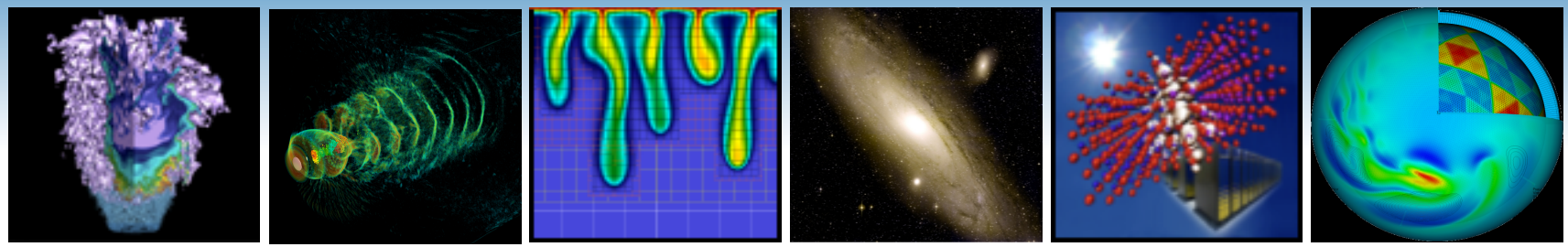


NERSC Science Highlights

A selection of science results produced by NERSC users

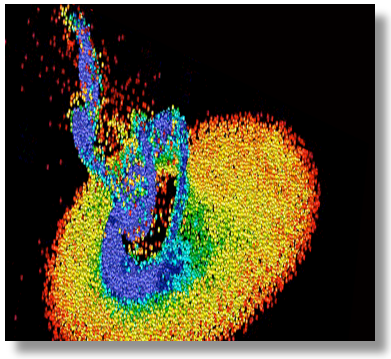
March, 2011

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC National Energy Research Scientific Computing Center

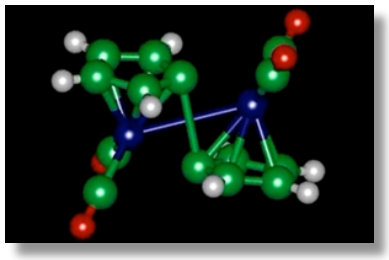
BERKELEY LAB

NERSC User Scientific Accomplishments March, 2011



Dark Matter

Simulations done at NERSC helped validate a key new method that reveals a dark companion to the Milky Way.
(S. Chakrabarti, UC Berkeley)

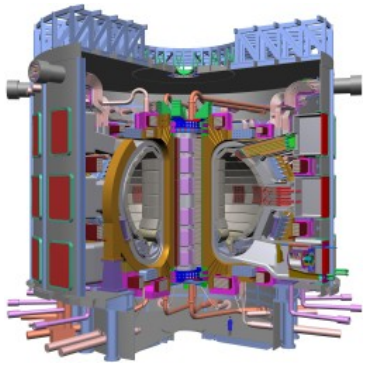


Energy Resources

Simulations suggest substantial promise for creating batteries from molecules that can reversibly store solar energy as heat.
(J. Grossman, MIT)

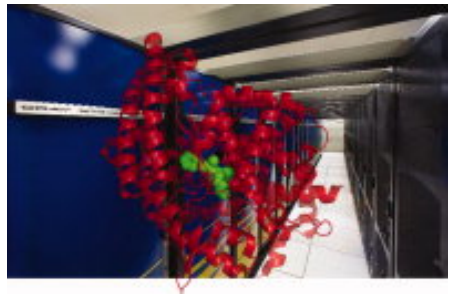
Fusion

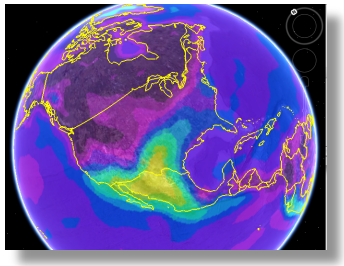
Study supported by NERSC NISE award suggests ITER might require an alternate mitigation strategy for "runaway electron" current.
(V. Izzo, General Atomics)



Proteins

Franklin is used to analyze a new parallel autodocking technique; on Hopper the technique helps identify environmental pollutants.
(B. Collignon, ORNL)





Climate

Huge historical weather database provides "time machine" for climate scientists.
(G. Compo, U. Colorado)

Catalysis

Calculations show why a nanocluster may be "just right" for recycling carbon dioxide by converting it to methanol.
(P. Liu, BNL)

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Dark Galaxy Detected

***Objective*: Validate a new method for detecting undiscovered galactic entities by analysis of their gravitational imprint**

