Immersive Molecular Visualization and Interactive Modeling with Commodity Hardware

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http://www.ks.uiuc.edu/Research/vmd/

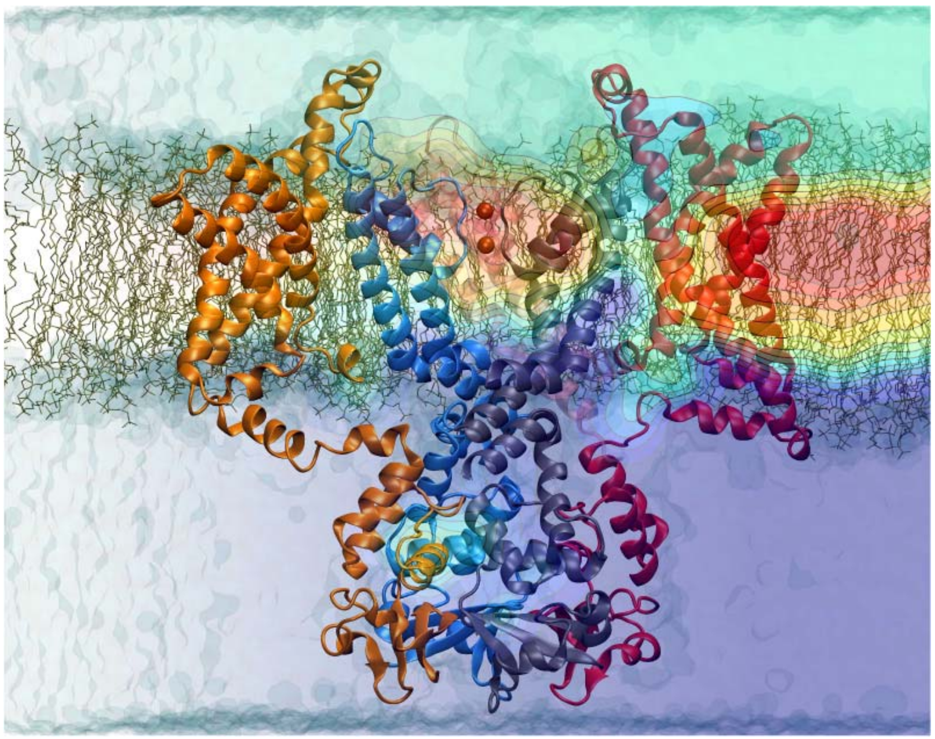
6th International Symposium on Visual Computing

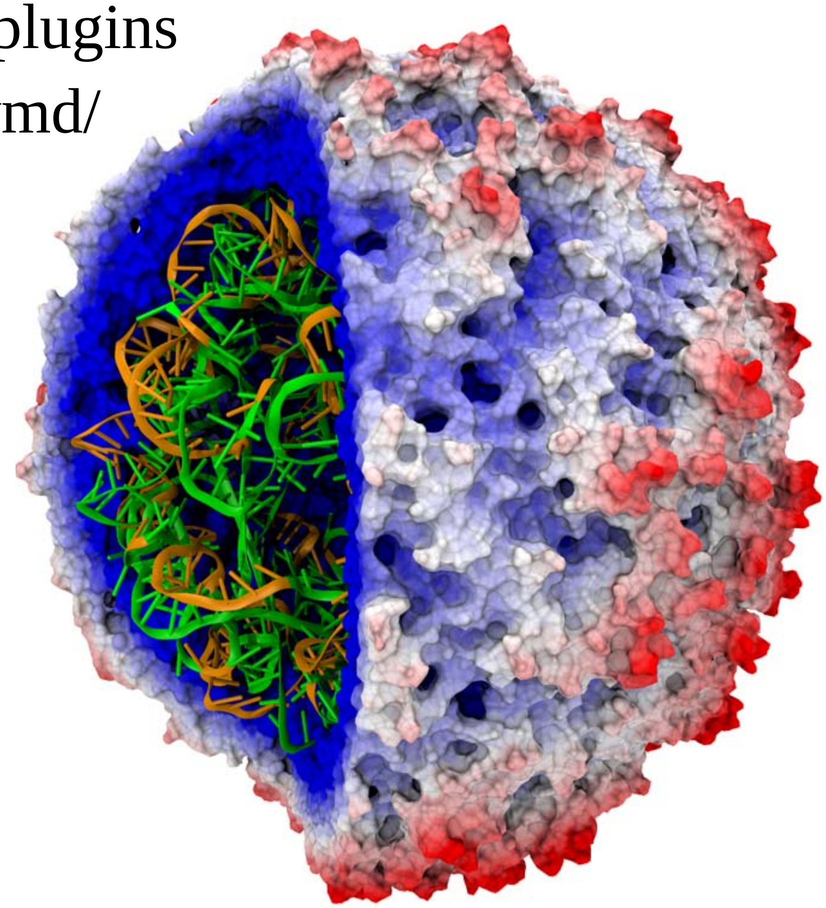
Special Track: Low Cost Virtual Reality: Expanding Horizons

Las Vegas, NV, December 1, 2010

VMD – “Visual Molecular Dynamics”

- Visualization and analysis of molecular dynamics simulations, sequence data, volumetric data, quantum chemistry simulations, particle systems, …
- User extensible with scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/

