Massive Dataset Visualization

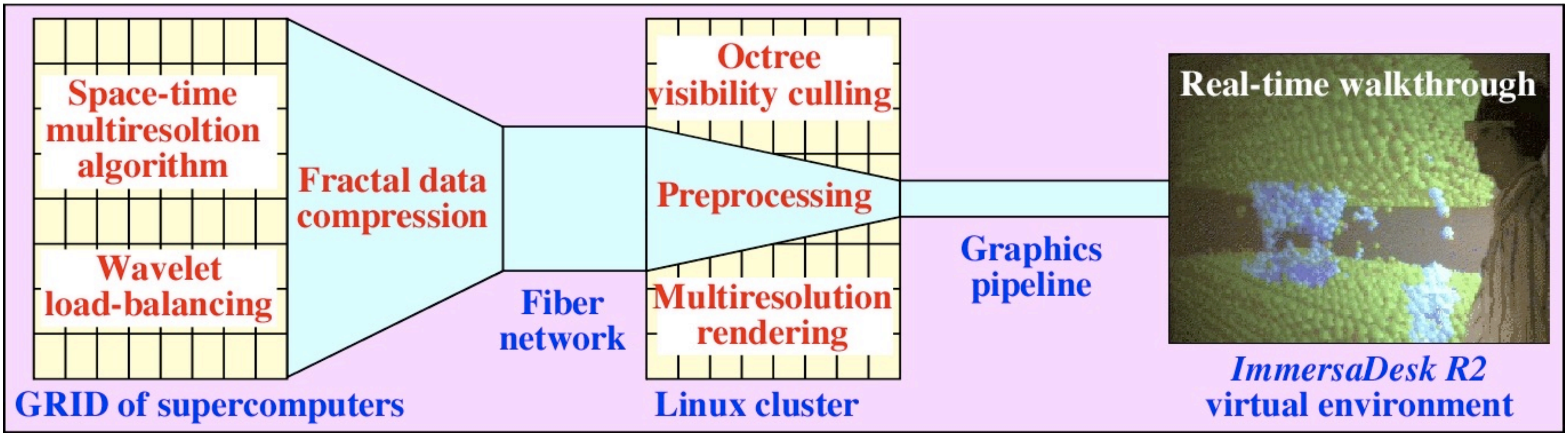
Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Quantitative & Computational Biology
University of Southern California

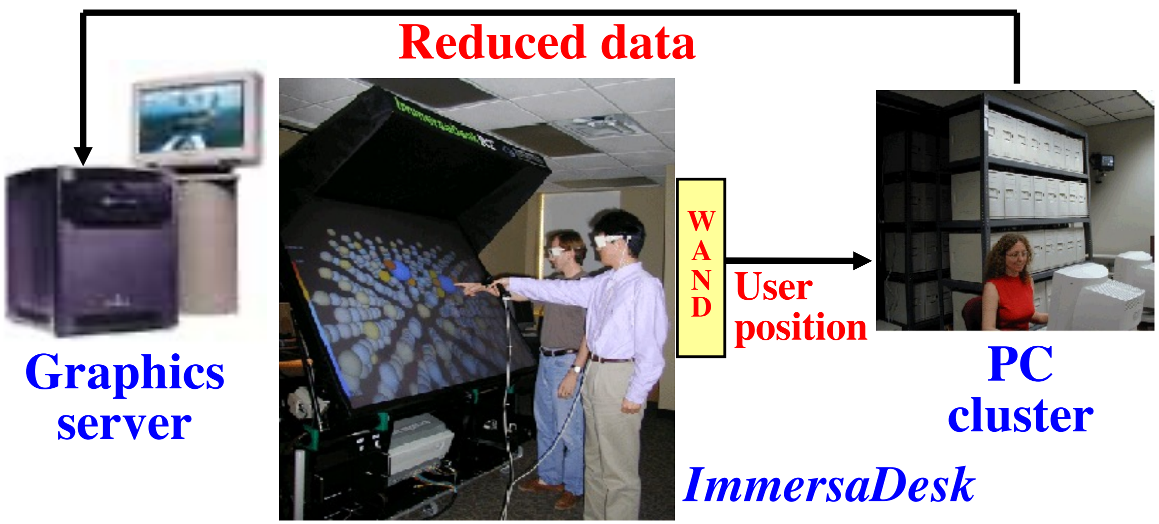
Email: anakano@usc.edu

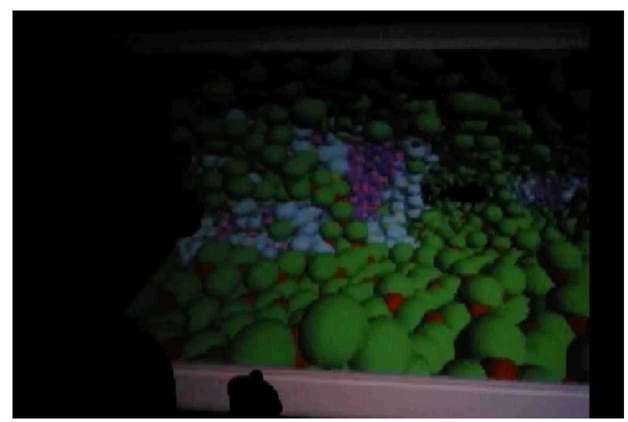
Immersive & Interactive Visualization

Challenge: billion-atom walkthrough



Solution: parallel & distributed Atomsviewer





Locality in Data Compression

Massive data transfer via wide area network:
75 GB/step of data for 1.5 billion-atom MD!

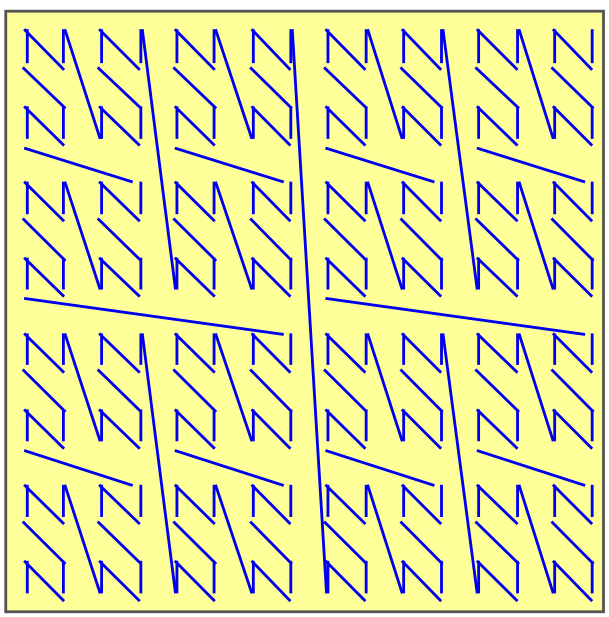
→ Compressed software pipeline

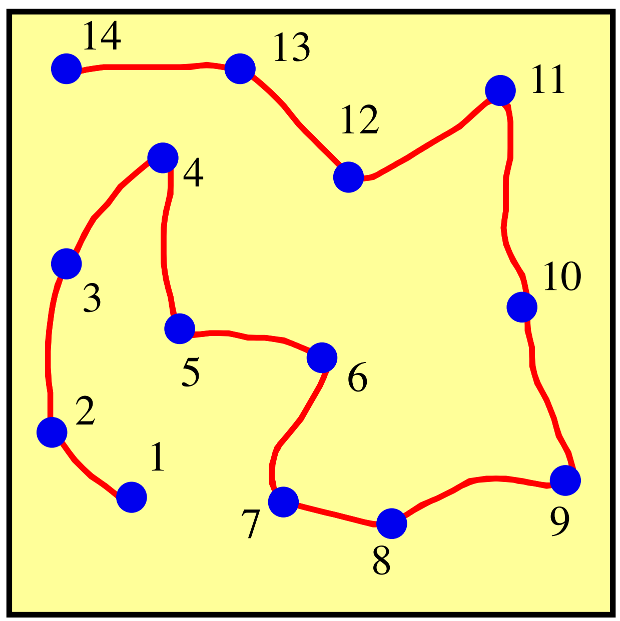
Scalable encoding:

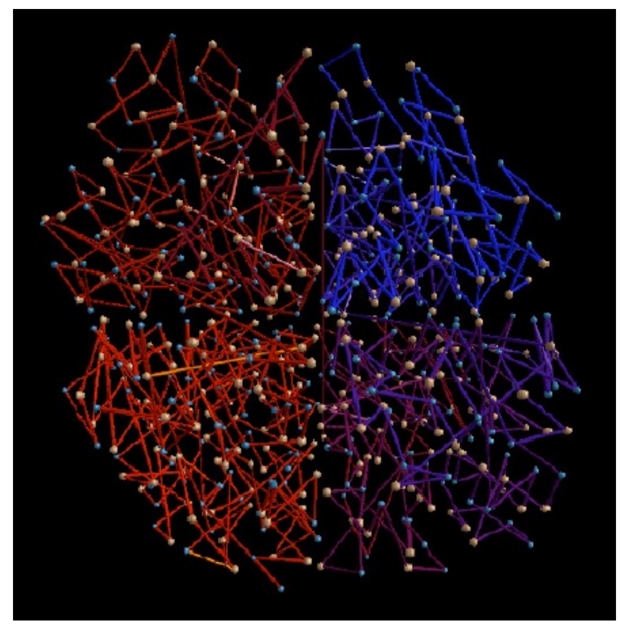
- **Store relative positions on spacefilling curve: $O(N\log N) \rightarrow O(N)$**

Result:

- **Data size, 50Bytes/atom → 6 Bytes/atom**







Data Compression for Scalable I/O

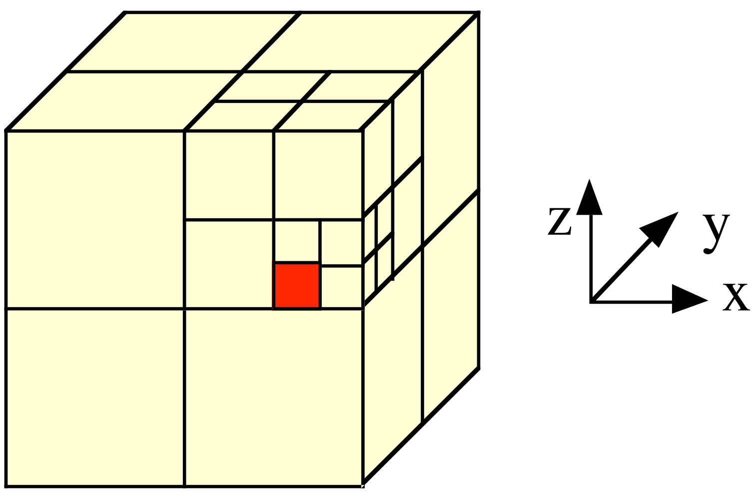
Challenge: Massive data transfer via OC-12 (622 Mbps)

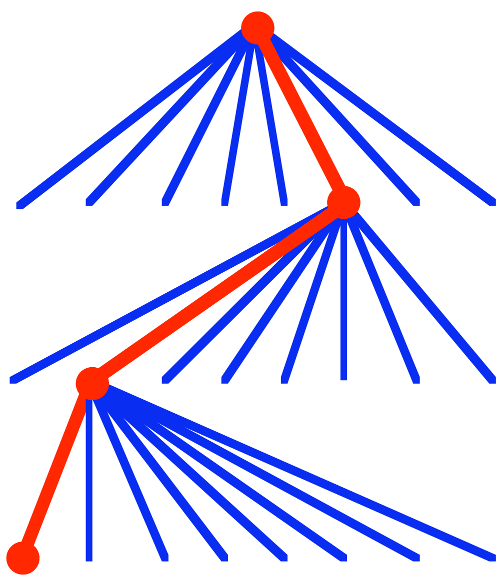
75 GB/frame of data for a 1.5-billion-atom MD!