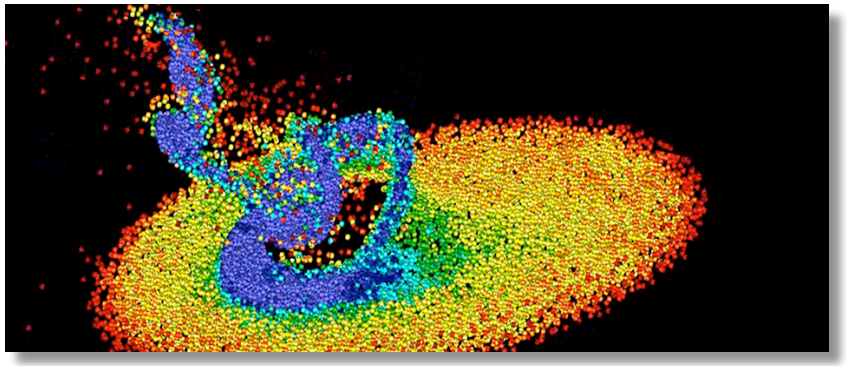
***Implications*: First discovery of a dark companion to our Milky Way galaxy.**

***Accomplishments:* Simulated the tidal interaction between two galaxies using GADGET-2 (an "N-body" code to model gravitation) and smooth particle hydrodynamics to model a gas.**

- **Analysis of cold gas ripples on galactic outskirts suggests mass and location of neighboring satellites.**
- **New method to detect dark matter.**

- ***NERSC:* Key visualization support; NERSC Global Filesystem support.**

S. Chakrabarti, L. Blitz (UC Berkeley)



Results from a simulation using the new method to show how the Whirlpool Galaxy M51 interacts with its known satellite galaxy. The new method is expected to have broad implications for astronomy and astrophysics.

The Astrophysical Journal, 731:40 (9pp), 2011 April 10

U.S. DEPARTMENT OF ENERGY | Office of Science | HEP

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Rechargeable Heat Batteries

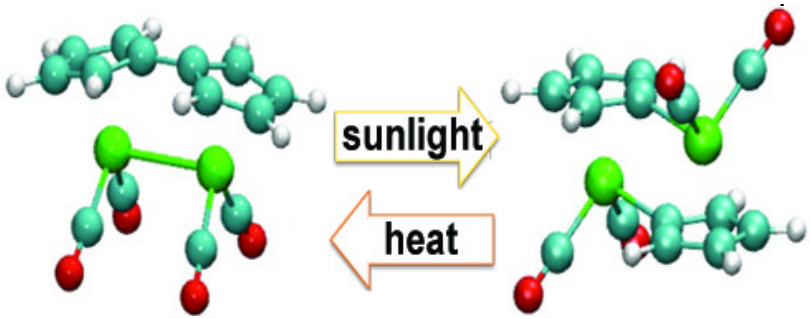
***Objective*: Investigate electronic structure of novel materials to harvest solar power**

***Implications*: Batteries that reversibly trap solar energy in the form of chemical bonds would improve energy storage & transportability.**

***Accomplishments*: Performed first-principles Density Functional Theory calculations on a highly promising solar fuel candidate.**

- **Provided detailed atom-scale awareness of key conversion and storage mechanisms limiting its performance.**
- **Findings indicate substantial promise for this class of molecule for both energy capture and storage.**

J. Grossman (MIT)



A model of the molecule that reversibly changes it structure when it absorbs heat. Red = oxygen; blue = carbon; green = iron; white = hydrogen. Simulations at NERSC suggest substantial promise for creating batteries from molecules that can reversibly store solar energy as heat.

Angewandte Chemie International Edition
Vol 49 (47) 8926–8929,
October 14, 2010

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Runaway Electrons Affect ITER

