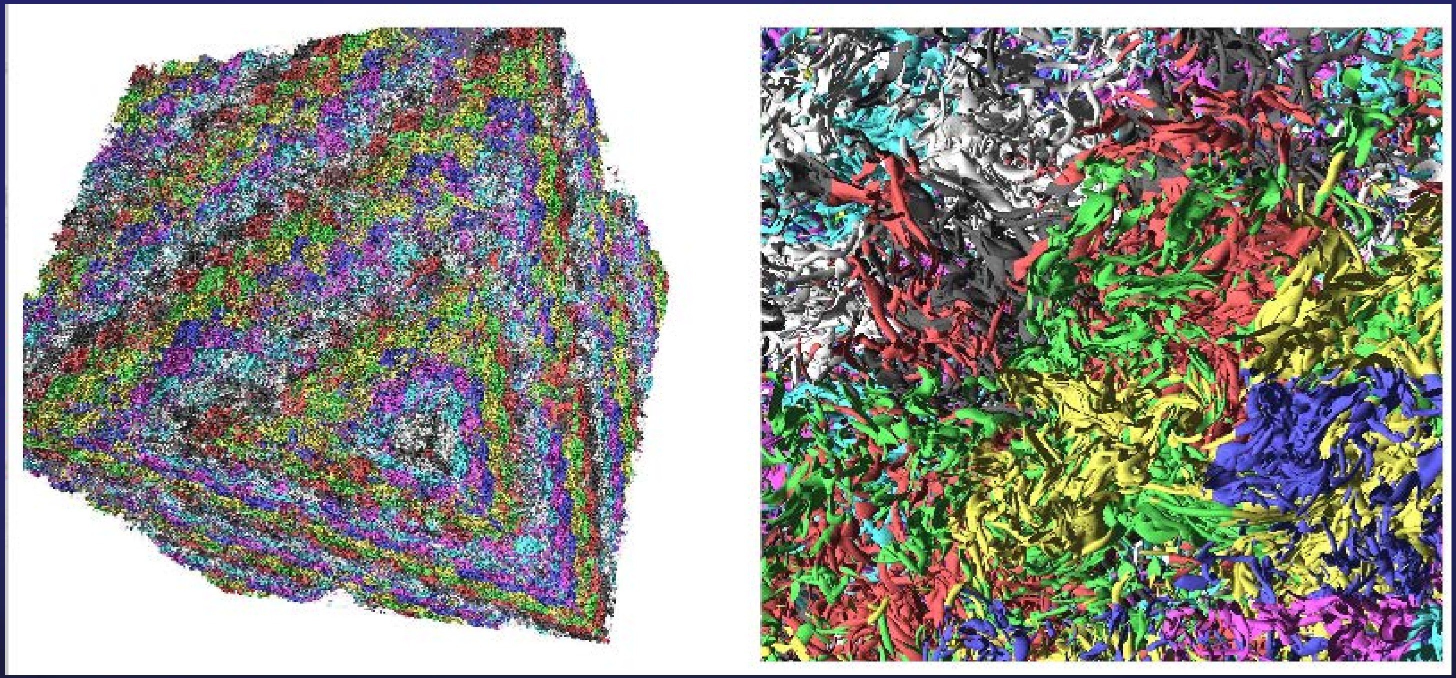
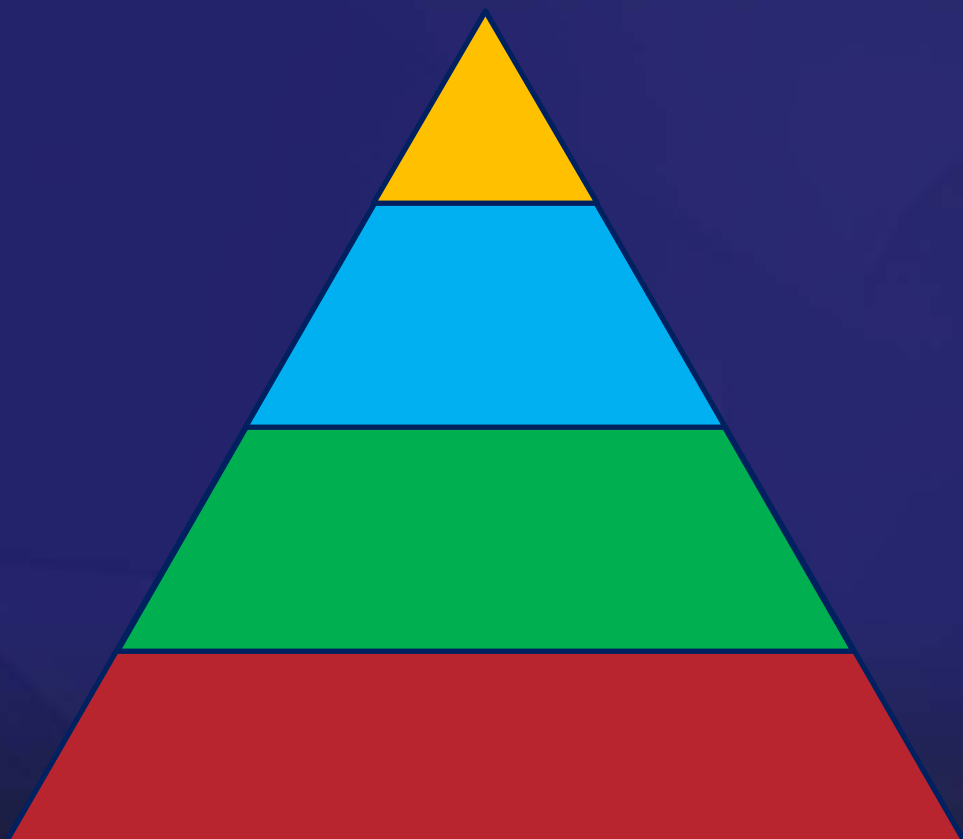
Parallel Visualization At TACC

Greg Abram



Visualization Problems



Huge problems:

- Data cannot be moved off system where it is computed
- Visualization requires equivalent resources as source HPC system

Large problems:

- Data are impractical to move over WAN, costly to move over LAN
- Visualization requires parallel systems for enough memory, CPU and GPU

Medium problems:

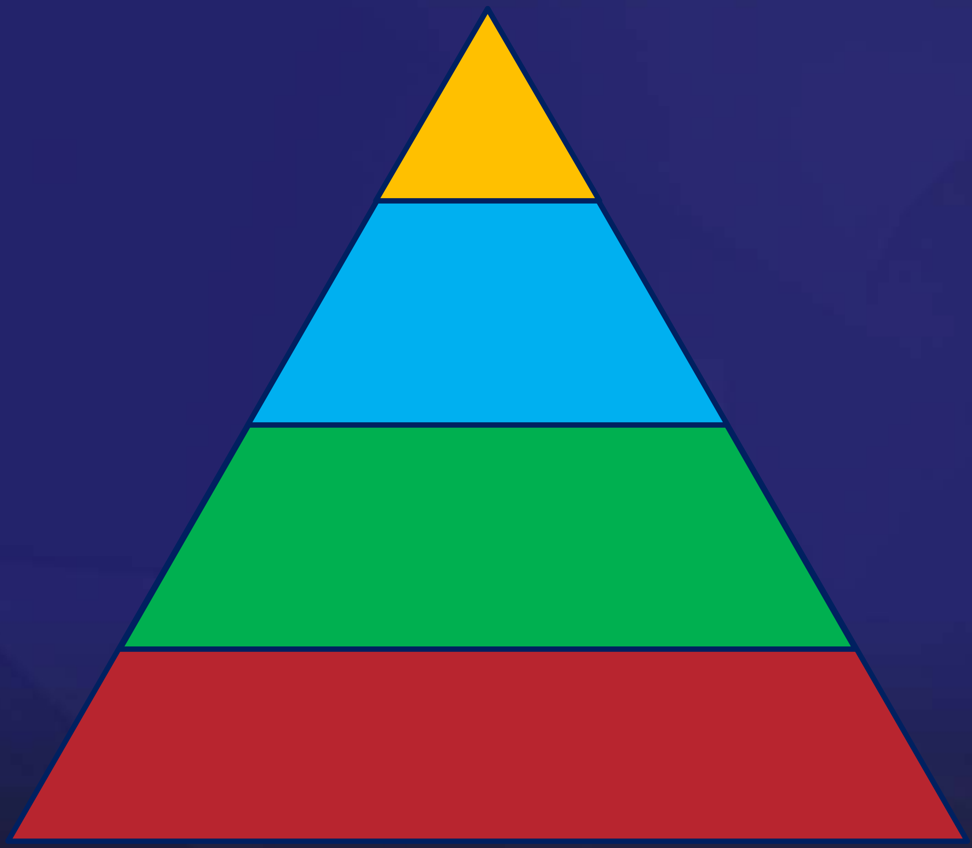
- Data are costly to move over WAN
- Visualization requires lots of memory, fast CPU and GPU

Small problems:

- Data are small and easily moved
- Office machines and laptops are adequate for visualization

* **With thanks to Sean Ahern for the metaphor**

Visualization Problems



Huge problems

Don’t move the data; in-situ and co-processing visualization minimizes or eliminates data I/O

Large problems

Move your data to visualization server and visualize using *parallel* high-performance systems and software at TACC

Medium and small problems

Move your data to visualization server and visualize using high-performance systems at TACC

* **With thanks to Sean Ahern for the metaphor**

Visualization Servers: Maverick

- Maverick (TACC) - HP
  - 132 20-core Ivy Bridge nodes
  - 256GB system memory per node
  - Nvidia Tesla K40 GPU
  - FDR InfiniBand interconnect
  - Designed for interactive visualization

Visualization Servers: Stampede

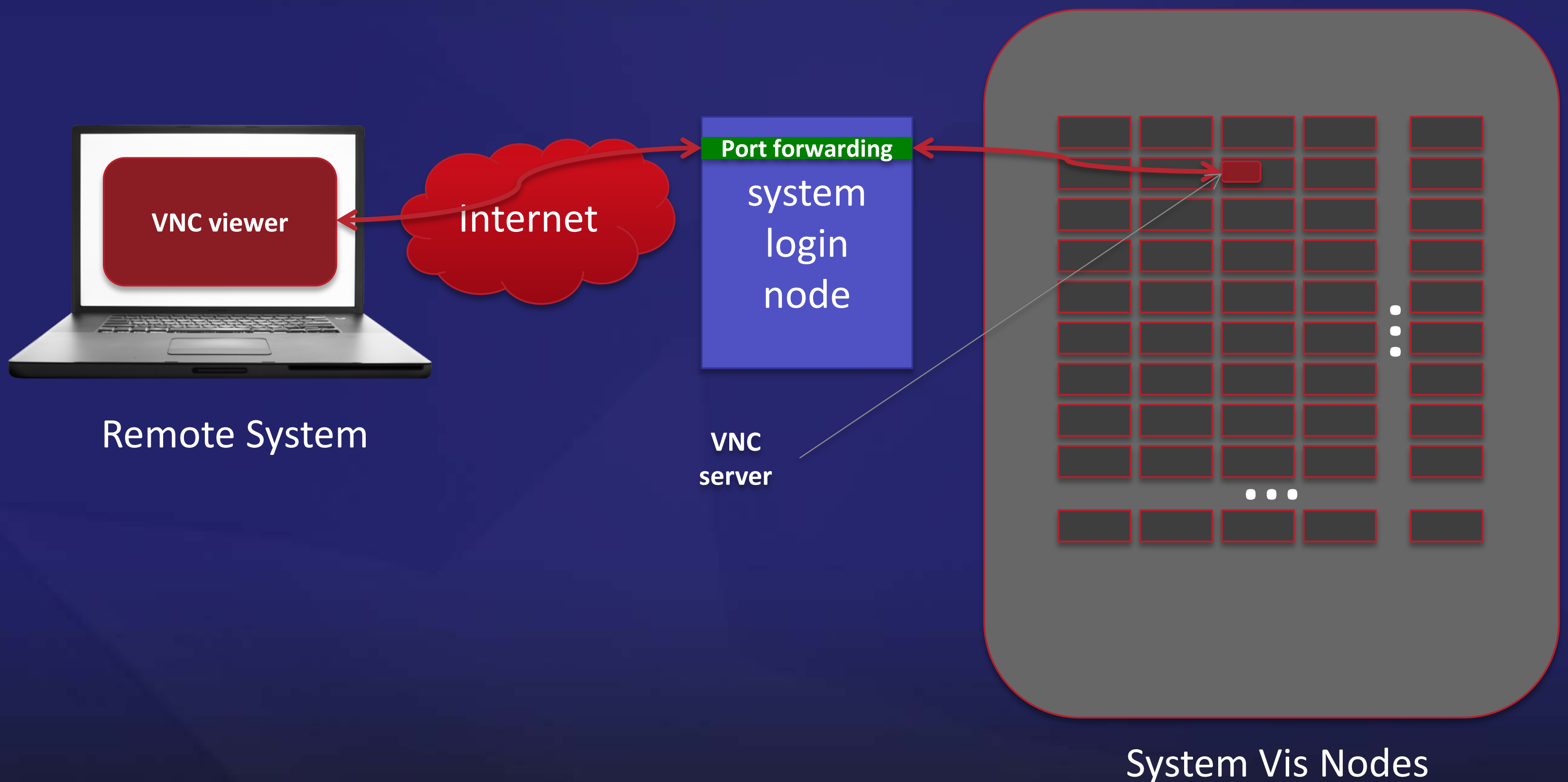
- Access to Stampede file systems
- 128 Vis nodes:
  - 16 Intel Sandy Bridge cores
  - 32 GB RAM
  - 1 Nvidia K20 GPU
- 16 Large Memory Nodes
  - 32 Intel Sandy Bridge cores
  - 1 TB RAM
  - 2 Nvidia K20 GPU
- Access (see Stampede User Guide):

