



Computational Visualization

- 1. Sources, characteristics, representation
- 2. Mesh Processing
- 3. Contouring
- 4. Volume Rendering
- 5. Flow, Vector, Tensor Field Visualization
- 6. Application Case Studies











Computational Visualization: Application Case Studies

Lecture 6

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Outline

Center for Computational Visualization

Case Studies

- Computational Cosmology
- Computational Medicine
- Computational Biology
- Computational Engineering



To significantly elevate the science and technology base of computational visualization techniques and tools for rapid scientific discovery on key and fundamental grand challenges and achieve a lasting impact on mankind.



Holy Grail of Visualization I

Beyond the Picture

- Interaction
- Interrogation
- Exploration







Visualization for Simulation

- •The Visible Living Species
- •The Visible Earth
- •The Visible Universe
- at multiple scales Copyright: Chandrajit Bajaj, CCV, University of Texas at Austin



The Auralization Era: **Beyond 3D Silent Movies**





Holy Grail of Visualization II

The Human Experience

- Visual Fidelity
- Audio Fidelity
- Audio-Video Immersion
- Tactile, Olfactory, ...





Simulation for Visualization

- Light scattering and absorption (Better Optical Models)
- Sound scattering and absorption (Helmholtz's Equation)
- Other Human Cognitive Inferences



- 1. High performance computers
- 2. High speed networking
- 3. High access data storage
- 4. High throughput graphics and sound cards
- 5. High resolution projectors and display screens
- 6. High sampling rate audio-visual trackers
- 7. Human ingenuity on demand!



What are the Barriers ?

HARDWARE LIMITATIONS

- I/O bound ---disks to memory slow…InfiniBand
- Buses are not fast enough

 --- memory to graphics
 cards
- Networking needs to get faster for distributed data caches or remote access
- Pixel Bound,,, pixel resolution and fill rates are not fast enough

SOFTWARE LIMITATIONS

- •Feature detection methods....local/global
- •Visibility calculations especially for time dependent
- •Image/audio processing techniques
- •Roadmaps for exploration
- •Seesaw strategies for remote access and visualization
- •Collaborative interaction metaphors

Human Ingenuity is Unlimited!!

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The Comprehensive Attack



- 1. Compressed Data Streams Everywhwere
- 2. Multi-resolution and Time Critical Processing at Both Ends
- 3. Scalability of parallel graphics, sound and distributed data stores
- 4. Closing the Loop \rightarrow Human Perception and Interaction



Visualization Holodeck for Scientific Discovery



Living Tomorrow Today!

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Visualization Inspirational Launchpads





Improved Teaming through Shared Workspaces & Collaboration

Remote Interactive Visualization Pods

Focus is on improved Human in the Loop

NOT Technology ! Copyright: Chandrajit Bajaj, CCV, University of Texas at Austin



The Visualization Educational Studio

AUTHORING & BROADCASTING !

•Vt-books of visualization technology advances

• Iv-books that tell an interactive story of scientific discovery and impact





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Center for Computational Visualization

Projects:

Shastra

collaborative architectures

- VisualEyes
- integrated simulations & interrogative visualization
- DiDi
- data intensive & display intensive computations
- Angstrom Structure determination

Proteomics



Interdiscplinary Team

- UT Faculty (3+)
- PostDocs (2)
- Graduate Students (12)
- Undergraduate Students (2)
- Staff (1)

Our Resources

SGI Onyx2

June of the second seco

- Twenty four
 400 MHz
 R12000
 processors
- Six Infinite
 Reality2 engine
 graphics
 pipeline
- 25 GB of main memory
- Large disc array





Our Resources (cont)

- PC cluster
 - 128 Compaq PC
 - Each node has
 256 MB main
 memory









Visualization Lab

Immersive environments

 Three front CRT projection
 Ten rear LCD projection







Motivation

- Large data-sets
 - multi-resolution data-structures
 - for dynamic settings little or no preprocessing
- Viability of data analysis for a wide class of inputs

 unified techniques for data of different dimension
- Guaranteed interactivity and scalability
 - highly flexible adaptivity
- Distributed computing resources
 - loose coupling between successive computation stages



Scalable Parallel Rendering

- Scalable Display Wall (Princeton)
 Myrinet & sort-first
- WireGL (Stanford)
- Sepia (Compaq)
 - ServerNet II & custom compositing
- Meta-Buffer (UT)
- Lighting 2 (Stanford)



Metabuffer Features

- Independently scalable number of renders and display tiles
- The viewport of a render can locate anywhere in the display space
- Viewports can overlap
- Viewports can be different size (multiresolution)





Configuration I





Configuration I

- Each Renderer has the same viewport
 - Polygons can be assigned to any renderer
 - Display has the same resolution as a rendering process
- Load balance for isosurface rendering
 - Each processor generates similar number of triangles
 - No need to redistribute triangles
 - Efficiently use memory as cache for change of viewpoint

_____ _



Configuration II





Configuration II

- Each renderer has a viewport with the size of a tile
 - Faster rendering and higher resolution on large display
 - Independent number of renderers and tiles
 - Combination of sort-first and sort-last
- Load Balance
 - Polygons cannot be assigned arbitrarily
 - Viewports are positioned with constraints
 - Load balance among the viewports
 - Different viewport locations for different view parameters



Movie



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Time-Varying Oceanography Data Visualization a

Multi-volumes

enter

- surface height (**PS**)
- salinity (**S**)
- temperature (*T*)
- velocity (*U*, *V*, *W*)
- convection (CV)
- 2160 x 960 x 30 x 4 bytes
- One time step has 300 seconds interval from 16-FEB-1991 12:00:00







- 2160×960×30×4(bytes) = 237 MB
- 237(MB)×115(timestep) = 27 GB





Combining Method

• Volume rendering + Isocontouring



Combining Tech vs Colormap





OpenGL Volumizer





OpenGL Performer





Mineralwasserrrr!!





