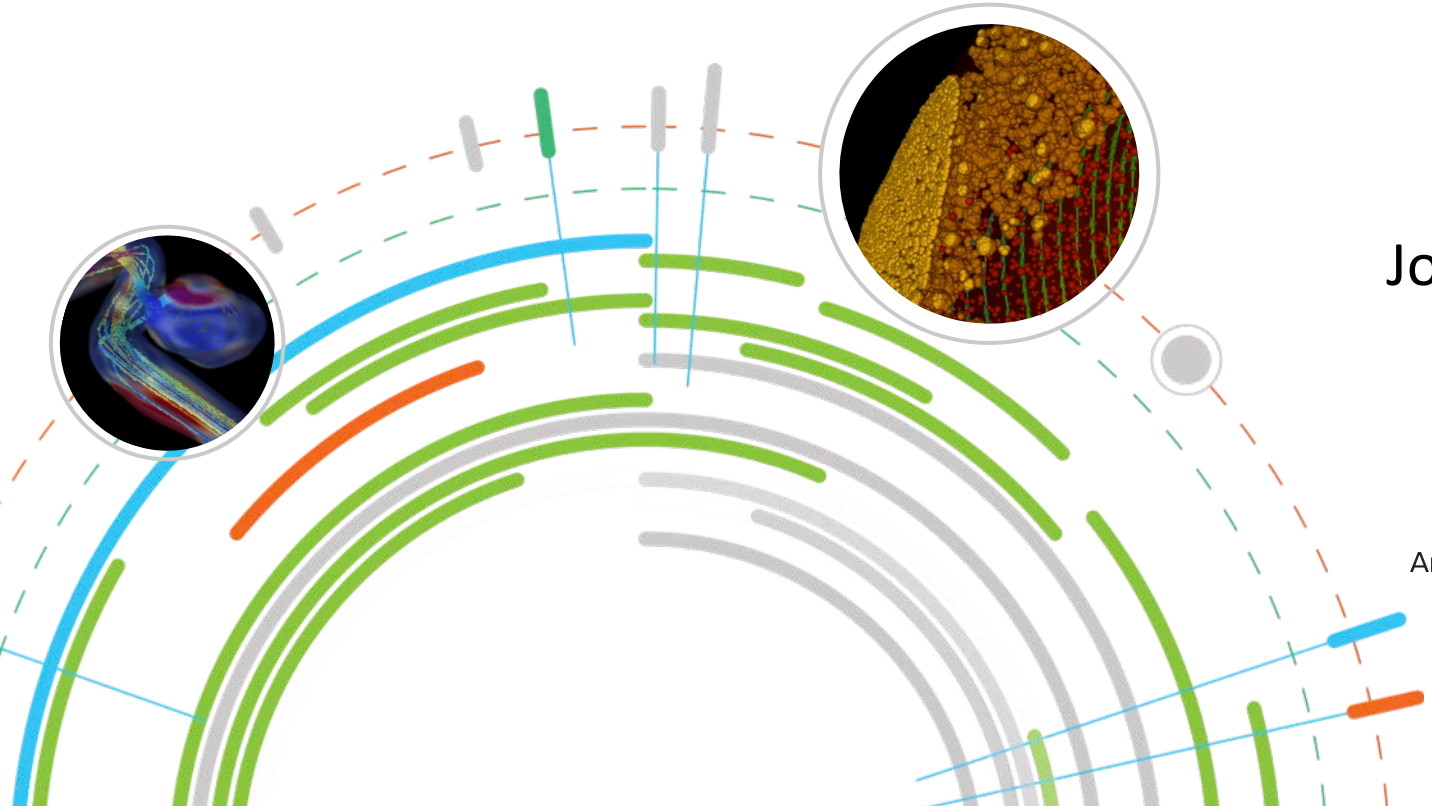
Perspectives on 10 years of Ultrascale Visualization Collaboration



Joseph A. Insley

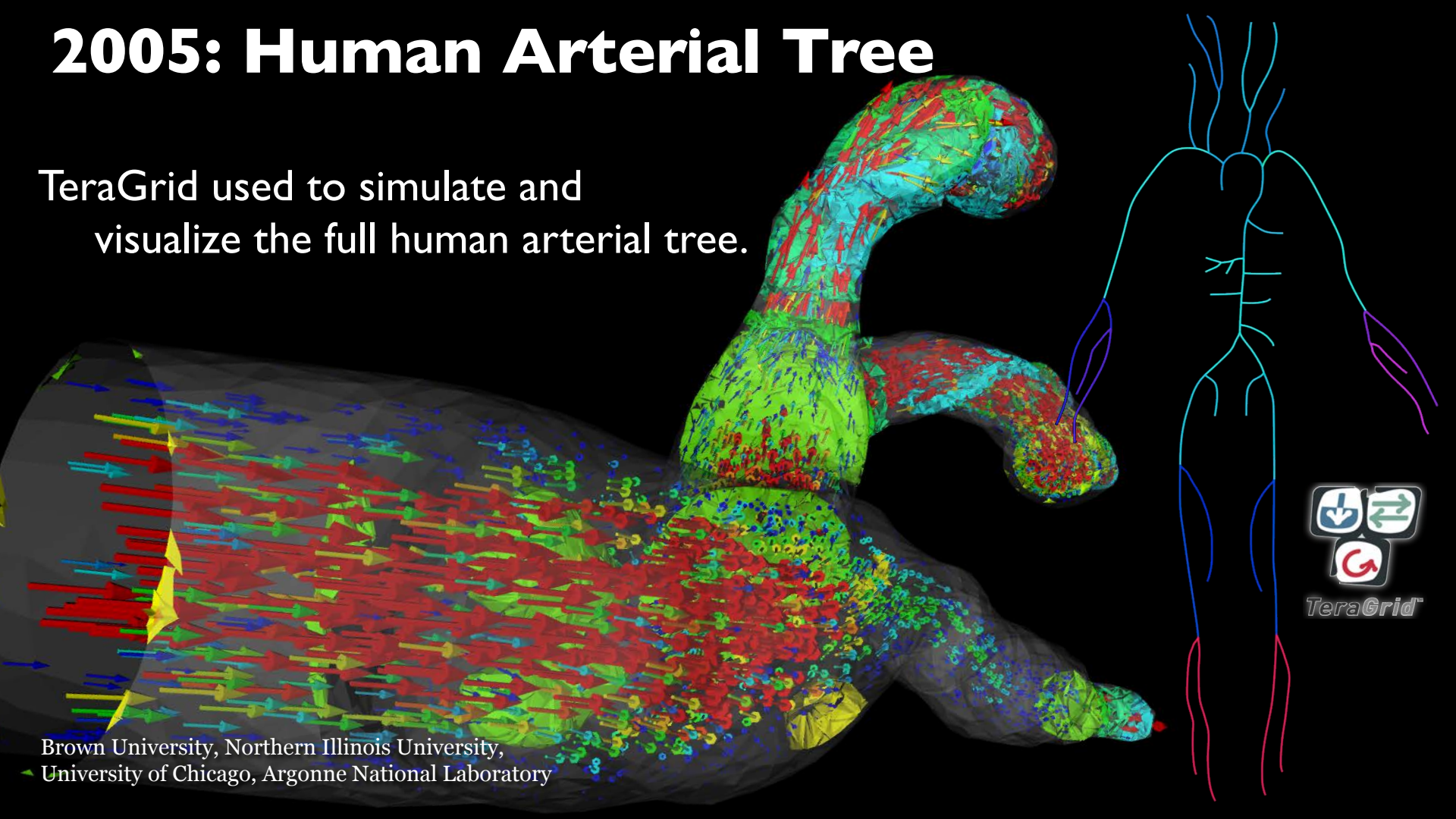
Ultravis '15
November 16, 2015

Argonne **Leadership Computing** Facility

Argonne NATIONAL LABORATORY

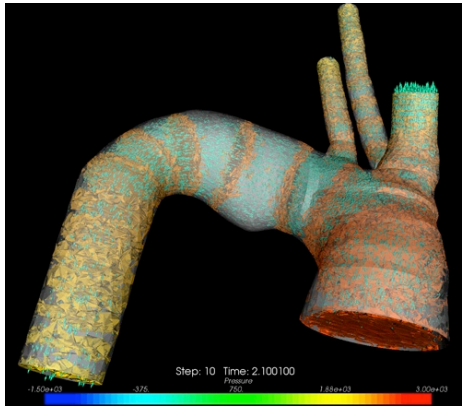
2005: Human Arterial Tree

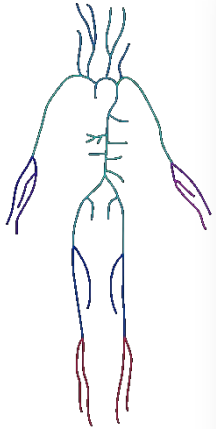
TeraGrid used to simulate and visualize the full human arterial tree.