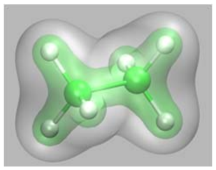


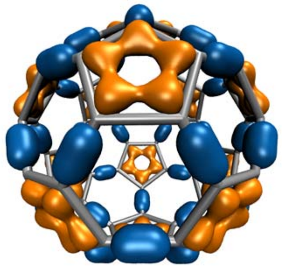


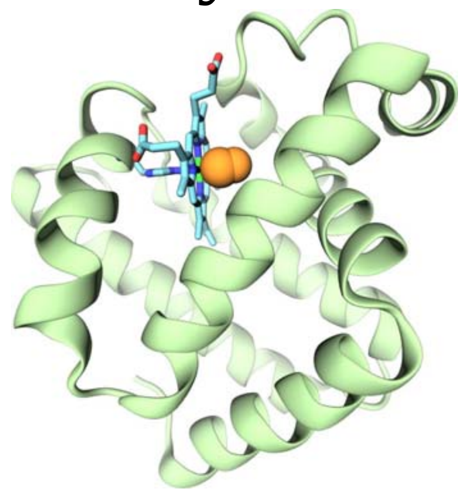
Visualizing Biomolecules

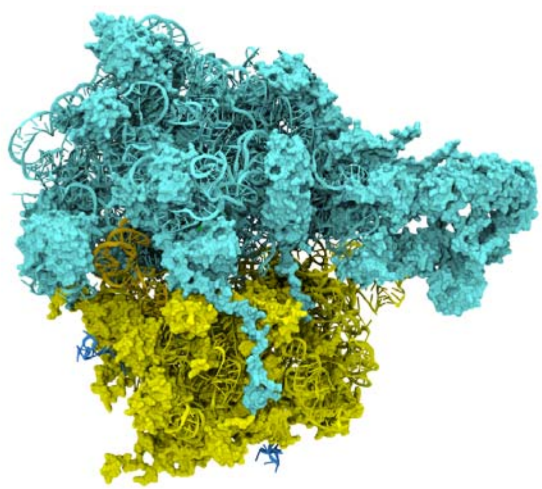
- Aids to understanding of biomolecules:
  - Simplified structure representations
  - High quality shading, depth cueing, ambient occlusion lighting
  - Stereoscopic display
  - Motion, animation of molecular dynamics

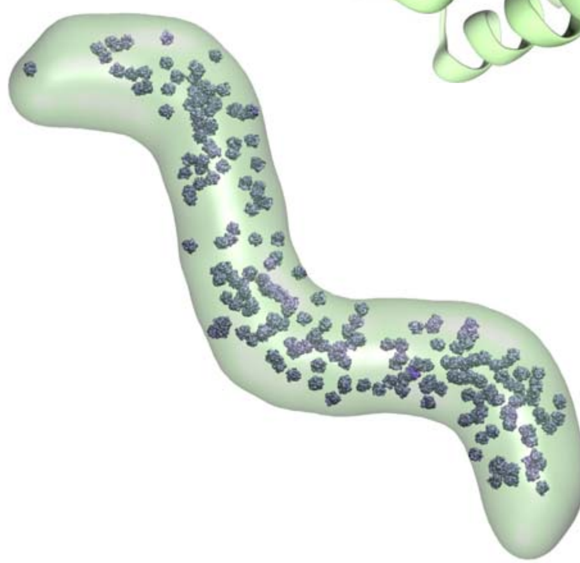
VMD Visualizes Scales from Molecules to Cells, and Beyond …

