Sculptor

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Overview

- Sculptor
  - Multi-resolution modeling software package
- Emphasis on visualization
  - Efficient (“real-time”), high-quality visualization
- Sculptor Architecture
- Tutorials

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Visualization

- Volumetric
  - DVR
  - Iso surfaces
  - Cross section
- Atomic Models
  - Static and dynamic scenes
- Global lighting
  - SSAO

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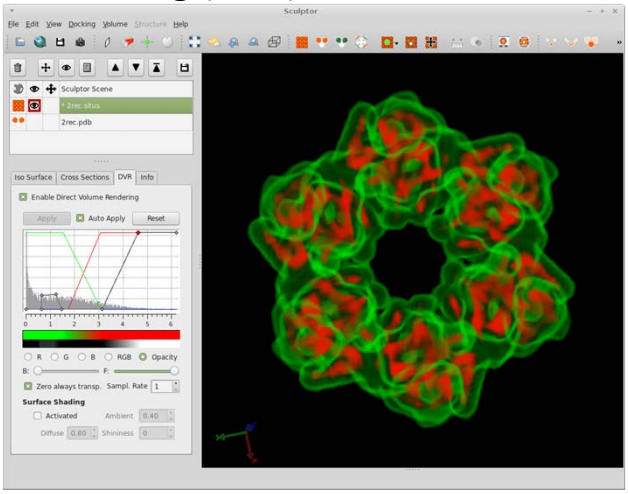
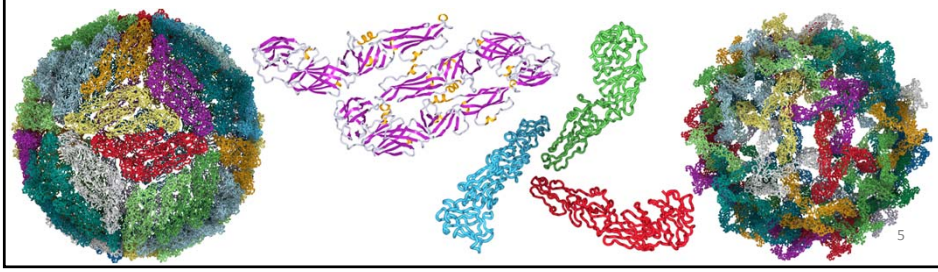
Volume Rendering

- Direct volume rendering (DVR)
  - Transfer function
  - Surface shading



Atomic Models

- Conventional geometry based
- Efficient vertex- and pixel-shader based
  - Large complexes
  - Protein dynamics
  - Cartoon, tube, VDW



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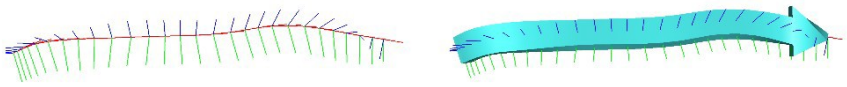
Dynamic Atomic Models

- Large time-varying structures not trivial to visualize
  - Geometry changes with every frame
  - CPU is bottleneck while GPU underutilized
- So: move computation from CPU to GPU
  - CPU computes path, GPU extrudes geometry



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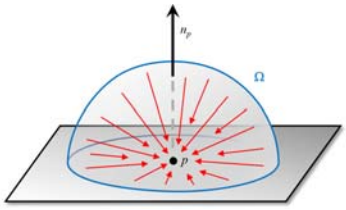
SSAO



- Ambient occlusion
  - Surface features like creases, pockets prevent areas from receiving light
  - Some regions appear darker than other
- However, standard lighting is local
  - Computed at every vertex for view and light position(s) -> parallelizable and fast
  - Ignores other geometry
- Global lighting is too expensive for real-time
  - Ray casting

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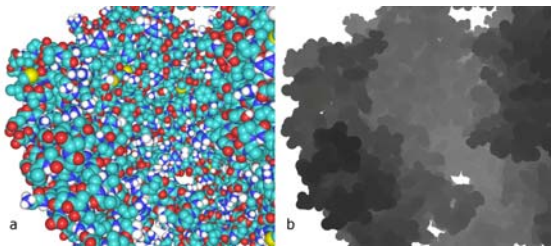
SSAO