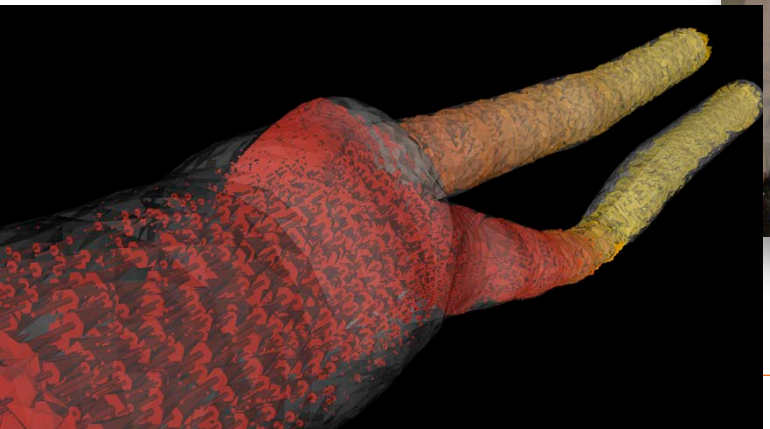


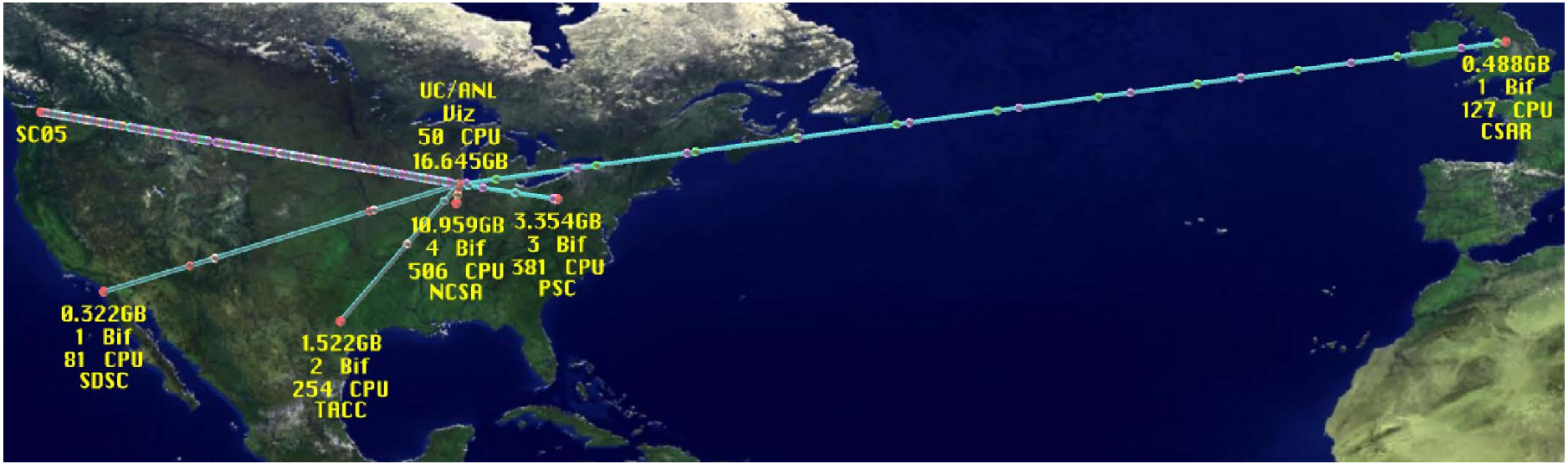
Brown University, Northern Illinois University,
University of Chicago, Argonne National Laboratory

SC'05: Arterial Tree Simulation and Visualization









Simulation:

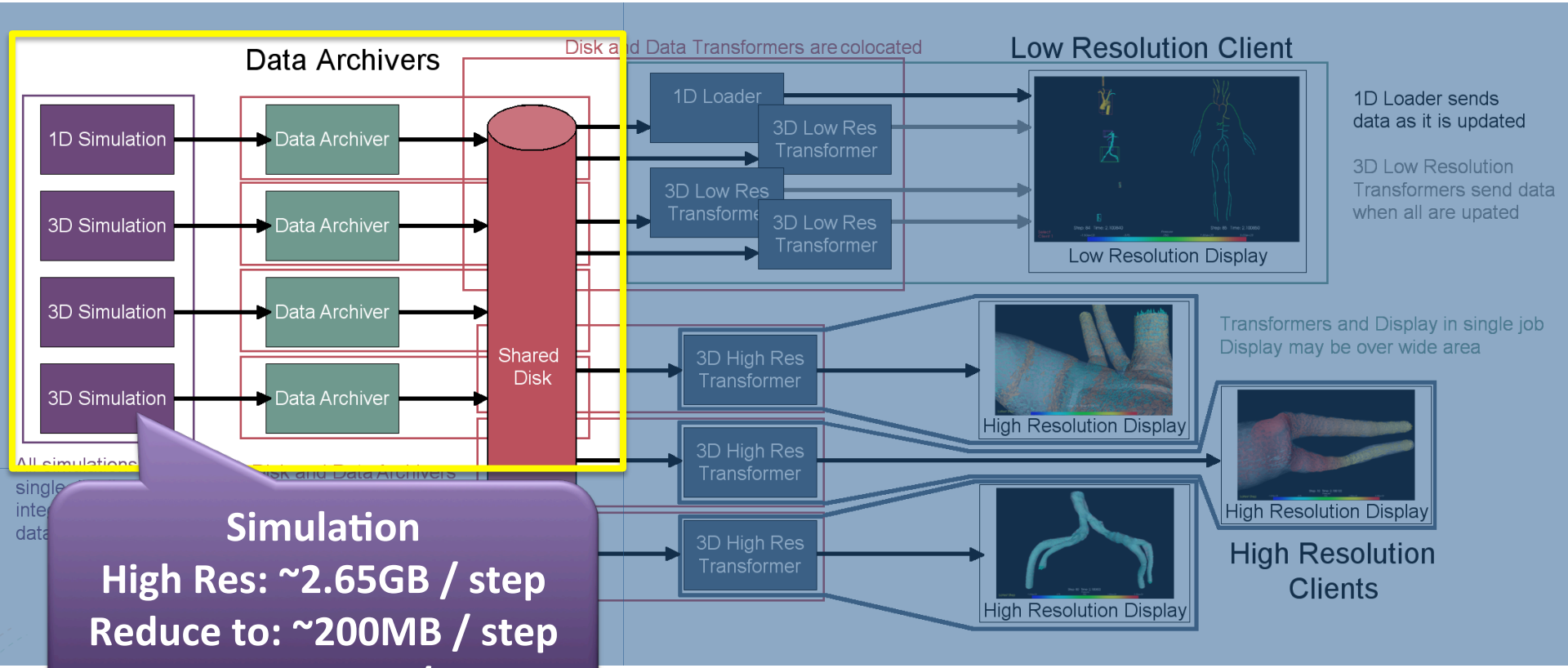
- 55 arteries, 17 bifurcations
- 11 Meshes
  - 20K – 200K finite elements / mesh
- 1,349 total processors, 5 sites
  - 64 to 128 processors each

Visualization:

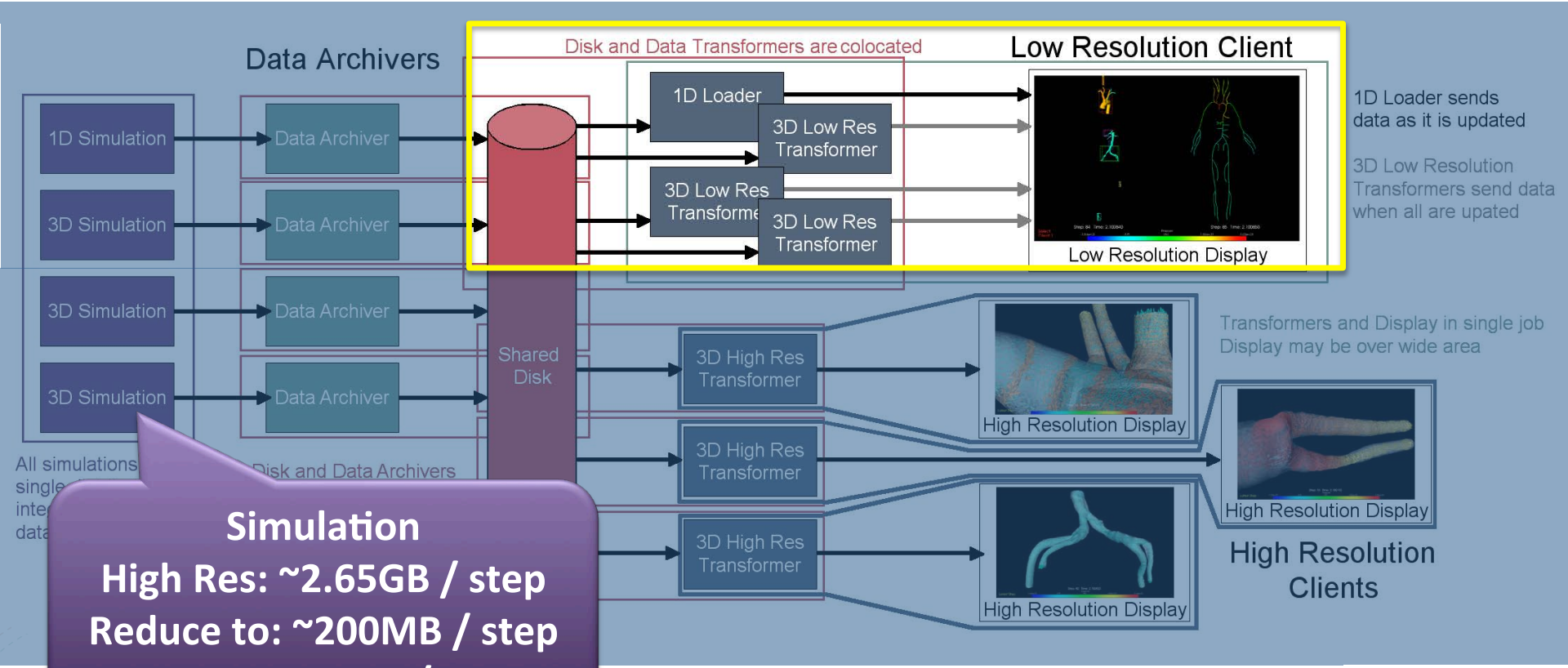
- 12 Data Archivers
- 1 Low resolution client
- 7 High resolution clients
- Monitoring

