A System for Interactive Molecular Dynamics Simulation

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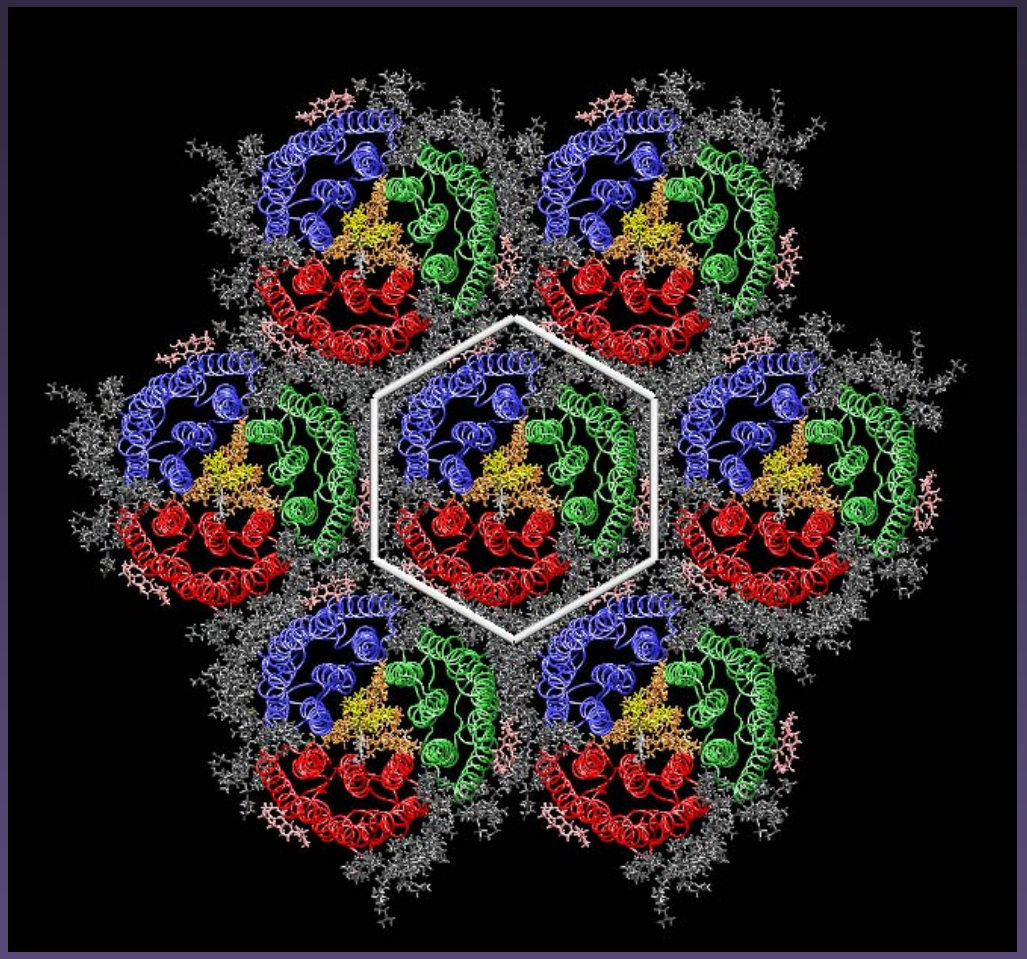
Scientific Visualization in Structural Biology

- Simplified structural representations reduce user confusion for large molecules.
- Many atoms move every frame, structural representations must be regenerated every frame.

Biomolecular Simulation

- All-atom models of protein, DNA, water.
- 10k-100k interacting particles.
- Time scales of 10-100 ns are accessible, still much shorter than experiment.



Steered Molecular Dynamics

- Moving restraints pull selected atoms along specified paths.
- Slow processes can be accelerated.
- New flexibility leads to new challenges: how can proteins be manipulated?

Previous Work

- UNC Nanomanipulator, PIT
- UIUC MDScope
- Haptic Sculpting [Dachille et al, I3D ’99]

A Haptic Interface

- Haptic devices allow multidimensional manipulation and force feedback.
- Pathways for steered molecular dynamics simulations can be identified interactively.

