Overview of NLCF FY 2006 Allocations

NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES

presented by

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NCCS – Scientific Computing Group

OUTLINE OF PRESENTATION

- Background of Center
- Brief Overview of Projects
- Summary of CCSE and Super Nova Core-Collapse Projects
- Conclusions

Background

- 1992 - The National Center of Computational Sciences (NCCS) was established
- 2004 - NCCS was designated a Leadership Computing facility by the Secretary of Energy Spencer Abraham
- 2005 - Opened for Computational Scientific Research
- Present day - Core NCCS computational resources:
  - Phoenix (Cray X1E): 1024 multi-streaming vector processors (MSPs), where each MSP has 2 MB of cache and a peak computation rate of 18 GF
  - Jaguar (Cray XT3): 5294 nodes, each with a 2.4-GHz, AMD, Opteron processor and 2 GB of memory. 5212 nodes are available in the compute partition

Phoenix

Jaguar

Allocations

- LCF
  - Open to scientific research consistent with the missions of the Department of Energy (DOE) Office of Science
- Incite
  - Open to scientific research for DOE, other government agencies, academia, or industry.

Overview of Allocations

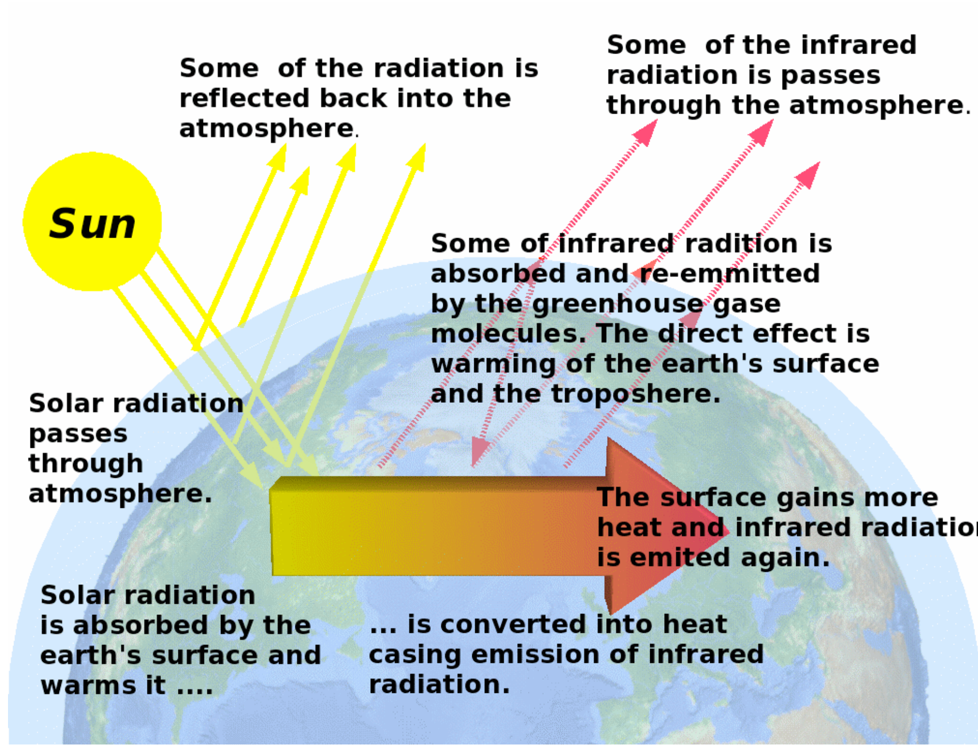
- **Climate and Carbon Research (3)**
  - Climate-Science Computational End Station Development and Grand Challenge Team; PI - W. Washington; National Center for Atmospheric Research (LCF)
  - The Role of Eddies in the Thermohaline Circulation; PI - P. Cessi; Scripps Institution of Oceanography (LCF)
  - Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean; PI - S. Peacock, University of Chicago (LCF)
- **Astrophysics (3)**
  - Multi-dimensional Simulations of Core-Collapse Supernovae; PI - A. Mezzacappa; Oak Ridge National Laboratory (LCF)
  - Multi-dimensional Simulations of Core-Collapse Supernovae; PI - A. Burrows; University of Arizona (LCF)
  - Ignition and Flame Propagation in Type Ia Supernovae; PI – S. Woosley; University of California, Santa Cruz (LCF)
- **Fusion (4)**
  - Gyrokinetic Plasma Simulation; PI - W. W. Lee; Princeton Plasma Physics Laboratory (LCF)
  - Exploring Advanced Tokamak Operating Regimes Using Comprehensive GYRO Gyrokinetic Simulations; PI - J. Candy; General Atomics (LCF)
  - Simulation of Wave-Plasma Interaction and Extended MHD in Fusion Systems; PI - D. B. Batchelor; Oak Ridge National Laboratory (LCF)
  - Interaction of ETG and ITG/TEM gyrokinetic turbulence; PI - R. Waltz; General Atomics (I)
- **Combustion (1)**
  - High-Fidelity Numerical Simulations of Turbulent Combustion - Fundamental Science Towards Predictive Models, PI – J. Chen, Sandia National Laboratories (LCF)
- **Nuclear Physics (1)**
  - *Ab-initio* Nuclear Structure Computations; PI – D. J. Dean; Oak Ridge National Laboratory (LCF)

