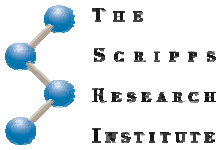


Haptic Rendering and Volumetric Visualization with SenSitus

Stefan Birmanns, Ph.D.

Department of Molecular Biology
The Scripps Research Institute
10550 N. Torrey Pines Road, Mail TPC6
La Jolla, California, 92037

Situs Modeling Workshop, San Diego, CA, Feb. 3-5, 2003

Outline

- **Virtual Reality**
- **Haptic Rendering**

- **Haptic Rendering for interactive molecular modeling**
  - Vector quantisation
  - Force calculation
  - Application

- **SenSitus**
  - Visualization of molecular structures and volume data

Virtual Reality

- **Ivan Sutherland – 1965 „ultimate display“**

*The **ultimate display** would be a room within the computer can control the existence of matter. […] Handcuffs displayed in such a room would be confining, and a bullet displayed in such a room would be fatal.*

- **Several definitions today**

*Virtual Reality is a **computer generated** simulated environment which users perceive as real with their **natural senses** and with which they can **interact**.*

- **Replace reality by virtual reality?**
  - Necessary/useful for visualization of scientific datasets?

Virtual Reality

- **Stereoscopic Viewing**
  - Head Mounted Displays
  - Shutter LCD glasses
  - Polarized Light

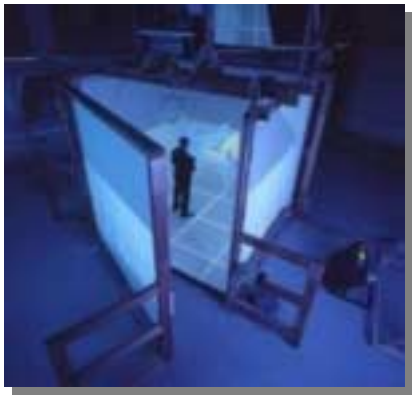
- **Head Tracking**
  - Magnetic
  - Ultrasonic
  - Optical

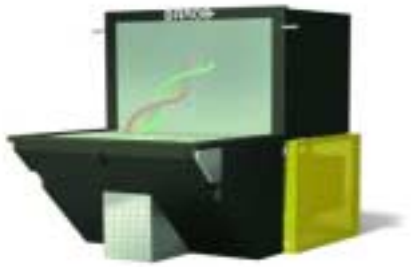
Virtual Reality

- **Head Mounted Devices (HMD)**
  - Stereoscopic viewing
  - Measurement of head orientation
  - Very immersive
  - Isolation from reality can cause sickness

Virtual Reality

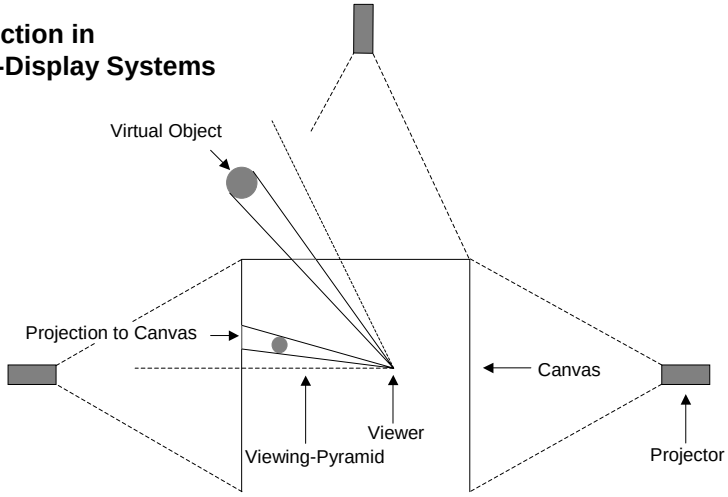
- **Multi-Display Systems**
  - CAVE, VR workbench





Virtual Reality

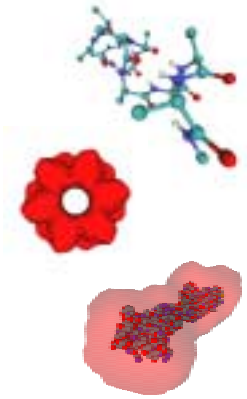
- **Projection in Multi-Display Systems**



