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**Flash Center**  
The University of Chicago



**TeraGrid**



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# *Challenges of a Terascale Turbulence Simulation*

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# Outline

- Simulation
- Challenges
  - Data
  - Visualization
  - Communication
- Summary and moving forward

## *Simulation Introduction*

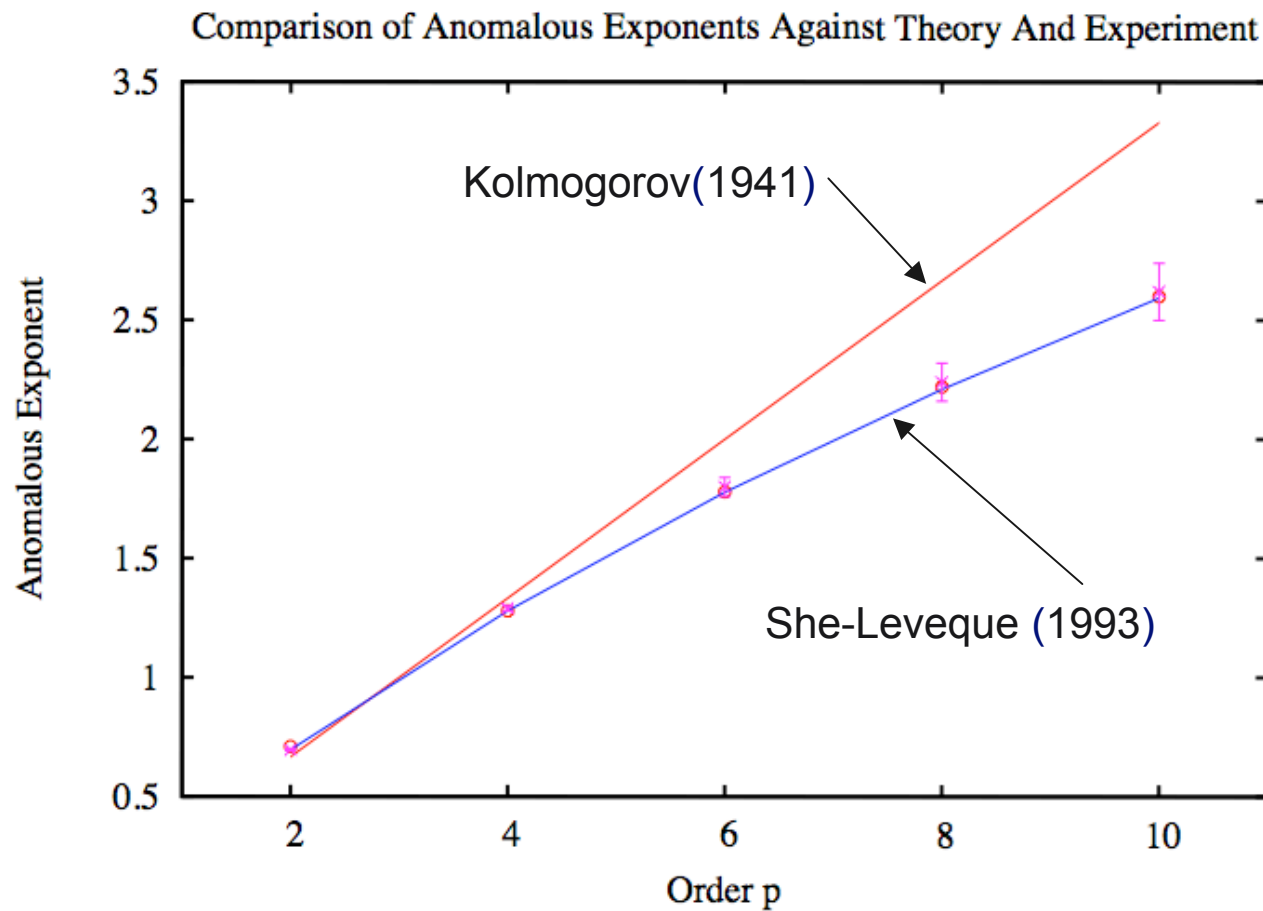
- Simulation done by ASC / Alliance Center  
Astrophysical Thermonuclear Flashes at The  
University of Chicago
- Ran on the LLNL BG/L machine during December  
2005 - January 2006
- Produced 14TB of analysis data
  - 13.3 TB grid data (1 vector, 3 scalar)
  - 0.7 TB particle data (2 vectors, id)
- Produced 150TB+ of checkpoint/restart files
- Each time-step produced 32K files

