National Energy Research Scientific Computing Center (NERSC)

Science Driven Analytics

Wes Bethel, Cristina Siegerist, Cecilia Aragon
Visualization Group, LBNL
02 May 2006

Science Driven Analytics

- Simulations and experiments are generating data faster than it can be analyzed and understood.
- Science bottleneck: information analysis and understanding.

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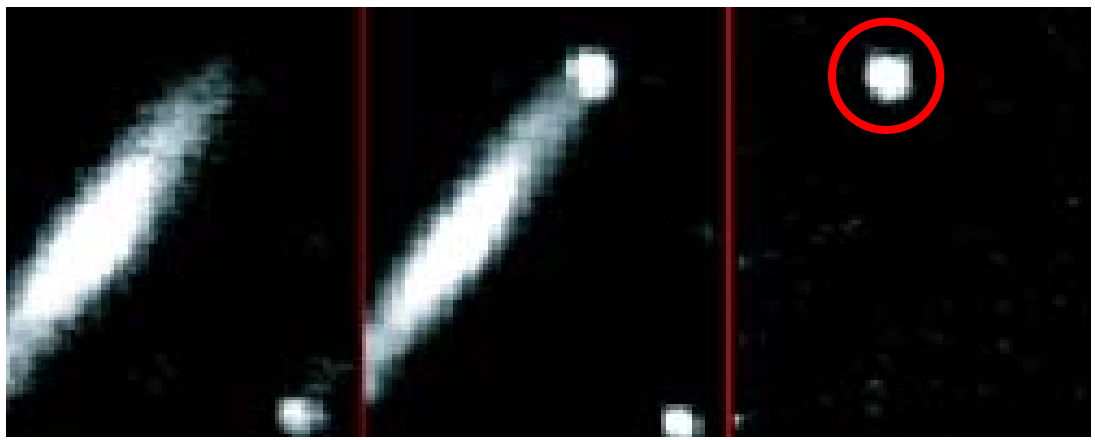
What is Analytics?

- **Science of reasoning.**
  - **Insight and understanding from large, complex, disparate, conflicting data.**
- **Visual Analytics**
  - **Science of reasoning facilitated by visual interfaces.**
- **Why at NERSC?**
  - **Data, data and more data.**

Distributed Analytics Workflow Example: SNFactory

Distributed Analytics Workflow serves an entire community.

- **Images collected from NEAT (Near- Earth Asteroid Tracking) telescopes.**
- **Images sent from telescope to network via custom wireless network.**
- **Images sent to NERSC for analysis on PDSF. Digital processing (registration, differencing) to locate potential targets.**
- **Potential Type 1a supernovae targets identified and broadcast to observation community (24-hour turnaround).**



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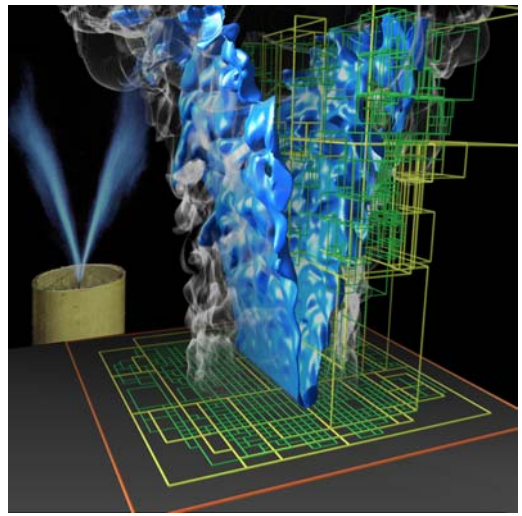
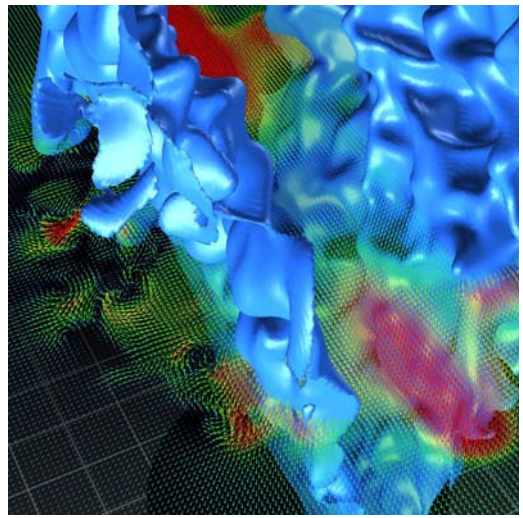
Iterative, Query-Driven Analytics Example