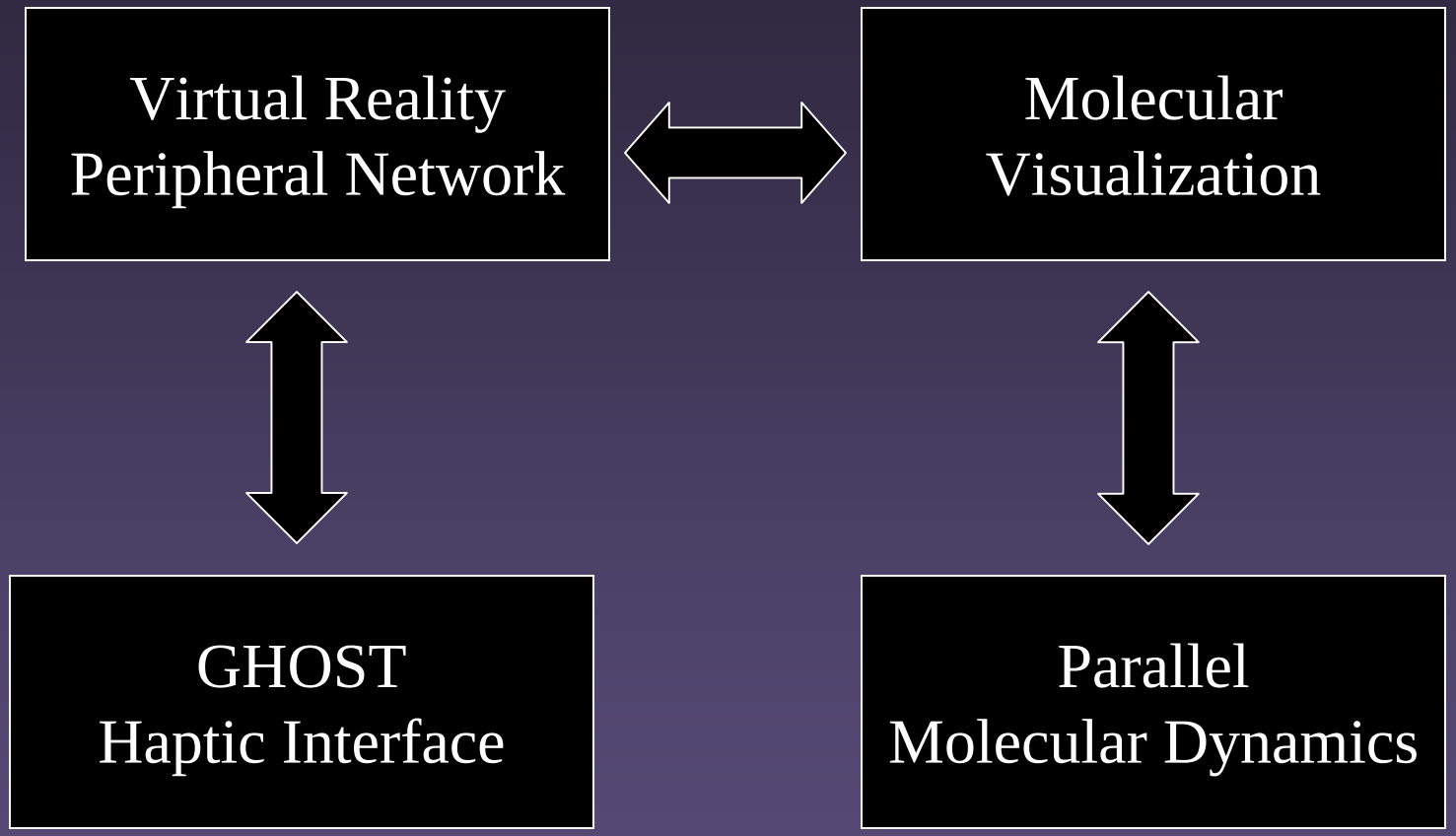
Interactive Molecular Dynamics

- Replaces pre-determined constraint point and spring with interactive user input and run-time configurable spring parameters;
- Provides user with real-time force feedback through the use of a haptic device;
- Allows user to direct simulation and gain insight by interactive exploration of structure and mechanical properties of molecular system.

