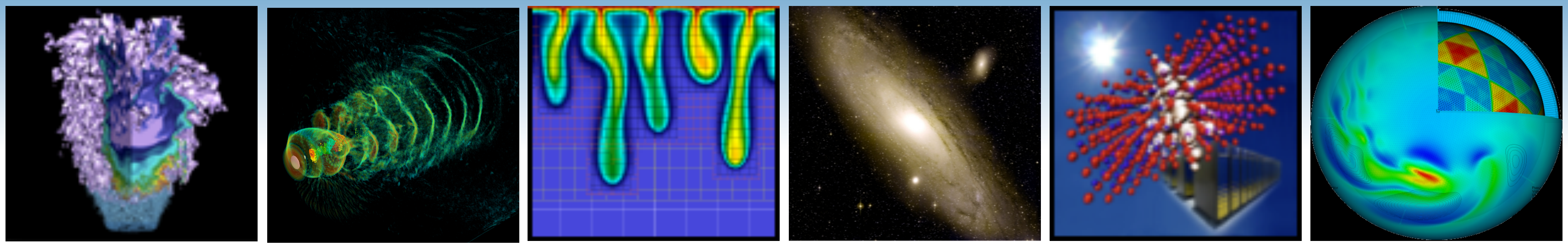

Workshop Goals & Process

Large Scale Computing and Storage Requirements for Advanced Scientific Computing Research

Joint ASCR / NERSC Workshop
January 5-6, 2011
Oakland Scientific Facility

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC National Energy Research Scientific Computing Center

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Logistics: Schedule

- **Agenda on workshop web page**
  - http://www.nersc.gov/projects/science_requirements/ASCR/agenda.php
  - Need your presentation slides
- **Mid-morning / afternoon break, lunch**
- **Self-organization for dinner**
- **5 "science areas," one workshop**
  - Science-focused but cross-science discussion
  - Explore areas of common need
- **Breakout sessions Weds AM**

Why is NERSC Collecting Computational Requirements?

- **Requirements help ASCR and NERSC make informed decisions for technology and services.**
- **Input is used to guide procurements, staffing, and to improve the effectiveness of NERSC services.**
  - Includes hardware, software, support, data, storage, analysis, work flow
  - Time frame: 2014
- **Result: NERSC can better provide what you (& other NERSC users) need**

Logistics: What is a Case Study?

- **One case study for each presentation.**
  - Table with quantitative estimates of needs
  - Narrative to justify the quantitative estimates
    - Describe <u>science</u> goals, methods
      - Audience is NERSC, DOE program managers
    - Current NERSC requirements
    - How science goals may change (2014)
    - Future NERSC requirements as a result
    - NERSC service requirements (and changes)
    - How you are dealing with architecture changes and what you need from NERSC
- ***<u>Not</u>* about justifying the science, methods, funding**

Logistics: Case Studies

- **Two kinds of research represented:**
  - Simulation
  - Simulation infrastructure
- **Two Themes for Some Case Studies**
  - NERSC requirements for your work.
  - Your estimate of how changes in your field may result in resource requirement changes for the broader NERSC workload.

Some Reference Material

- **Previous NERSC Workshop reports:**
  - BER
  - HEP
  - www.nersc.gov/projects/science_requirements/ASCR
    - Reference Material

Questions?

THANK YOU.

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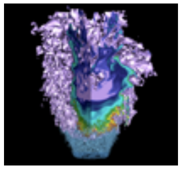
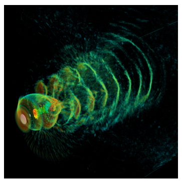
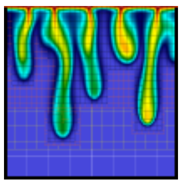
About the Cover



Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.

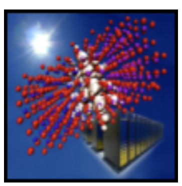


Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL. Image courtesy of Cameron Geddes.

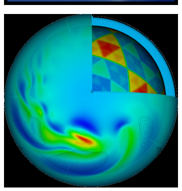


Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving the security of CO_2 storage. Image courtesy of George Pau, LBNL

False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PFT) camera in February 2009. NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod. Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



Simulation of a global cloud resolving model (GCRM). This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.