Haptic Rendering and Volumetric Visualization with SenSitus

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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

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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

![Diagram](image-url)
Virtual Reality

- **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

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**Virtual Reality**

![Diagram of VR system components: Application, Core, Util, System, Operating System]
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 acceleration 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

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

- **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

![Diagram showing the structure of L.I.V.E.](image)

- Device driver interface

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

- 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

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

SenSitus – Reduced Fitting Criterion

- Reduced Model:

\[ \rho_{\text{calc}}(\mathbf{r}) \equiv \sum_{i=1}^{k} \delta(\mathbf{r} - \mathbf{w}_i) \]

- Simplified Correlation Coefficient:

\[ C(R, T) \propto \sum_{i=1}^{k} \rho_{\text{em}}(\mathbf{w}_i(R, T)) \]
**SenSitus – Force Calculation**

- **Molecule:** Rigid body in conservative force field
- **C negative potential energy:**
  \[ U(x) = -c(x) \]
- **Force field:**
  \[ F(x) = -\nabla U(x) \]
- **Force on CV:**
  \[ f(w_i) = F(w_i) \]
- **Force on COM:**
- **Torque about COM:**
  \[ T = \sum_{i=1}^{k} w_i \times f(w_i) \]

**SenSitus - Speed**

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

![Graphs showing force updates per second over time for 1CPU and 2CPU scenarios.](image)
SenSitus – Codebook Vectors

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

SenSitus – Translational Accuracy

![Graph showing deviation in Ångström for different force levels and model complexities.](image)
SenSitus

- Overview

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

- 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
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