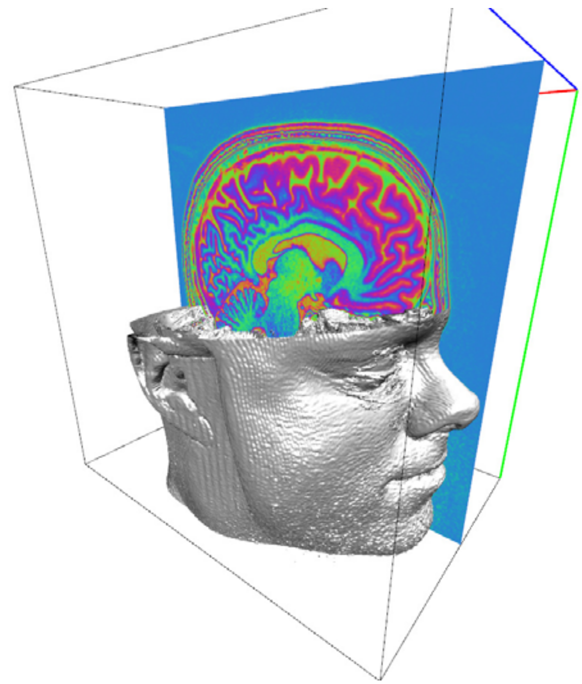








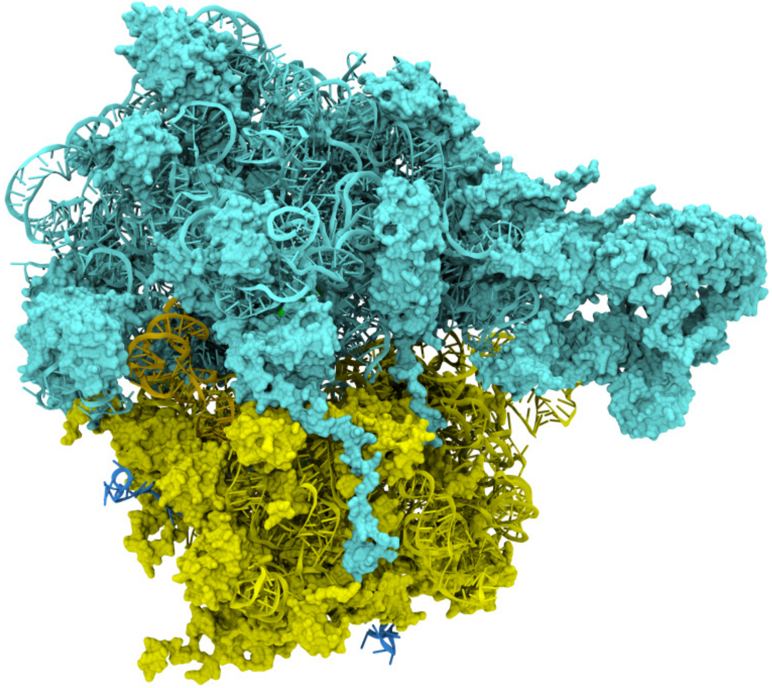




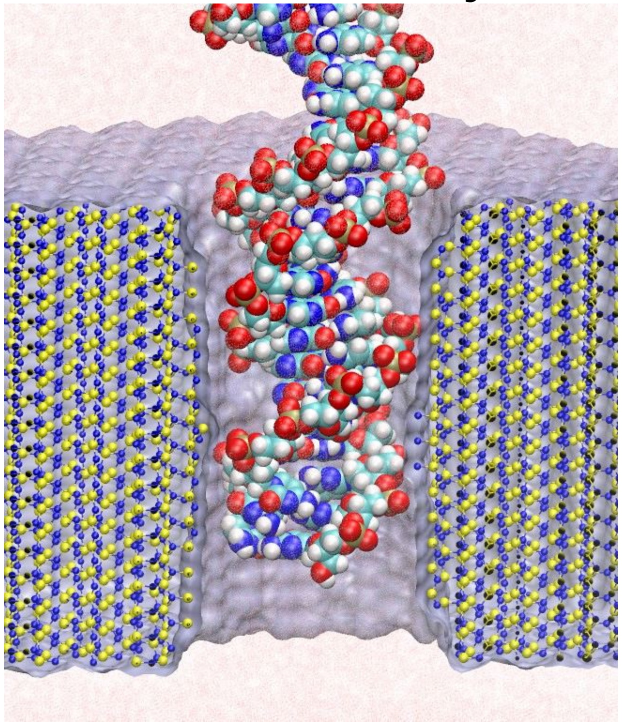
Goal: A Computational Microscope

- Study the molecular machines in living cells

Ribosome: synthesizes proteins from genetic information, target for antibiotics



Silicon nanopore: bionanodevice for sequencing DNA efficiently



Profile of VMD User Community

- 47,400 registered users of latest VMD, ver. 1.8.7
- Molecular scientists are:
  - Highly intelligent experts in their domain
  - Proficient computer users
  - Focused on using tools that get them results
  - Willing to try new things and are very interested in using technology to further their scientific pursuits
- They are NOT:
  - System administration, VR, or HPC cluster hackers
  - Interested in technology for its own sake

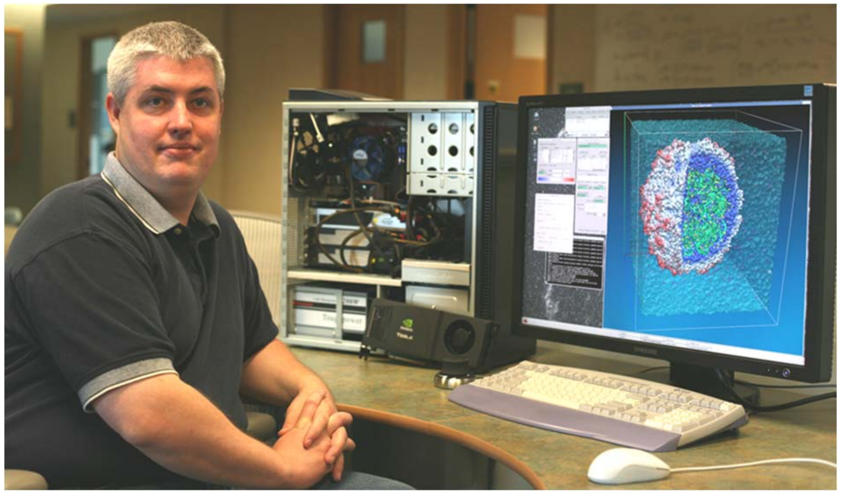
User Expectations and Challenges

- Want to spend majority of budget on fundamental equipment, e.g. CPUs, GPUs, RAM, disk storage
- Easy installation, full-featured pre-compiled binary distribution for mainstream platforms
- Want it in their office, on their desk…
- VMD auto-detects and uses multi-core CPUs, GPU computing w/ CUDA and OpenCL, advanced OpenGL shading, tiled displays, etc…
- As administrative complexity and costs increase, users lose interest in advanced technologies, software features…

Interactive Modeling on Low-Cost Hardware

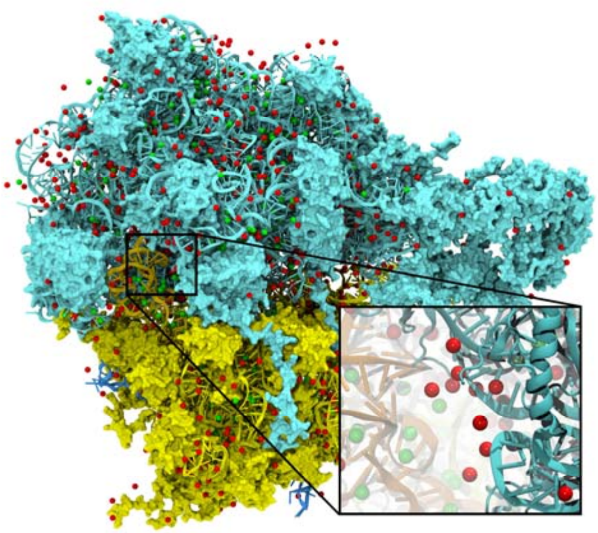
- Opportunities:
  - Hardware costs for stereo displays plummeting
  - GPU computing enables interactive MD simulation on desktop hardware without clustering for the first time
  - Increasing availability and decreasing cost of high-function 6DOF input devices
- Remaining challenges: make immersive display and input devices automatic, plug-and-play, universally understood