Let $\Omega \subset R^3$ denote a bounded domain with boundary surface Γ that is split into Γ_1 and Γ_2 . We assume Γ be a smooth closed surface.





Given an incident pressure p^{inc} . We wish to determine a (complex-valued) total pressure $p = p^{inc} + \hat{p}^s$ in $\hat{\Omega} = IR^3 - \Omega$ Satisfying the following Helmholtz equation $\nabla^2 p + k^2 p = 0$ in $\hat{\Omega}$ and rigid boundary condition on Γ_1 $\frac{\partial p}{\partial n} = 0,$ Impedance boundary condition on Γ_2 $\frac{\partial p}{\partial m} = 0$

With scattered pressure satisfying Sommerfeld radiation condition

$$\left|\frac{\partial p^s}{\partial R} - ikp^s\right| = O(\frac{1}{R^2}) \text{ for } R \to \infty$$



i	Imaginary Unit	ω	Frequency
$k = \omega / c$	Wave number	С	Sound speed
R	Distance from the origin	E	Impedance
ρ	Density of air	n	Outward unit normal



Acoustic Pressure Solution for a Plane Incident Wave



















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 Consider the molecular interaction energy between a receptor and a ligand.
 Assuming rough axial symmetry of the ligand this is a scalar field *SF* defined on a five-dimensional configuration space (three translational degrees of freedom and two rotational degrees of freedom).



Can we look at SF?

RED	= attraction	
BLUE	= repulsion	
GREEN = free configuration		



Can we look at **SF**?





Some Related Approaches

Charnoff faces

(Charnoff '73)

- Grand Tour (Asimov '85)
- Parallel Coordinates (Inselberg & '90)
- Hyperslices (VAN Wijk & VAN Liere '93)
- Animation



Sound definition of a "view"

- User interface
- Hardware acceleration

Multi-resolution
 representation

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View Definition





View Definition

The view is defined by a N×2 matrix M



The "direction of projection" π is the kernel of M.

For N>3 there is no total order in π



We do not consider occlusion

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- A straightforward generalization of the typical 3D GUI requires to provide rotational widgets (rotating a certain wheel you rotate the object in a certain 2D coordinate subspace).
- Problem 1: How many 2D coordinate subspaces exist ?

 $\binom{n}{2} = \frac{n(n-1)}{2}$

• Problem 2:

without any previous experience of ND navigation do you know which rotation you want to apply ?



- In our approach we do not want to force the user to "think in ND space" to be able to select a view.
- The user navigates the scene by adjusting the view of the reference system.

- The number of parameters used to adjust the view grows linearly with the dimension N
- There is no redundancy in the selection of the view (other than a scaling factor)





 The user associates also each color with a particular range of the scalar field value space (two sliders per color).









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STEP1

Compute the elementary footprint (the splat)

• STEP2

For each voxel in the (hyper)volume do:

- compute its position in screen space
- copy in its place the splat scaled by color/transparency.



Splatting Approach

- The exact luminosity distribution of the elementary footprint (splat) is a bivariate box-spline (expensive to compute exactly).
- The approximated splat is computed by the same volume rendering routine using a square as splat (bootstrapping).





The Curse of Dimensionality

• The size/complexity of a data-set grows exponentially with its dimension N.

• To achieve real time interaction we need to optimize for speed.



- Multi-resolution representation with 2ⁿ tree:
 - either guaranteed frame rate;
 - or guaranteed error bound.

- Hardware acceleration:
 - Textured polygons used to draw the splats;
 - Mipmapping used to perform automatically the splat selection in the multi-resolution approach.



Back to our SF

- 5-dimensional scalar field SF given by the interaction energy between a small ligand and a large receptor (three translational degrees of freedom and two rotational degrees of freedom).
- The display is performed by direct projection (splatting) form 5D space to 2D space.
- No slicing/isocontouring is performed to preserve the "global view" of the dataset.



RED = attraction BLUE = repulsion GREEN = free configuration



5D Molecular Interaction

- The axis of one degree of freedom is much longer than the others to highlight the relevance of such rotation.
- From the top picture it is clear that low or high angles (large red spots) are more favorable for the dockingof the two molecules.
- Removing all colors but red as in the bottom figure you can also see how the two large regions are connected by a narrow tunnel.





5D Molecular Interaction





—On the bottom right one can notice an interesting site in green where the ligand can move along the interface with the receptor without being subject to a repulsion force.

—Leaving only the red component one can see that the center has no attraction region.





5D Molecular Interaction





DankeSchon

http://www.ticam.utexas.edu/CCV