Visualization on TeraGrid at TACC

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TeraGrid-Scale Visualization at Texas Advanced Computing Center

- Ranger: Sun cluster, 3936 nodes, 62976 cores
- Spur: Sun vis. Cluster, 128 cores, 1TB MEM, 32 GPU

- TeraGrid scale
- Run remotely
- Modern tools
Ranger Job Batch System

- You give the scheduler a script. It goes, runs it when it has time.
- You don't get to login to the compute nodes where the work is done.
#!/bin/bash

#$ -V # Inherit the submission environment
#$ -cwd # Start job in submission dir
#$ -N visit.job # Job name
#$ -j y # stderr and stdout into stdo
#$ -o $HOME/$JOB_NAME.o$JOB_ID # Name of the output file
#$ -pe 16way 16 # Request 1 Ranger node
#$ -q normal # Queue name
#$ -A TG-MyTGAcct # Account
#$ -l h_rt=01:00:00 # runtime (hh:mm:ss) - 1 hour

# configure environment for visit
module purge
module load TACC
module delete pgi mvapich CTSSV4
module load intel mvapich
module load vis mesa visit/1.10.0

# run visit
visit -cli -nowin -s myVisItScript.py
• ssh to spur.tacc.utexas.edu
• Submit a job to get access to vis[1-7,big] node.
• Run many ways
  – Ssh to spur, then ssh to the node from spur.
  – Run VNC to the node, through spur.
  – Do something in the job script.
  – Let the application connect to the node, through spur.
Spur Nodes

- Each node has multiple GPUs.
- The batch job can assign a GPU to your processes.
- 4 quad-core AMD Opteron processors
- 4 GPUs, NVIDIA FX 5600
- 128 GB RAM (visbig has 256 GB)

No GPU on Ranger nodes.
32 GB memory on Ranger node.
What Software is on Spur?

- Paraview
- VisIt
- Ensight
- Amira (on vis6)
- IDL

General purpose
Capable of complicated 3D
Parallel processing capable
VisIt Example
Paraview Example

Orange: Isosurface at $T = 1000$ K  
Blue: Isosurface at $n_e = 5 \times 10^{-3}$ cm$^{-3}$
VTK

```python
# create sphere geometry
vtkSphereSource sphere
sphere SetRadius 1.0
sphere SetThetaResolution 18
sphere SetPhiResolution 18
# map to graphics library
vtkPolyDataMapper map;
map SetInput [sphere GetOutput]
# actor coordinates geometry, properties, transformation
vtkActor aSphere
aSphere SetMapper
map[aSphere GetProperty] SetColor 0 0 1; # blue
# create a window to render into
vtkRenderWindow renWin
vtkRenderer ren1
renWin AddRenderer ren1
# create an interactor
vtkRenderWindowInteractor iren
iren SetRenderWindow renWin
# add the sphere
ren1 AddActor aSphere ren1 SetBackground 1 1 1;
renWin Render
```

Scripting (Python, Java) + C++
LOTS of algorithms
Free, basis for Paraview
Buy a book to learn it.
Spur Software Supporting Players

- Mesa – Software OpenGL alternative.
- Imagemagick – 2D image manipulation.
- Netpbm – Converts all sorts of images.
- Qt – Windowing toolkit
- CUDA SDK – To program GPUs.
- **Regular cluster stuff** (anything you can do I can do better)
  - MPI, OpenMP in many versions.
  - Hmmer, Amber, Charm
  - Petsc, fftw3,metis, scalapack, gotoblas
- Whatever you install in your home directory.
Large Data, Remote Systems

Problems with speed, responsiveness, available memory, access to GPUs, security, data formats...

The Pipeline is the Key.
Visualization Pipeline Starts with a Conversion

- Dim: 0D, 1D, 2D, 3D
- Support

From *The Visualization Toolkit* by Schroeder et al.

03/11/09

www.cac.cornell.edu
Then Put Data on that Support

- Scalar / Vector / Tensor
- Point pairs, materials
- Discrete, pseudo-cont.
- Nominal, ordinal, interval, ratio.
- Node-centered or links.

Input datasets will have lists of scalar, vector, and tensor data associated with given supports.
Graph Layout: Visualization of the hierarchical topology of the international web cache. Developed by B. Huffaker at the Cooperative Association for Internet Data Analysis

Different data formats
Information Visualization.

Parallel Coordinates
http://www.comp.leeds.ac.uk/richardh/astro/index.html
The Pipeline Begins

- Read Data
- Translate it to application format
- Execute Module A
- Execute Module B
- Write result to file or screen

How large is the data after each step?
What are your goals for doing it better?
What can be done in parallel?
Example: Molecular Dynamics

• Start with x,y,z, atom type at each timestep.
• One pipeline associates a colored sphere with each atom. Displays it to a 1024x768 image.
  – atoms -> scalar (atom type) in space -> polygons w/scalar -> polygons w/color -> rendered pixels
  – Polygons larger than atom file. Rendered smaller than either.
• Another pipeline computes electronic energy, finds isovalues in it, and shows semi-transparent surfaces around the atoms.
  – Atoms -> scalar on a regular 3D grid -> polygons w/scalar
  – Some of calculation is scientific, some visualization.
Parallel Visualization Pipeline

• With many processors, split up the data when you read.
• Each process works on its part of the dataset.
• Aggregate for display.
Running an MPI-parallel isosurface algorithm on several nodes is less efficient than running it on a single node, although it takes longer. Task parallelism can offer more speed if it is balanced.
Pipeline Parallelism