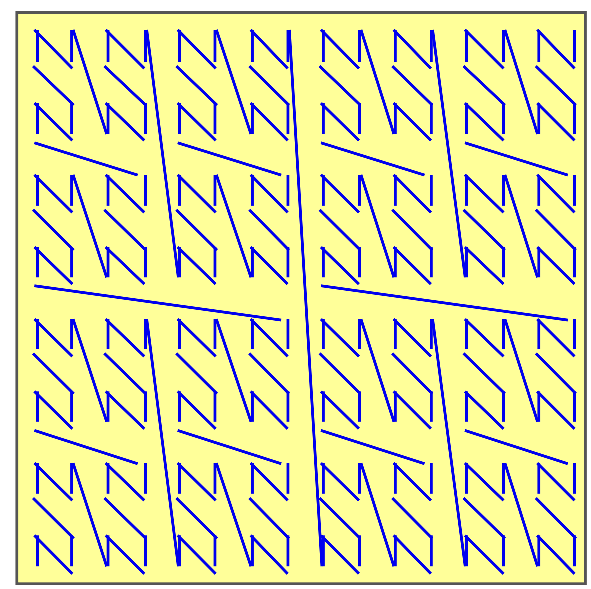
Scalable encoding:

- **Spacefilling curve based on octree index**

```
x =    1    1    0
y =   0    0    0
z =  1    0    0
-------------------
R =  101  001  000
```







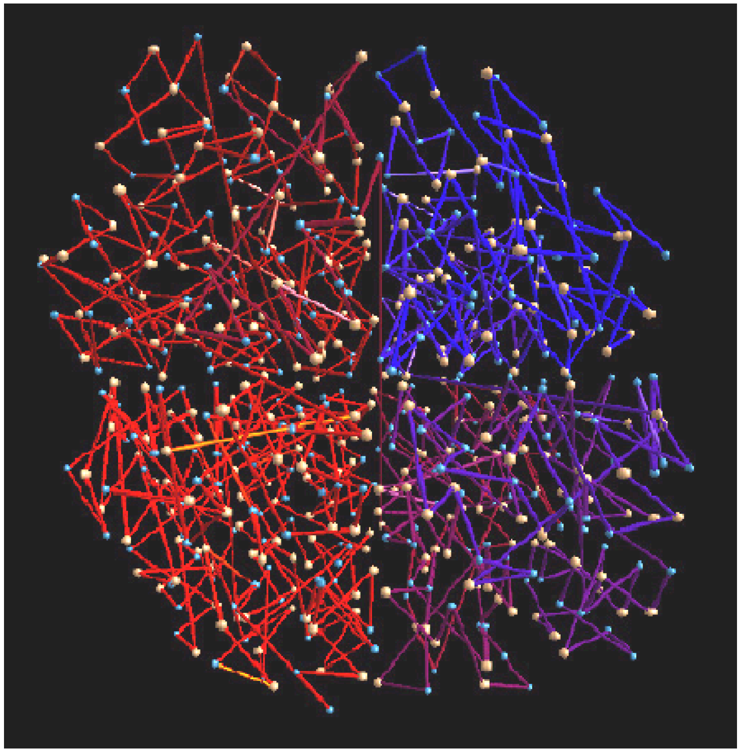
3D → list map preserves spatial proximity

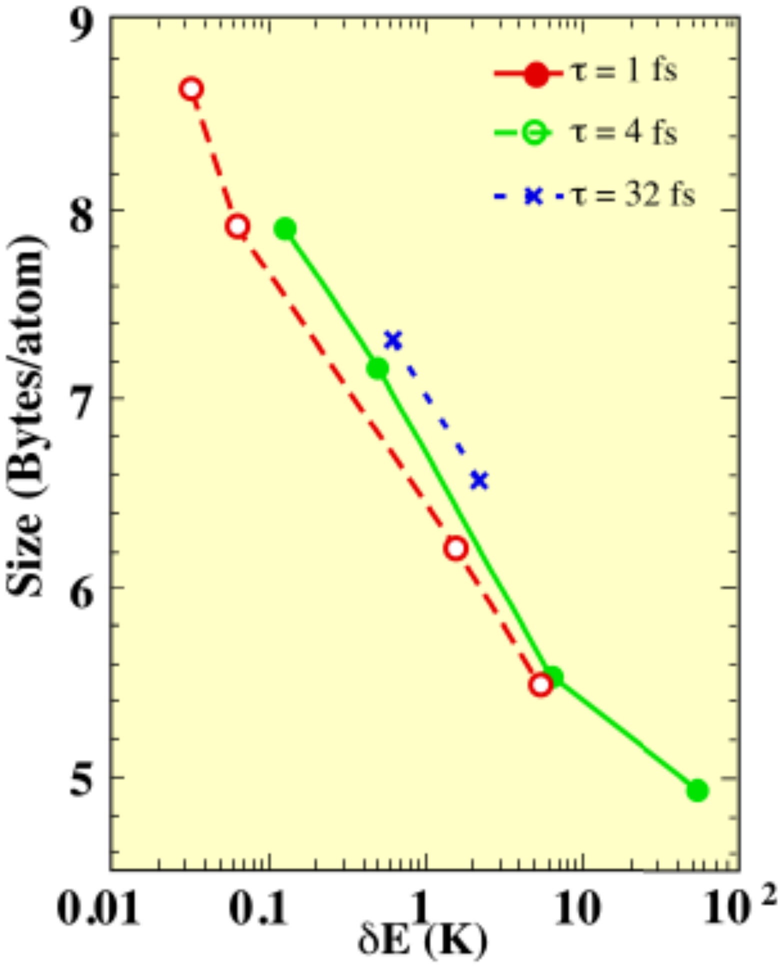
Spacefilling-Curve Data Compression

Algorithm:

1. Sort particles along the spacefilling curve
2. Store relative positions: $O(N\log N) \rightarrow O(N)$

- Adaptive variable-length encoding to handle outliers
- User-controlled error bound



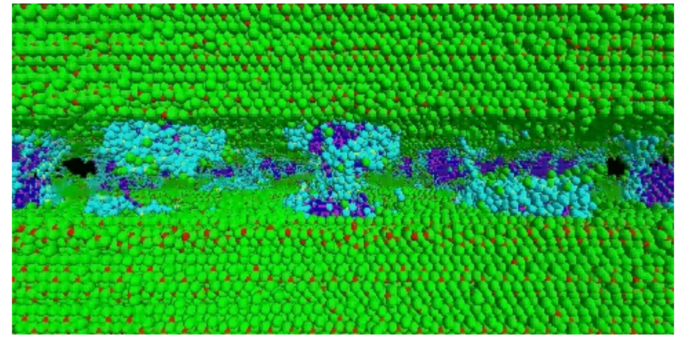


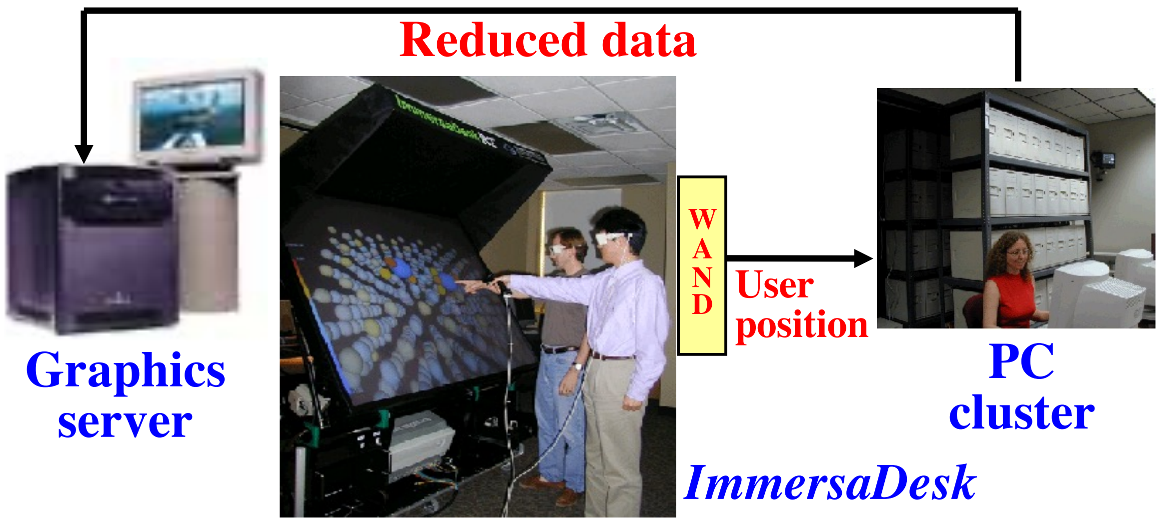
Result:

- An order-of-magnitude reduction of I/O size: 50 → 6 Bytes/atom

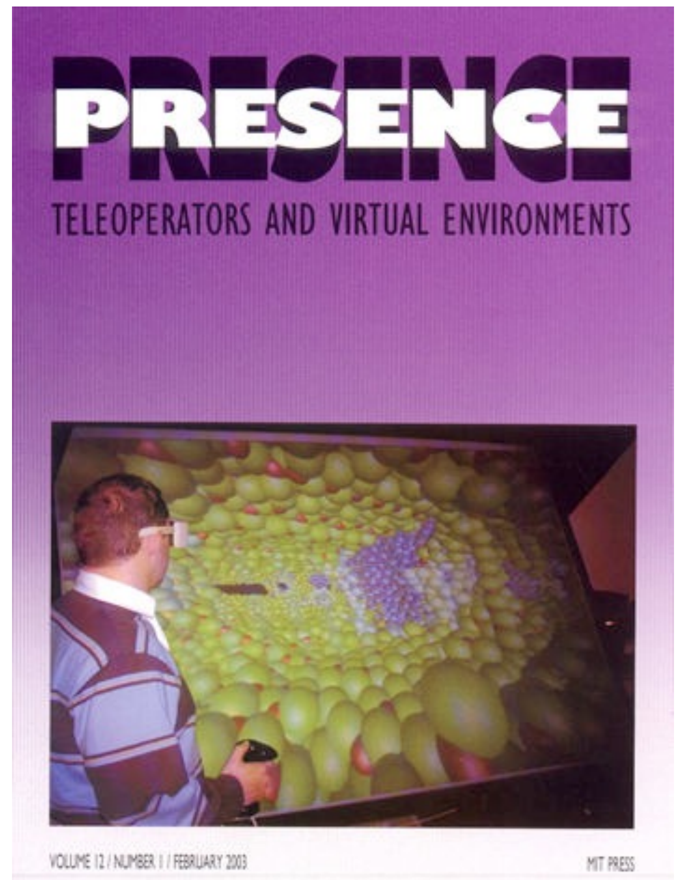
Data Locality in Visualization

- Octree-based fast view-frustum culling
- Probabilistic occlusion culling
- Parallel/distributed processing

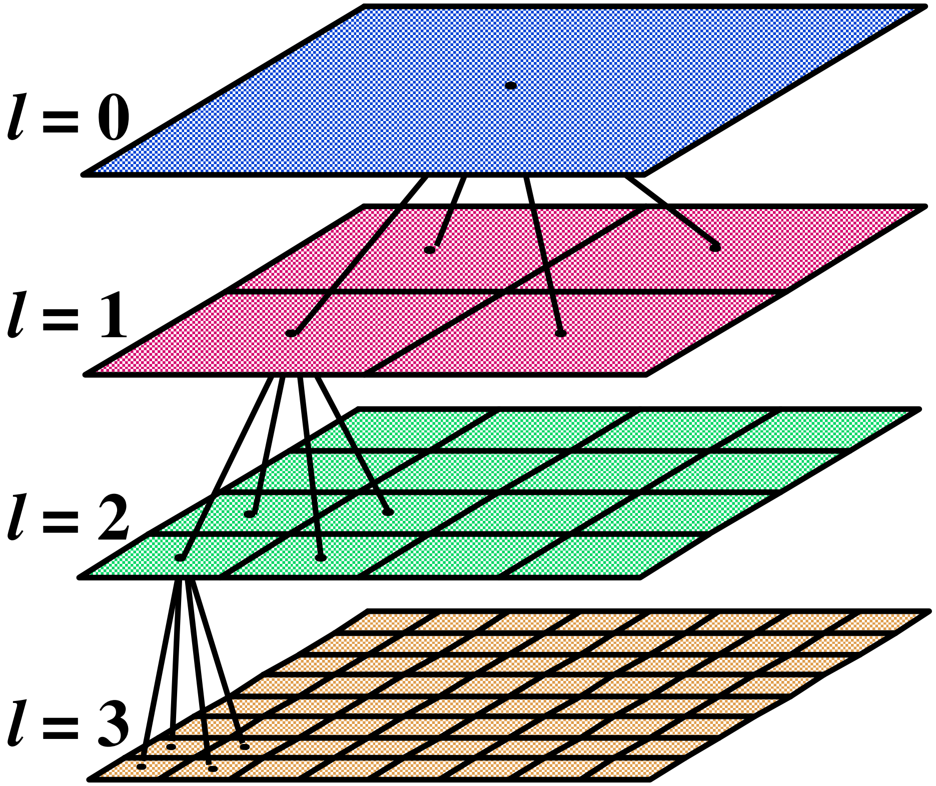




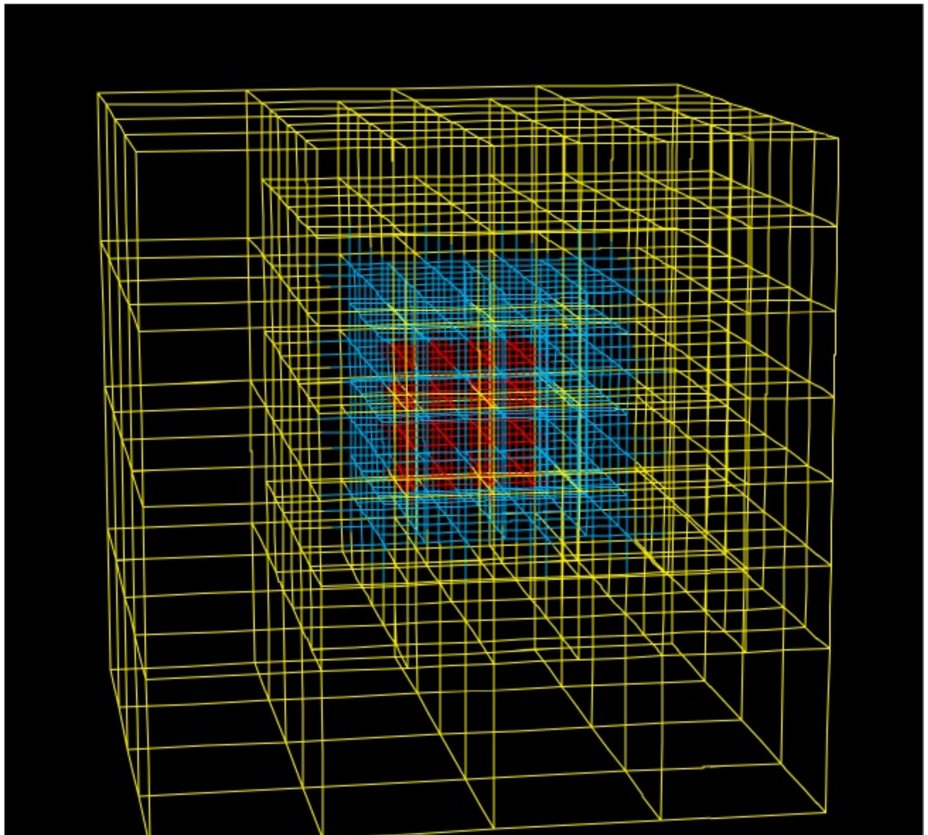
- Interactive visualization of a billion-atom dataset in immersive environment