Virtual Reality

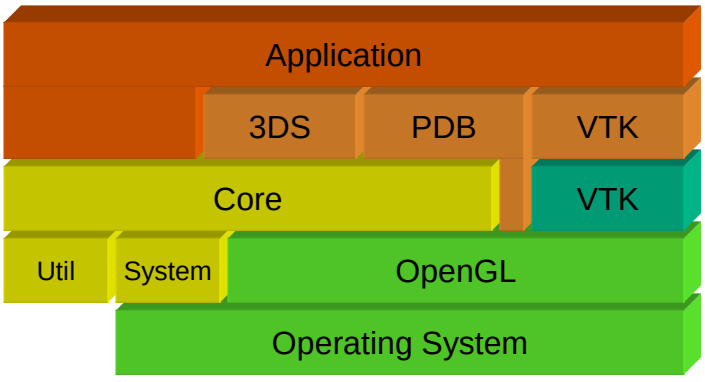
SVT

- **SVT**
  - Visualization of Molecular Structures
    - VDW, CPK, etc.
    - Combination of drawing modes within one molecule
    - Trajectory files from MD simulations
  - Visualization of Volume Data
    - Isosurface
    - Volume rendering (2D/3D Textures)
  - VR Systems
    - Multi-display systems
    - Standard PC and graphics workstations



Virtual Reality

SVT



Haptic Rendering

- **Haptic: *haptesthai* (greek) – to touch**
- **Haptic Rendering**
  - Create an artificial tactile sensation
- ***Haptic* feedback**
  - Skin receptors
  - Measures temperature, pressure, vibration, slip
- ***Kinesthetic* feedback**
  - Receptors in muscles and tendons
  - Measures perceived and produced force
- ***Proprioceptive* feedback**
  - Joint position receptors
  - Measures accelleration and position

Haptic Rendering

- **Receptor properties**
  - Adaptation, spatial and temporal resolution, …
  - Important research issue
- **High temporal resolution**
  - For realistic kinesthetic feedback force updates with 500hz – 1000hz frequency necessary
- **Problem:**
  - Visual system needs only 15-30 updates per second
  - Programs tuned to update inner loop with 15-30hz
  - Forces difficult to calculate

Haptic Rendering

- **Devices:**
  - 195x Argonne Remote Manipulator
  - 196x GROPE (2D)
  - 196x exoskeleton designs
  - …
  - 199x commercial devices:
    - Immersion
    - SensAble
- **Used here:**
  - SensAble Phantom 6DOF

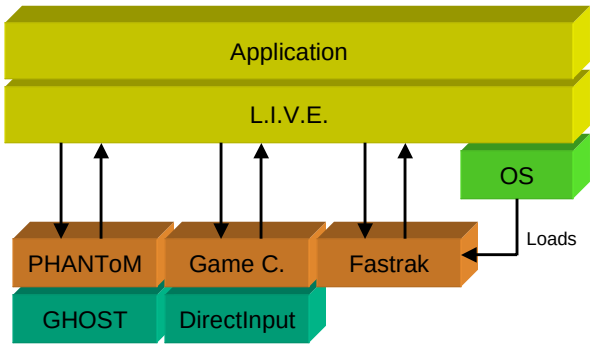
L.I.V.E.

Library for **I**nput Devices in **V**R **E**nvironments

- **Countless VR devices**
  - Different programing interfaces
  - OS dependencies
  - Application bound to expensive libraries
- **Abstract Layer necessary**
  - Layer between application and VR devices
- **L.I.V.E.**
  - Compact C library

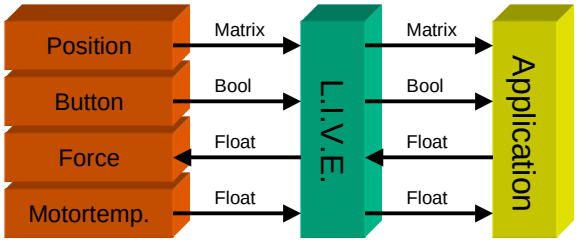
L.I.V.E.
Library for Input Devices in VR Environments

