Welcome to UPPMAX Workshop on *Scientific Visualization with*

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UPPMAX

- Uppsala Multidisciplinary Center for Advanced Computational Science
- http://www.uppmax.uu.se/
- *"UPPMAX provides resources and a common environment for an extensive community of researchers in a wide range of high performance computing (HPC) research fields."*

UPPMAX

- Director *Sverker Holmgren*
- Application experts:
  - Quantum Chemistry: *Hans Karlsson*
  - Algorithm & Code Development: *Jarmo Rantakokko*
  - Scientific Visualization: *Ingela Nyström*
  - Molecular Dynamics: *Daniel Spångberg*
  - Bioinformatics: *Ann-Charlotte Sonnhammer*
- System experts

UPPMAX

- Interdisciplinary resource for projects in
  - Astronomy
  - Bioscience
  - Chemistry
  - Geoscience
  - Mathematics
  - Physics
  - Computer Science
  - and others

Dictionary

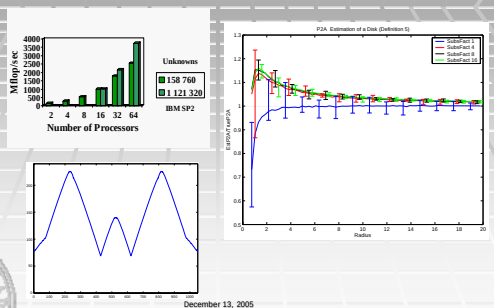
- **vi·su·al·ize**
  - To form a mental image of; envisage: *tried to visualize the scene as it was described*
  - To make visible

"Visualization offers a way to see the unseen"

Interpreting data in visual terms

- When data is complex: Collected/Computed
- When numerous data
- Visualization is not a substitute to, but *in addition to*, statistical analysis and other quantitative methods
- Visualization takes advantage of human sensory abilities
  - Pattern recognition, Trend discovery, etc.

Graphs are one type of visualization



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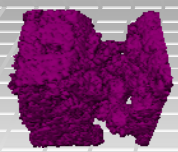
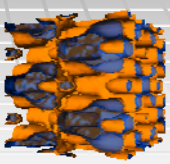
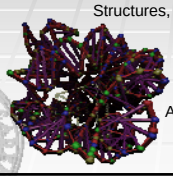
Some more sophisticated examples



Nuclear, Quantum, and Molecular Modeling



Structures, Fluids and Fields



Advanced Imaging and Data Management

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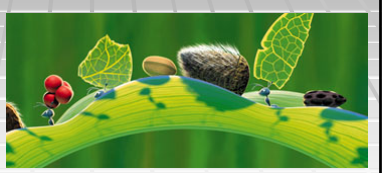
Computer Graphics

- Creating images with a computer – 3D



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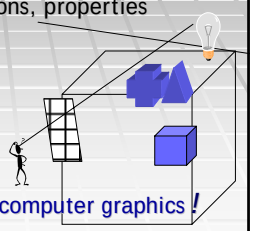
Computer Graphics

- Components
  - Model: geometry, surface properties, …
  - Lighting: number, positions, properties
  - Viewpoint
  - Projection



Visualization is more than computer graphics!

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Scientific Visualization

- Scientific visualization is the process of exploring, transforming, and viewing data as images
- The dimensionality of the data is generally larger than or equal to 3
- Visualization is often **interactive**
- We are not trying to create realistic images, but to visualize the data in an informative way
- Dependent on the task given

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Visualization serves many purposes

- ”Pretty pictures”
- For further analysis
- Debugging
- …

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Visualization can be used in every step of most processes

- Problem formulation
- Mathematical modelling
- Software/Hardware
- Simulation
- Result
- Interpretation

General development of visualization

- Rather new discipline that still is developing into sub-areas
- Tool users vs tool developers
- Collaboration among computer scientists and computational scientists
- Faster computers, high-speed networks, new user-interfaces

VTK – The Visualization ToolKit

- What is VTK?
- What can VTK be used for?
- How to actually use VTK?