2001: 32-node molecular dynamics cluster



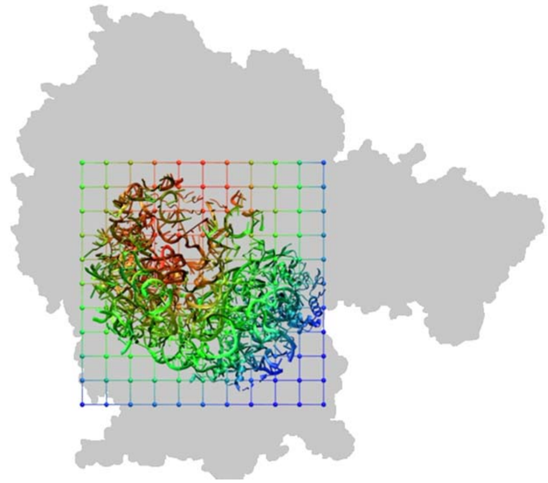
2010: Multi-GPU workstation

CUDA Algorithms in VMD



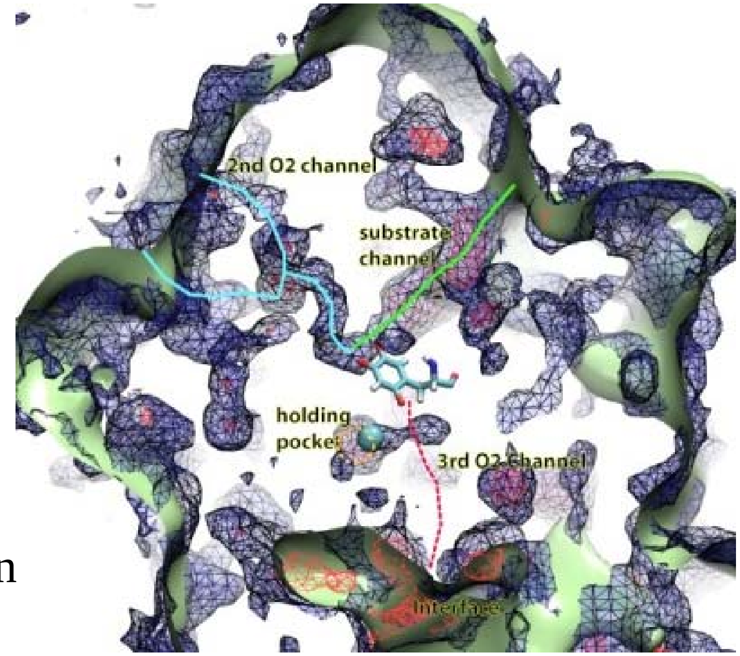
Ion placement

20x to 44x faster



Electrostatic field calculation

31x to 44x faster

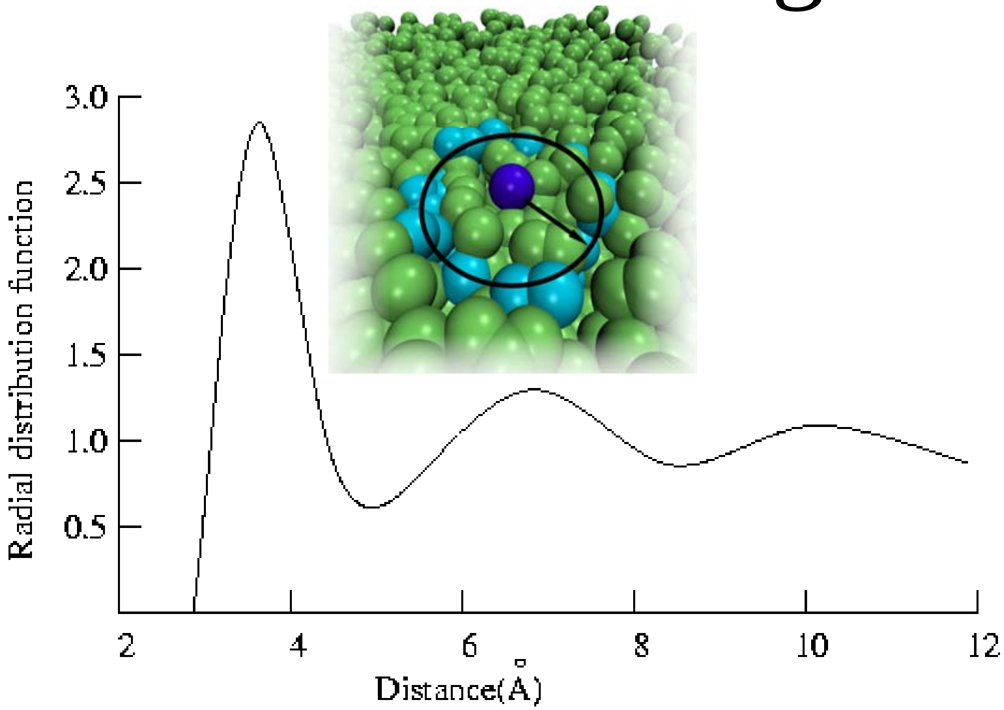


Imaging of gas migration pathways in proteins with implicit ligand sampling

20x to 30x faster

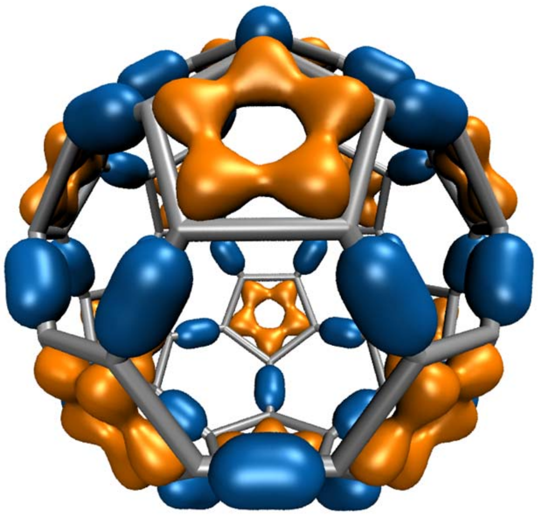
GPU: massively parallel co-processor

CUDA Algorithms in VMD



Radial distribution functions

30x to 92x faster



Molecular orbital