Hierarchical Abstraction



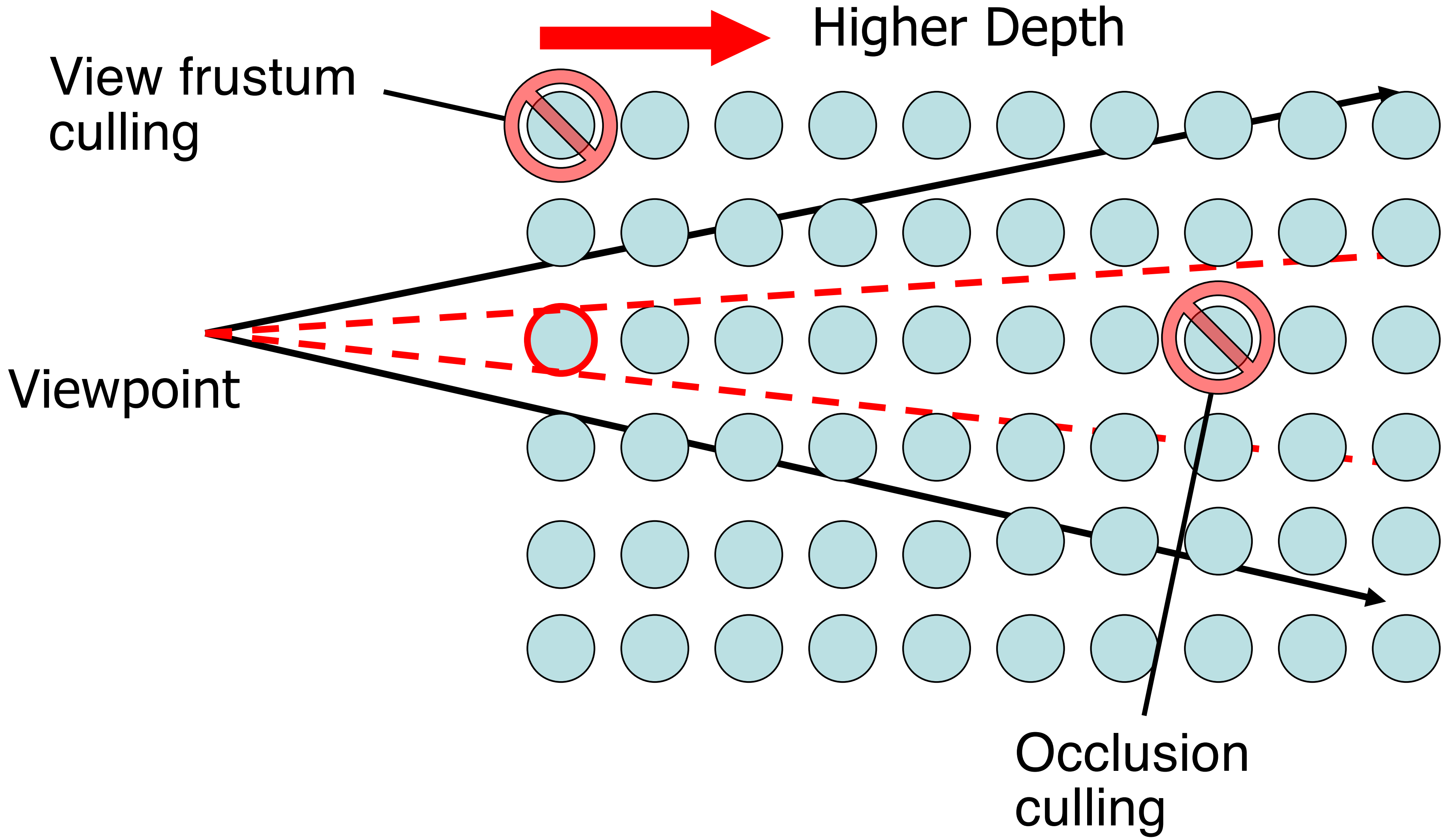
2D example



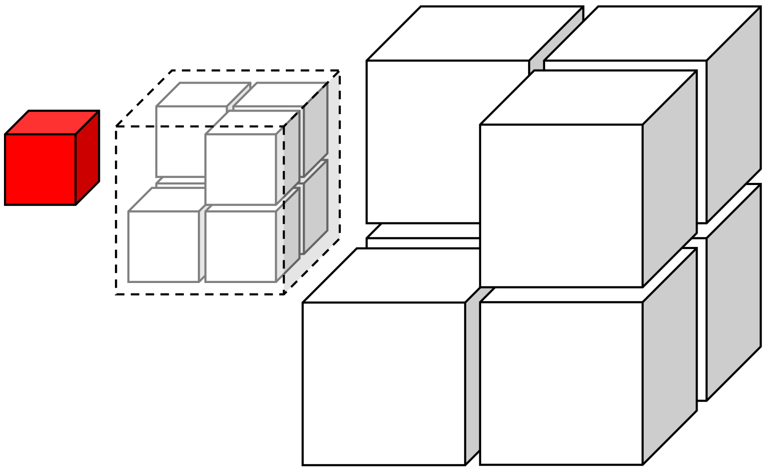
Use of an octree

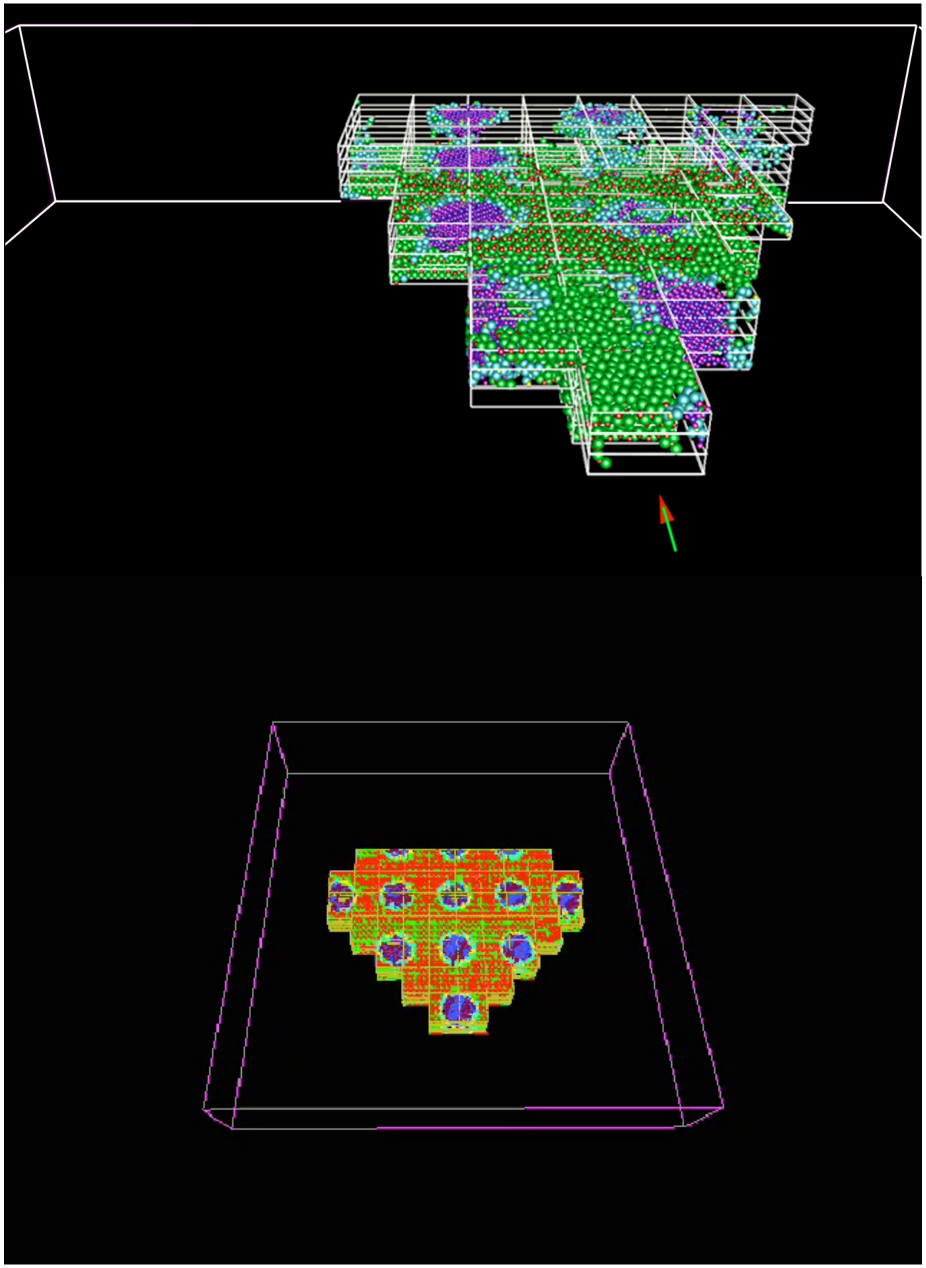
- Larger clusters for longer distances
- Recursively subdivide the 3D space to form an octree

Visibility Culling



Octree-based View-Frustum Culling

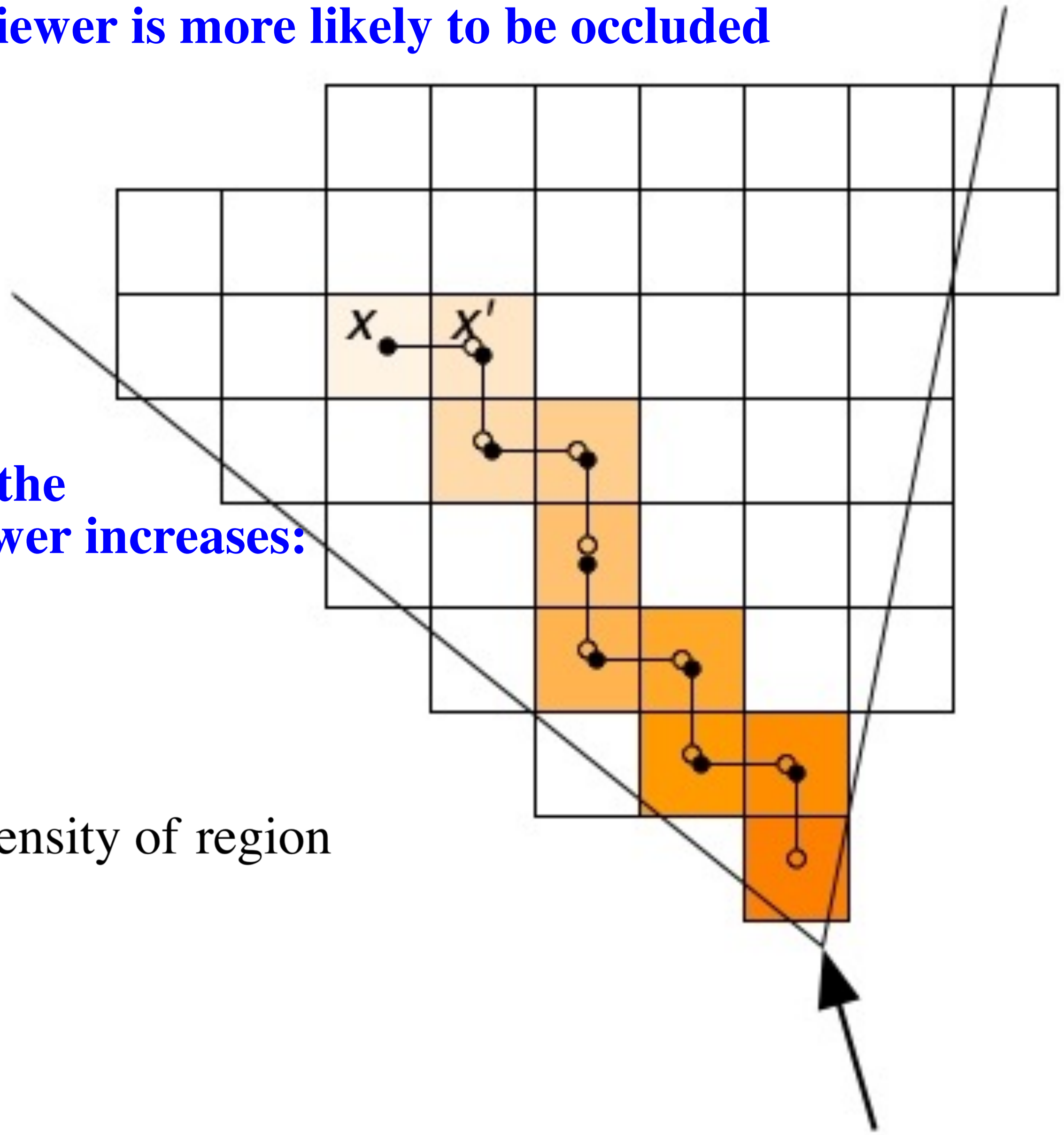




- Use the octree data structure to efficiently select only visible atoms
- Complexity
  Insertion into octree: $O(N)$
  Data extraction: $O(\log N)$

Probabilstic Occlusion Culling

- Remove atoms that are occluded by other atoms closer to the viewer
- Regions farther away from the viewer is more likely to be occluded than one in front of the viewer