Overview of Allocations

- Computational Biology (2)
  - Next Generation Simulations in Biology: Investigating Biomolecular Structure; Dynamics and Function through Multi-scale Modeling; PI - P. K. Agarwal; Oak Ridge National Laboratory (LCF)
  - Molecular dynamics simulations of molecular motors; PI - M. Karplus; Harvard University (I)
- Theoretical Chemistry (1)
  - An Integrated Approach to the Rational Design of Chemical Catalysts; PI - R. Harrison; Oak Ridge National Laboratory & University of Tennessee; (LCF)
- Materials and nanomaterials theory (2)
  - Predictive Simulations in Strongly Correlated Electron Systems and Functional Nanostructures; PI - T. Schulthess; Oak Ridge National Laboratory (LCF)
  - Direct Numerical Simulation of Fracture; Fragmentation and Localization in Brittle and Ductile Materials; PI - M. Ortiz; California Institute of Technology (I)
- High Energy Physics (2)
  - Monte Carlo Simulation and Reconstruction of CompHEP-produced Hadronic Backgrounds to the Higgs Boson Diphoton Decay in Weak-Boson Fusion Production; PI - H. Newmann; California Institute of Technology (LCF)
  - Computational Design of the Low-loss Accelerating Cavity for the ILC; PI - K. Ko; Stanford Linear Accelerator Center (LCF)
- Computer Science (1)
  - Performance Evaluation and Analysis Consortium (PEAC) End Station; PI - P. H. Worley; Oak Ridge National Laboratory (LCF)
- Industry (2)
  - Real-Time Ray-Tracing; PI - Evan Smyth; Dreamworks (I)
  - Development and Correlations of Large Scale Computational Tools for Flight Vehicles; PI - M. Hong; The Boeing Company (I)