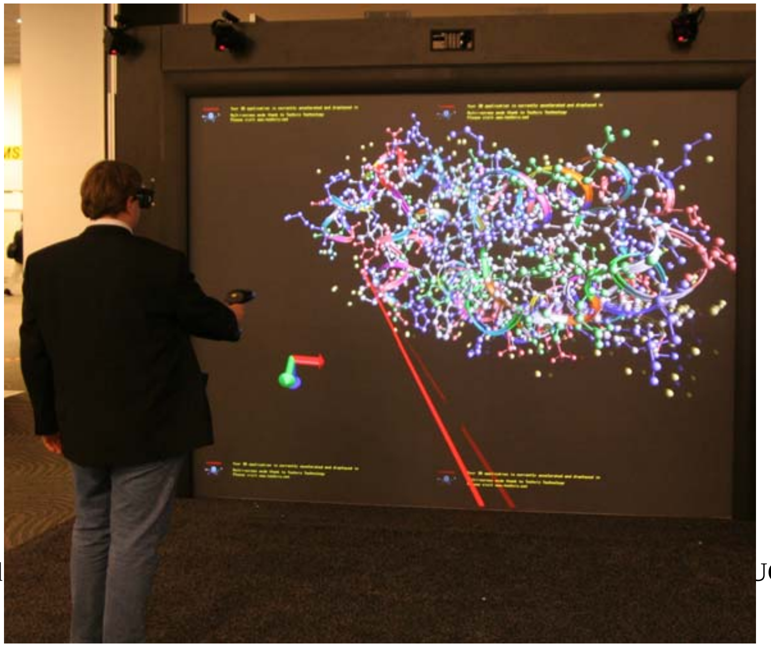
calculation and display

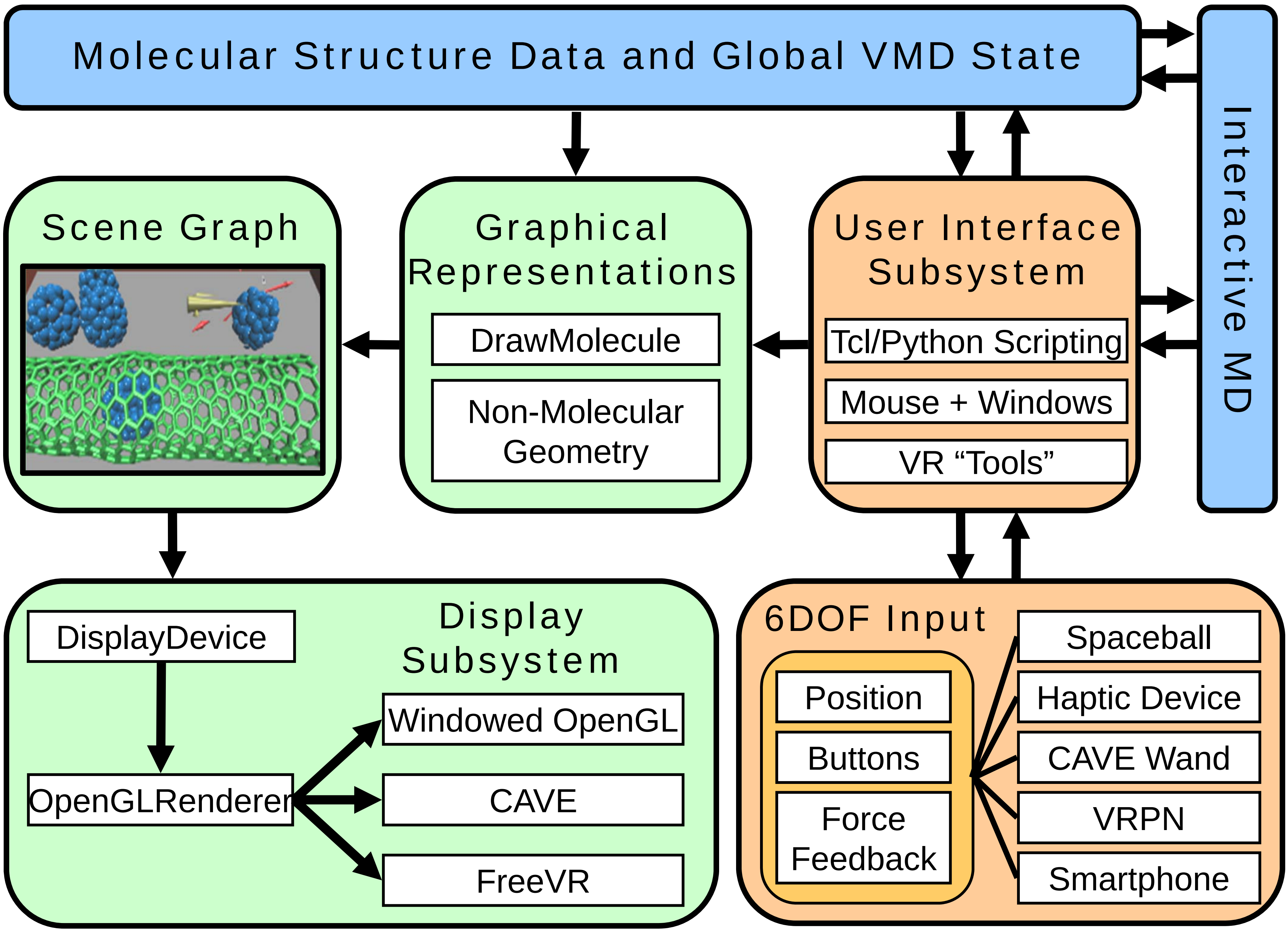
100x to 120x faster

GPU: massively parallel co-processor

Immersive Visualization in VMD

- Earliest versions of VMD ca. 1993: C++ src, CAVE w/ IRIS GL
- VMD rendering and UI engines allow support for diverse APIs and hardware, via C++ subclassing
- VMD currently supports OpenGL, CAVElib, FreeVR, VRPN for immersive interaction
- Experimental versions have supported VR Juggler, distributed memory viz clusters, various custom systems, Direct3D, other VR, UI , and rendering APIs