- Solution: screen space ambient occlusion
  - Approximation to global lighting
- Computed not on the geometry, but using data within the image plane (pixel data)
  - Taking advantage of rendering pipeline



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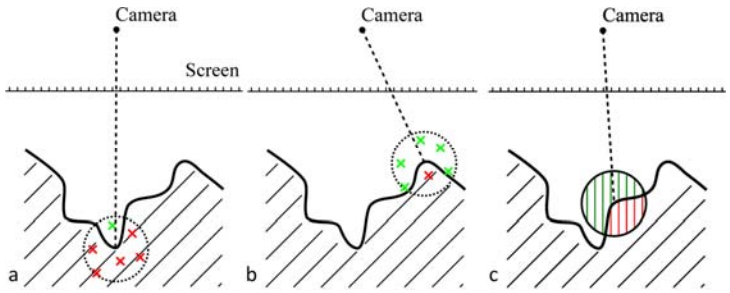
SSAO

- Rendering pipeline computes per-pixel color and depth during rasterization
- Back project from viewpoint through each pixel
- Sample points/lines in a sphere for occlusion ratio



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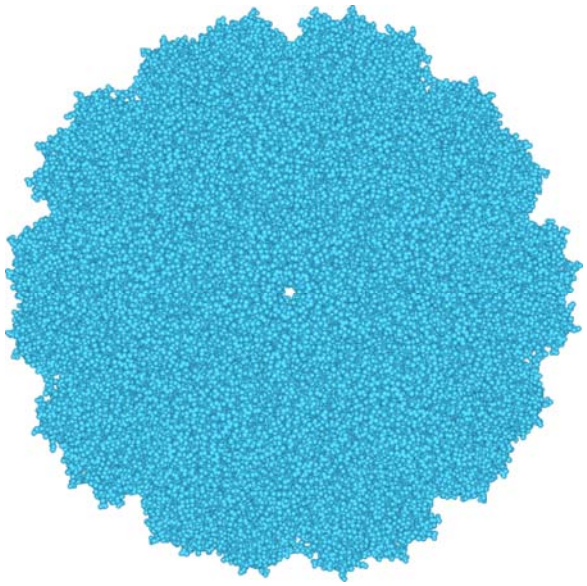

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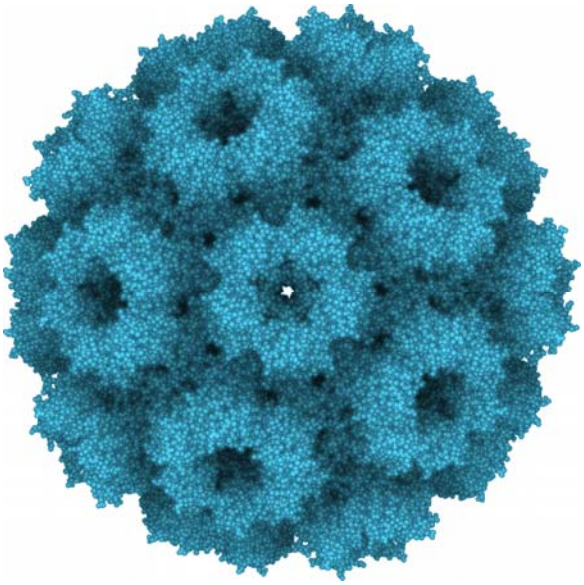

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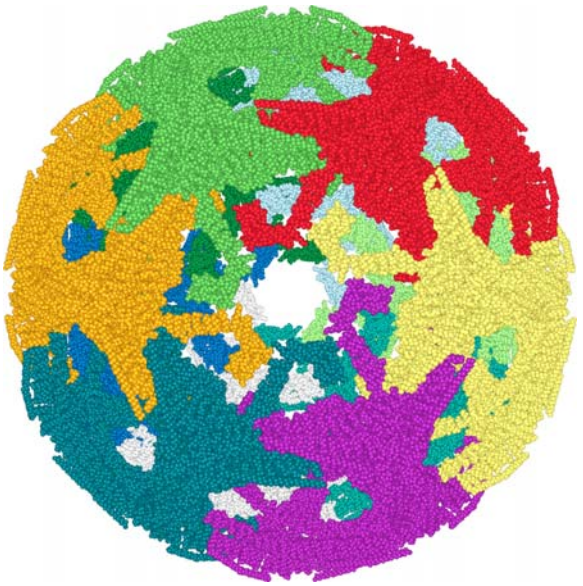