- **L.I.V.E.**
  - Device driver concept



L.I.V.E.
Library for Input Devices in VR Environments

- **Device driver interface**

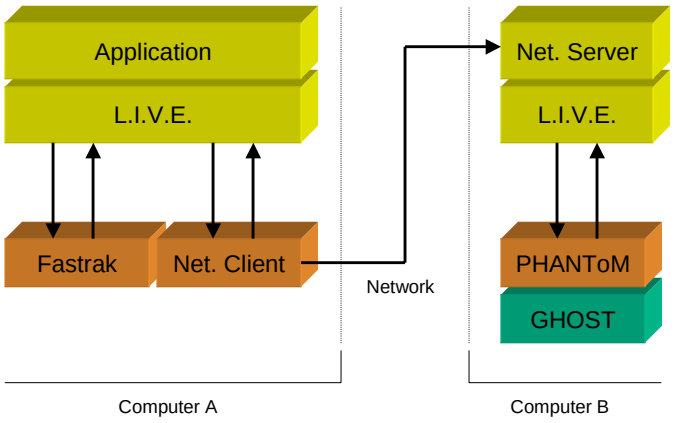


- **Modularity**
  - OS independent
  - Replace device without recompilation of application
  - Simplified development process

L.I.V.E.

Library for **I**nput Devices in **V**R **E**nvironments

- **Network**

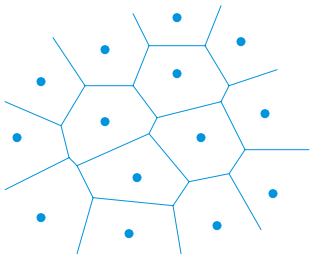


SenSitus

- **Haptic rendering for interactive fitting of xtal structures into EM density maps**
- **Idea: Correlation coefficient used for force calculation**
  - Guide user to better fitting location
  - Additional source of information beside visual information
  - User can overcome force
  - User = global maximum, force = local maximum
- **Problem: Too slow!**
- **Simplification of structural information**

SenSitus – Vector Quantization

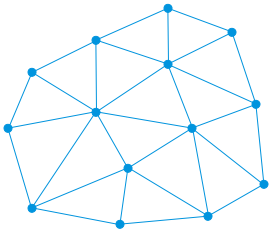
- **Vector Quantization**
  - Array of “codebook vectors”, describing a signal
  - Signal-values replaced by nearest CV



Voronoi tessellation

SenSitus – Vector Quantization

- **Error: Sum of distance**
- **Problem: Find CV set with minimal error**
- **Solution: Topology Representing Networks**
  - Martinez, Schulten
  - Neuronal network
    - training process creates a Voronoi tessellation and Delaunay triangulation



SenSitus – Reduced Fitting Criterion

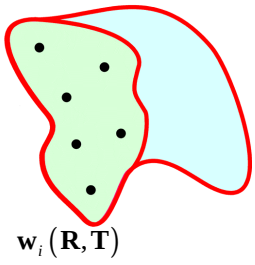
- **Correlation coefficient**

$$C(R,T) \propto \int \rho_{calc}(\mathbf{r},R,T) \cdot \rho_{em}(\mathbf{r})\, d^3\mathbf{r}$$

SenSitus – Reduced Fitting Criterion

- **Reduced Model:**

$$\rho_{calc}(\mathbf{r}) \equiv \sum_{i=1}^{k} \delta(\mathbf{r} - \mathbf{w_i})$$



- **Simplified Correlation Coefficient:**

$$C(R,T) \propto \sum_{i=1}^{k} \rho_{em}(\mathbf{w_i}(R,T))$$

SenSitus – Force Calculation

- **Molecule: Rigid body in conservative force field**
- **C negative potential energy:**

$$U(\mathbf{x}) = -c(\mathbf{x})$$

- **Force field:**

$$\mathbf{F}(\mathbf{x}) = -\nabla U(\mathbf{x})$$

Force on CV:

$$\mathbf{f}(\mathbf{w_i}) = \mathbf{F}(\mathbf{w_i})$$

- **Force on COM:**

$$\mathbf{F} = \sum_{i=1}^{k} \mathbf{f}(\mathbf{w_i})$$

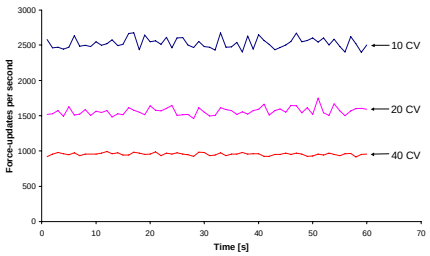
Torque about COM:

$$\mathbf{T} = \sum_{i=1}^{k} \mathbf{w_i} \times \mathbf{f}(\mathbf{w_i})$$

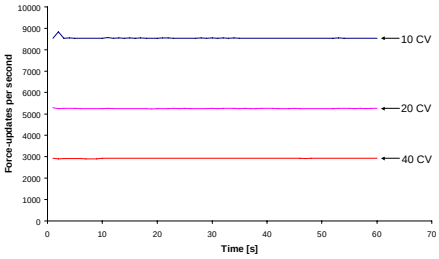
SenSitus - Speed

- **Speed of force calculation**
  - Force calculation thread runs parallel to visual rendering
  - Achievable force update rates 1kHz – 10khz

1CPU



2CPU

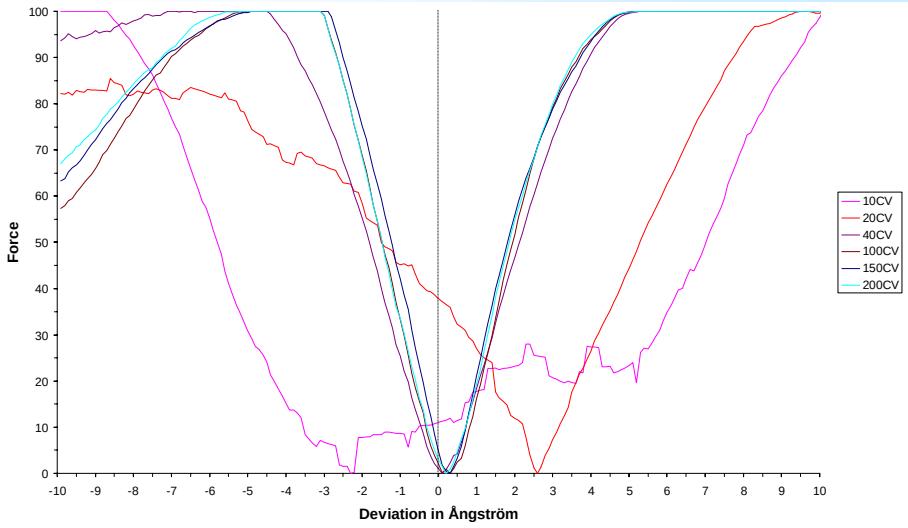


SenSitus – Codebook Vectors

- **Precision of the force calculation as a function of model complexity**
  - Actin Deoxyribonuclease I Complex (1ATN) - 5020 atoms