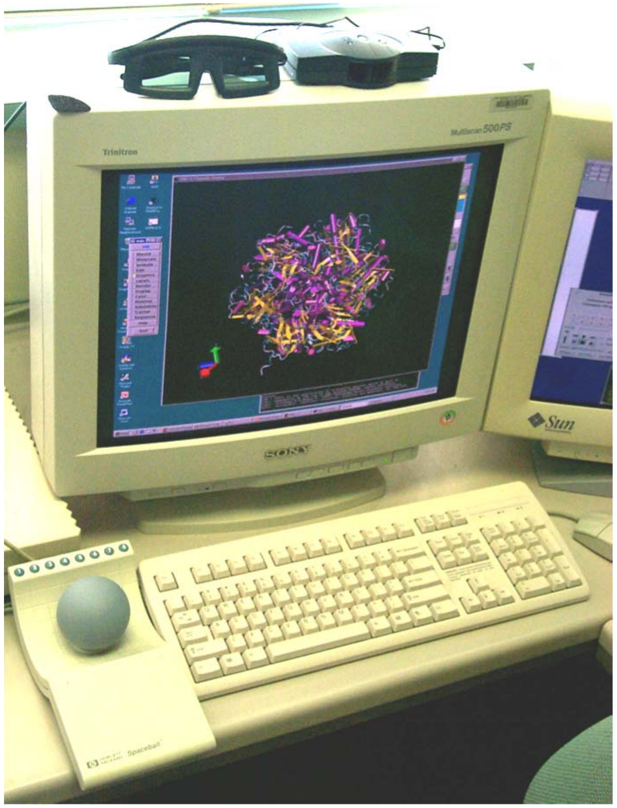


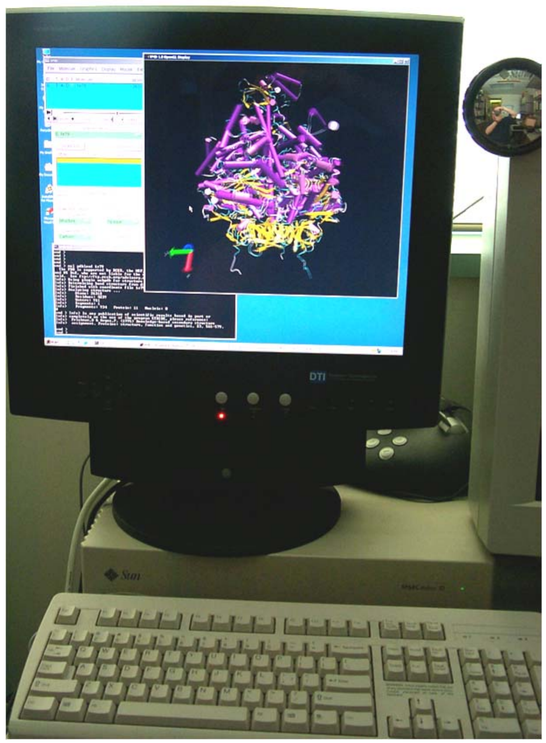
Molecular Structure Data and Global VMD State
Interactive MD
Scene Graph
Graphical Representations
DrawMolecule
Non-Molecular Geometry
User Interface Subsystem
Tcl/Python Scripting
Mouse + Windows
VR “Tools”
DisplayDevice
Display Subsystem
OpenGLRenderer
Windowed OpenGL
CAVE
FreeVR
6DOF Input
Position
Buttons
Force Feedback
Spaceball
Haptic Device
CAVE Wand
VRPN
Smartphone

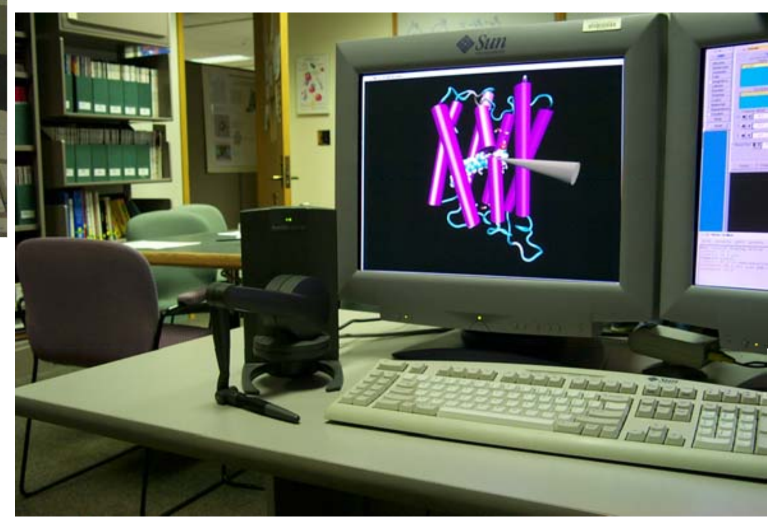
Rendering and Display Engine

- Multiple levels of abstraction from native windowing system and graphics hardware
- Custom scene graph purpose-built for molecular visualization
  - Subclasses use shared memory or cluster communication, e.g. for CAVE/FreeVR/VRJuggler
  - Abstractions allow >90% of OpenGL code to be re-used for VR and non-VR code paths
- Renderer abstractions also make it easy to write scene export modules for ray tracing and other special rendering paths

Support for Diverse Display Hardware







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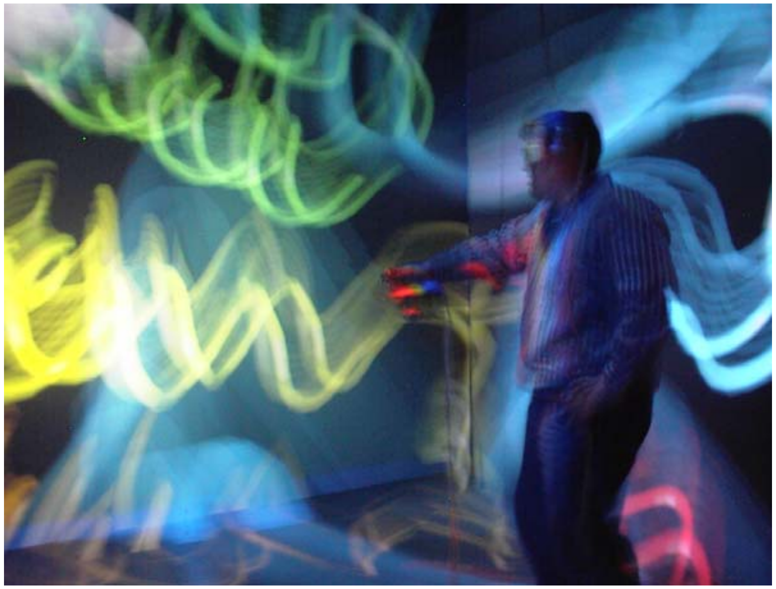