***Objective*: Understand safe termination of fusion plasmas that undergo rapid unexpected discharges**

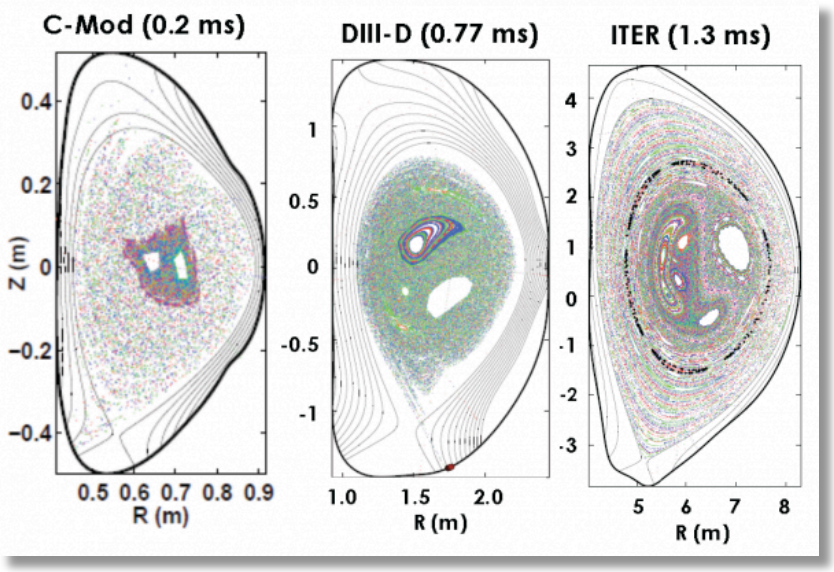
***Implications*: Will help predict scenarios requiring quick tokamak shut down to avoid damaging reactor components.**

***Accomplishments*: Simulated "runaway electron" (RE) current on ITER and two smaller tokomaks; results showed big differences in RE confinement.**

- **Demonstrated that magnetohydrodynamic (MHD) effects appear to transport REs out of the plasma for smaller devices; not so for ITER.**
- **Alternate strategies for RE mitigation and control may be needed in ITER.**

- ***NERSC*: NISE award in 2010 enabled this work; Franklin runs used up to 6,480 cores**

Valerie Izzo (General Atomics)



NERSC simulation results from three tokomak devices clearly showing that runaway electron current losses due to disruption related MHD fluctuations decrease with increasing vessel size and that **alternate strategies for RE mitigation/control may be needed in ITER.**

23rd IAEA Fusion Energy Conference, Daejon, Korea, (2010)

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20th Century Reanalysis

Objective: **Reconstruct global weather conditions in 6-hour intervals, 1871 – 2010**

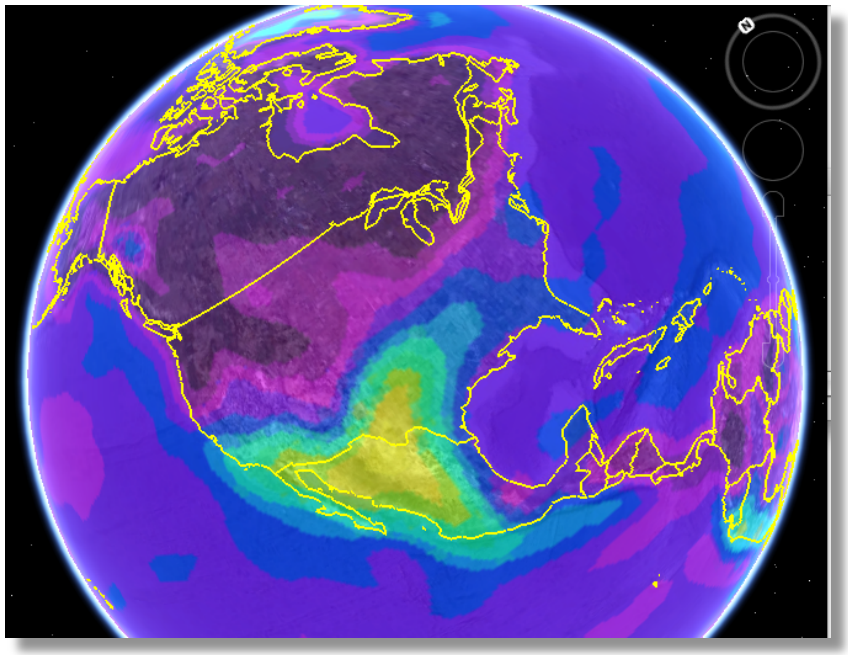
Implications: **Help explain long-term impact of extreme weather by recreating and explaining past climate anomalies.**

Accomplishments: **Completed the first 3-D global weather database covering 150 yrs.**

- **Provided missing information about extreme climate events that may have misinformed earlier policy decisions.**
- **Will be an important validation tool for climate models used in making 21st Century climate projections.**

NERSC: **NERSC NISE award, 2010; Selected fields from the dataset are made available via a NERSC science gateway; key long-term NERSC Global Filesystem and user services roles.**

G. Compo (U. Colorado)



1000mb Relative Humidity (%) Composite Mean for 1920-1929, from 20th Century Reanalysis V2. Visualized by GoogleEarth.