  Run sbatch job.vnc on Longhorn using vis, largemem queues

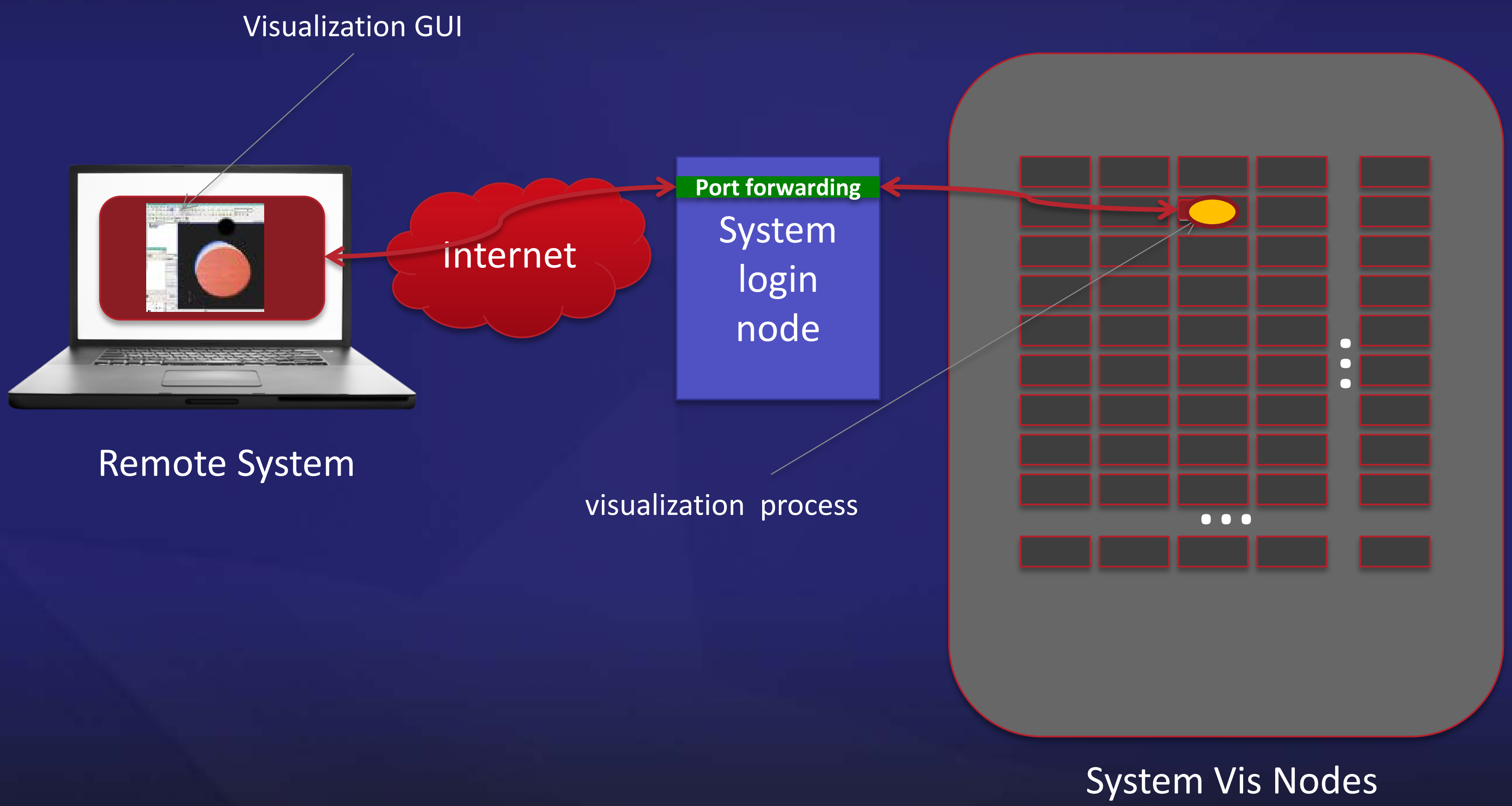
Parallel Visualization Software

- Good news! Paraview and Visit both run in parallel on and look *just the same!*
- Client/Server Architecture
  - Allocate multiple nodes for vncserver job
  - Run *client* process serially on root node
  - Run *server* processes on all nodes under MPI

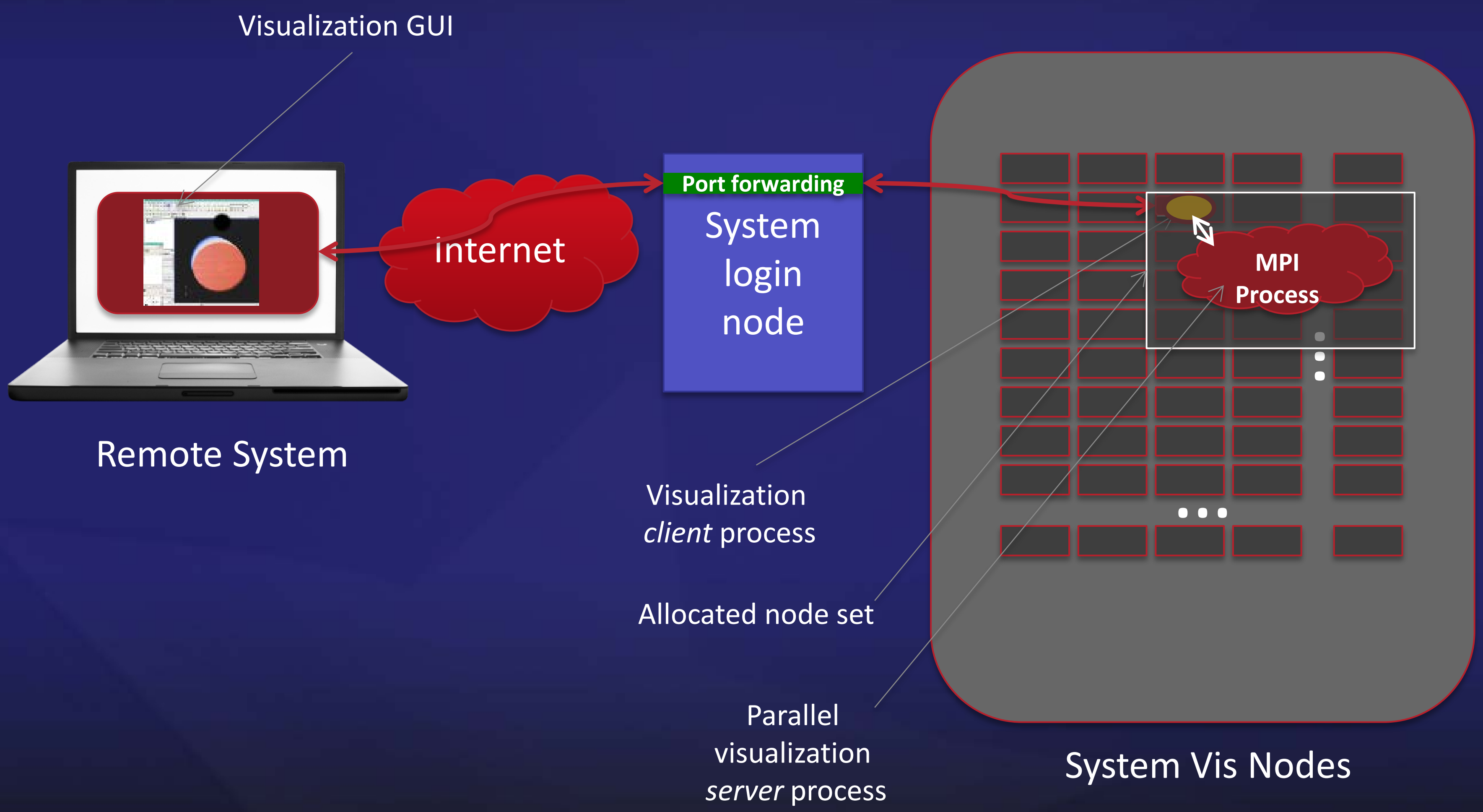
Interactive Remote Desktop



Remote *Serial* Visualization



Remote *Parallel* Visualization



Parallel Session Settings

- Number of nodes *N*
  - more nodes gives you:
    - More total memory
    - More I/O bandwidth (up to a limit determined by file system and other system load)
    - More CPU cores, GPUs (though also affected by wayness)
- Number of *processes* *n*
  - Total processes to run on each node
  - Paraview and Visit are not multi-threaded
  - *N* < *k* gives each process more memory, uses fewer CPU cores for k = number of cores per node
- Longhorn portal:
  - Number of Nodes and processes are pulldowns
- sbatch –N [#nodes] –n [#processes]   *job*