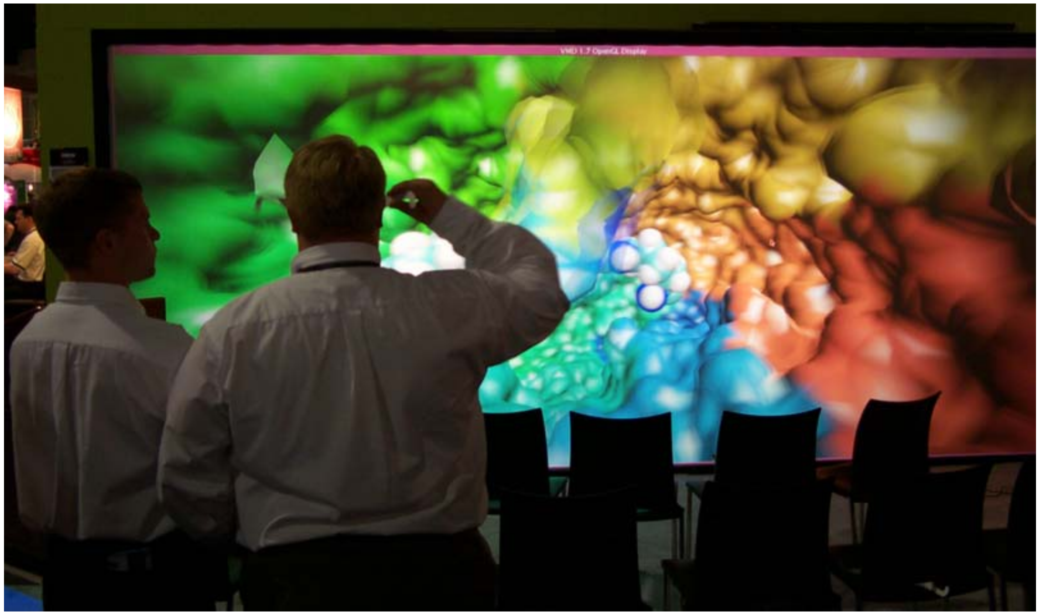

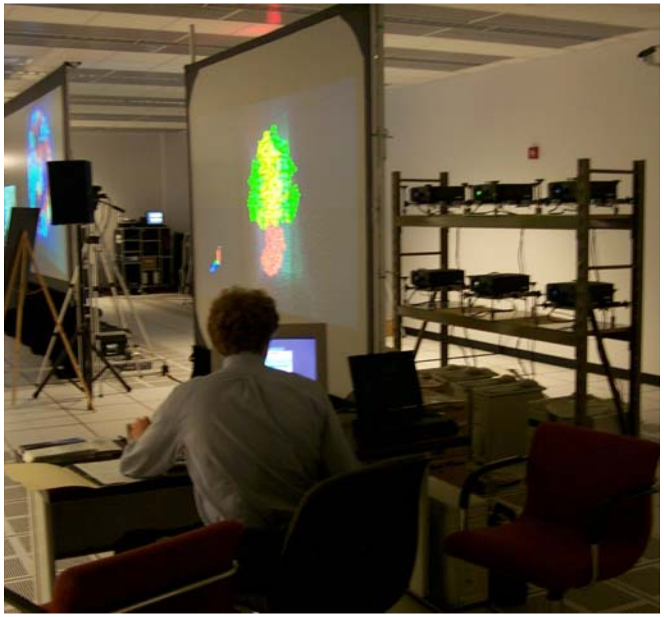

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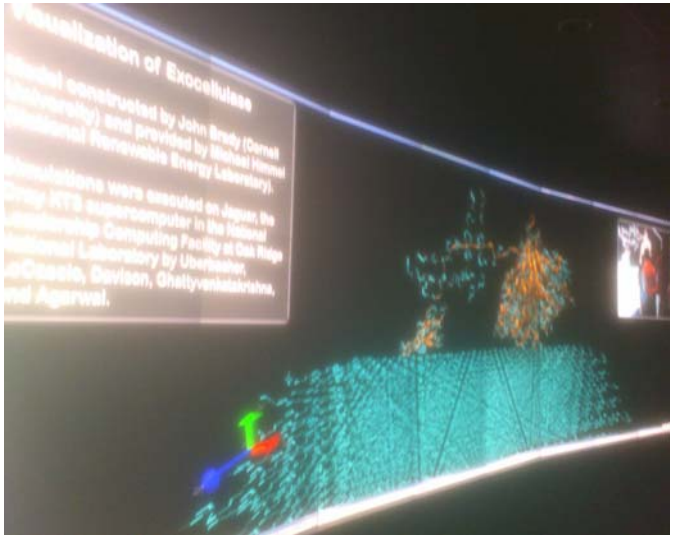
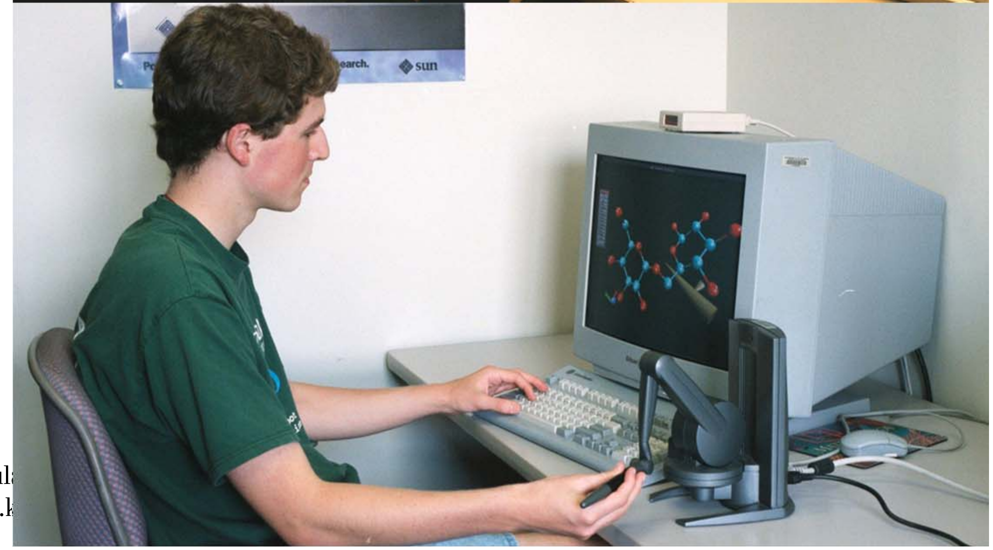


Window System Input, 6DOF, and Haptic Interaction

- VMD accepts input from all modalities concurrently
- Window system devices are “zero configuration”, auto-detected and used in a “first-person” mode like a mouse
- VR, and haptic devices require some configuration and interface through user interface “Tools”, used more like a CAVE wand
- Internal scripting interface: customized interactions through callback APIs