TeraGrid™

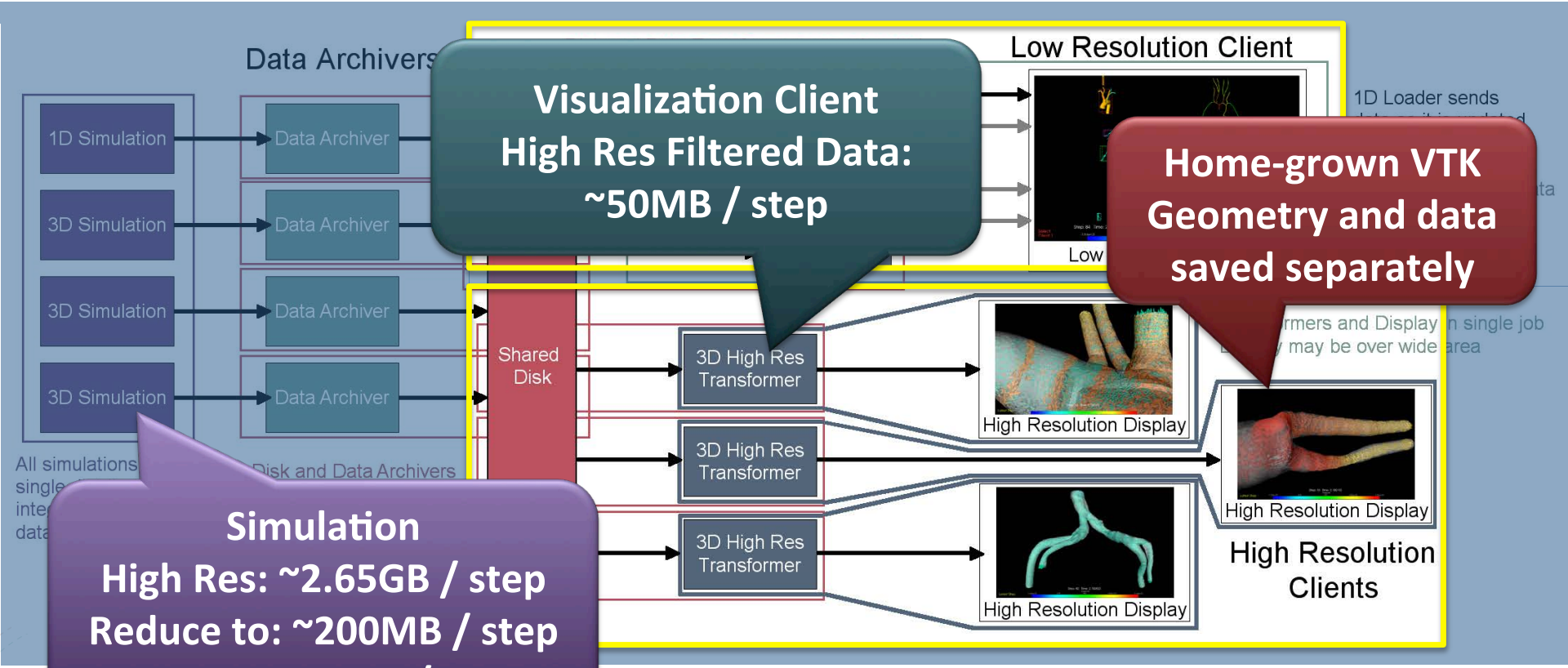
System Architecture

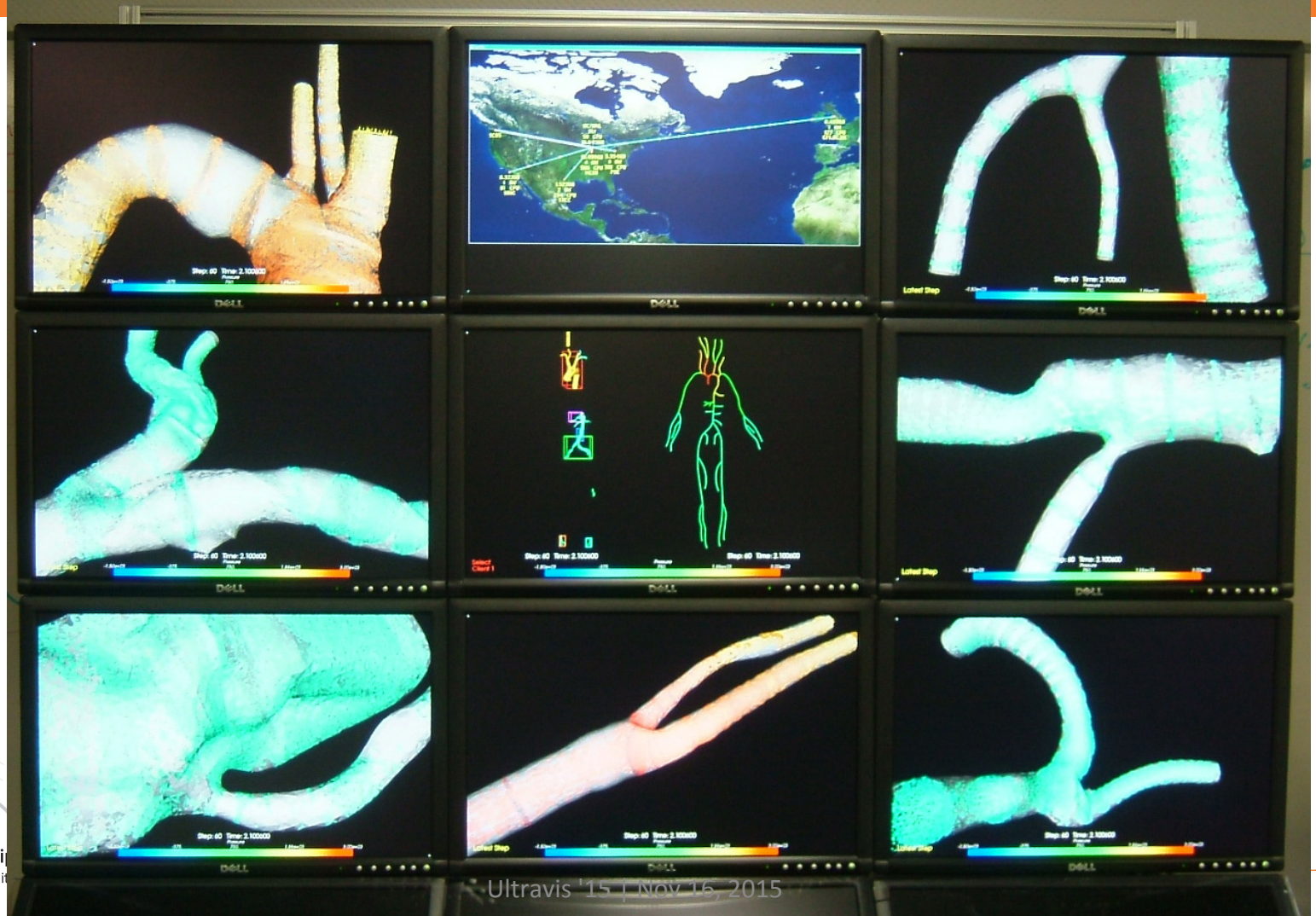


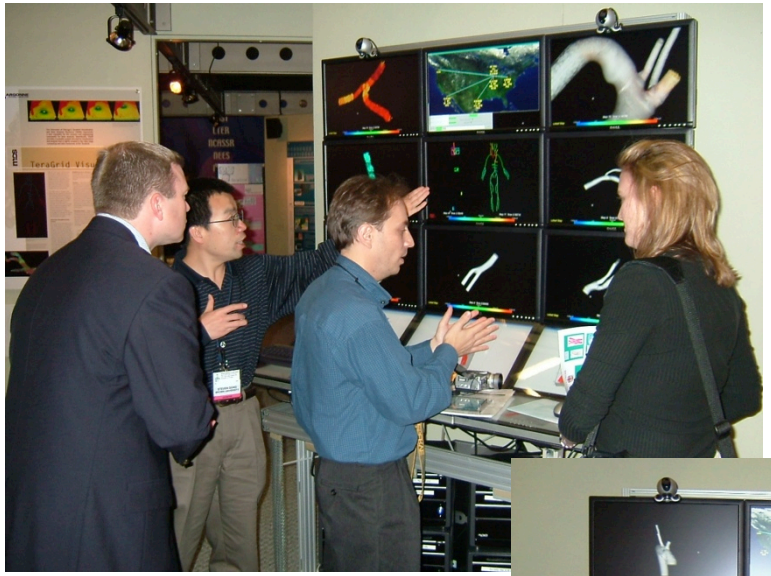
System Architecture



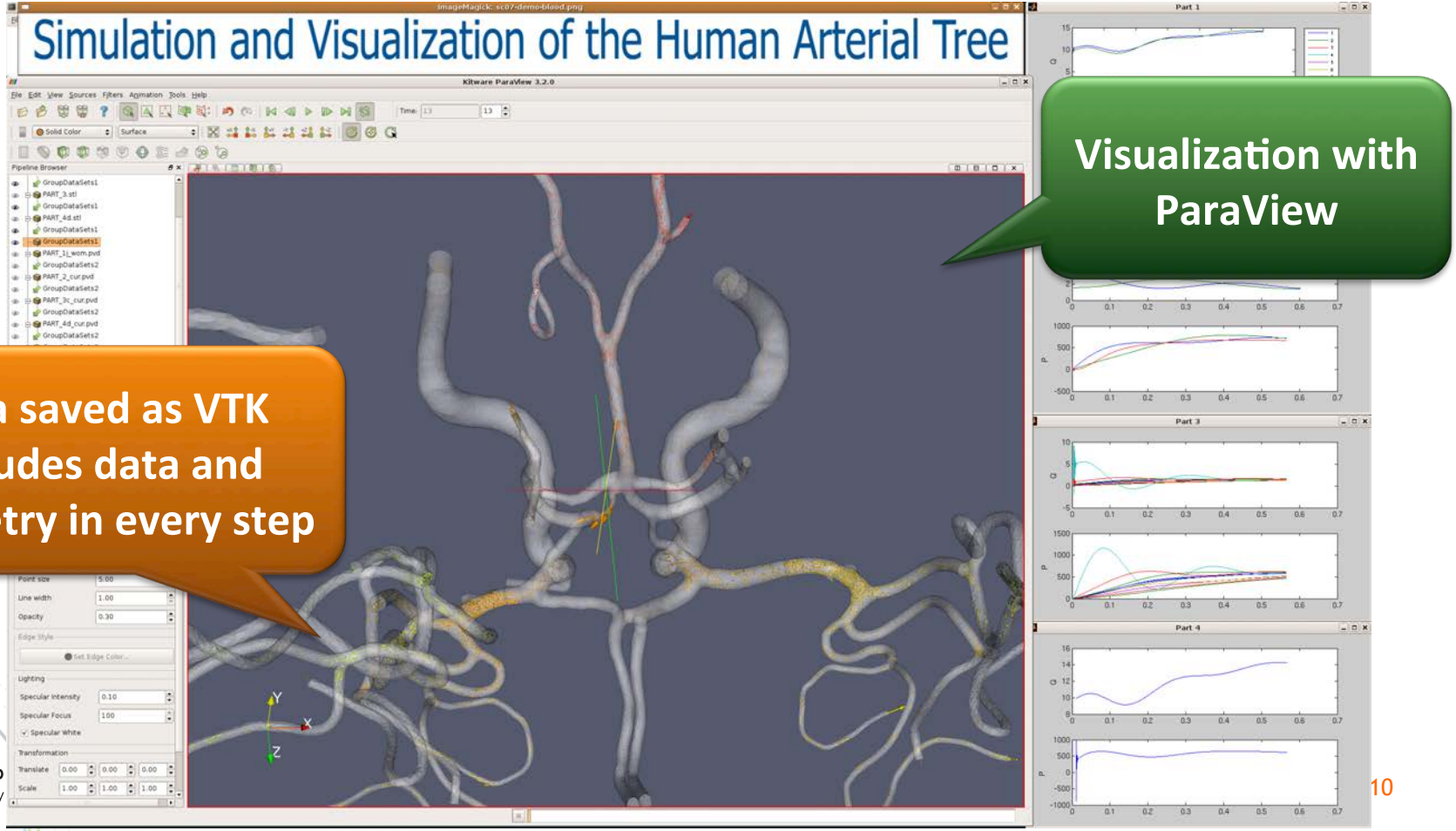