# *Simulation Specifics*

- Homogeneous, isotropic compressible turbulence run with Lagrangian tracers on BG/L using FLASH 3
- Computation Size
  - $1856^3$  base grid size ( $928^3$  used for analysis files)
  - $256^3$  Lagrangian tracer particles
- Computation Specifics
  - MILES-based approach solving Euler equations using PPM
  - Driven using stochastic driver (Eswaran & Pope, 1988)
  - 3D turbulent RMS Mach number = 0.3 (1D = .17) in steady-state
  - $Re_\lambda \sim 500 - 1000$
  - Full eddy-turnover time in steady-state
- Roughly one week wall clock on 65,536 processors in CO mode



# Anomalous Scaling Exponents



Circles = Experiment  
(Benzi et al, 1993)  
Crosses = FLASH

# Challenges

## ■ Data

- Data transfer
- Data storage
- Data integrity

## ■ Visualization

- Real-time analysis
- Filtering

## ■ Communication

- Effective communication with scientific team

## *Data Transfer*

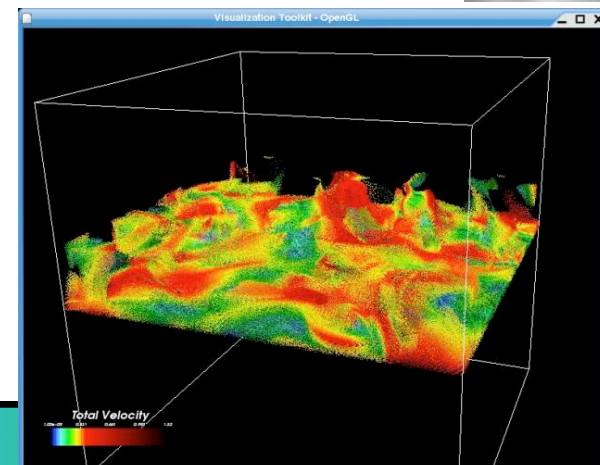
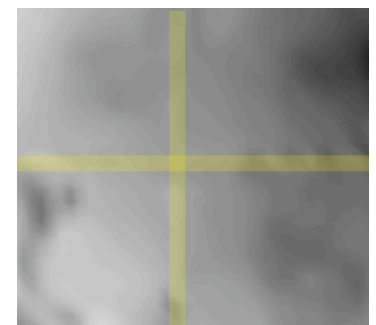
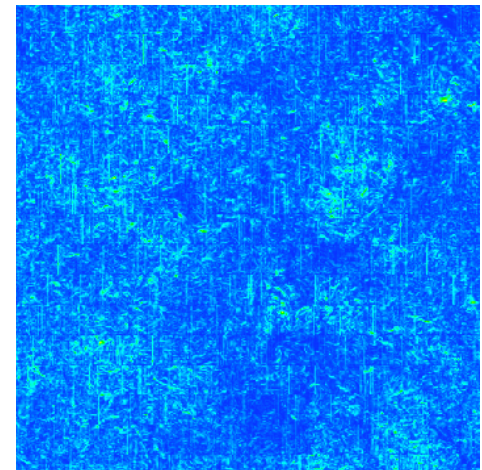
- Tarred directories to transfer as a single 18GB chunk
- GridFTP from LLNL to UC
  - Data got moved to HPSS before all could be transferred so added additional work in transfer
  - Expect scripts to manage transfers from HPSS to scratch space
  - Python scripts to manage transfers from scratch to UC
  - Screen sessions to manage overall effort
- 28 days to get 13.3 TB (grid data) to UC