VTK – The Visualization ToolKit

- Open source, freely available software for
  - 3D computer graphics
  - image processing
  - visualization
- Managed by Kitware, Inc.
- Object-oriented design (C++)
- High-level of abstraction
- Use C++, Tcl/Tk, Python, Java

True visualization system

- Visualization techniques for visualizing
  - scalar fields
  - vector fields
  - tensor fields
- Polygon reduction
- Mesh smoothing
- Image processing
- *Your own algorithms*

Additional features

- Parallel support
  - message passing
  - multi-threading
- Stereo support
- Integrates with Motif, Qt, Tcl/Tk, Python/Tk, X11, Windows, …
- Event handling
- 3D widgets

3D graphics

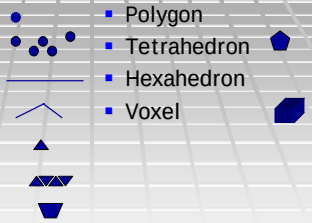
- Surface rendering
- Volume rendering
  - Ray casting
  - Texture mapping (2D)
  - Volume pro support
- Lights and cameras
- Textures
- Save render window to .png, .jpg, … (useful for movie creation)

Data Representation

- *Cells & Points*
- Topology
  - Shape such as triangle, tetrahedron
- Geometry
  - Point coordinates assigned to a topology
- Data attributes
  - Data associated with topology or geometry

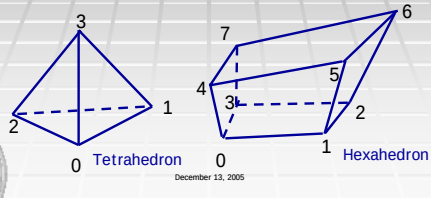
Cells specify Topology

- Vertex
- Poly-vertex
- Line
- Poly-line
- Triangle
- Triangle strip
- Quadrilateral
- Polygon
- Tetrahedron
- Hexahedron
- Voxel



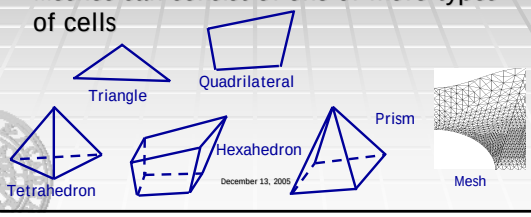
Cells

- A Cell is defined by an ordered list of points
  - Triangle and quadrilateral vertices specified counter clockwise



Meshes consist of Cells

- Cells can have different shapes and sizes
  - 2D: Triangles, Quadrilaterals, etc.
  - 3D: Tetrahedra, Hexahedra, Pyramids, etc.
- Meshes can consist of one or more types of cells

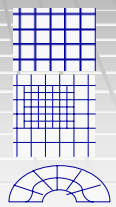


VTK Dataset Types

- vtkStructuredPoints, vtkImageData
- vtkRectilinearGrid
- vtkStructuredGrid
- vtkPolyData
- vtkUnstructuredGrid
- Methods for reading and writing

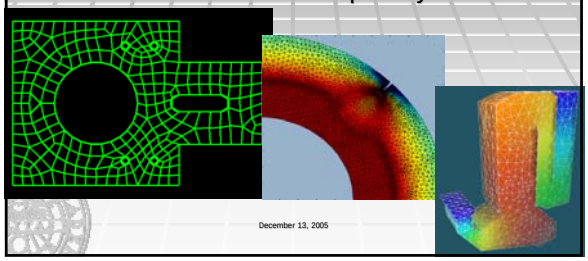
Datasets

- Organizing structure plus attributes
  - Structured Points
  - Rectilinear Grid
  - Structured Grid



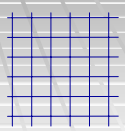
Unstructured Grid

A collection of vertices, edges, faces, and cells whose connectivity information must be explicitly stored



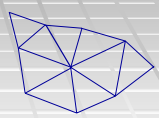
How are unstructured meshes different than regular grids?

- **Regular Grids**
  - mesh info accessed implicitly using grid point indices
  - efficient in both computation and storage
  - typically use finite difference (FD) discretization
  - Cartesian grids or logically rectangular grids



How are unstructured meshes different than regular grids?