System Architecture



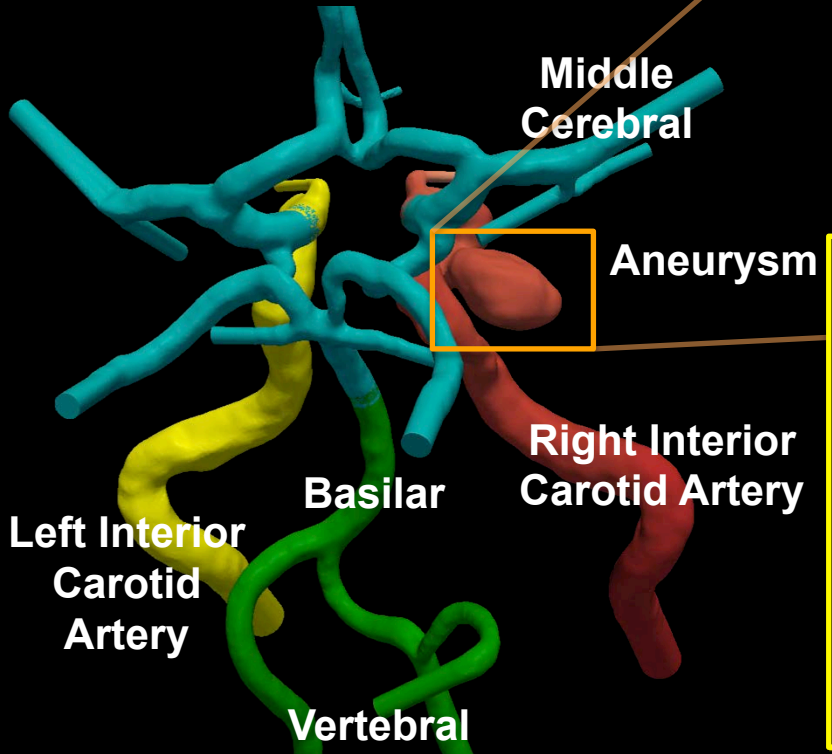


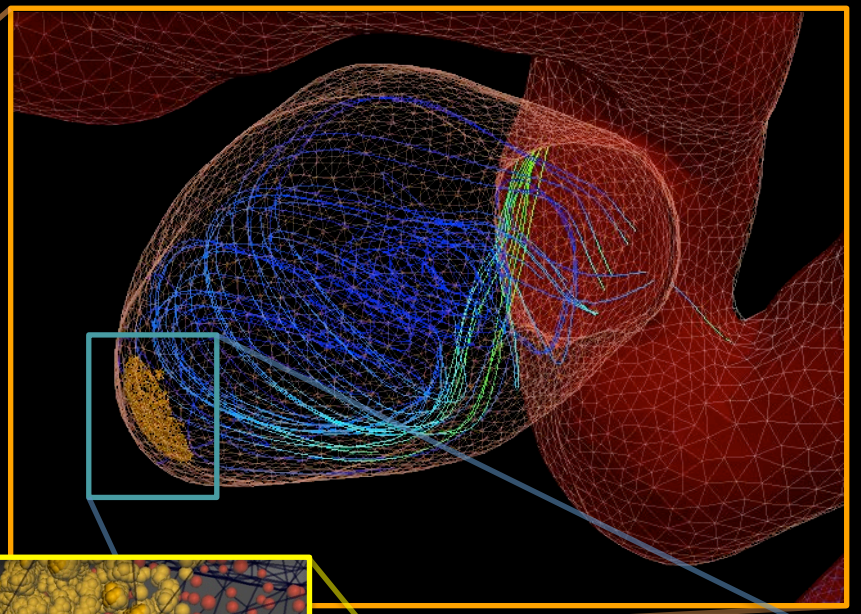


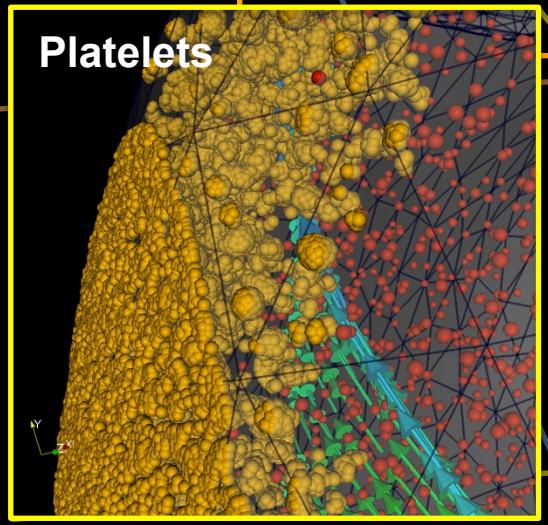
SC'07: Cranial Arterial System Simulation and Visualization