## *Data Storage*

- How do you keep 14TB around?
- Represents 28% of all data the center has on disk
- Spread across multiple different volumes
- Augmented data compounds issue

# Data Integrity

- Whose fault is it?
- Enstrophy calculation problems
  - Calculate vorticity from analysis data
- Possible block boundary issues
  - Verify using different tools
  - Ghostcell issues
- Particle ids
  - Corrected midway through run
  - Track reconstruction



# *Visualization Tools*

## ■ Community tools

- ParaView
- VisIt
- POVRay

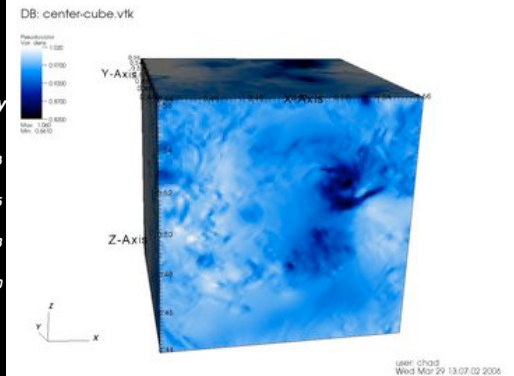
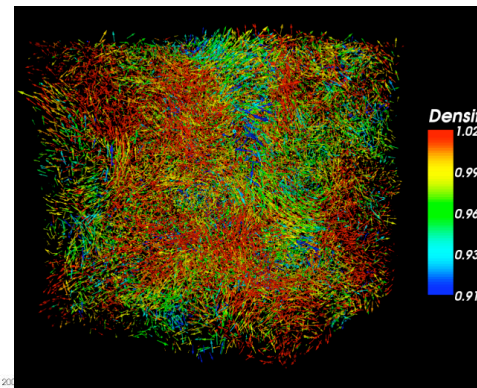
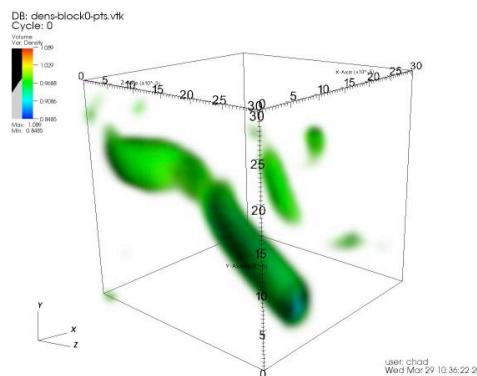
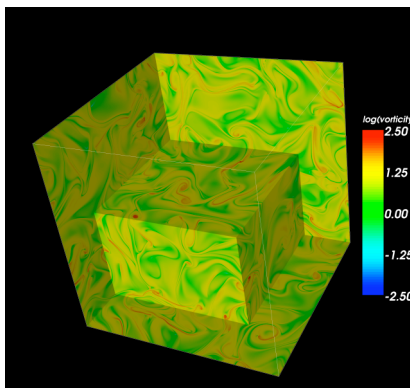
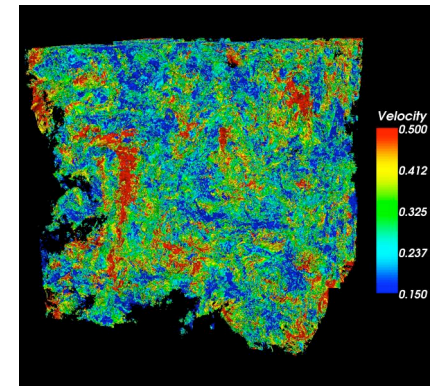
## ■ Group developed tools

- Volume rendering
- Particle rendering (built with vtk)