- **Combustion research.**
  - **Compare simulation with experiment.**
  - **Need analysis in regions defined by data- and topologically defined features.**
  - **10s of TB of simulation data, but only small portions interesting for any given analysis problem.**
  - **Several NERSC projects: Bell (LBNL), Chen (SNL-CA).**
  - **Need for remote analytics capability.**

  (Data courtesy M. Day, J. Grcar, and J. Bell, LBNL)





Analytics Challenges

- Cellular simulation: integrate and analyze data from multiple sources: proteins, multimolecular assemblies, metabolic pathways, and scale codes to complexity of living organisms.
- Fusion: analysis and comparison of multiple-code simulations and experiments leads to tokomak plasmas with improved energy confinement, and that are predictable and repeatable.
- Astrophyics: CMB/Planck – satellite mission to collect data; size estimated at 100s TB per year; needs to be stored and analyzed; workflow serves a community of over 80 researchers.

What is Analytics, Really?

- Intersection of:
  - Visualization, analysis, scientific data management, human-computer interfaces, cognitive science, statistical analysis, reasoning, …
- No such thing as Microsoft Analytics v1.0.
- Solutions are domain-specific combinations of above technologies.

Why Analytics, Really?

- All sciences need to find, access, and store and understand information.
- In some sciences the data management (and analysis) challenge already exceeds the compute-power challenge in its needed resources.
- The ability to tame a tidal wave of information will distinguish the most successful scientific, commercial, and national security endeavors.
- It is the limiting or the enabling factor for a wide range of sciences.

Why Analytics at NERSC?

- Clear scientific need (next slide).
- Small change in program focus likely to have profound positive impact on science.
- High likelihood of success:
  - World-class support for computational science projects.
  - Excellent existing infrastructure and program.
  - Building upon well-established visualization program at NERSC.
  - Clear, focused analytics strategy.

2002 Visualization Greenbook

Analytics Topics

- Users highly value institutional visualization support.
- Establish a coherent program that focuses on remote visualization.
- Establish mechanisms whereby generally applicable visualization technology is developed and deployed in a centralized fashion.
- Develop new programs that:
  - Link visualization with data management.
  - Support multiresolution representations of large datasets.
  - Support simultaneous display from disparate sources.
  - Support the ability to generate and display derived quantities, and the ability to pose queries and display results.
- Develop a research program in interactive visualization with running codes that stresses the integrated design and development of coupled simulation-visualization methods.
- Establish a research program in the areas of multi-field and multidimensional data visualization.
- Automated data exploration for petascale datasets.
- Enhance life sciences visualization with particular emphasis upon the relationship with SDM.

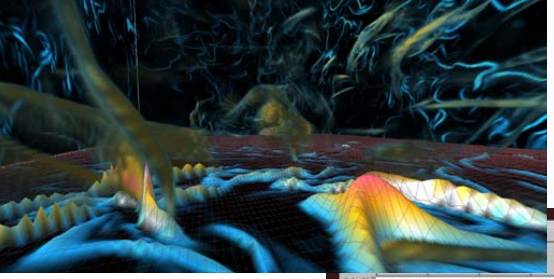
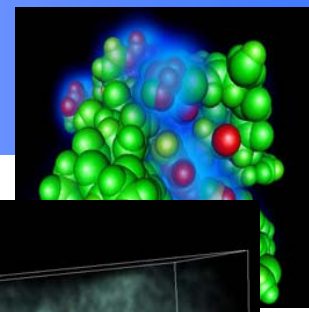
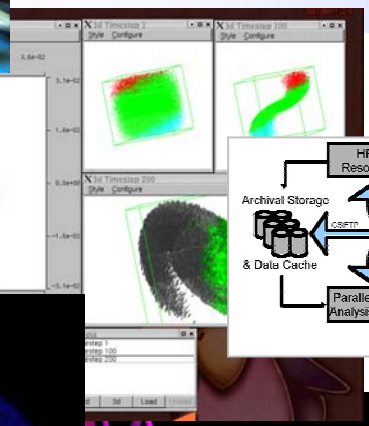
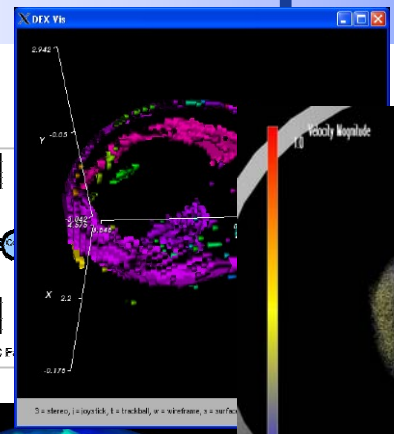
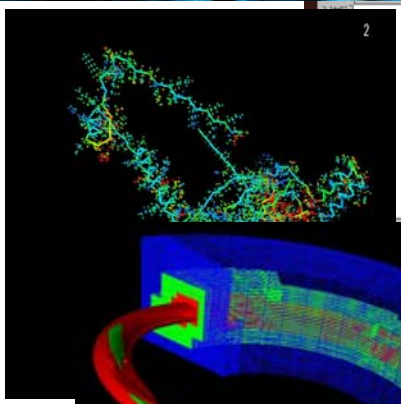
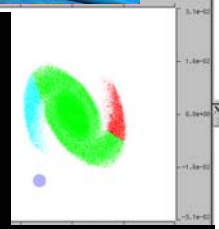
NERSC's Analytics Strategy