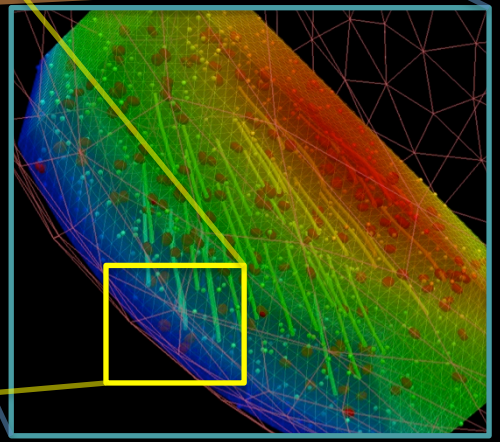


2010-2011: Multi-Scale Simulation/Visualization Arterial Blood Flow









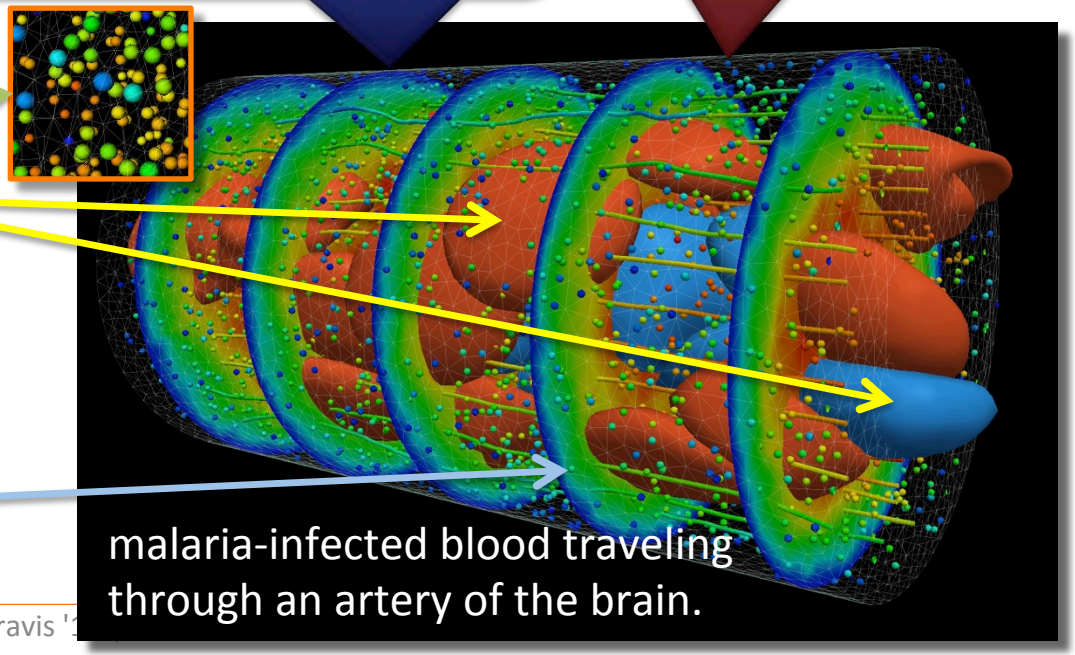
2010: PetaApps: Microscale Simulation

Modified version of LAMMPS

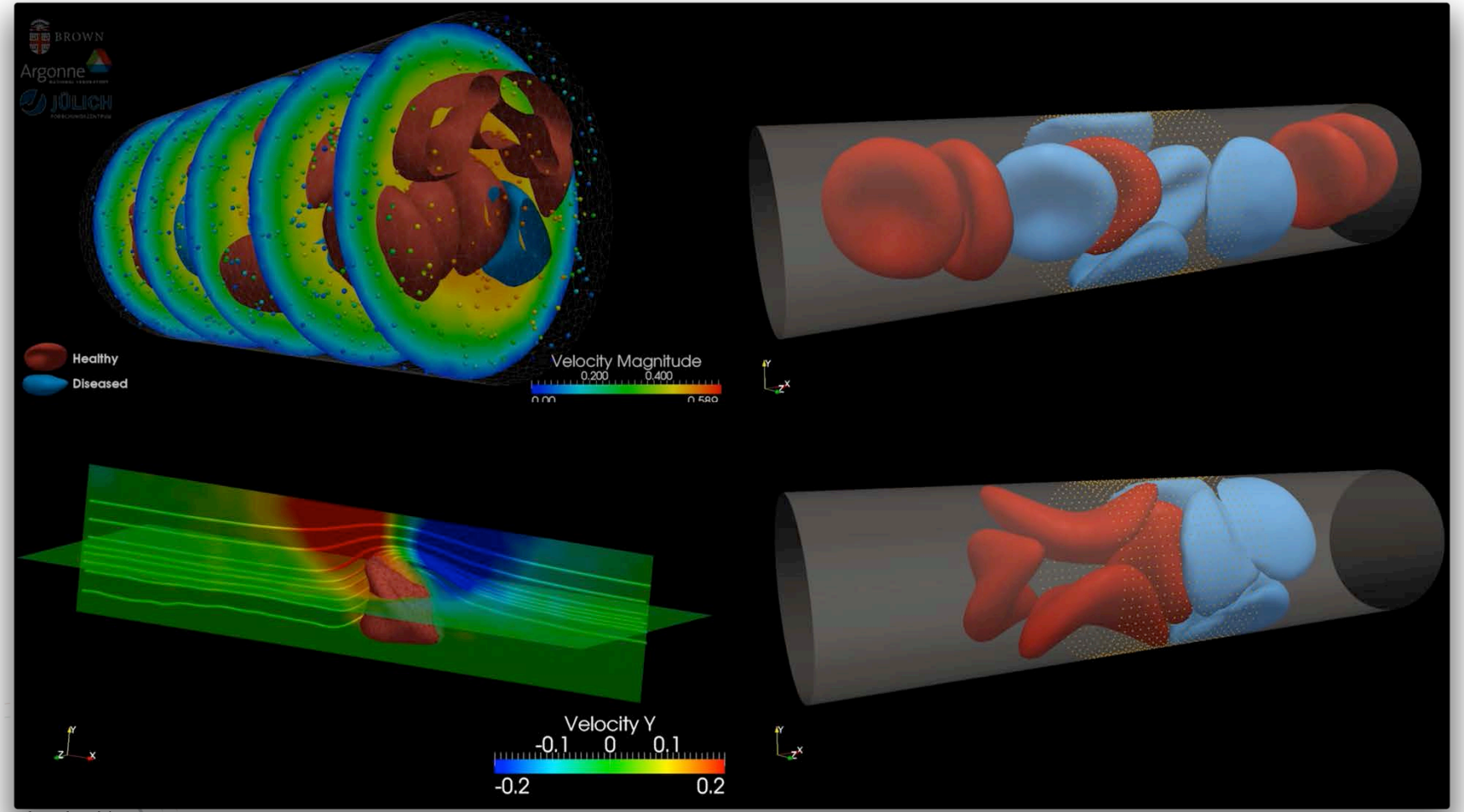
- Two types of data
  - Atomistic (particle) data
    - Plasma
    - Red Blood Cells (RBC)
    - Platelets
  - Field data
    - Ensemble average solution
    - Window Proper Orthogonal Decomposition (WPOD)

~30K particles
Couple of MBs / step
~2GB for ~400 time steps
VTK and ParaView

~30K cores of Kraken Cray XT5 (NICS)

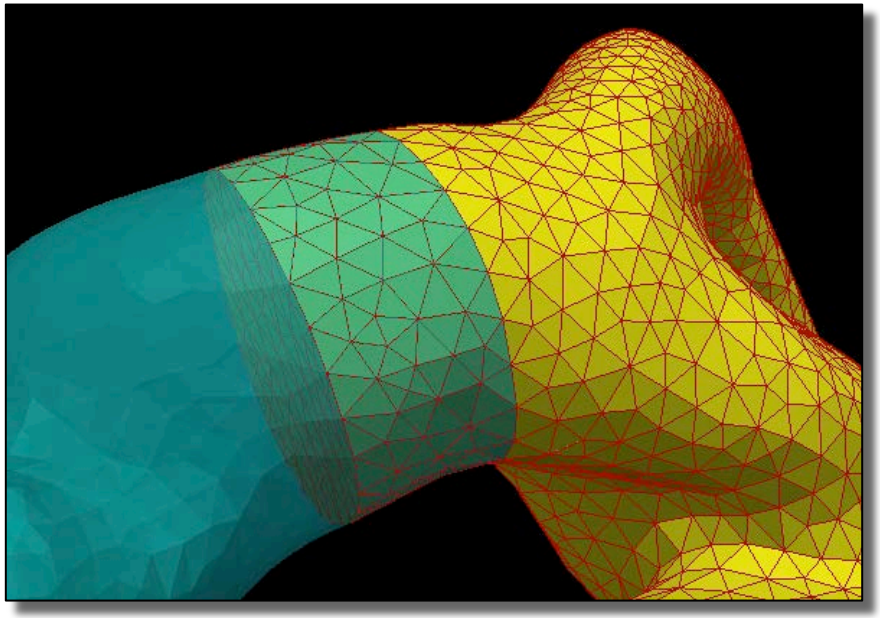


malaria-infected blood traveling through an artery of the brain.

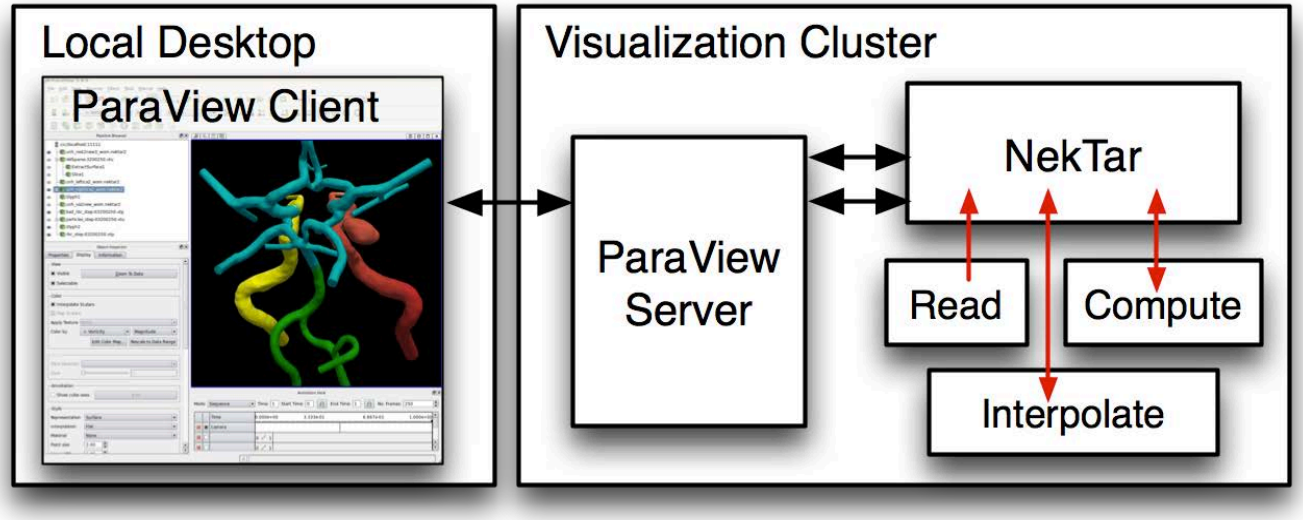

BROWN
Argonne
JÜLICH
Healthy
Diseased
Velocity Magnitude
0.200
0.400
Velocity Y
-0.1
0
0.1
-0.2
0.2

Macroscale Simulation (NekTar)

- NekTar Data
  - Saved in Modal space
  - Mesh (geometry)
  - Solution data
- Preserve high order
- Flexibility in visualization