Quarterly Journal of the Royal Meteorological Society, 137: 1 – 28, January 2011 Part A

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Faster Computational Docking

Objective: **Develop a faster version of a valuable molecular modeling technique known as protein-ligand docking**

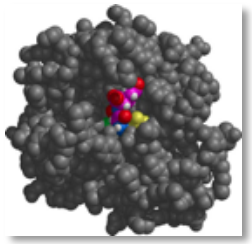
Implications: **Could speed development of new drug treatments and other products.**

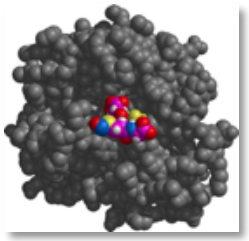
Accomplishments: **Developed an MPI-parallel method to scan the most widely-used molecular database (Autodock4).**

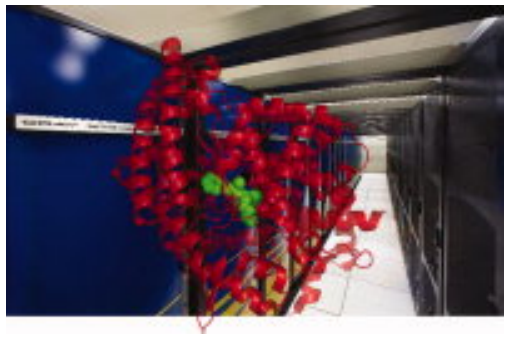
- **Allows rapid protein docking at unprecedented scale.**
- **Could provide a "missing link" between supercomputers and huge molecular databases like the Human Genome Project**

- ***NERSC:*** **3.7M early user Hopper hours were used for high-throughput screening of an EPA database to identify environmental pollutants that may have estrogenic properties; used 16 – 65k cores.**

B. Collignon, R. Schulz, J. Smith, J. Baudry (ORNL)







Conceptual view of a protein showing two possible docking orientations for a ligand. Docking programs try to identify the best of all possible orientations.

An illustration of a protein structure superimposed on NERSC's Franklin system, which was used to understand the scalability of the newly parallel Autodock method. This image appeared in the journal's table of contents.

Journal of Computational Chemistry, Vol 32(6) pp1202–1209, 30 April 2011

U.S. DEPARTMENT OF ENERGY | Office of Science | BER

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Recycling Carbon Dioxide

Ping Liu (BNL)

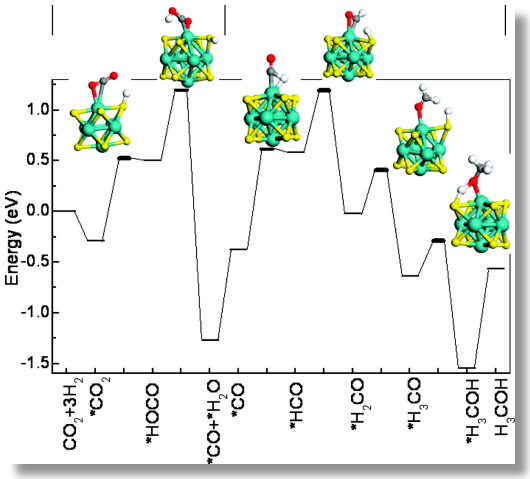
***Objective*: Study small metal clusters supported on nanoparticles to help design improved catalysts for key reactions**

***Implications*: Moves us a step closer to inexpensive conversion of waste gases into valuable chemical products and fuels.**

***Accomplishments:* Revealed the mechanism for catalytic activity of molybdenum-sulfur clusters in synthesis of alcohol from water and carbon dioxide.**

- **Explained the unexpected catalytic activity and why the clusters are more selective than bulk metal.**
- **May assist in real catalysis of reactions that can use waste carbon dioxide.**

***NERSC:* Accomplished with .ca 45,000 hours on Franklin using ~800 cores per job in 2009.**



Individual steps in the synthesis of methanol (CH_3OH) from CO_2 and H_2 on a Moly-sulfide cluster as discovered using Density Functional Theory calculations on Franklin at NERSC.