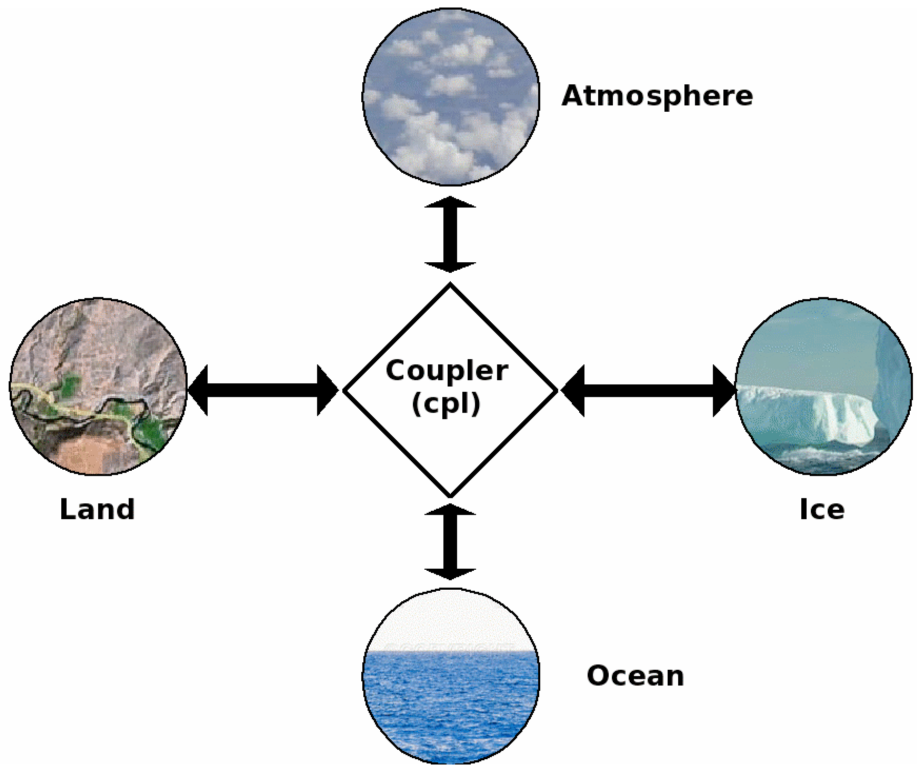
Climate-Science Computational End Station

- Climate science is the study of long term weather
- The greenhouse effect
- The Climate-Science Computational End Station (CCSE) project at the NCCS focuses on climate prediction based on various scenarios of anthropogenic emissions and energy policies.



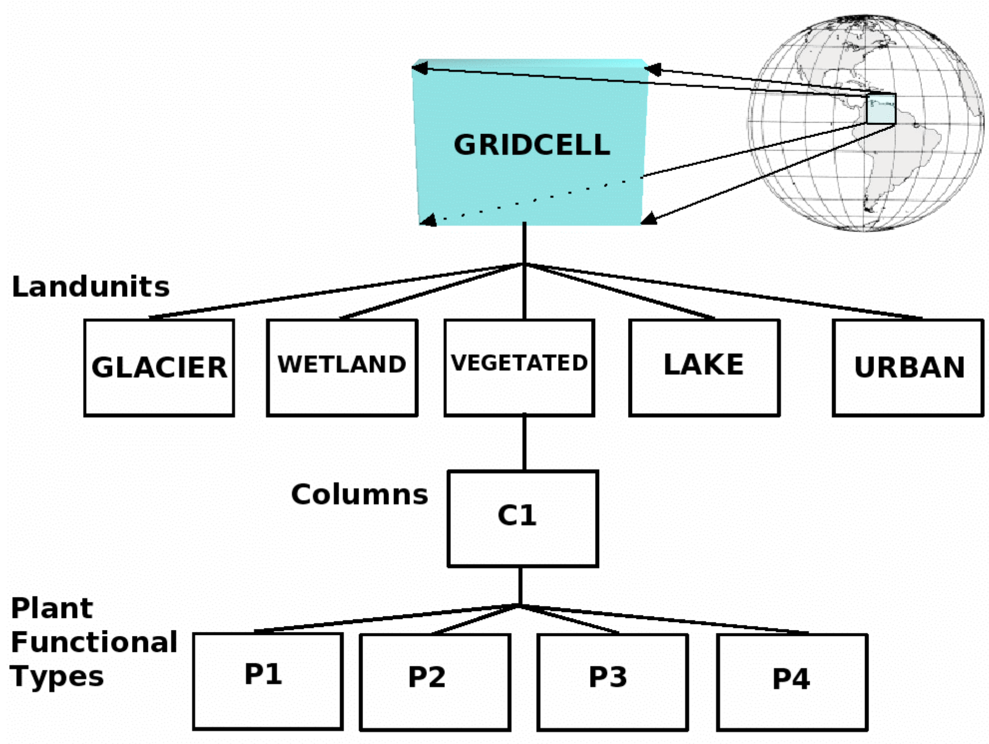
CCSM Framework

- The CCSM consists of four individual component models - representing the atmosphere, the land surface, the oceans, and sea ice - connected by a coupler