Running Paraview In Parallel

- Run Paraview as before
- In a separate text window:

  module load python paraview

  ibrun tacc_xrun pvserver
- In Paraview GUI:
  - File->Connect to bring up the Choose Server dialog
  - Set the server configuration name to *manual*
  - Click Configure and, from Startup Type, select Manual and Save
  - In Choose Server dialog, select *manual* and click Connect

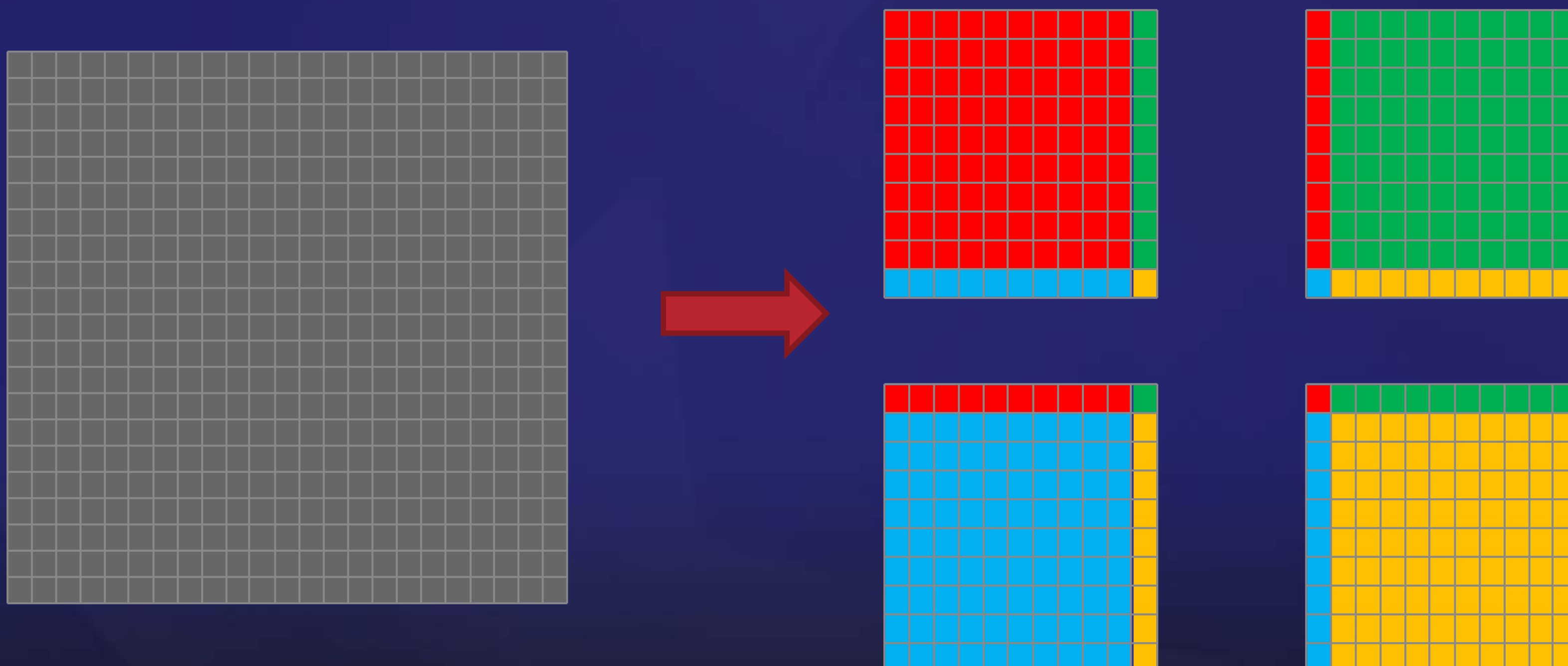
In client xterm, you should see Waiting for server… and in the server xterm, you should see Client connected.

Running Visit In Parallel

- Run Visit as before; it'll do the right thing

Data-Parallel Visualization Algorithms

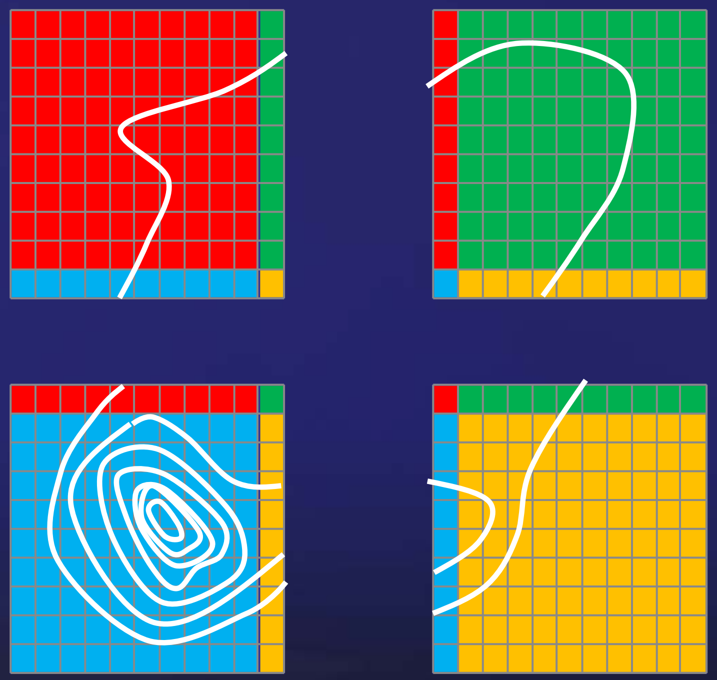
- Spatially partitioned data are distributed to participating processes…