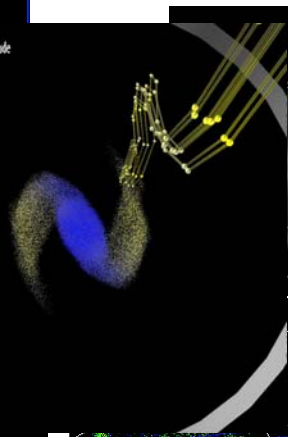
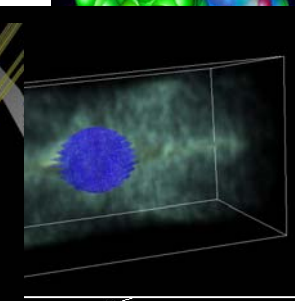
- **NERSC Analytics Strategy :**
  - **Objective: Improve scientific productivity by increasing analytics capabilities and capacity for NERSC user community.**
  - **Several key strategy elements: scientific data management, visualization, analysis, support and integrated activities.**
- **Tactics: How to Accomplish Objectives**

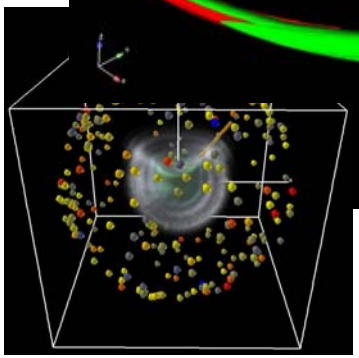
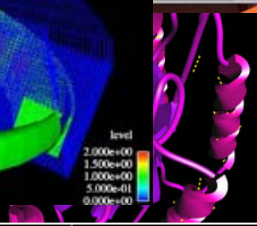
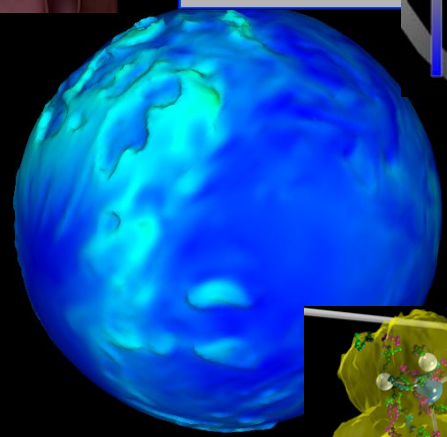
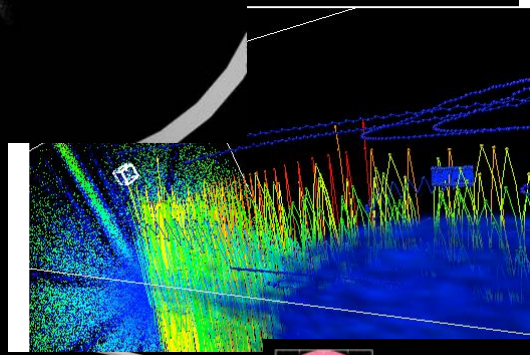
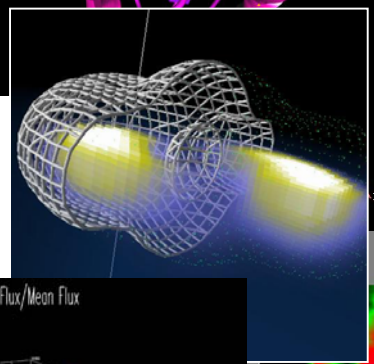
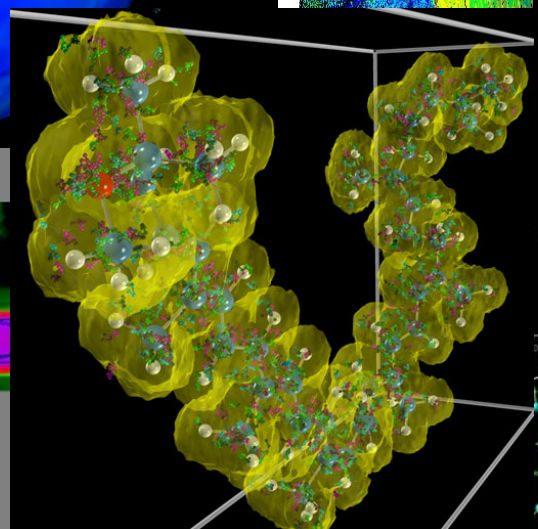
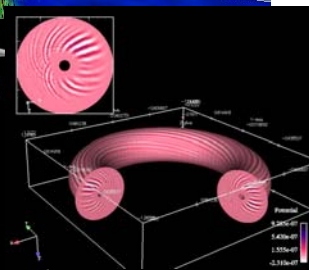
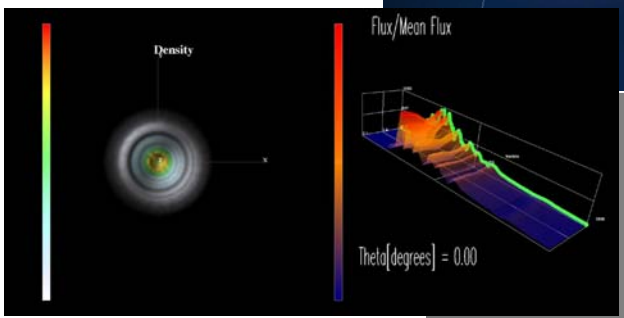
NERSC's Analytics Strategy