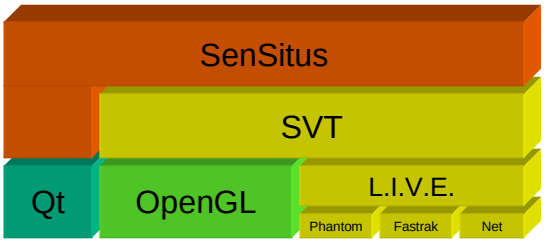
10CV 20CV 40CV 100CV

SenSitus – Translational Accuracy



SenSitus

- **Overview**

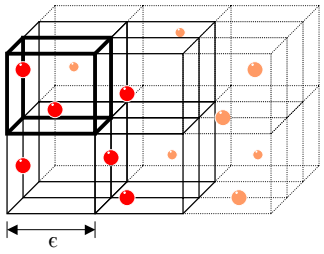


- **Portable: Versions for SGI, SUN, DEC, Linux, Windows**

SenSitus

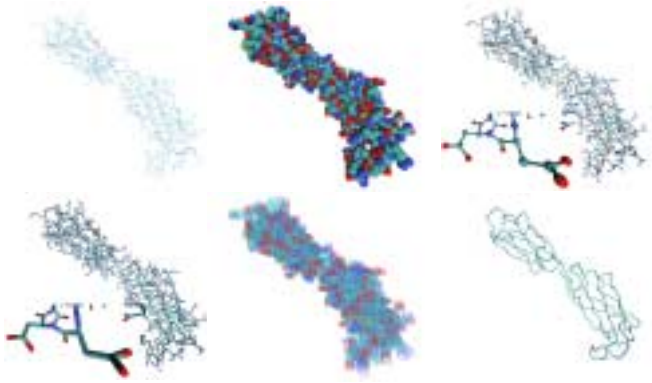
SenSitus – Molecular Structures

- PDB (Protein Data Bank) files
- Bond information often missing
- Guessing bonds by atom-atom distance criterion
- Problem: Calculation complexity $O(N^2)$!
- Space partitioning approach



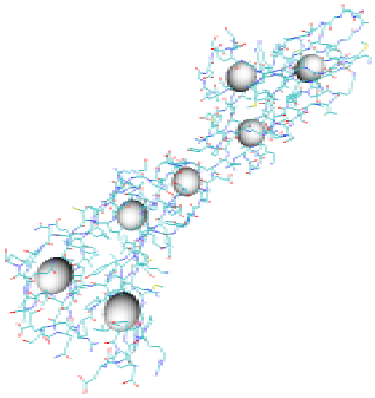
SenSitus – Molecular Structures

- PDB (Protein Data Bank) files



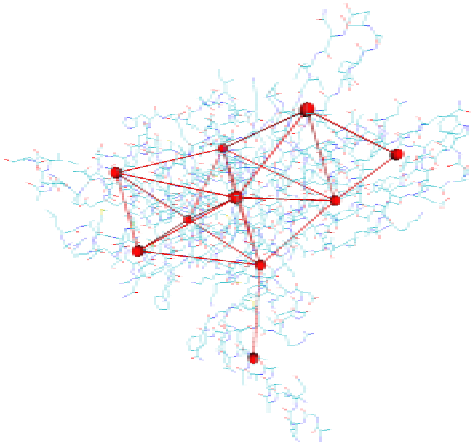
SenSitus – Molecular Structures

- **Combination of drawing modes**



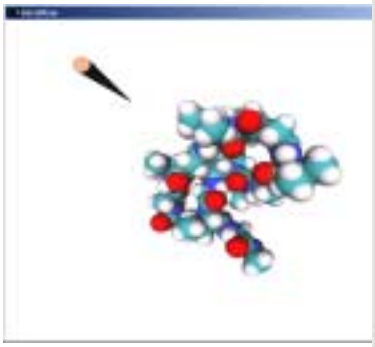
SenSitus – Structural Data

- **PSF (Protein Structure) files**
- **Can be used together with PDB files**
- **Used in Situs to store the codebook-vector connections**

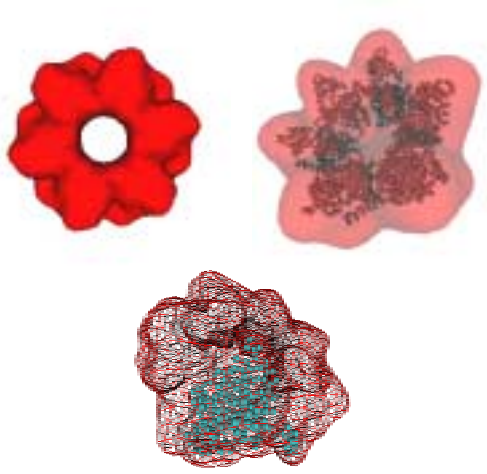


SenSitus – Molecular Dynamics

- **Visualizing computer simulations of molecular motion (DCD file format)**



SenSitus – Volumetric Data



SenSitus - Future Enhancements

- **Flexible fitting**
  - Interactive flexible fitting
  - Haptic rendering of the biophysical restrictions during flexible fitting
- **Integration of pure algorithmic solutions**
  - Online supervision
  - Editing of search space
  - Comparison of interactive and algorithmic results
- **Interactive manipulation of datasets**

SenSitus

- **Try it out yourself!**
- **Group I:**
  - Tuesday 2:45PM
- **Group II:**
  - Wednesday 2:45PM

Acknowledgements

- **Research Centre Jülich**
  - John von Neumann Institute for Computing

- **The Scripps Research Institute**
  - Computational Structural Biology Group