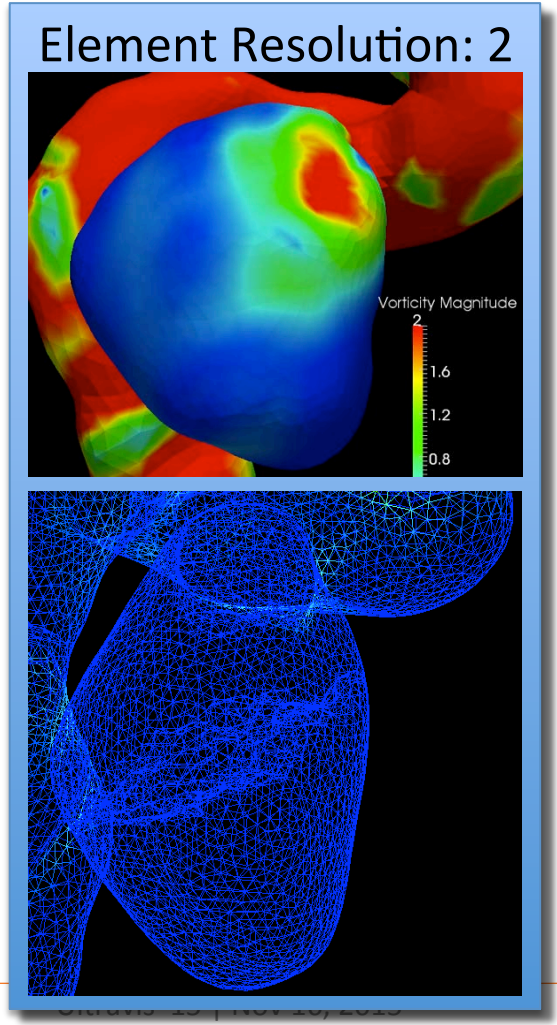
NekTar-ParaView Coupling

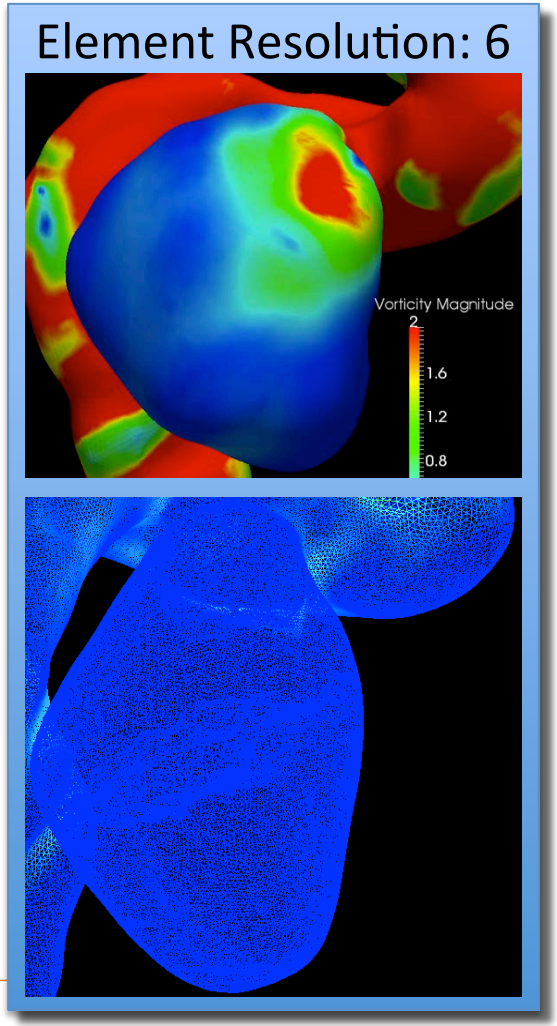


- NekTar for parallel I/O and computation
- ParaView for parallel visualization and rendering

Visualization Control

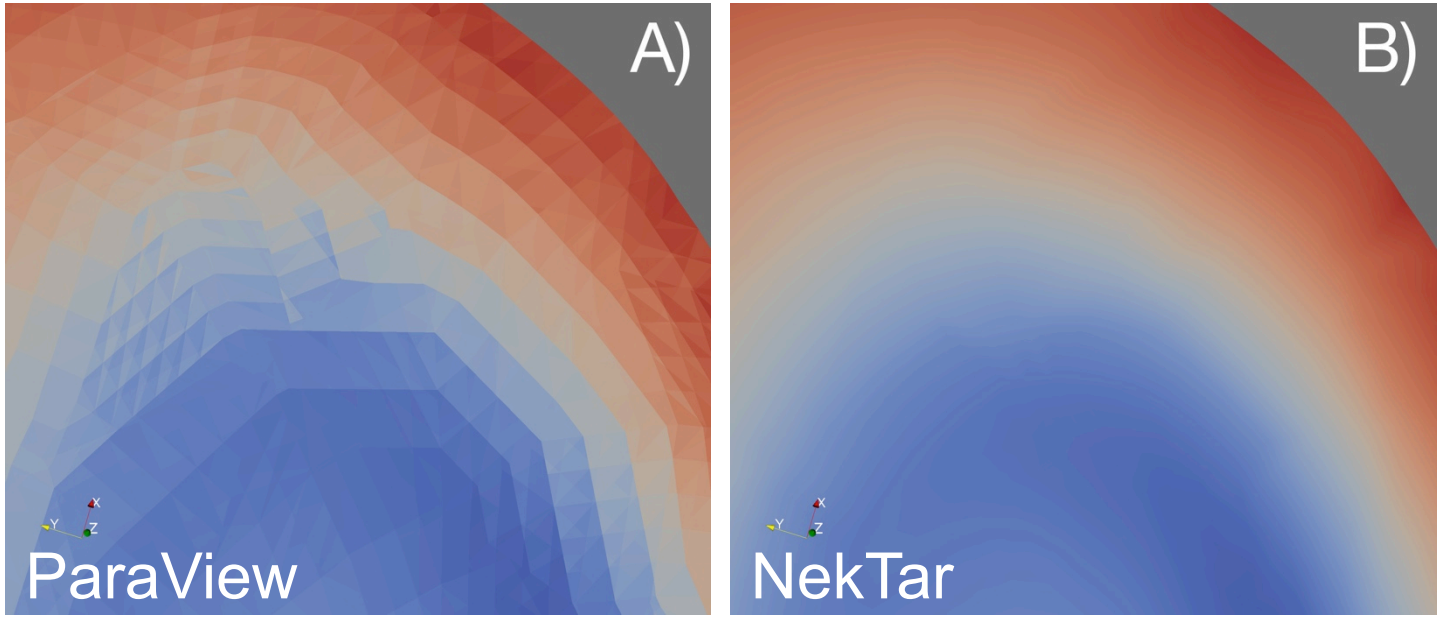
- Select variables / derived quantities
- Interactively set data resolution
  - No need to re-read mesh data from disk
- Time varying data
  - Only new data read from disk, not geometry





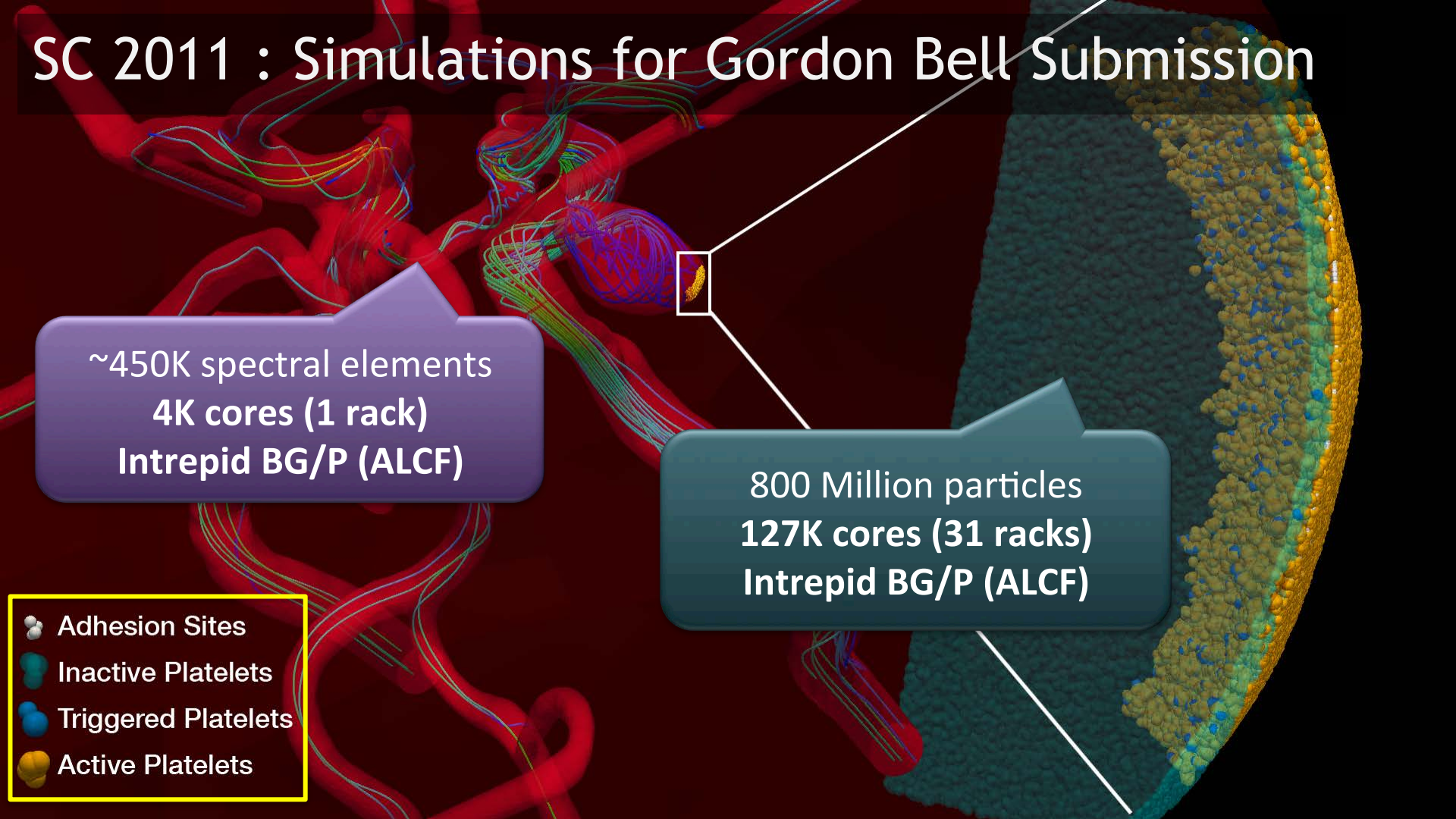
Process High-order Spectral Elements

- Data computed with high-order spectral accuracy
  - Grid consistent with simulation resolution