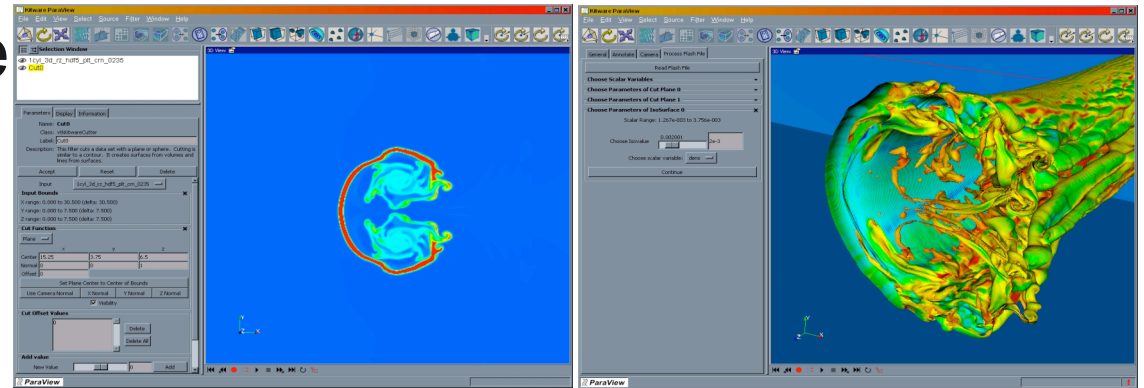
# ParaView and VisIt

- In use by both visualization team and scientist
- Addresses real-time analysis need
  - Parallel capabilities
  - Hides complexity
  - Supports additional computation