- **Unstructured Meshes**
  - mesh connectivity information must be stored
  - handles complex geometries and grid adaptivity
  - typically use finite volume or finite element (FE) discretization
  - mesh quality becomes a concern

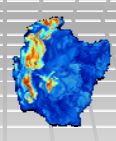


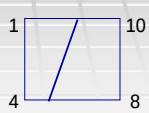
Data attributes assigned to points or cells

- Scalar
- Vector
  - magnitude and direction
- Normal
  - a vector of magnitude 1
  - used for lighting
- Texture coordinate
  - mapping data points into a texture space
- Tensor

Visualization of attributes

- Scalar
  - Color Mapping
  - Contouring
    - 3D isosurface

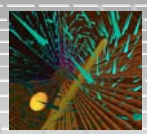


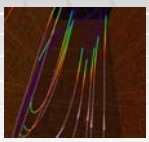


Contour value of 5

Visualization of attributes

- Vector
  - Oriented Line
  - Oriented Glyph
  - Streamline





Visualization continued

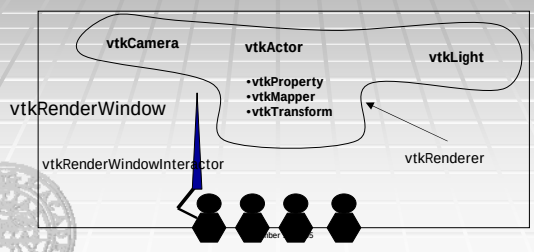
- Scalar algorithms
  - Iso-contouring
  - Colour mapping
- Vector algorithms
  - Hedgehogs
  - Streamlines / streamtubes
- Tensor algorithms
  - Tensor ellipsoids

Basic VTK objects to render a scene:

1. **vtkRenderWindow**
2. **vtkRenderer**
3. **vtkLight**
4. **vtkCamera**
5. **vtkActor**
6. **vtkProperty**
7. **vtkMapper**

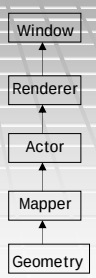
The Graphics Model

The purpose is to render the geometry (volume) on the screen



Example Program

```
main()
{
  create a window;
  create a renderer;     give the renderer
                         to the window;
  create procedural geometry;
  create a mapper;       give the geometry
                         to the mapper;
  create an actor;       give the mapper
                         to the actor;
  give the actor to the renderer;
  window->render();
}
```



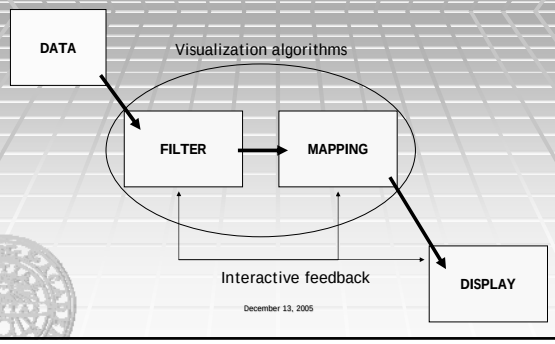
Summary +

- Free and open source
- Create graphics/visualization applications fairly fast
- Object oriented - easy to derive new classes
- Build applications using "interpretive" languages Tcl, Python, and Java
- Many (state-of-the-art) algorithms
- Heavily tested in real-world applications
- Large user base provides decent support
- Commercial support and consulting available

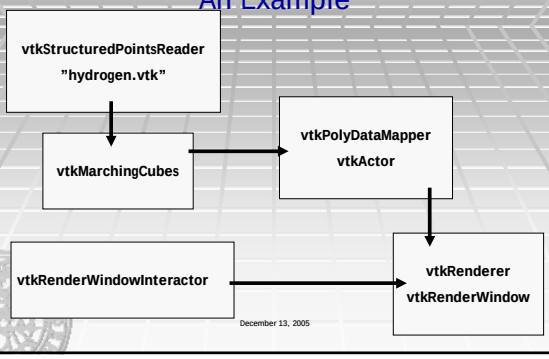
Summary -

- Not a super-fast graphics engine due to portability and C++ dynamic binding – you need a decent workstation
- Very large class hierarchy ➔ learning threshold might be steep

The Visualization Pipeline



The Visualization Pipeline – An Example



Objects

- Data objects
  - vtkPolyData
  - vtkImageData
- Process objects
  - Source objects (vtkReader, vtkSphereSource)
  - Filter objects (vtkContourFilter)
  - Mapper objects (vtkPolyDataMapper)