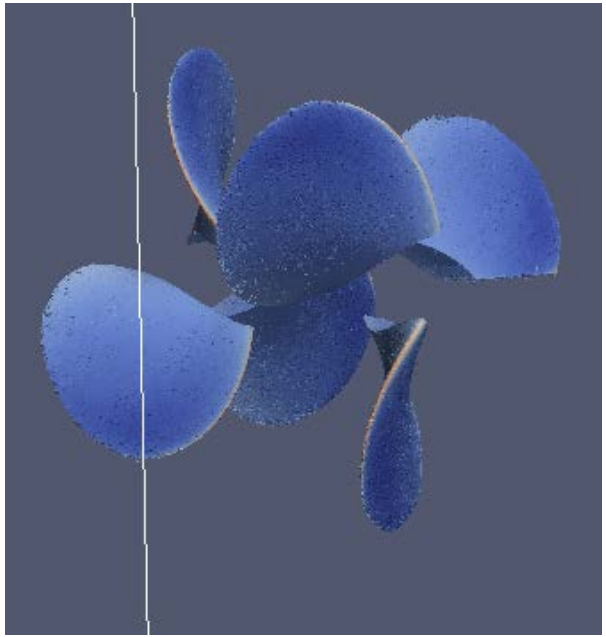


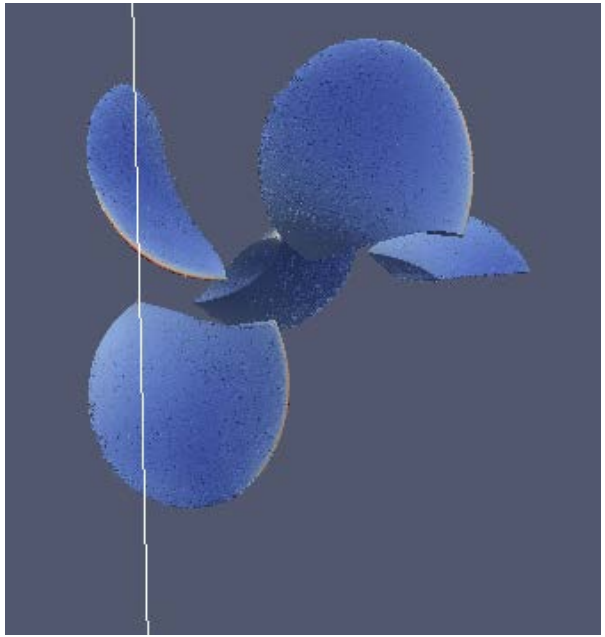
Derived Quantity: Vorticity

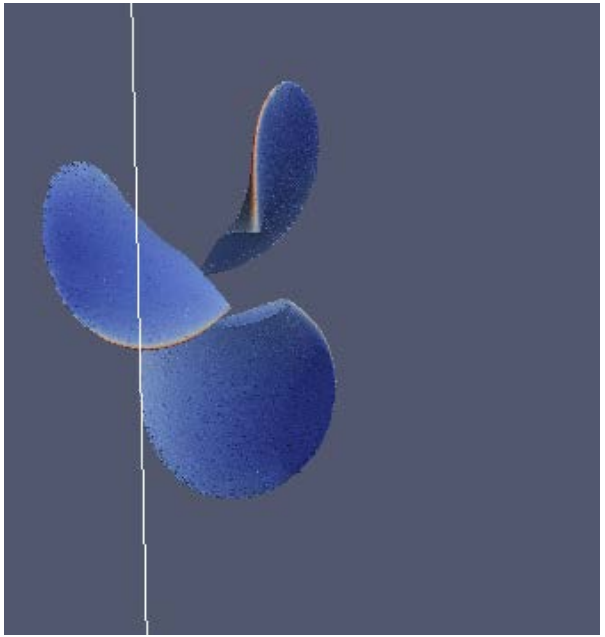
SC 2011 : Simulations for Gordon Bell Submission



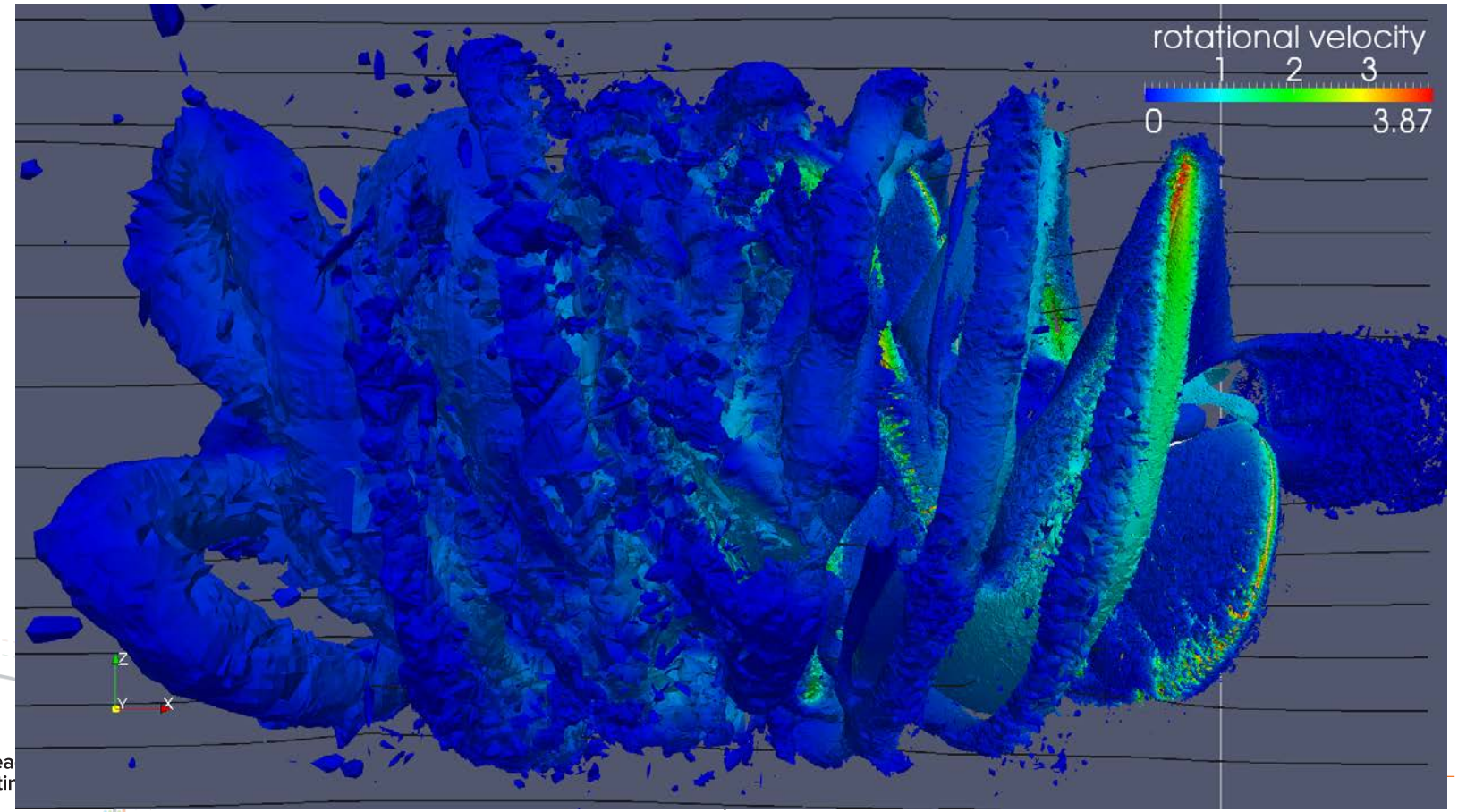
Visualization for Debugging





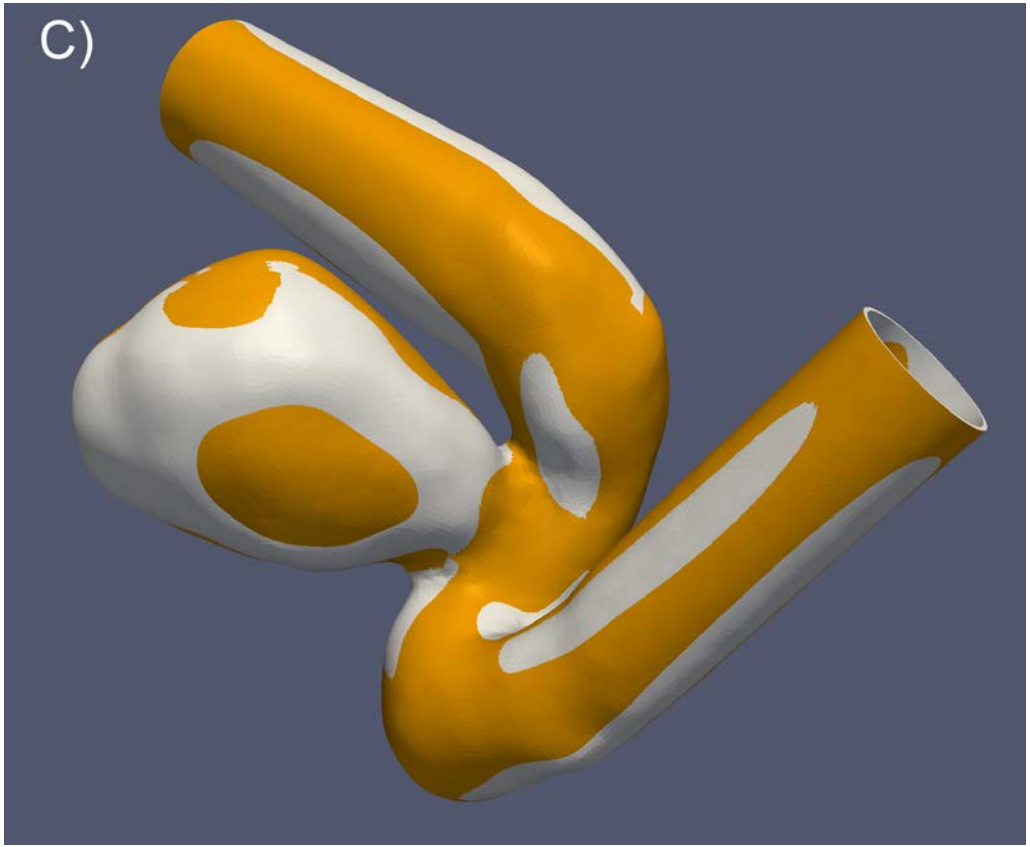


Visualization for Debugging



2013: Fluid-Structure Interactions (FSI)