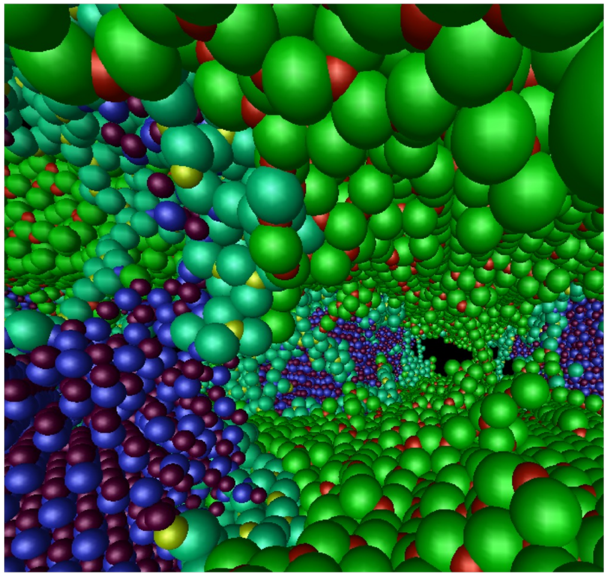
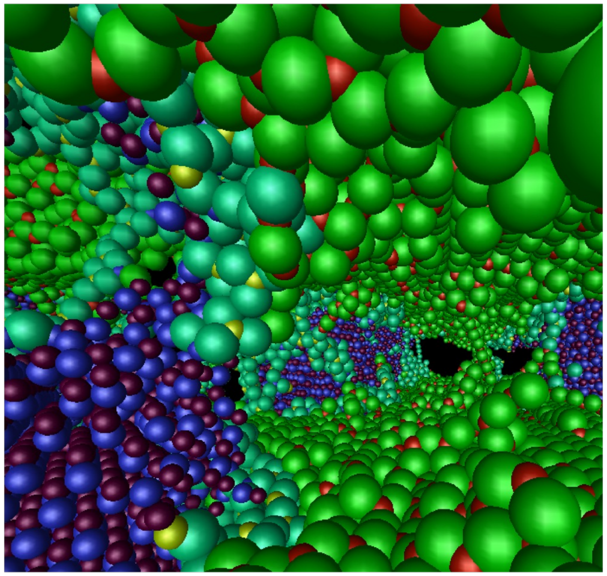
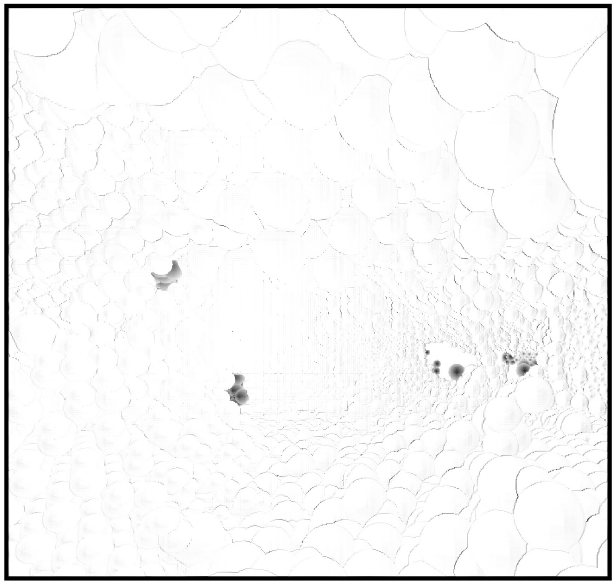
- Draw fewer atoms per region as the distance of a region from the viewer increases: visibility value $v(x)$ for region x
- Recurrence along the view line

$$v_x = \begin{cases} 1 & x = 0 \\ f(D_{x'}, v_{x'}) & \text{else} \end{cases} \qquad D_x = \text{density of region}$$

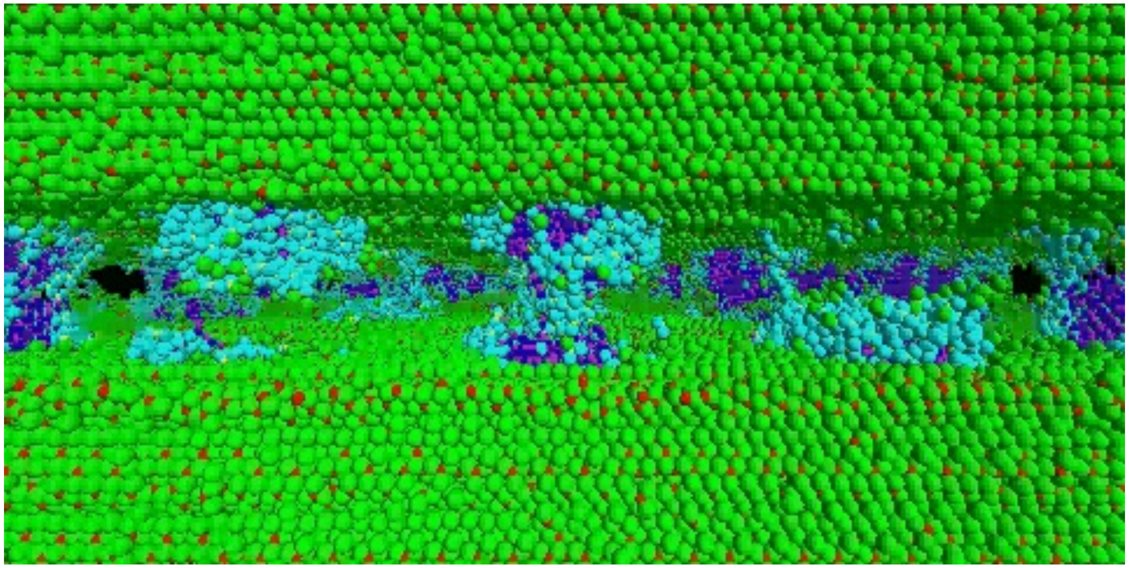
- Run-time adaptation

$$v'_x = f(\text{user speed}) \times v_x$$

Results of Probabilstic Occlusion Culling

Original	Probabilistic	Difference
		

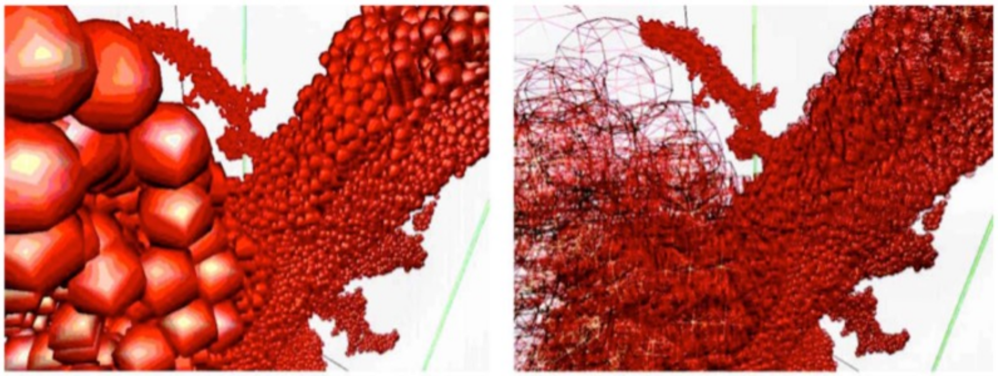
68% fewer objects; 3× frame rate



Multiresolution Culling & Rendering

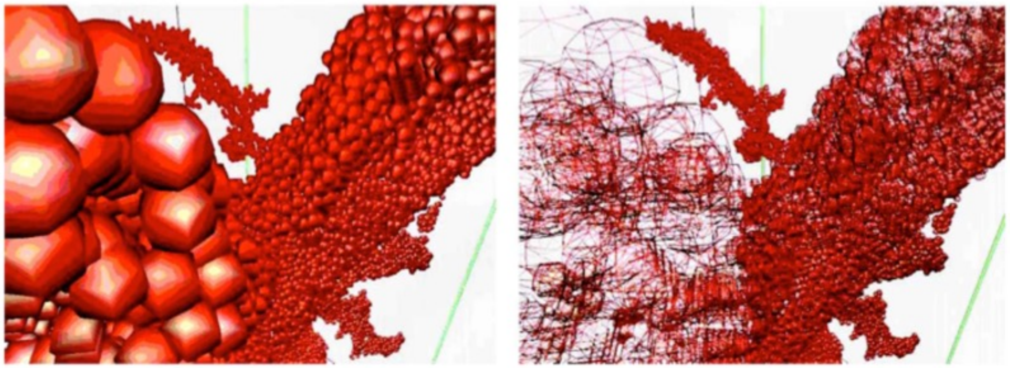
- Per-octree node operations:
  - Frustum culling
  - Probabilistic occlusion culling
- Per-atom operations
  - Multiple levels-of-detail
  - Occlusion culling (per-object, per-octree node)