- If process 1 can read faster, process 3 better at rendering.
- Increases render rate without decreasing efficiency

<table>
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<th>Processes</th>
<th>Timesteps</th>
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<tr>
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<td>1</td>
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<tr>
<td>1</td>
<td>Read file 1</td>
</tr>
<tr>
<td>2</td>
<td>Isosurface 1</td>
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<tr>
<td>3</td>
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Data Parallel

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- When one computer can't handle a filter's memory requirements.
- Some algorithms handle whole dataset with many CPUs.
- Others can be run completely independently on each CPU.
Domain Decomposition for Data Parallel

- Some algorithms need neighbors, called *ghosting*.
Decomposition Imbalance

- Irregular grids don't decompose nicely.
- Subsequent modules may worsen imbalance.
- Paraview uses D3: Distributed Data Decomposition to rebalance.
- Can be done anywhere in the pipeline.
Architecture for Parallel Visualization

- Data servers for numerics, render for graphics
- TCP to coordinate MPI
- "server" = data + render
- Start client then Start servers with MPI.
- Renderers like GPUs.

![Diagram showing client and servers connected via TCP and MPI]
Graphics Pipeline

- Given polygons, show them on the screen.
  - Point 0: x, y, z
  - Point 1: x, y, z
  - Point 2: x, y, z
  - Color

- OpenGL does this for you

```c
glColor3f(0.0, 1.0, 0.0); // blue
glBegin(GL_QUAD);
  glVertex2f(0.0, 0.0);
  glVertex2f(1.0, 0.0);
  glVertex2f(1.0, 1.0);
  glVertex2f(0.0, 1.0);
glEnd();
glTranslate(-1.5, 0.0, 0.0); // move object
```
Camera – Lighting – Object

Camera

Near and far clipping planes

Light

Object
What's Wrong?
Answers

- The camera can point the wrong way.
- Lights are off.
- Object beyond near and far clipping planes.
- OpenGL polygons can be one-sided, transparent from behind.
- Flickering polygons can happen when two polygons nearly overlap. May need to offset them artificially.
Who's In Front Is A Problem

- Z-buffer
- Sorting

Near and far clipping planes

Especially for transparency.
Sorting Among Servers

- Uses tree, binary methods for opaque polygons.
- Important for speed.
- Transparency can have artifacts.
- “Disable Ordered Compositing”
Graphics Pipeline

- Modeling Transformation
- Trivial Rejection
- Illumination
- Viewing Transformation
- Clipping
- Projection
- Rasterization
- Display
Graphics Pipeline In English

- Squeeze the world of your polygons into a normalized box.
- Rotate, translate, and scale them according to camera and model positions.
- Figure out what color they should be from lighting.
- Flatten them to a 2D world.
- Scan through the lines, turning them into pixels.
- (Along the way, cut out anything that won't be visible.)

Geometry, then Rasterization.
Big Data and Graphics

- Big data usually means lots of geometry.
- Rasterization is a function of the size of the display screen.

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Show this scientific data

Copy data from Ranger to your desktop.

Draw these polygons

Chromium
X Windows with GLX

Draw these pixels

VNC
X Windows and X Display Protocol

• Messages like:
  – Use Courier-New.
  – Make a Window.
  – Draw a Menu.
  – Show bitmap.

• GLX, OpenGL for X Windows
  – Gives a context to OpenGL programs.
  – Sends polygons over the wire.
  – Your workstation's card does drawing.
  – Xming, Exceed don't do it. Exceed3D does.

From wikipedia
Tunnel an X-Windows Session

- Enable X11 forwarding.
- Open a terminal (ssh) and run interactive programs.
- DISPLAY=localhost:10.0
VNC Virtual Network Computing

- Sends remote framebuffers = rectangle of pixels
- OpenGL done on remote machine.
- Starts a desktop on the remote machine (:1, :2).
- Listens on port 5901, 5902...
- Has its own vncpassword.
- Must use ssh tunnel for security.
Secure Shell Tunneling

YourMachine

SSH listens on port 5901

Your application connects to localhost:5901

Ssh connection

Spur

Server listens on port 5901.

Your application is actually talking to spur:5901.
Weigh Alternatives for the Last Mile

• Single screen, lots of triangles -> VNC
• Many screens -> Maybe Sage or Chromium
• Lots of processing, little output -> Paraview client locally, gets data from cluster.
• VNC is a generally good bet.
Parallelism in All Parts

- Memory limitations, transparency, network latency, GPUs, decomposition algorithms
What's Slow?

• Each click or spin of the model.
  – Under VNC, message to TACC and back has *latency*.
  – With X-Windows, rotation could be done locally.

• Watching a movie of data.
  – Depends more on bandwidth.
  – 1280×1024 pixels of 24 bits at 12 times a second = 360 MBps

• Lots of data.
  – Reading from disk.
  – Doing the actual calculation.
  – GPU always helpful rendering, sometimes helpful earlier.
Complications

• 62976 cores wrote your atom data.
  – Save to /scratch/tgusername to read from spur.
  – Do some processing by each core before writing that data.
  – Visualize it while it runs.

• Your data lives far from spur.
  – TeraGrid connections are much faster and cheaper.
  – What can you preprocess to make transfer smaller?

The line between analysis and visualization is blurry. Save / transfer what you need.
Human Pipeline

• Can you really see all those little triangles?
• 1x1 pixel has no color
• 3D + colors + movement? Funny glasses?
• Depth of understanding of complex data comes more from speed of interaction, ability to shift focus, than from increasing complexity of what we see.