- Dynamic mesh
- Compute stress tensor at high-order

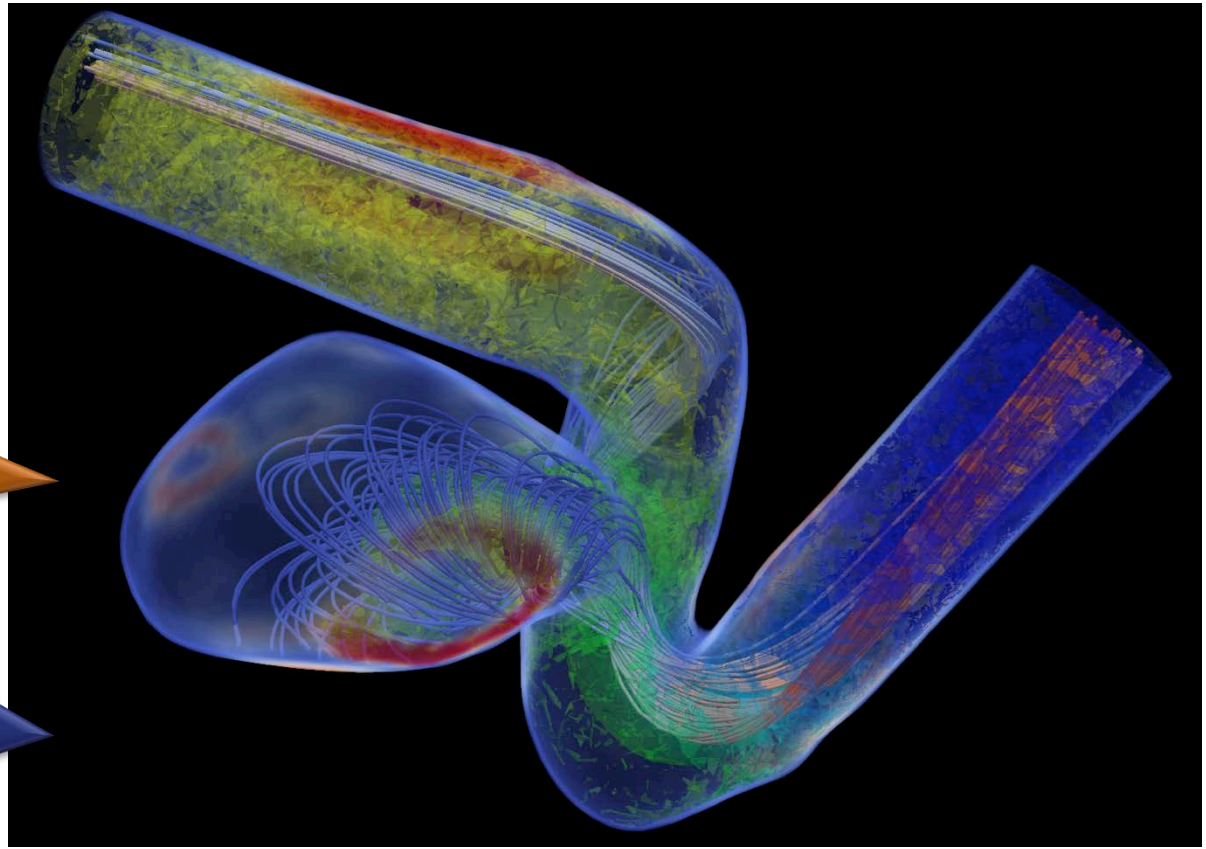


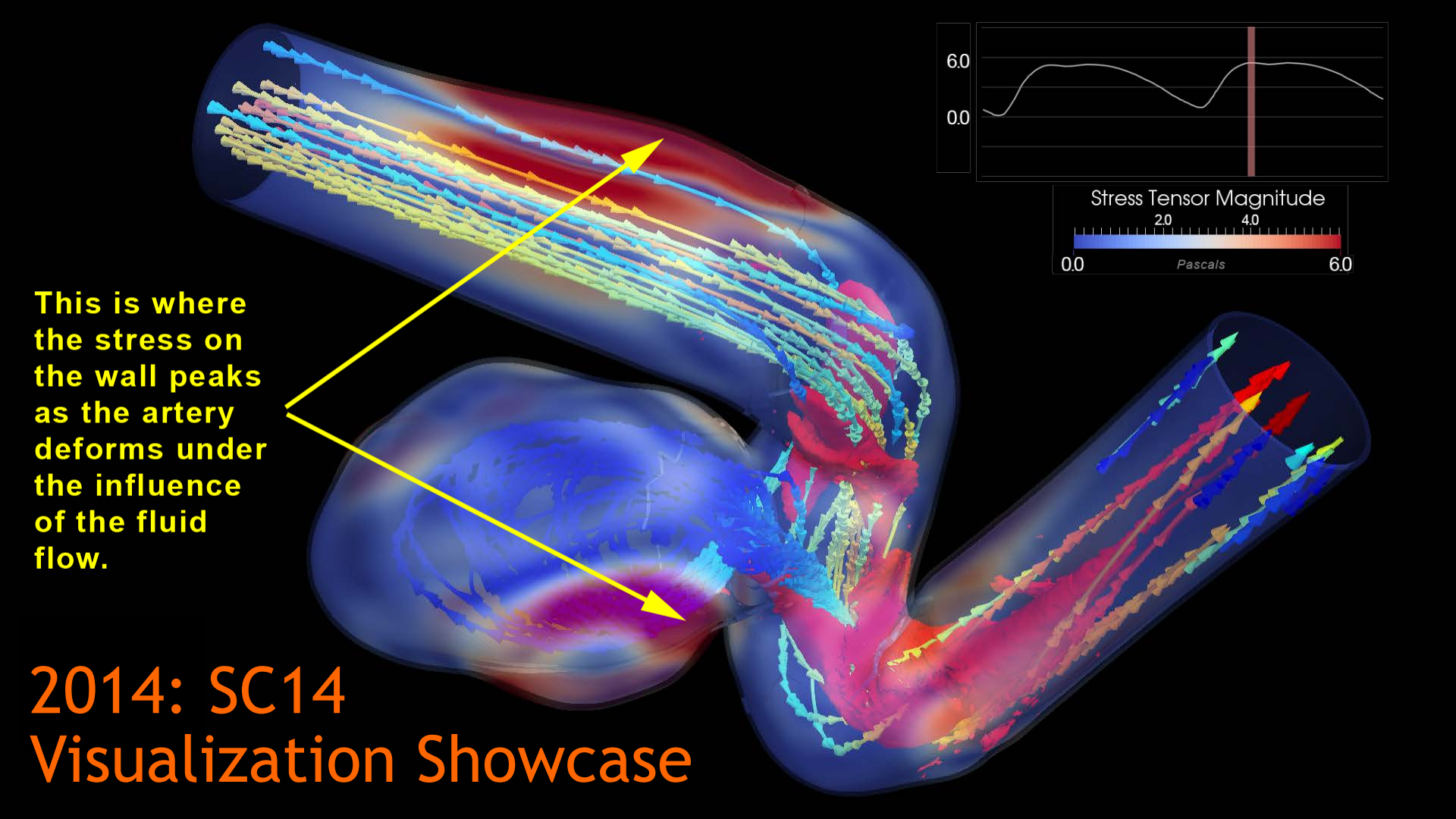
2013: Fluid-Structure Interactions (FSI)

- Dynamic mesh
- Compute stress tensor at high-order

Fluid: ~42K elements
Solid: ~17K elements

~1K cores
Mira BG/Q (ALCF)

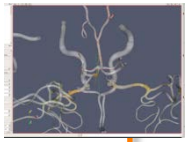



6.0
0.0
Stress Tensor Magnitude
2.0
4.0
0.0
Pascals
6.0
This is where the stress on the wall peaks as the artery deforms under the influence of the fluid flow.
2014: SC14
Visualization Showcase

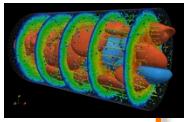
Demos and Publications

SC05
demo

SC07
demo

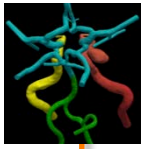


SC10
poster
vis showcase



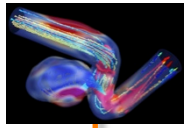
SciDAC
2011
vis showcase

SC11
Gordon Bell paper
poster
vis showcase



XSEDE
2012
paper

SC14
vis showcase

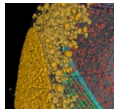


2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015

FGCS
(2006)
article

TVGC
(2007)
article

TeraGrid
2011
paper
vis showcase



LDAV
2011
paper

CISE
(2012)
article

PARCO
(2015)
article

So… What have I learned?

- Work closely with scientists
  - Cyclical process – learn from each other what is important and possible (and not possible)
- Problems at (Ultra)scale haven't fundamentally changed all that much
  - Managing / reducing / filtering data
- We've aged surprisingly well..



Thanks

- ALCF Visualization and Analysis Team
  - Michael Papka, Mark Hereld, Venkat Vishwanath, Thomas Uram, Silvio Rizzi, Preeti Malakar
- Collaborators at Brown University
  - George Karniadakis, Steve Dong, Leopold Grinberg, Paris Perdikaris
- Nick Karonis (Northern Illinois University)
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    - TeraGrid
    - PetaApps

Thank you!