Data-Parallel Algorithms

- Sometimes work well…

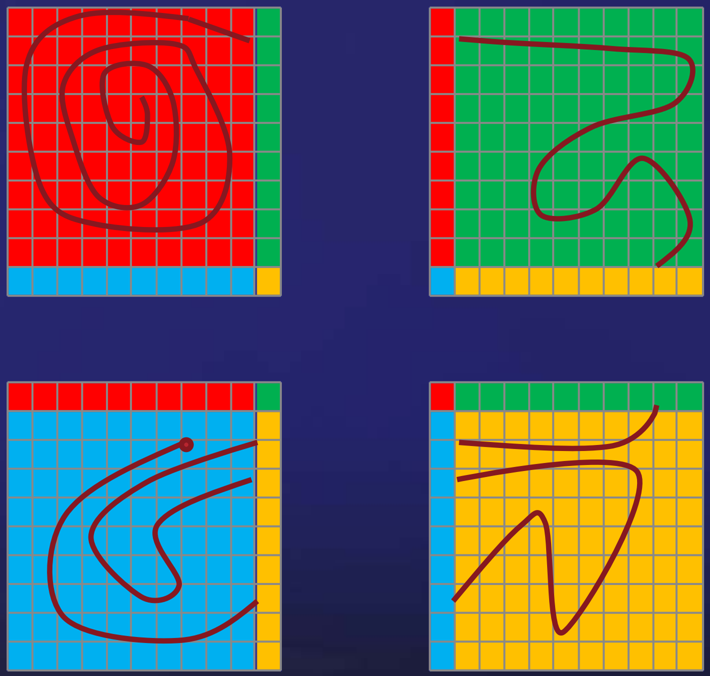
- Iso-contours
  - Surfaces can be computed in each partition concurrently and (with ghost zones) independently
  - However, since surfaces may not be evenly distributed across partitions, may lead to poor load balancing



Data-Parallel Algorithms

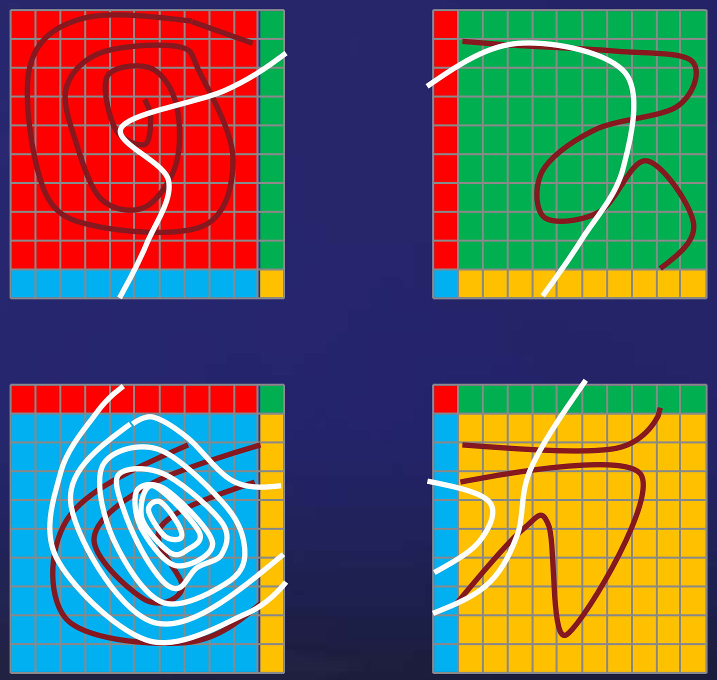
- Sometimes not so much…

- Streamlines are computed incrementally



Parallel Rendering

- Collect-and-render
  - Gather all geometry on 1 node and render
- Render-and-composite
  - Render locally, do depth-aware composite
- Both PV and Visit have both, offer user control of which to use



Parallel Data Formats

- To run in parallel, data must be distributed among parallel subprocess' memory space
- *Serial* formats are "data-soup"
  - *Data must be read, partitioned and distributed*
- *Parallel* formats contain information enabling each subprocess to import its own subset of data simultanously
  - *Maximize bandwith into parallel visualization process*
  - *Minimize reshuffling for ghost-zones*
- Network file system enables any node to access any file

Paraview XML Parallel Formats

- Partition data reside in separate files:
  - .vti regular grids, .vts for structured grids …
  - Example: One of 256 partitions of a 2040^3 volume: c-2_5_5.vti

```
<?xml version="1.0"?>
<VTKFile type="ImageData" version="0.1" byte_order="LittleEndian">
 <ImageData WholeExtent="510 765 1275 1530 1275 1530" Origin="0 0 0" Spacing="1 1 1">
 <Piece Extent="510 765 1275 1530 1275 1530">
  <PointData Scalars="Scalars_">
   <DataArray type="Float32" Name="Scalars_" format="binary" RangeMin="0.0067922524177" RangeMax="1.7320507765">
   ….. Encoded data looking lijke ascii gibberish
   </DataArray>
…
```

- *Global* file associates partitions into overall grid
  - .pvti regular grids, .pvts for structured grids …
  - Example: global file for 2040^3 volume: c.pvti

```
<?xml version="1.0"?>
<VTKFile type="PImageData" version="0.1" byte_order="LittleEndian" compressor="vtkZLibDataCompressor">
  <PImageData WholeExtent="0 2040 0 2040 0 2040" GhostLevel="0" Origin="0 0 0" Spacing="1.0 1.0 1.0">
    <PPointData Scalars="Scalars_">
      <PDataArray type="Float32" Name="Scalars_"/>
    </PPointData>
<Piece Extent="0 255 0 255 0 255" Source="c-0_0_0.vti"/>
<Piece Extent="0 255 0 255 255 510" Source="c-0_0_1.vti"/>
…
<Piece Extent="510 765 1275 1530 1275 1530" Source="c-2_5_5.vti"/>
…
```

SILO Parallel Format

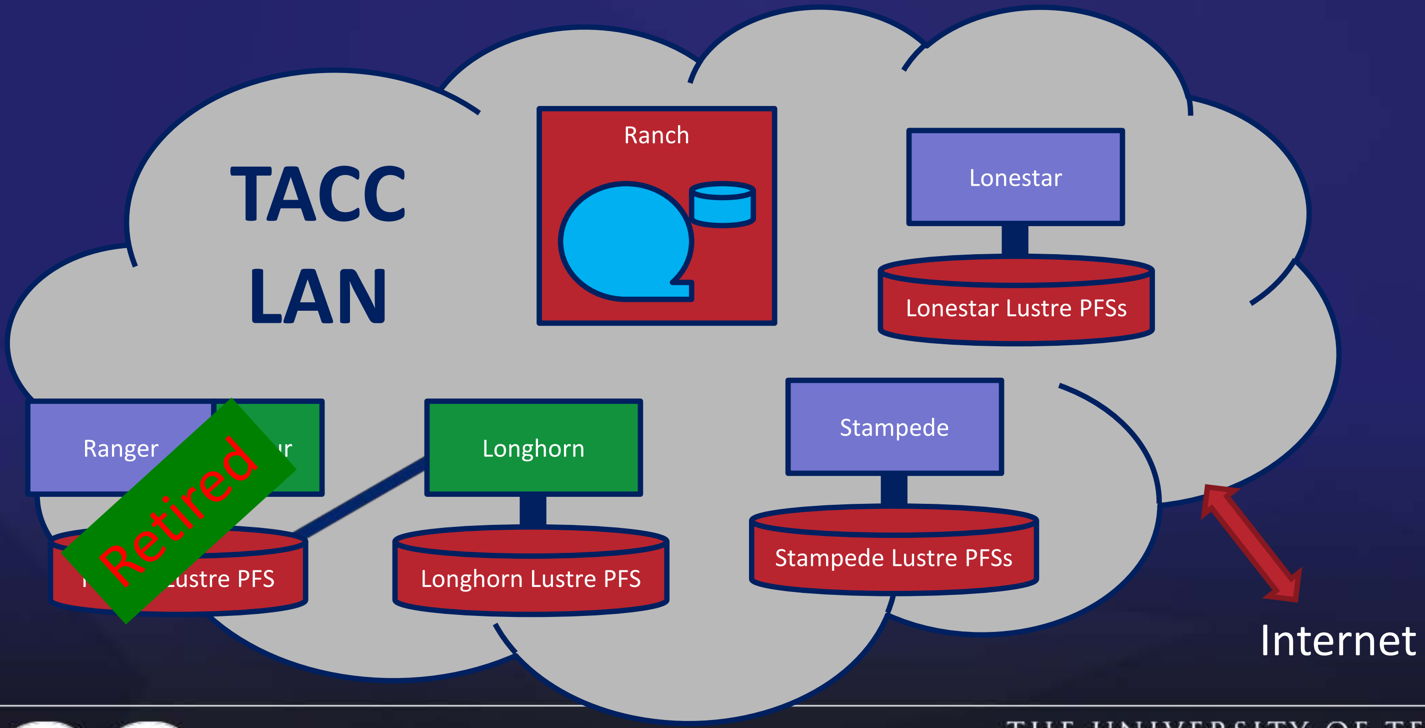
- "Native" VisIt format
  - Not currently supported by Paraview
- Built on top of lower-level storage libraries
  - NetCDF, HDF5, PDB
- Multiple partitions in single file simplifies data management
  - Directory-like structure
  - *Parallel* file system enables simultaneous read access to file by multiple nodes
  - *Optimal* performance may be a mix
    - note that *write* access to silo files is serial