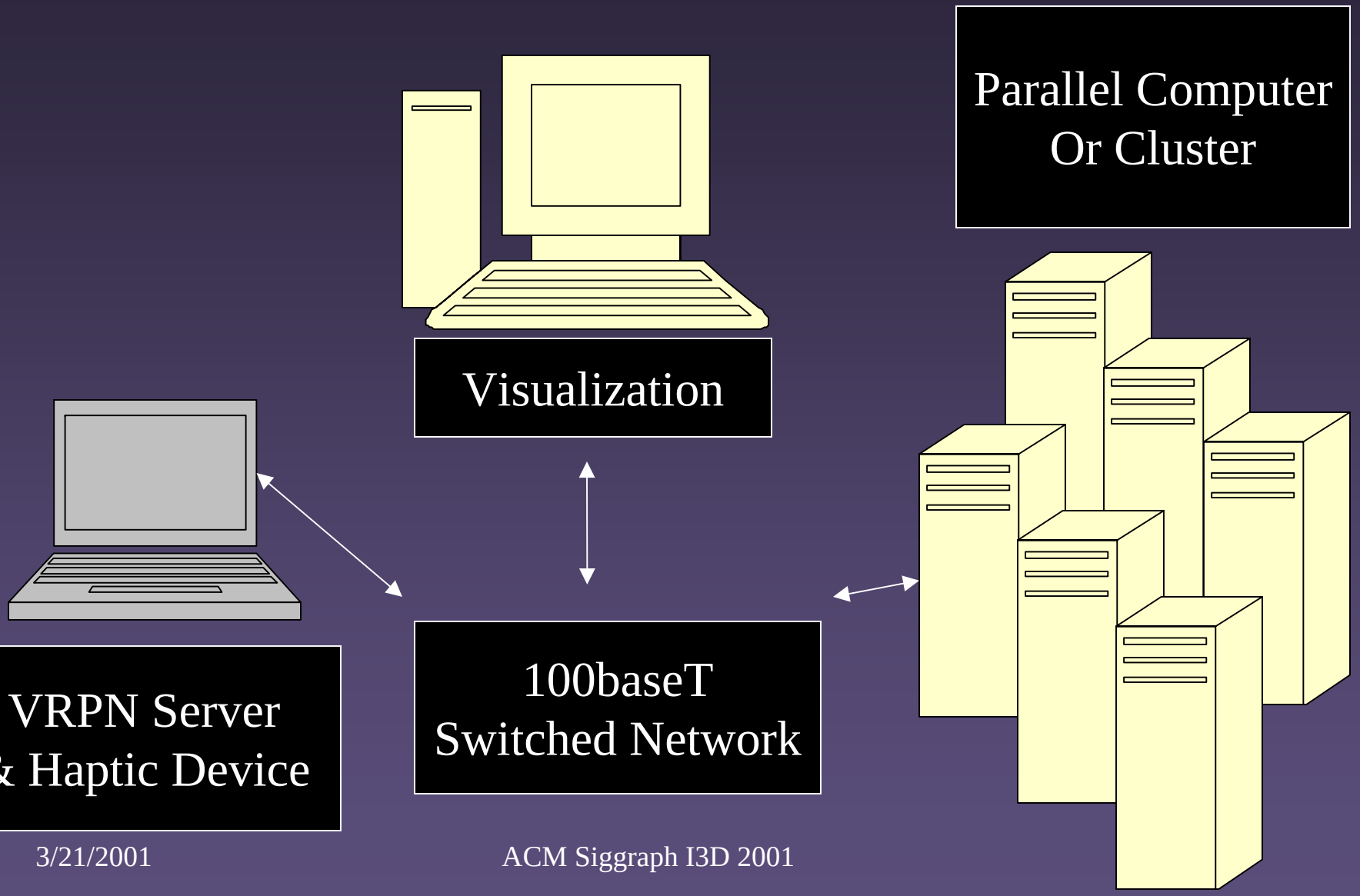
Challenges

- Achieving even modest interactive simulation rates requires parallel computing
- Latency is the enemy
- Many atom positions must be transmitted to visualization engine for every rendered timestep
- Molecular rendering is very geometry intensive
- Simulation, rendering, and haptic feedback necessarily occur at greatly differing time scales

IMD Software Architecture



IMD Hardware Architecture



IMD Hardware and Software

- Molecular visualization engine
- Parallel molecular dynamics simulation engine
- Virtual Reality Peripheral Network (VRPN)
- Haptic device
- Low-latency network with medium bandwidth
- High performance visualization and computation machines

Force Feedback Model: Parameters

- The response of the IMD system to user input is ultimately determined by three parameters:
- Ratio of wall clock time to simulation time.
- Ratio of user-applied force to simulation force.
- Ratio of atom coordinates to haptic coordinates.

Force Feedback Model: Results

- The sensitivity of the haptic interface to atomic interactions goes as the *square* of the speed of the simulation.
- Responsiveness can be improved by increasing the simulation force, but at the cost of sensitivity.
- Stiff restraints give better precision, but result in a noisier haptic interface.

Interactive Performance Results

- Current results used a cluster of 32 1.1GHz Athlons, and multithreaded communication.
- Dynamics were calculated at 79 timesteps/sec.
- Rendering and haptic restraint update rate of 30fps.
- Haptic feedback rate of 1000Hz.

Future Work

- Develop simplified dynamics integrators for higher interactivity at slight cost in accuracy
- Further decouple rendering process from haptic constraint point update rate with threads
- Apply IMD to larger, more interesting systems
- 6 Degree-of-freedom haptic feedback

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