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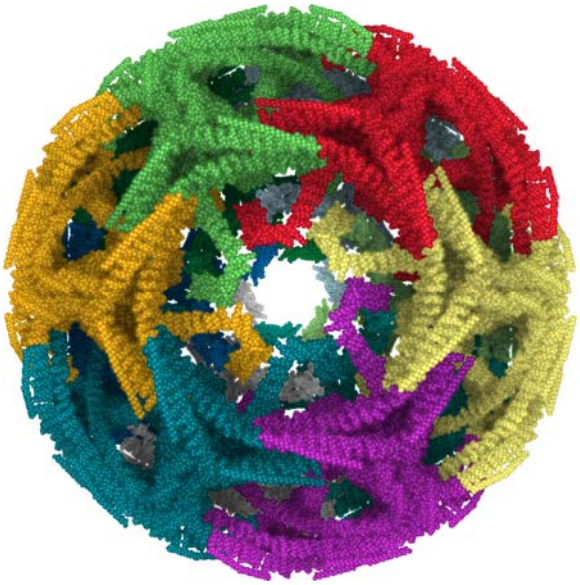

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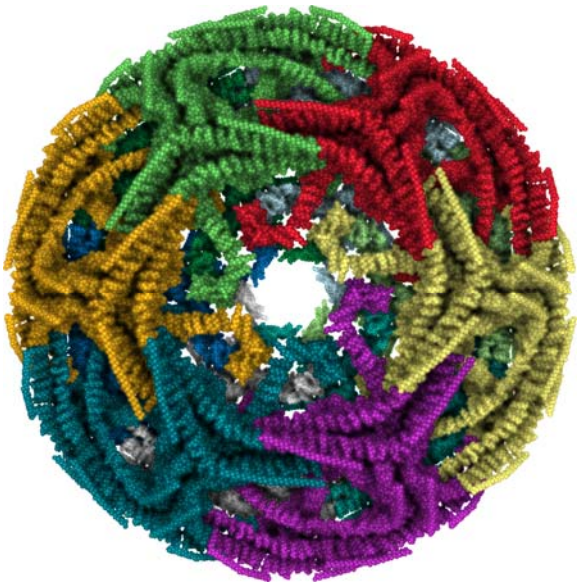

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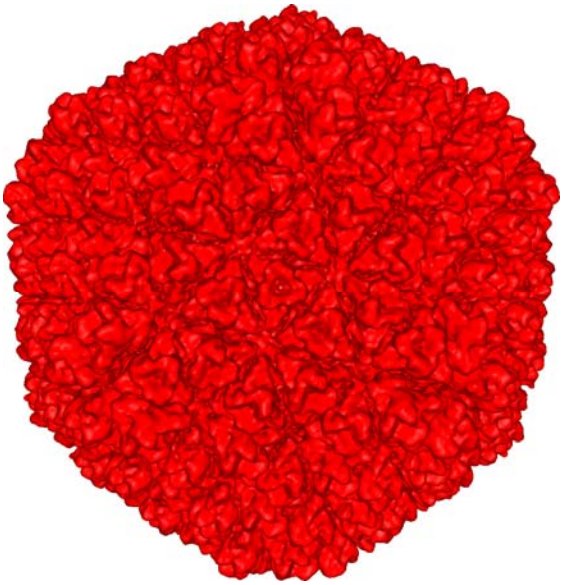

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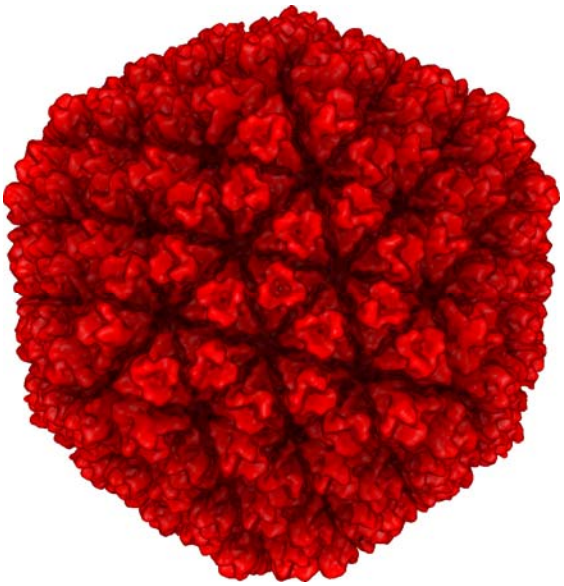