Community Land Component

- Spatial land surface heterogeneity in CLM is represented as a nested subgrid hierarchy in which grid cells are composed of multiple landunits, snow/soil columns, and PFTs.
- A grid cell can have a different number of landunits,
- A landunit can have a different number of columns.
- A column can have multiple PFTs.
- The landunit captures the broadest spatial patterns of subgrid heterogeneity. The specific landunits are glacier, lake, wetland, urban, and vegetated. Physical soil properties such as texture, color, depth, and thermal conductivity are defined at the landunit subgrid level and hence landunits can vary in soil properties.
- The columns are intended to capture potential variability in the soil and snow state variables within a single landunit.
- The PFT level is intended to capture the biogeophysical and biogeochemical differences between broad categories of plants in terms of their functional characteristics.

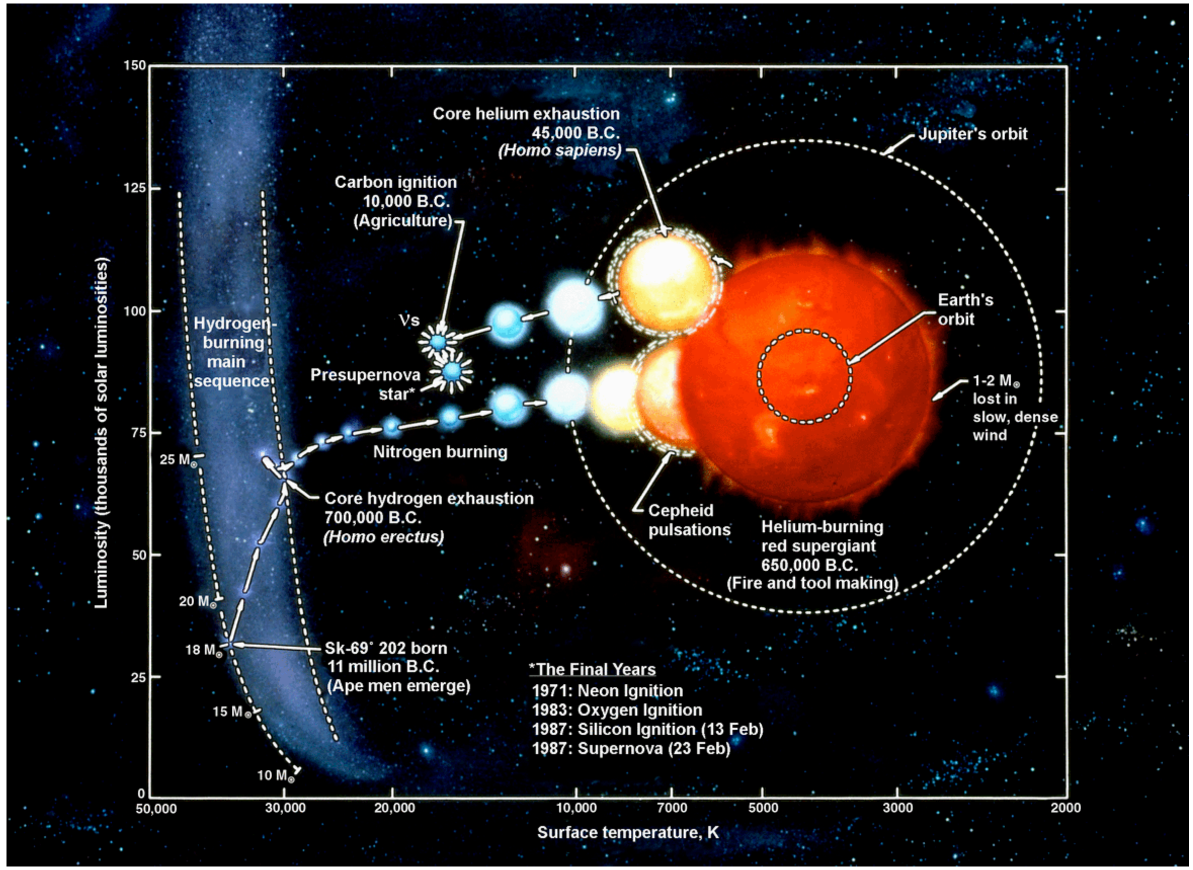


Significance of Research