Xdmf Parallel Format

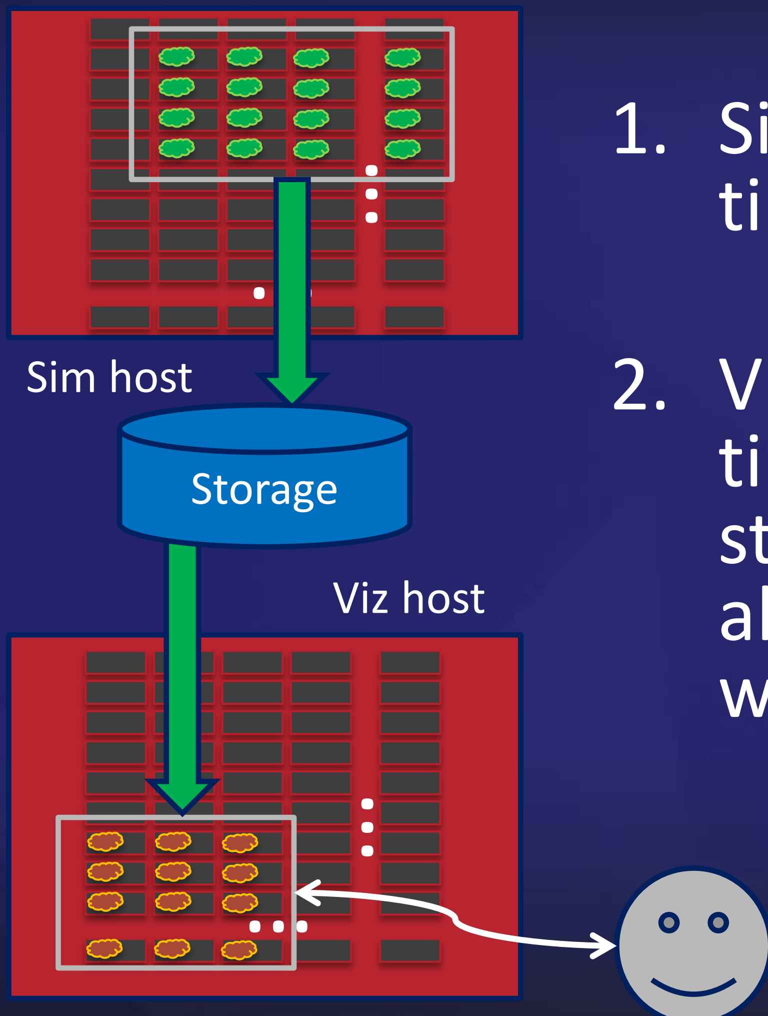
- Common parallel format
  - Seen problems in VisIt
- Also built on top of lower-level storage libraries
  - NetCDF, HDF5
- Multiple partitions in single file simplifies data management
  - Also directory-like structure
  - Also leverages Parallel File System
  - Also optimal performance may be a mix

Data Location

- Data must reside on accessible file system
- Movement *within* TACC faster than across Internet, but can still take a long time to transfer between systems