Without multiresolution



.94fps - 90,000 particles

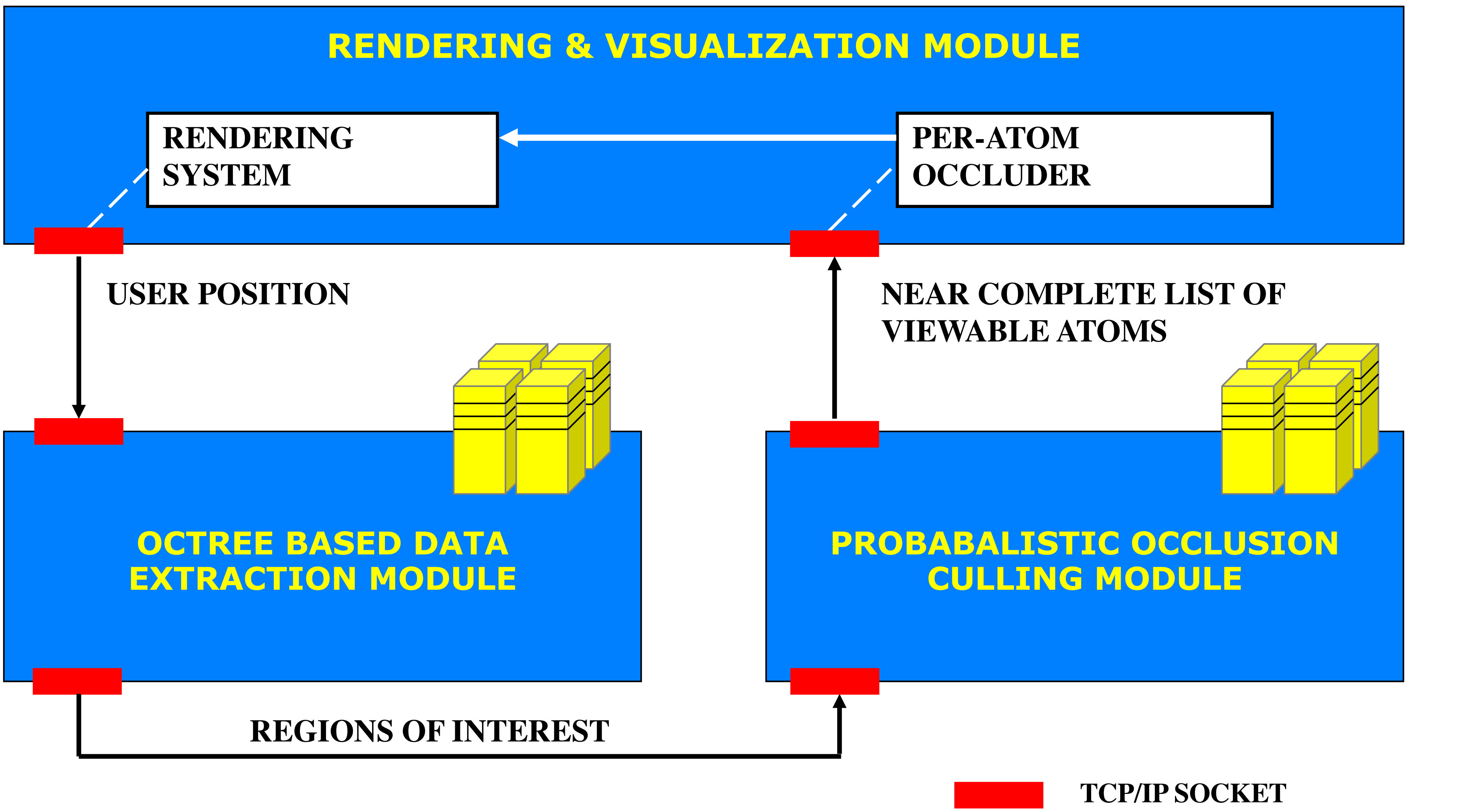
With multiresolution



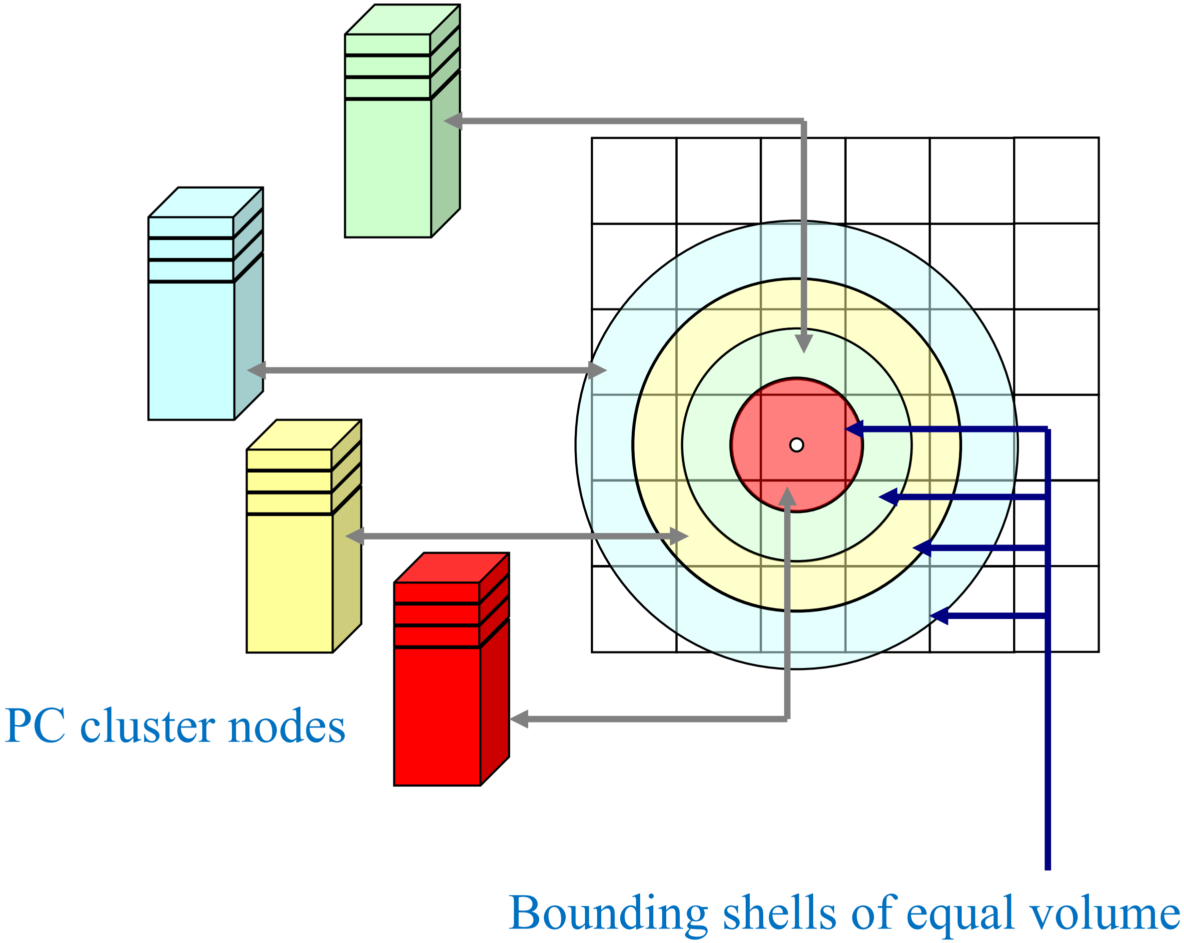
3.2fps - 4,500 particles

Outflow pathways of optic nerves from the retina of a rabbit eye
(Experimental data by C. Burgoyne & R. Beuerman, *LSU Eye Center*)

Distributed Architecture



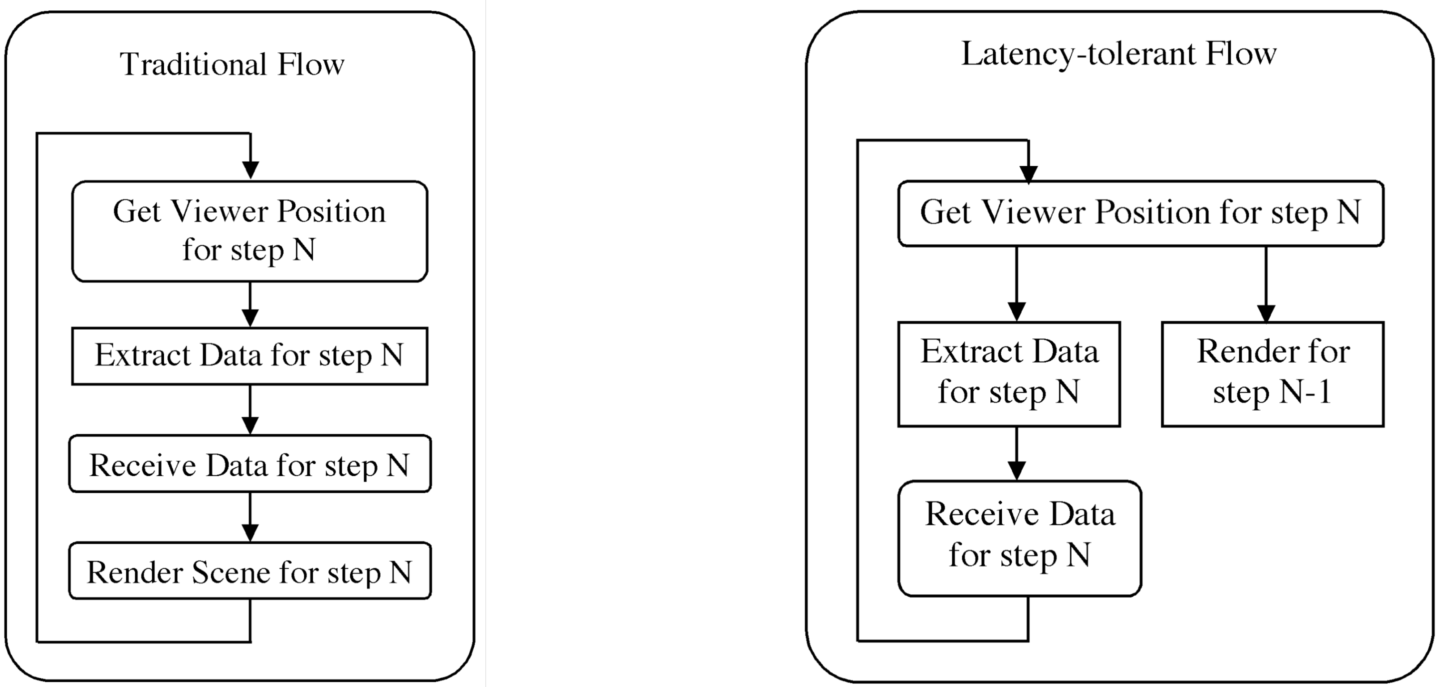
Parallel Octree Extraction



- Individual copies of the octree with each node
- Spherical extraction using shells of equal volume
- Load balancing due to the equal use of each processor for extraction

Latency Hiding

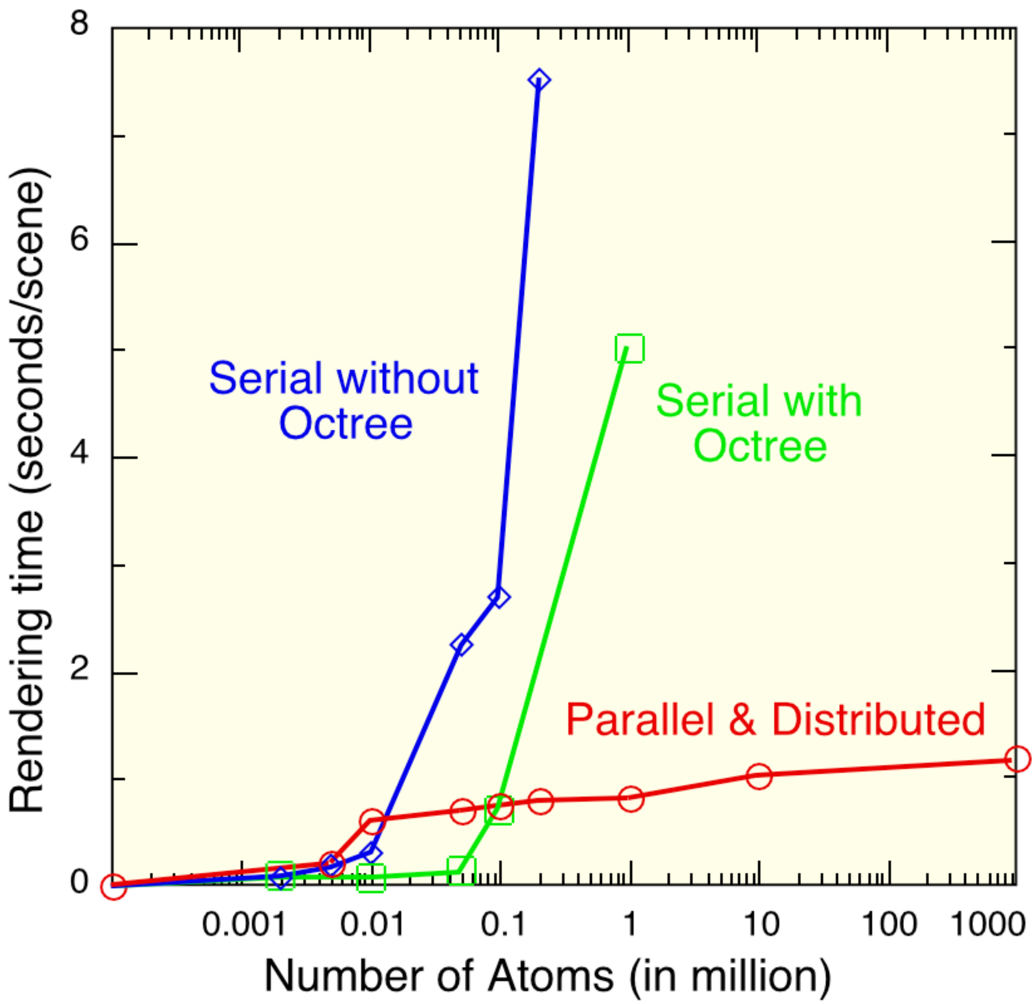
- **Individual modules are multithreaded to reduce network or module latency**
- **Minimize latency due to inter-modular dependencies by overlapping the inter-module communication and module computation**