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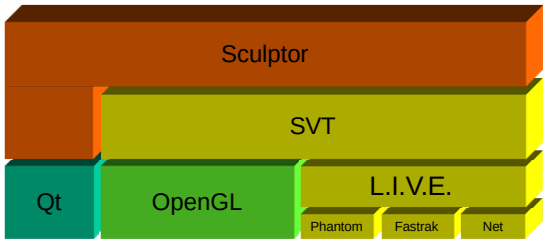
Sculptor Architecture

- C++, OpenGL, Cg
- Sculptor almost only UI
  - About 50k SLOC
- SVT – Scientific Visualization Toolkit
  - About 100k SLOC



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Tutorials

Available at http://sculptor.biomachina.org/tutorials.html

We will cover:

1 - Visualization of Molecular Structures

2 - Visualization of Volumetric Data

4 - Manual Docking and Correlation-based Refinement

8.2 - Detecting Alpha Helices in Intermediate Resolution Maps

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1 Visualization of Molecular Structures

- Load 1OS5.pdb
  - Switch to new tube
  - Add to graphics mode stack
    - Select residue seq. from 371 to 563
    - Change to VDW mode, structure coloring
  - Get rid of water atoms:
    - Add to graphics mode stack
      - Select either “water atoms” or “residue name” HOH
      - Change mode to off

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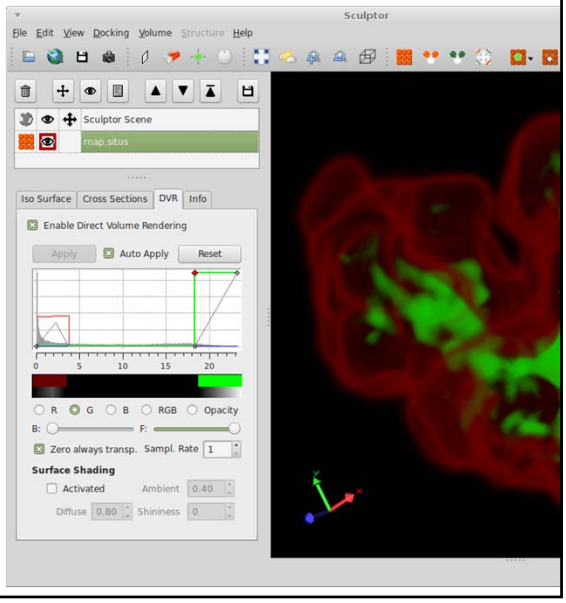
2 Visualization of Volumetric Data

- Load rnap.situs
  - Play with iso surface
  - Go to DVR tab
    - Try to create transfer function
    - Grey line is opacity



4 Manual Docking and Correlation-based Refinement

- Load 2rec15.situs, 2recmon.pdb, 2REC
  - Set 2rec15 to iso surface level 1.0, half transparent
  - Set 2recmon to “New Tube” graphics mode and to a “Solid” bright color
  - Set 2REC to New Tube, different color, and hide it
- 2recmon initially placed perfectly, so misalign *a little*
- Make 2recmon the probe, then select Docking-> Refinement
  - Set resolution to 15
- Load 2recmon again, change to new tube, then try to align to next position, make probe, then refine

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8.2 Detecting Alpha Helices in Intermediate Resolution Maps

- Load emd_1740_AI.situs
  - Volume -> Threshold (minimum 2.5, max OK)
  - Volume -> Local normalization (sigma 2.5)
  - Volume -> Gaussian (1.5)
- Docking -> Volume Tracer
  - 11 “Traced Objects”, “Resolution” 6.8
  - Show “Search Template”
  - Windows 1 thread, others 4
  - “Execute”

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