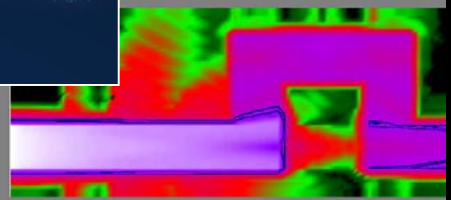
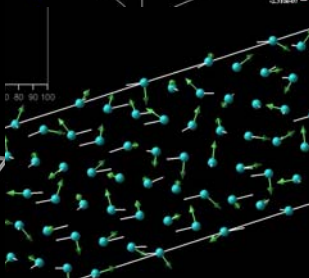
- **Broad strategic program objectives:**
  - **Clear picture of user needs.**
  - **Leverage existing and provide new visualization and analysis capabilities.**
  - **Enhance data management infrastructure.**
  - **Enhance distributed computing infrastructure.**
  - **Realizing analytics: support for the NERSC user community.**

Leverage Existing Visualization Capabilities

Enhance Data Management Infrastructure

- Strategic objective: increase capability and capacity of NERSC's data management infrastructure.
- Tactics:
  - Store and retrieve more bytes more quickly: global unified parallel filesystem, storage expansion.
  - Project-driven data management infrastructure:
    - Store and find data: RDBMs (record), SRM (file), FastBit (cell), others.
    - Move data: SRM (file), Logistical Networking (file), Tsunami (protocol), switched lambdas (link).
    - Share data: MDSPlus (field, variable), SRM (file).
- Leveraging experience: HPSS, PPDG, MDSPlus, Logistical Networking.

Programmatic Comments

- Analytics is a new term and a new field.
  - It is a problem-rich research environment.
- The focus of NERSC Analytics program is not research. Program focus is on:
  - Adapting, tuning, and deploying research prototypes along with hardened technology.
  - Close interactions with CS research community figure prominently in achieving tactical objectives.
  - Working with research-grade software is often a groundbreaking activity.
- Ongoing evolution of user needs.

Conclusion

- **Analytics:**
  - **Intersection of analysis, scientific data management, visualization, …**
  - **Addresses the fundamental problem of information understanding that faces modern science.**
- **NERSC Analytics Strategy**
  - **Deploy and apply constituent analytics technologies.**
  - **Project- and community-centric targeted impact.**

Conclusion

- **Objective**
  - **Increase scientific productivity.**