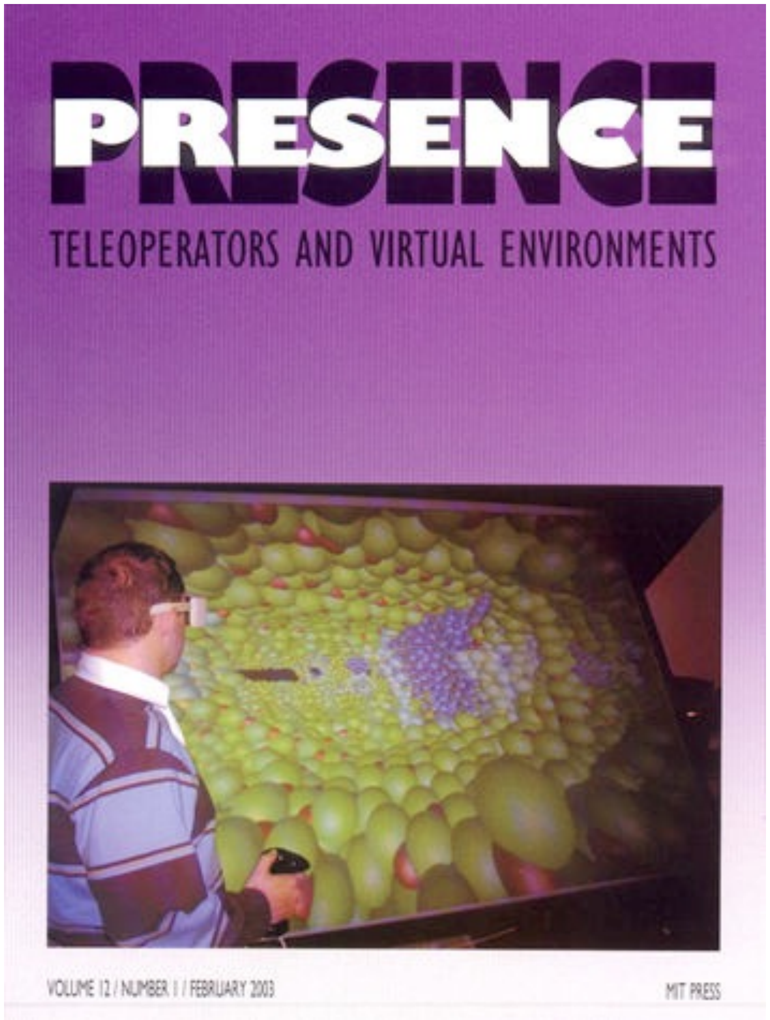


- **Instantaneously trained neural network (CC4** [Tang & Kak, *CSSP'98*]**) predicts the user's next position** [Liu *et al.*, *PDPTA'02*]

Parallel & Distributed Atomsviewer

Real-time walkthrough for a billion atoms on an SGI Onyx2 (2 × MIPS R10K, 4GB RAM) connected to a PC cluster (4 × 800MHz P3)





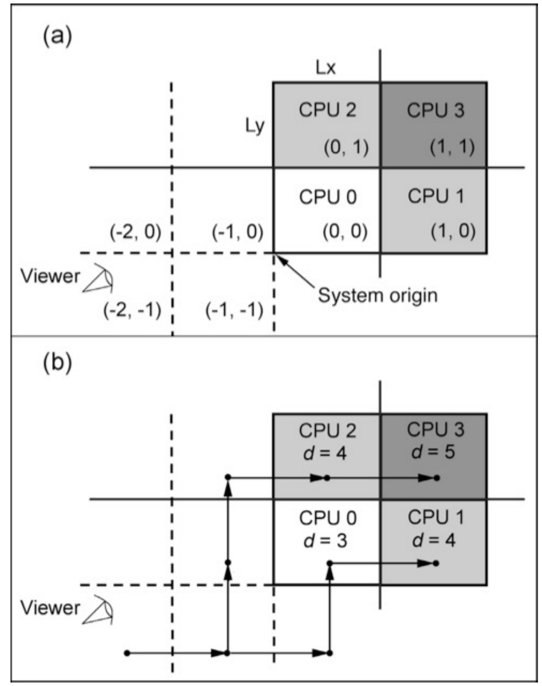
IEEE Virtual Reality Best Paper

Parallel *In Situ* Rendering

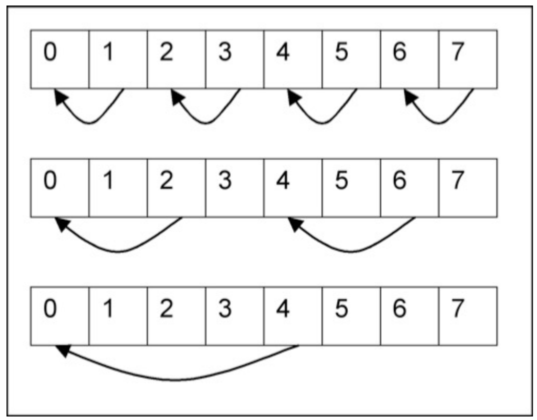
International Journal of Computational Science
1992-6669 (Print) 1992-6677 (Online) © Global Information Publisher
2007, Vol. 1, No. 4, 407-421

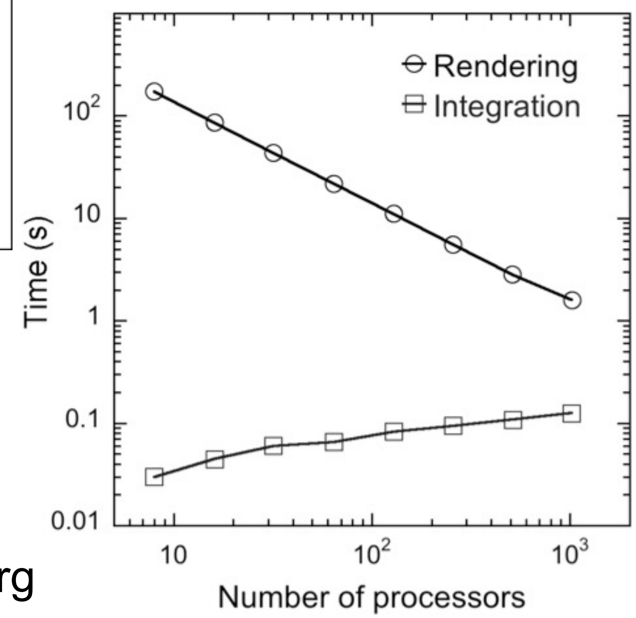
ParaViz: A Spatially Decomposed Parallel Visualization Algorithm Using Hierarchical Visibility Ordering

Cheng Zhang[1], Scott Callaghan[2], Thomas Jordan[2], Rajiv K. Kalia[1],
Aiichiro Nakano[1*], Priya Vashishta[1]



- **Parallel (software) rendering of spatially distributed data: hybrid sort-first/sort-last**
- **Scalable depth buffer by domain-level distributed visibility ordering**
- **On-the-fly visualization of parallel simulation without data migration**
- **Parallel efficiency 0.98 on 1,024 processors for 16.8 million-atom molecular-dynamics simulation**