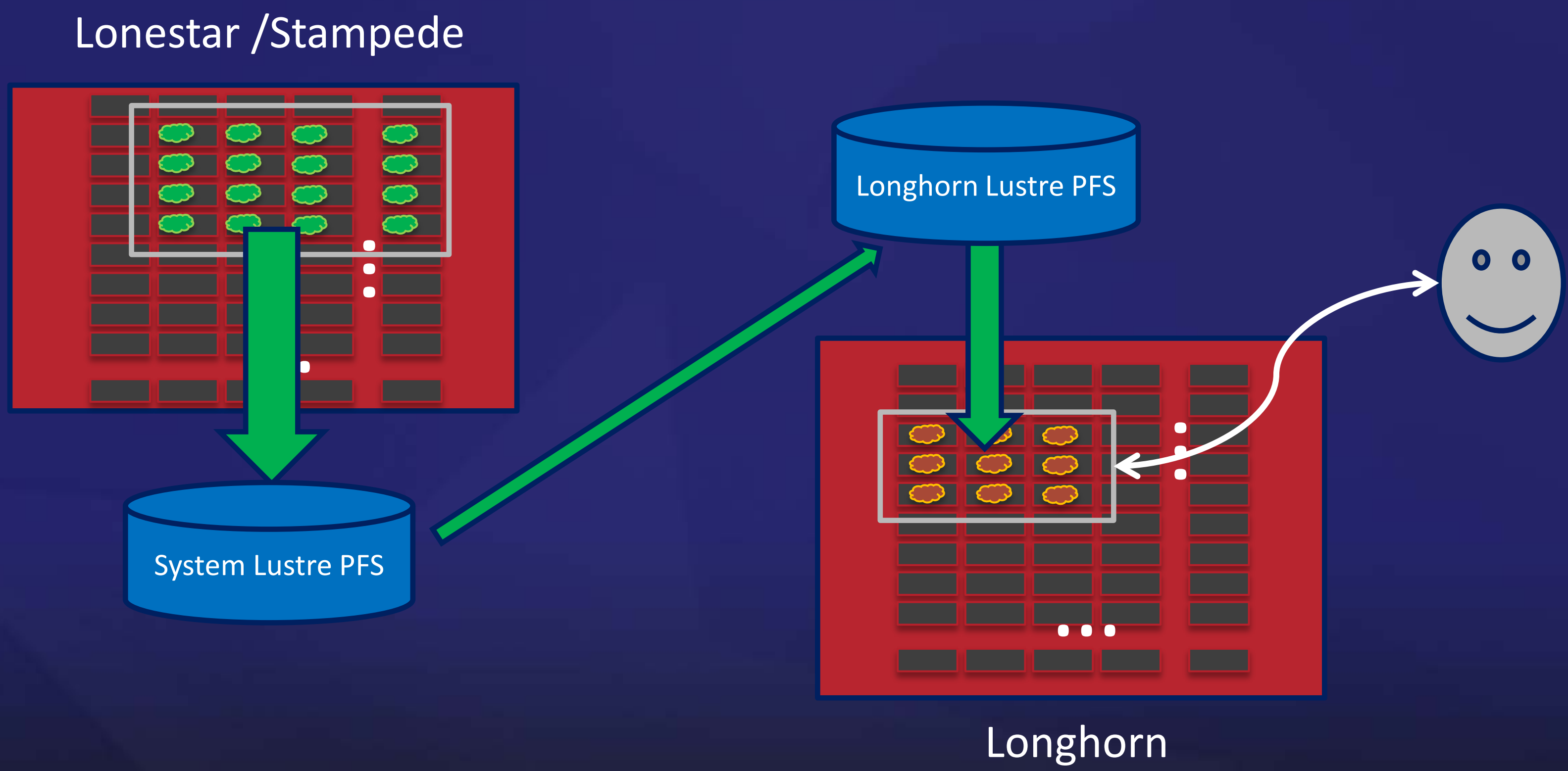
Post-Processing



1. Simulation writes periodic timesteps to storage

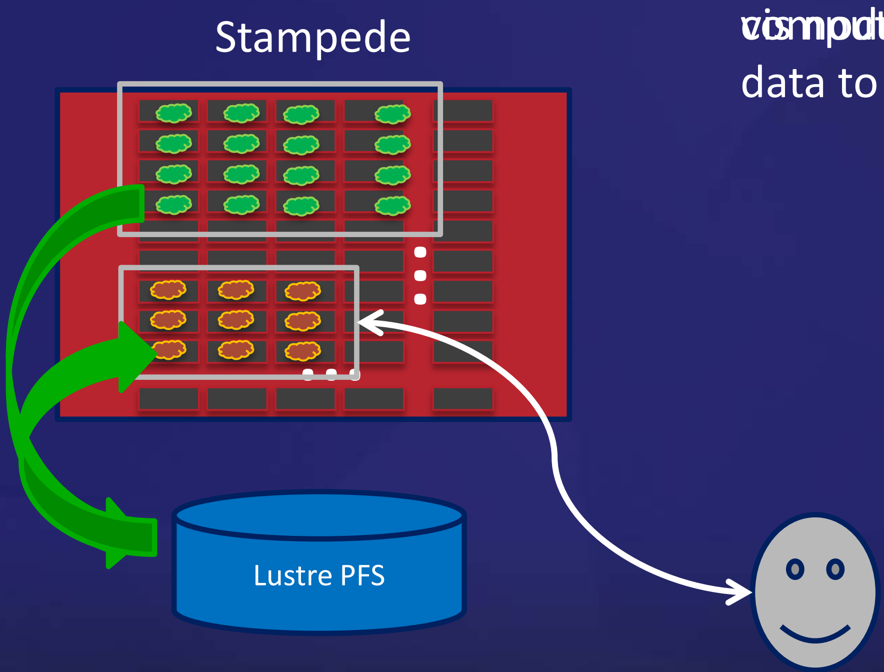
2. Visualization loads timestep data from storage, runs visualization algorithms and interacts with user

Postprocessing On HPC Systems and Longhorn



Postprocessing On Stampede

1. Simulation runs on compute nodes, writes data to Lustre file system
2. Data is read back into vis nodes for visualization



Huge Data: *Co- and In-Situ* Processing

- Visualization requires equivalent horsepower
  - Not ***all*** visualization computation is accelerated
  - Increasingly, HPC platforms include acceleration
- I/O is *expensive:* simulation to disk, disk to disk, disk to visualization
  - I/O is not scaling with compute
  - Data is not always written at full spatial, temporal resolution

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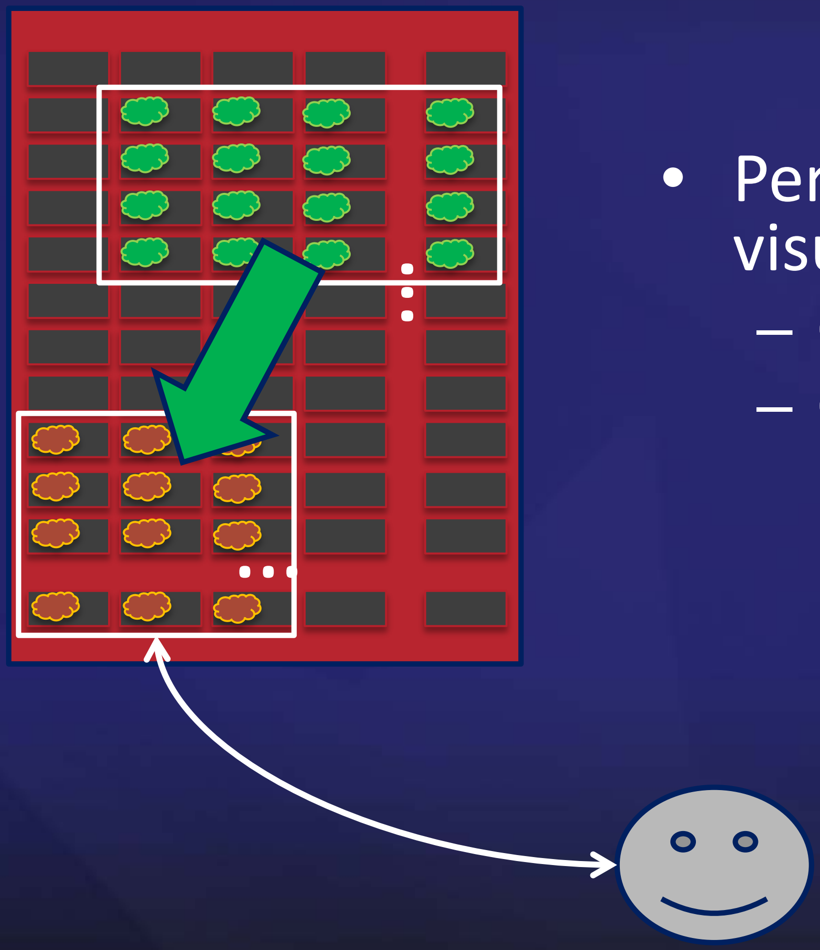
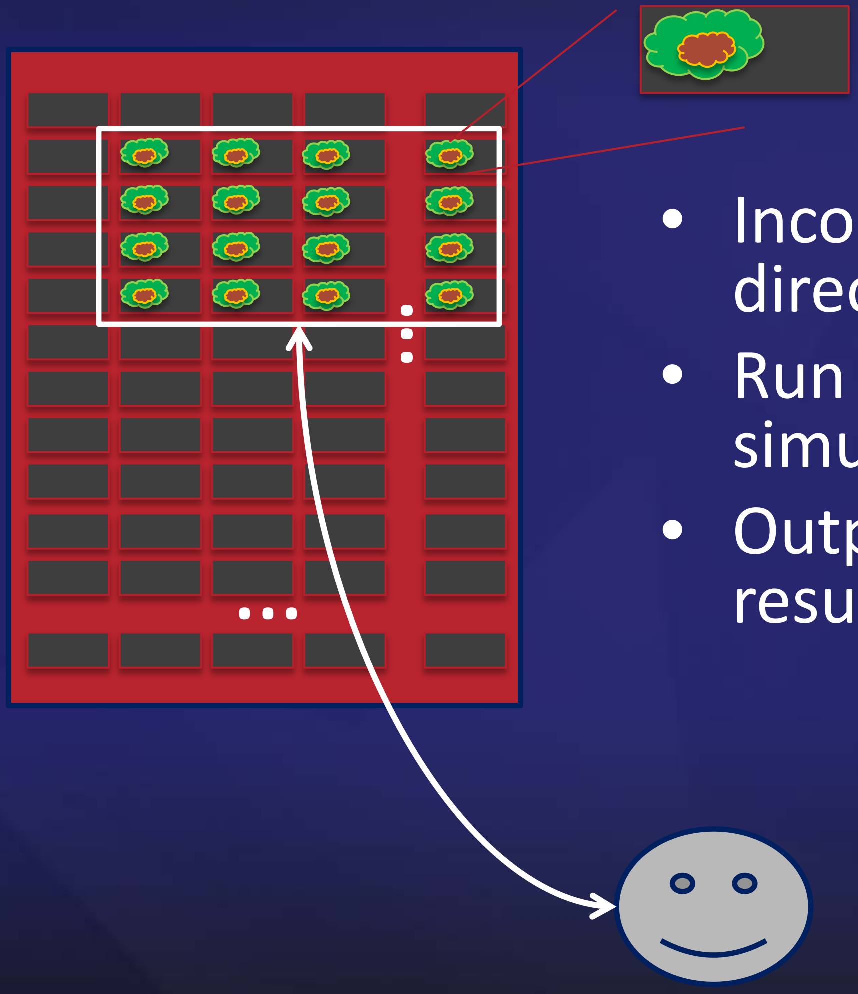
Co-Processing