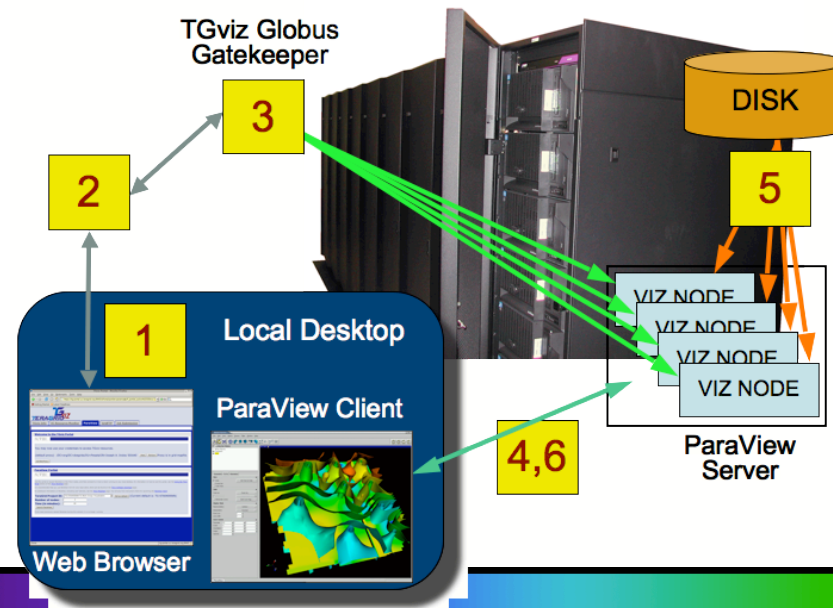


# ParaView Efforts

## ■ Simplified interface



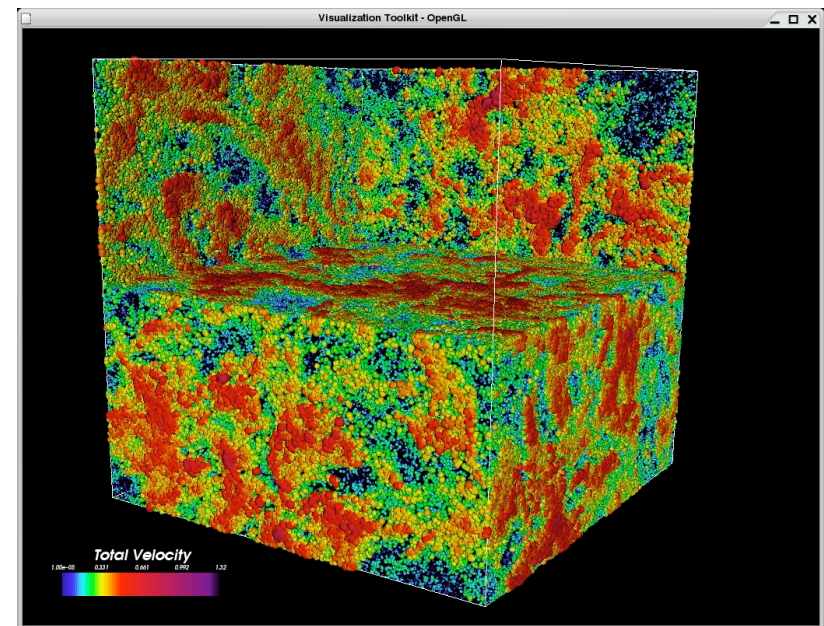
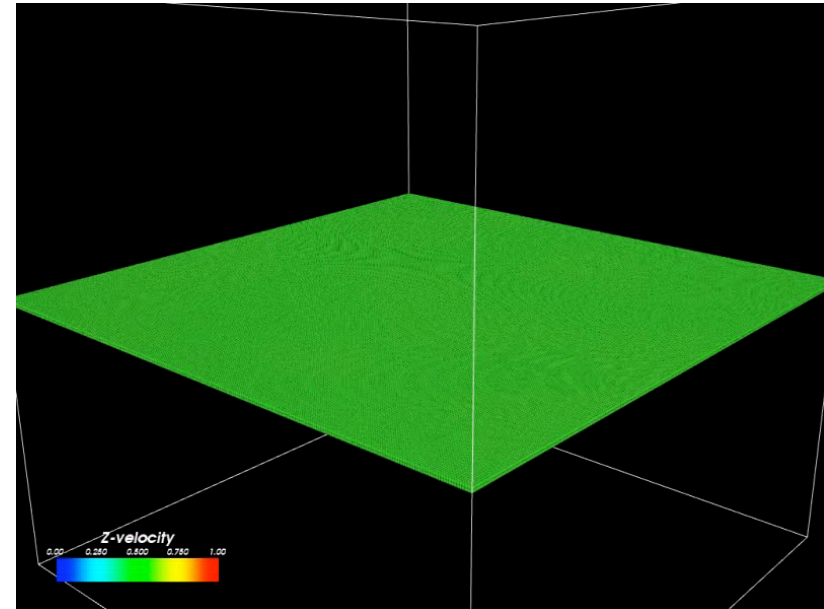
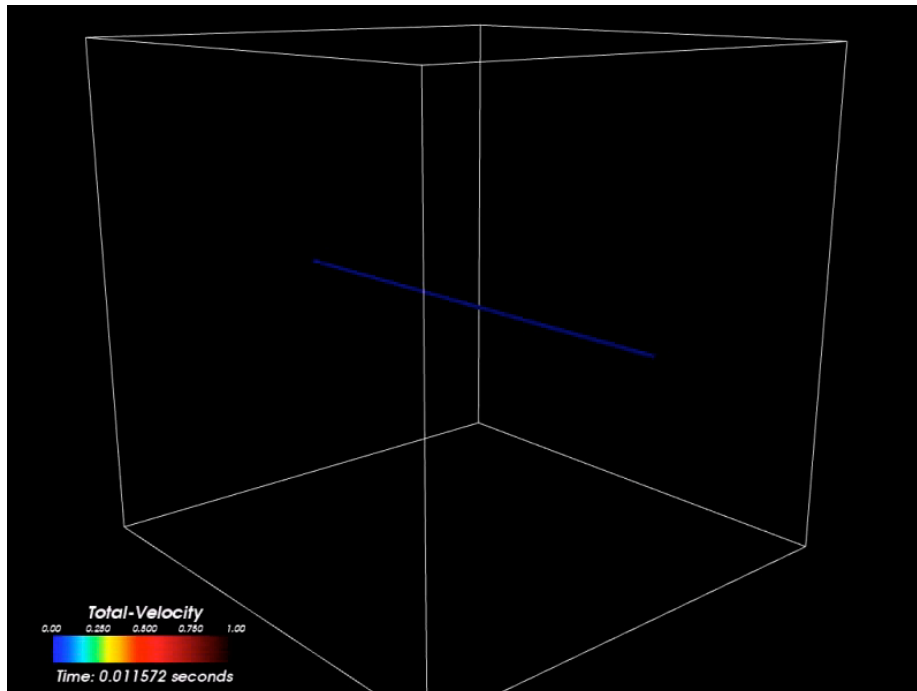
## ■ TeraGrid visualization gateway