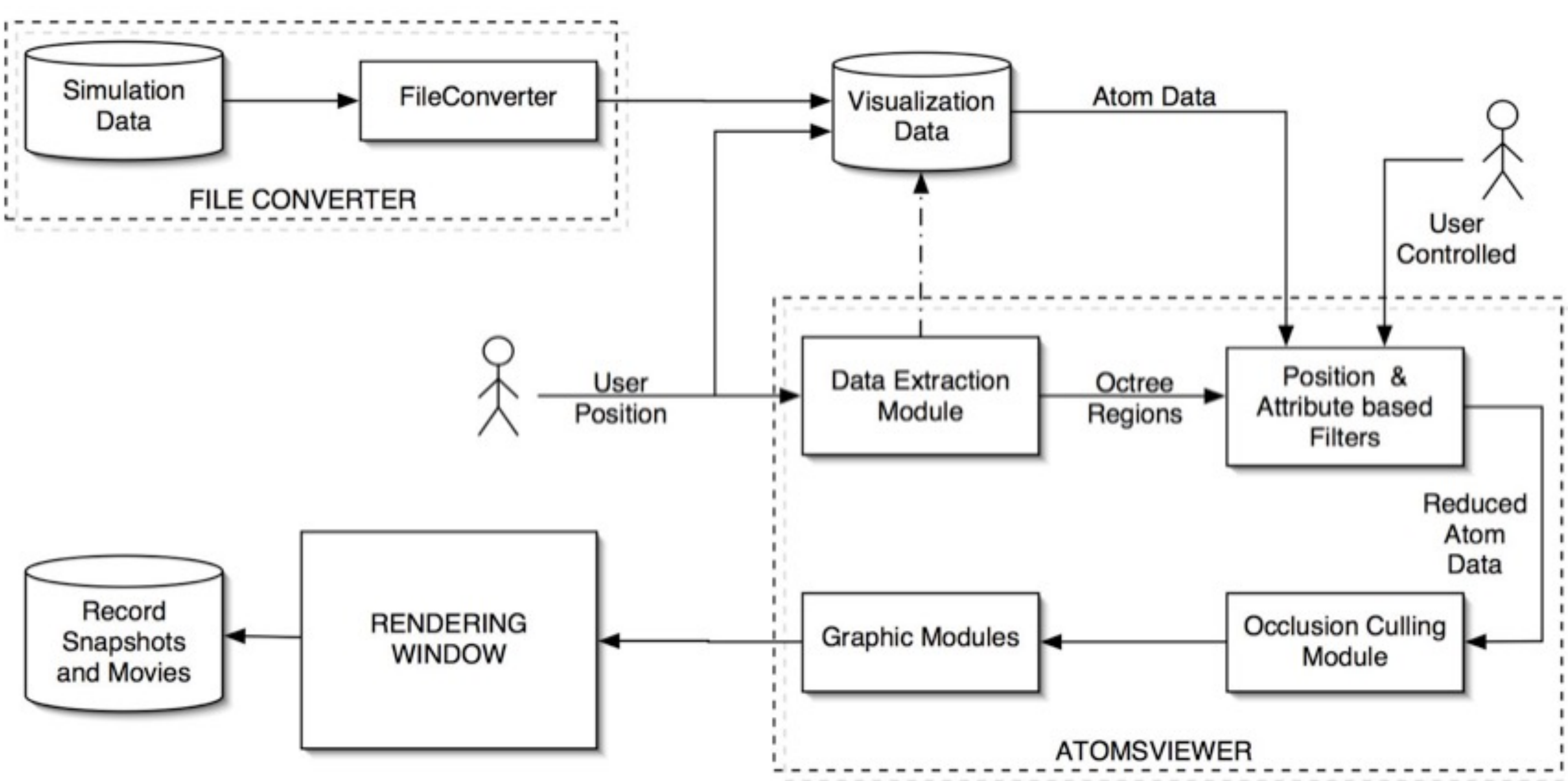


Soft rendering
http://www.mesa3d.org

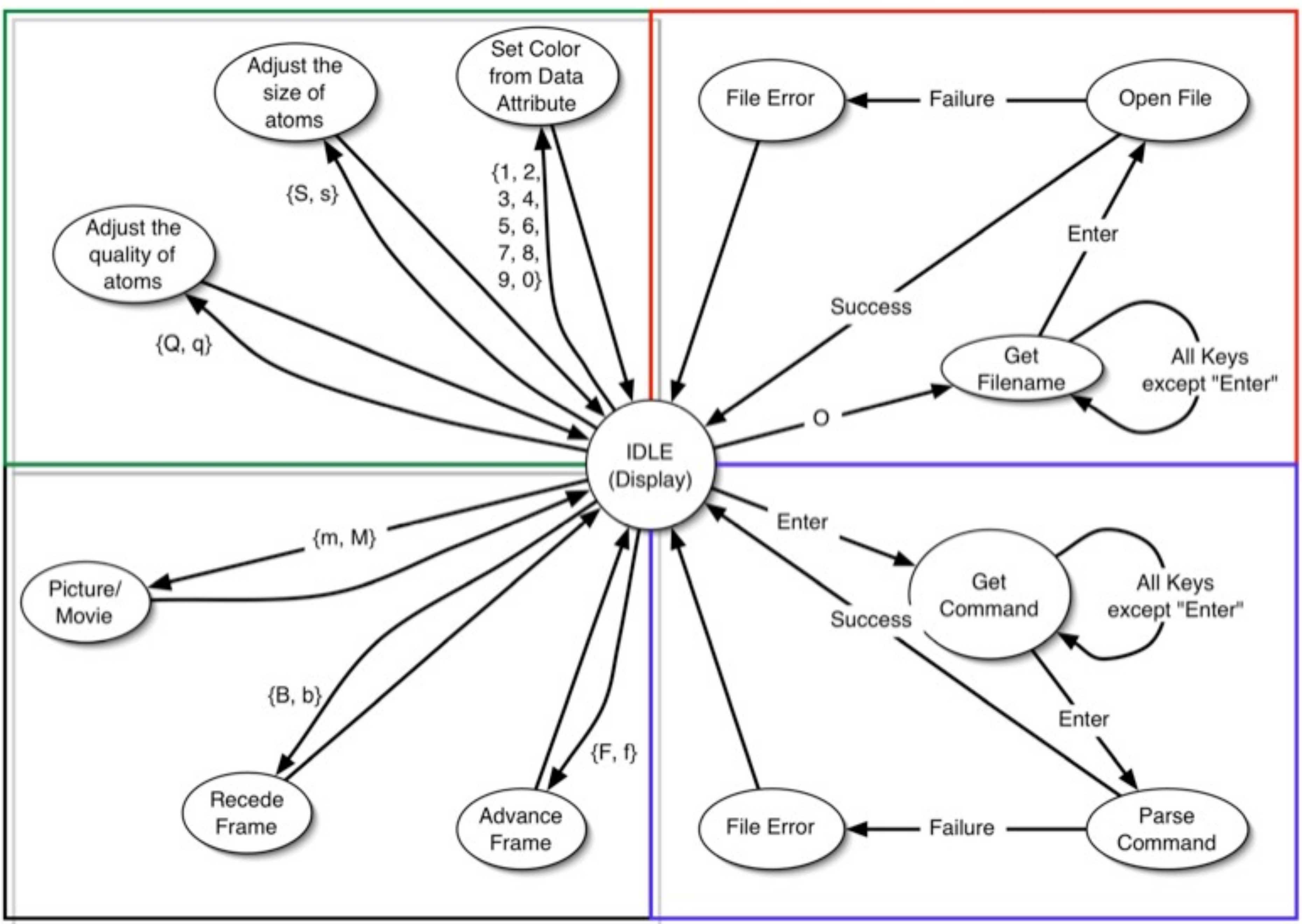
Atomsviewer Code

- Programming language
  - > C++
- Graphics
  - >OpenGL
  - >CAVE Library (optional)
- Platforms
  - >Windows
  - >Macintosh OS X
  - >SGI Irix

Atomsviewer System



Atomsviewer Commands



Atomsviewer Code Dissemination

Computer Physics Communications Program Library

Available online at www.sciencedirect.com

SCIENCE @ DIRECT®

ELSEVIER

Computer Physics Communications 163 (2004) 53–64

Computer Physics Communications

www.elsevier.com/locate/cpc

Scalable and portable visualization of large atomistic datasets ☆

Ashish Sharma *, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta

Collaboratory for Advanced Computing and Simulations, Department of Computer Science, Department of Physics & Astronomy, Department of Material Science & Engineering, University of Southern California, Los Angeles, CA 90089-0242, USA

Received 15 June 2004; accepted 8 July 2004

Available online 16 September 2004

Abstract

A scalable and portable code named Atomsviewer has been developed to interactively visualize a large atomistic dataset consisting of up to a billion atoms. The code uses a hierarchical view frustum-culling algorithm based on the octree data structure to efficiently remove atoms outside of the user's field-of-view. Probabilistic and depth-based occlusion-culling algorithms then select atoms, which have a high probability of being visible. Finally a multiresolution algorithm is used to render the selected subset of visible atoms at varying levels of detail. Atomsviewer is written in C++ and OpenGL, and it has been tested on a number of architectures including Windows, Macintosh, and SGI. Atomsviewer has been used to visualize tens of millions of atoms on a standard desktop computer and, in its parallel version, up to a billion atoms.

Program summary

Title of program: Atomsviewer
Catalogue identifier: ADUM
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADUM
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Computer for which the program is designed and others on which it has been tested: 2.4 GHz Pentium 4/Xeon processor, professional graphics card; Apple G4 (867 MHz)/G5, professional graphics card
Operating systems under which the program has been tested: Windows 2000/XP, Mac OS 10.2/10.3, SGI IRIX 6.5
Programming languages used: C++, C and OpenGL
Memory required to execute with typical data: 1 gigabyte of RAM
High speed storage required: 60 gigabytes
No. of lines in the distributed program including test data, etc.: 550 241
No. of bytes in the distributed program including test data, etc.: 6 258 245
Number of bits in a word: Arbitrary

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

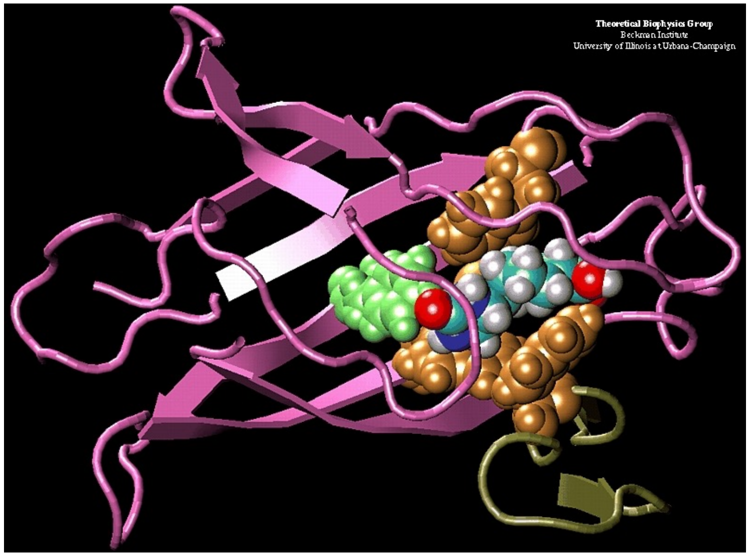
* Corresponding author.
E-mail address: anakano@usc.edu (A. Sharma).

doi:10.1016/j.cpc.2004.07.008

http://www.cpc.cs.qub.ac.uk/cpc

Scientific Visualization Tools

- **Atomsviewer: Billion-atom visualizer**
  http://cpc.cs.qub.ac.uk/summaries/ADUM_v1_0.html
- **VMD: Molecular-dynamics data**
  http://www.ks.uiuc.edu/Research/vmd
- **OVITO: Open visualization tool**
  https://ovito.org
- **VisIT: General visualization system**
  https://visit.llnl.gov
- **ParaView: General visualization system**
  http://www.paraview.org



OVITO
Open Visualization Tool