- Perform simulation and visualization on same host
  - Concurrently
  - Communication:
    - Many-to-many
    - Using high-performance interconnect to communicate

In-Situ Processing



- Incorporate visualization directly *into* simulation
- Run visualization algorithms on simulation's data
- Output only visualization results

Co- and In-Situ Processing

- *Not* a panacea
  - Limits scientist's exploration of the data
    - Can't go back in time
    - May pay off to *re-run* the simulation
  - Impacts simulation
    - May require source-code modification of simulation
    - May increase simulation node's footprint
    - May affect simulation's stability
  - Simulation host may not have graphics accelerators
    - … but visualizations are often not rendering-limited
    - … and more and more HPC hosts are *including* accelerators

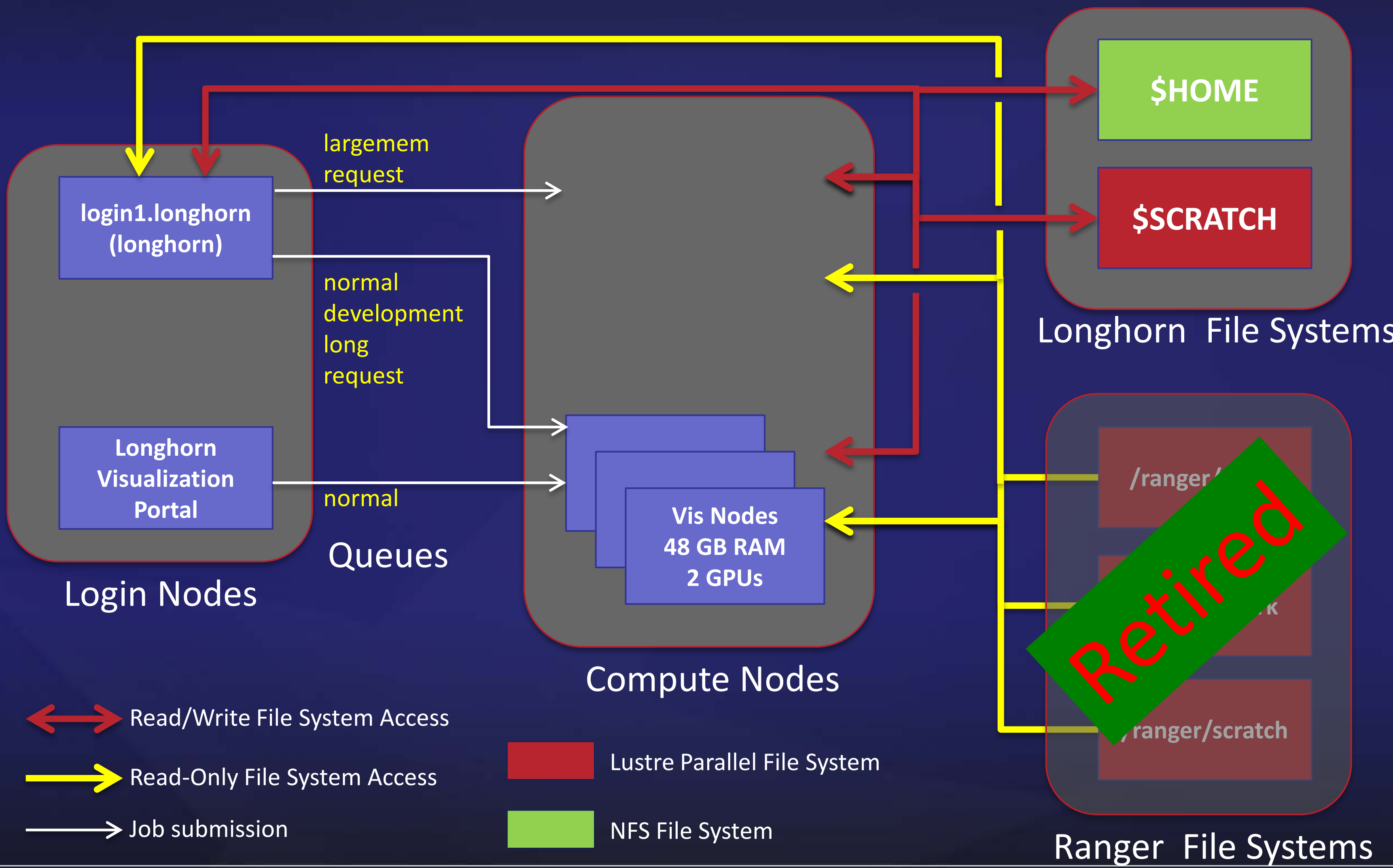
Co- and In-Situ Status

- *Bleeding* edge
- Coprocessing capabilities in Paraview, VisIt
  - Did I say bleeding edge?
- In-Situ visualization is not simple
- We can help

Summary

- Parallel visualization is only *partly* about upping the compute power available, its also about getting sufficient memory and I/O bandwidth.
- I/O is a *really big* issue. Planning how to write your data for parallel access, and placing it where it can be accessed quickly, is critical.
- The TACC visualization groups are here to help you!

Longhorn Architecture



Stampede Architecture