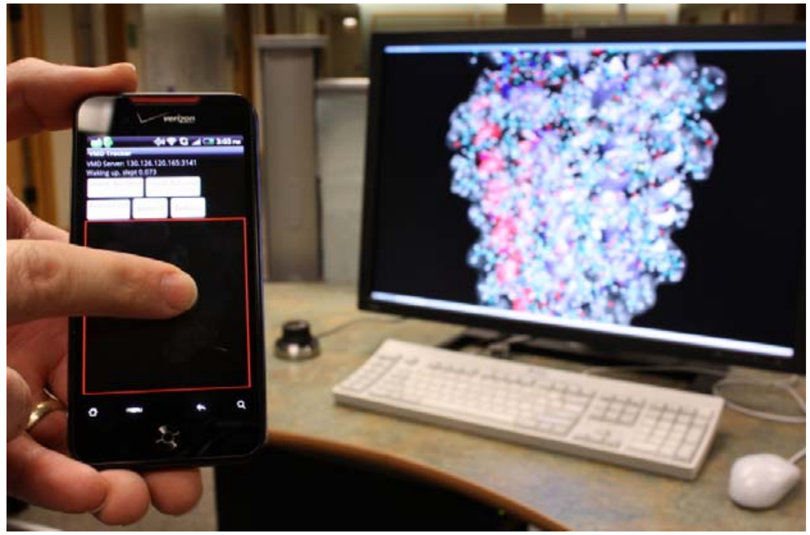


Experiences with Existing VMD Input Devices, Interfaces

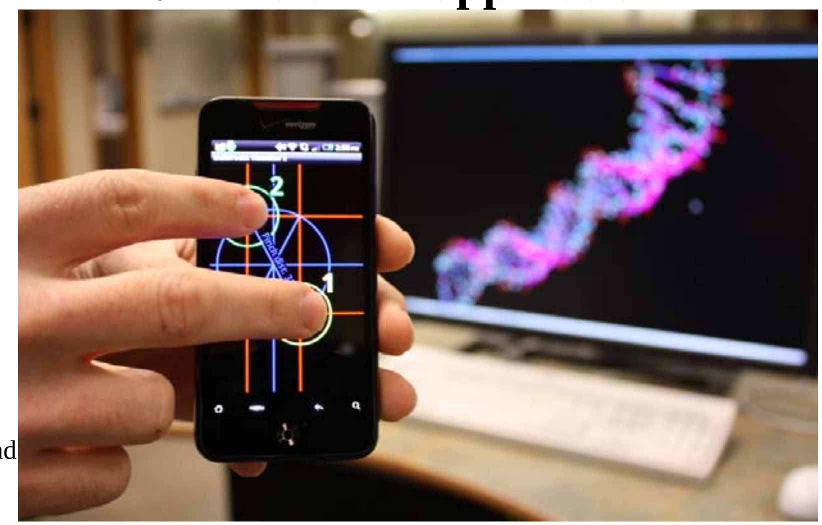
- Users want inexpensive, easy-to-use devices that don't need special drivers or extensive configuration
- Cheap 6DOF SpaceNavigator USB devices are popular
- Haptic devices, e.g., Sensable Phantom, Novint Falcon:
  - More usable for challenging tasks
  - Not nearly as widely used, yet…
  - Price has come down by 2 orders of magnitude in 10 yrs
  - Still require more configuration (drivers, VRPN daemons, etc)
- Ideal devices are cheap, ubiquitous, convenient, something users own and always have with them…

Ongoing Work: Smartphones as Wireless Multi-modal Input Devices

- Ubiquitous commodity devices, ideal for impromptu 6DOF motion control and interaction in meetings, offices
- Programmable in Java, C, C++
- Multi-touch display
- Built-in camera, accelerometer, magnetometer, gyroscope sensors
- Audio and vibration feedback
- On-board preprocessing of input
- 802.11 wireless ethernet enables TCP/UDP sockets to VMD session
- Challenges: variation in on-board sensors, precision/quality by vendor



HTC Incredible w/ Android running VMD tracker application



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GPU Computing Publications

http://www.ks.uiuc.edu/Research/gpu/

- **Fast Analysis of Molecular Dynamics Trajectories with Graphics Processing Units – Radial Distribution Functions.** B. Levine, J. Stone, and A. Kohlmeyer. 2010. (submitted)
- **Quantifying the Impact of GPUs on Performance and Energy Efficiency in HPC Clusters**. J. Enos, C. Steffen, J. Fullop, M. Showerman, G. Shi, K. Esler, V. Kindratenko, J. Stone, J Phillips. *The Work in Progress in Green Computing*, 2010. In press.
- **GPU-accelerated molecular modeling coming of age**. J. Stone, D. Hardy, I. Ufimtsev, K. Schulten. *J. Molecular Graphics and Modeling,* 29:116-125, 2010.
- **OpenCL: A Parallel Programming Standard for Heterogeneous Computing**. J. Stone, D. Gohara, G. Shi. *Computing in Science and Engineering*, 12(3):66-73, 2010.
- **An Asymmetric Distributed Shared Memory Model for Heterogeneous Computing Systems**. I. Gelado, J. Stone, J. Cabezas, S. Patel, N. Navarro, W. Hwu. *ASPLOS '10: Proceedings of the 15th International Conference on Architectural Support for Programming Languages and Operating Systems*, pp. 347-358, 2010.

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- **Probing Biomolecular Machines with Graphics Processors**. J. Phillips, J. Stone. *Communications of the ACM,* 52(10):34-41, 2009.
- **GPU Clusters for High Performance Computing**. V. Kindratenko, J. Enos, G. Shi, M. Showerman, G. Arnold, J. Stone, J. Phillips, W. Hwu. *Workshop on Parallel Programming on Accelerator Clusters (PPAC)*, In Proceedings IEEE Cluster 2009, pp. 1-8, Aug. 2009.
- **Long time-scale simulations of in vivo diffusion using GPU hardware**. E. Roberts, J. Stone, L. Sepulveda, W. Hwu, Z. Luthey-Schulten. In *IPDPS'09: Proceedings of the 2009 IEEE International Symposium on Parallel & Distributed Computing*, pp. 1-8, 2009.
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- **Multilevel summation of electrostatic potentials using graphics processing units**. D. Hardy, J. Stone, K. Schulten. *J. Parallel Computing*, 35:164-177, 2009.

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- **Adapting a message-driven parallel application to GPU-accelerated clusters**. J. Phillips, J. Stone, K. Schulten. *Proceedings of the 2008 ACM/IEEE Conference on Supercomputing*, IEEE Press, 2008.
- **GPU acceleration of cutoff pair potentials for molecular modeling applications**. C. Rodrigues, D. Hardy, J. Stone, K. Schulten, and W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.
- **GPU computing**. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.
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- **Continuous fluorescence microphotolysis and correlation spectroscopy**. A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.