J. Phys. Chem. A, 2010, 114 (11), pp 3888–3895
(featured on the journal cover)

U.S. DEPARTMENT OF ENERGY | Office of Science | BES

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Computational Chemistry for Better Batteries

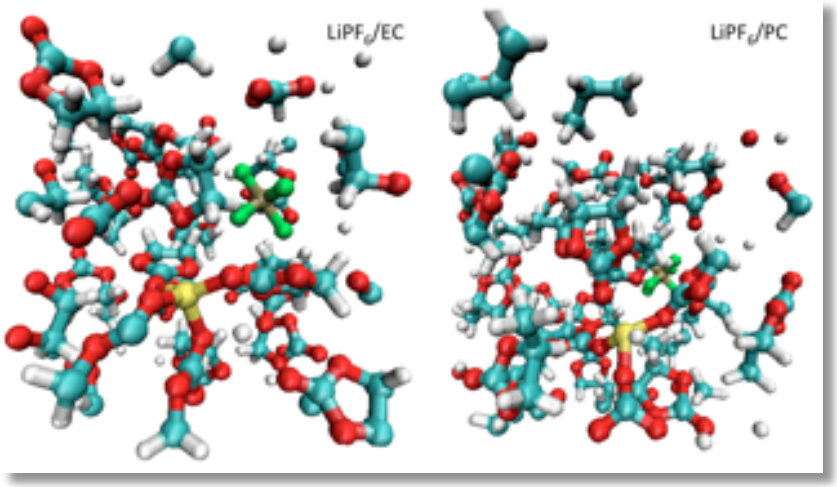
***Objective*: Predict & optimize the structure of fluid-solid electrolyte interfaces that are important in future energy technologies**

***Implications*: Lithium-ion batteries are an example; finding the right electrolyte for them could revolutionize transportation.**

***Accomplishments*: Used molecular dynamics simulation to determine, for the first time, accurate solvation models, diffusion coefficients, and solvation energies for lithium ion in two contrasting electrolytes.**

- **Another key example of simulation/ experiment interplay; helps explain neutron, X-ray, NMR, and optical data.**
- **Simulations are more accurate than "classsical" simulations and agree well with experiments.**

P. Kent, P. Ganesh, De-en Jiang (ORNL)



Simulation results for lithium ion in two solvents, ethylene-carbonate (left) and propylene-carbonate (right).

J. Phys. Chem. B, 115 (12), pp 3085–3090 (2011)

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Nanofluids Change Phase

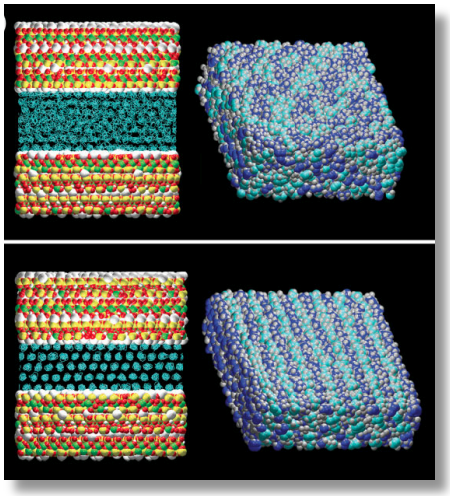
***Objective*: Atomistic simulations to understand structural and rheological properties of nanoconfined fluids - fluids confined between surfaces separated by just a few nanometers**

***Implications*: Could aid in rational design and control of lubricants for disk drives and microelectromechanical systems (MEMS).**

***Accomplishments:* Convincingly demonstrated that certain nanofluids undergo an abrupt, reversible phase transition into a solid (that would render it useless as a lubricant).**

- **Showed how increasingly high fidelity molecular simulations provide the ability to understand complex experimental findings, particularly at the nanoscale.**

Peter Cummings (Vanderbilt U)



Results of molecular dynamics simulations run on Franklin showing an organic molecule (blue) confined between two surfaces (red, white, green, and yellow). At a separation of about 41 nanometers (top) the molecule remains fluid-like but at about 30 nanometers (bottom), the molecule undergoes a rapid and abrupt transition to an ordered solid-like structure.

American Institute of Chemical Engineers Journal, Vol 56(4) April 2010 842-848 (cover story)

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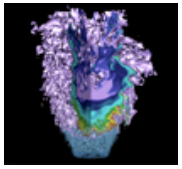
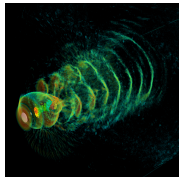
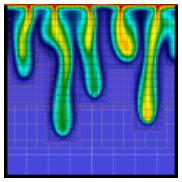
About the Cover Images



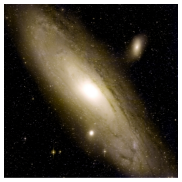
Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive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



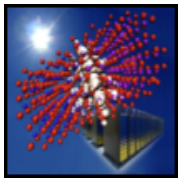
Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour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



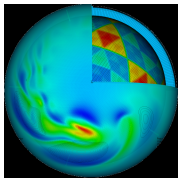
Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving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