The Hydrogen example - Python

```
# File: isosurface.py
import vtk

# image reader
reader = vtk.vtkStructuredPointsReader()
reader.SetFileName("hydrogen.vtk")
reader.Update()

# bounding box
outline = vtk.vtkOutlineFilter()
outline.SetInput( reader.GetOutput() )
outlineMapper = vtk.vtkPolyDataMapper()
outlineMapper.SetInput( outline.GetOutput() )
outlineActor = vtk.vtkActor()
outlineActor.SetMapper( outlineMapper )
outlineActor.GetProperty().SetColor(0.0,0.0,1.0)
```

call update to read

pipeline connections

Example continued

vtkContourFilter chooses appropriate method for the dataset

```
# iso surface
isosurface = vtk.vtkContourFilter()
isosurface.SetInput( reader.GetOutput() )
isosurface.SetValue( 0, .2 )
isosurfaceMapper = vtk.vtkPolyDataMapper()
isosurfaceMapper.SetInput( isosurface.GetOutput() )
isosurfaceMapper.SetColorModeToMapScalars()
isosurfaceActor = vtk.vtkActor()
isosurfaceActor.SetMapper( isosurfaceMapper )

# slice plane
plane = vtk.vtkImageDataGeometryFilter()
plane.SetInput( reader.GetOutput() )
planeMapper = vtk.vtkPolyDataMapper()
planeMapper.SetInput( plane.GetOutput() )
planeActor = vtk.vtkActor()
planeActor.SetMapper( planeMapper )
```

Example continued

create a legend from the data and a lookup table

```
# a colorbar
scalarBar = vtk.vtkScalarBarActor()
scalarBar.SetTitle("Iso value")

# renderer and render window
ren = vtk.vtkRenderer()
ren.SetBackground(.8, .8, .8)
renWin = vtk.vtkRenderWindow()
renWin.SetSize( 400, 400 )
renWin.AddRenderer( ren )
```

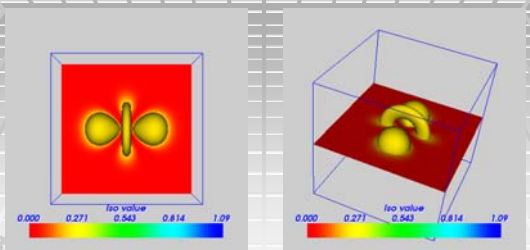

Example continued

vtkRenderWindowInteractor contains functions for mouse/keyboard interaction

renWin.Render() calls Update() on the renderer, which calls Update() for all its actors, which calls...

```
# render window interactor
iren = vtk.vtkRenderWindowInteractor()
iren.SetRenderWindow( renWin )

# add the actors
ren.AddActor( outlineActor )
ren.AddActor( isosurfaceActor )
ren.AddActor( planeActor )
ren.AddActor( scalarBar )

# this causes the pipeline to "execute"
renWin.Render()

# initialize and start the interactor
iren.Initialize()
iren.Start()
```


Renditions



Would you like an icecream?

User interaction

- vtkRenderWindowInteractor
  - allows the user to interact with the objects
- Try the following key presses

w wireframe mode	s surface mode
j joystick mode	t trackball mode
button1 rotate	button2 translate
button3 scale	r reset camera view
e, q exit	

The VTK file format

a converter from raw data to vtk file format is available on Erik's web-page

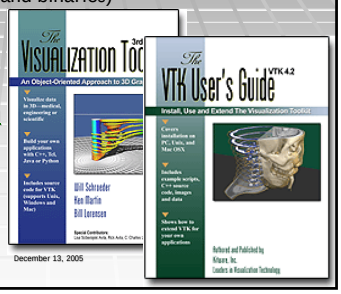
```
# vtk DataFile Version 2.0
Hydrogen orbital
ASCII
DATASET STRUCTURED_POINTS
DIMENSIONS 64 64 64
ORIGIN 32.5 32.5 32.5
SPACING 1.0 1.0 1.0
POINT_DATA 262144

SCALARS probability float
LOOKUP_TABLE default
0.0 0.0 0.01 0.01 .....
```

VTK and C++

- Build with CMake and your favorite compiler
- CMake generates makefiles or project files for your environment
- Use the resulting file(s) to build your executable
- With C++ you have full control and can derive own classes, but you need to write many lines of code…

VTK resources

- www.vtk.org
  - Download (source and binaries)
  - Documentation
  - Mailing lists
  - Links
  - FAQ, Search
- www.kitware.com
  - VTK Textbook
  - VTK User's guide
  - Mastering CMake



Questions?

Let's try VTK