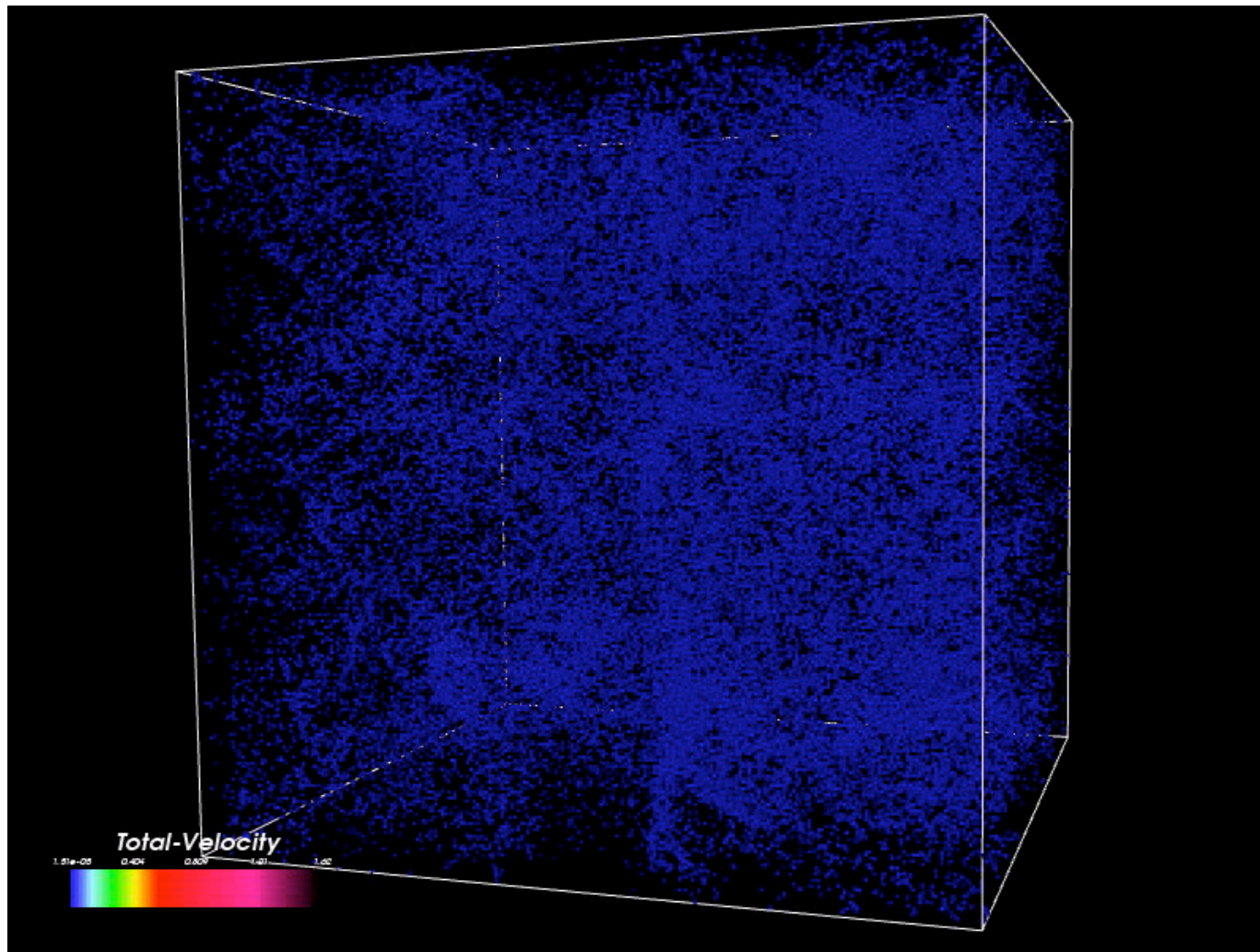


# Particle Rendering

- Filtering of data
  - Geometric extraction
  - Data cuts

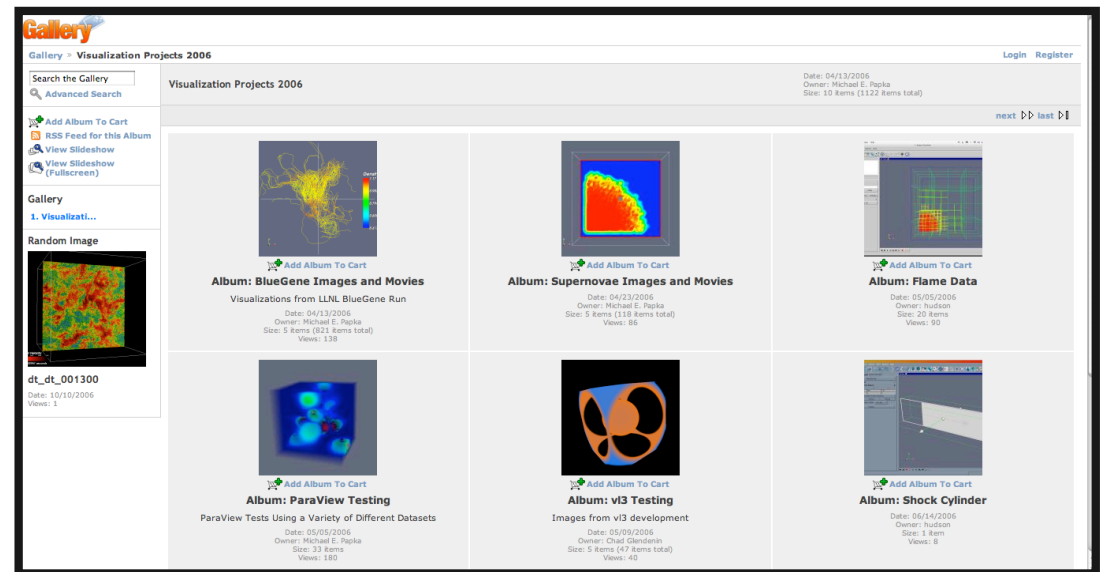
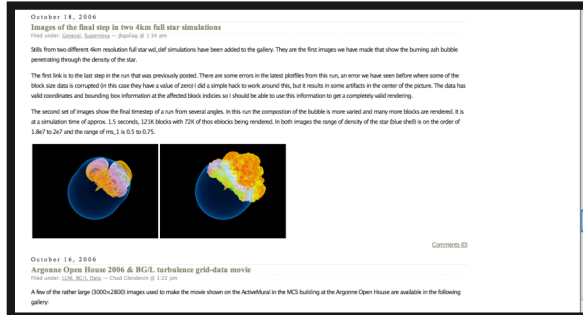
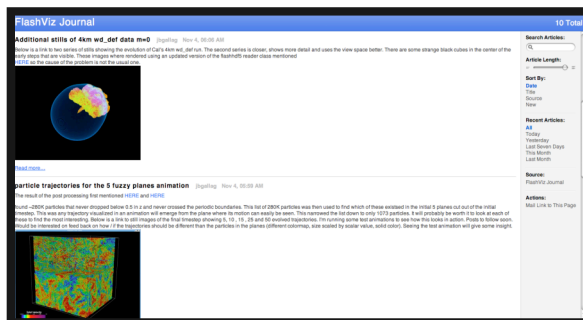


# *Particle Visualization with Data Filter*



# Communication Challenges

- Keeping scientist updated
- Informing fellow team members
- Organizing results



# *Challenges - Revisited*

- Visualization component is only a fraction of the challenge
  - Usability
  - Simplification
- Data issues dominate the process
  - Location
  - State
- Communication
  - Process moving

# *Moving Forward*

‘Turbulence is the most important unsolved problem of classical physics.’ - Richard Feynman

- Looking at ways to make data publicly available
- Exploring integration of workflows into the process



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