016	49149062	Trajectory analysis
03/15/2016	49148936	About various errors
03/15/2016	49148370	specifically: Milestoning, String Method with analysis
03/15/2016	49148367	Metalic Systems, Ceramics
03/15/2016	49147716	validating output is effectively modeling input request
03/15/2016	49147986	Simulation with thousands of small molecules
02/25/2016	48190063	Free energy calculations

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

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