- The primary end significance of this project is the culmination of large-scale data archives (100 TB) of climate simulations that will be available for the larger scientific community.
- Secondly, the CCSM model will be strengthened with greater spatial resolutions, integration of biogeochemistry, dynamic simulations, atmospheric chemistry, etc. – the simulations will become more realistic.
- Finally, climate change is important to nation and world. The simulations and model development proposed in this end station will provide the best tools as to date in making rational, energy policy decisions that will benefit the sustentation of planetary life.

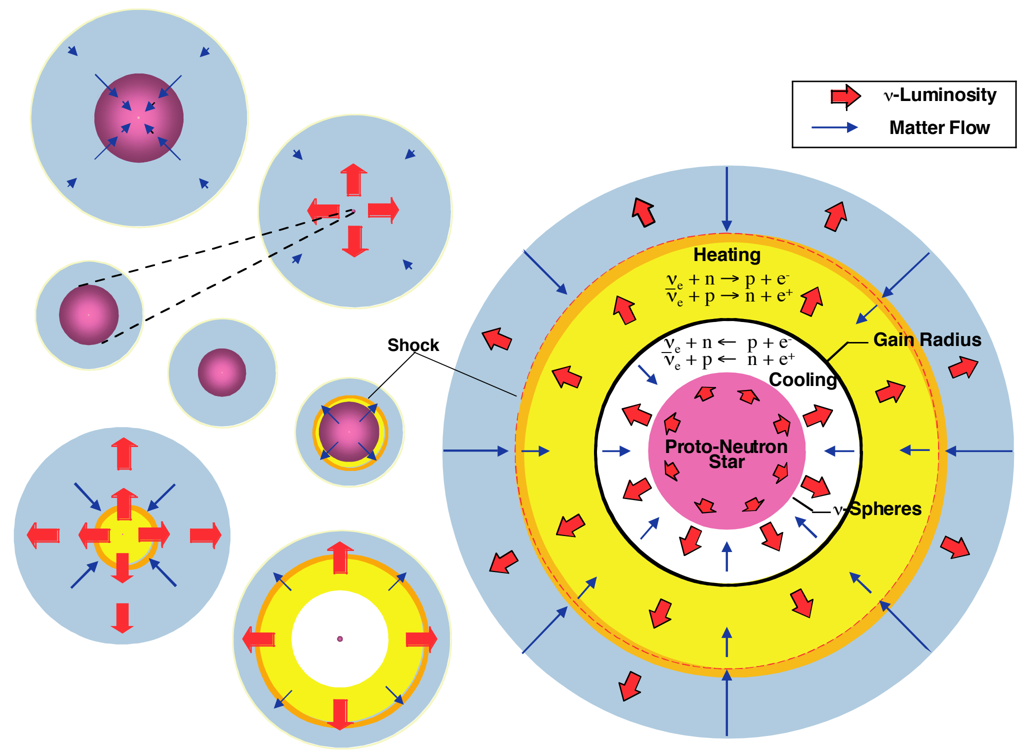
Multi-dimensional Simulations of Core-Collapse

- This project focuses on multi-dimensional simulations of the core collapse during their supernova stage.
- Large timescales associated with the formation of the stratified “onion skin” structure developed in massive stars - where an inner iron core is surrounded by shells of lighter elements, including, silicon, oxygen, helium, and hydrogen.



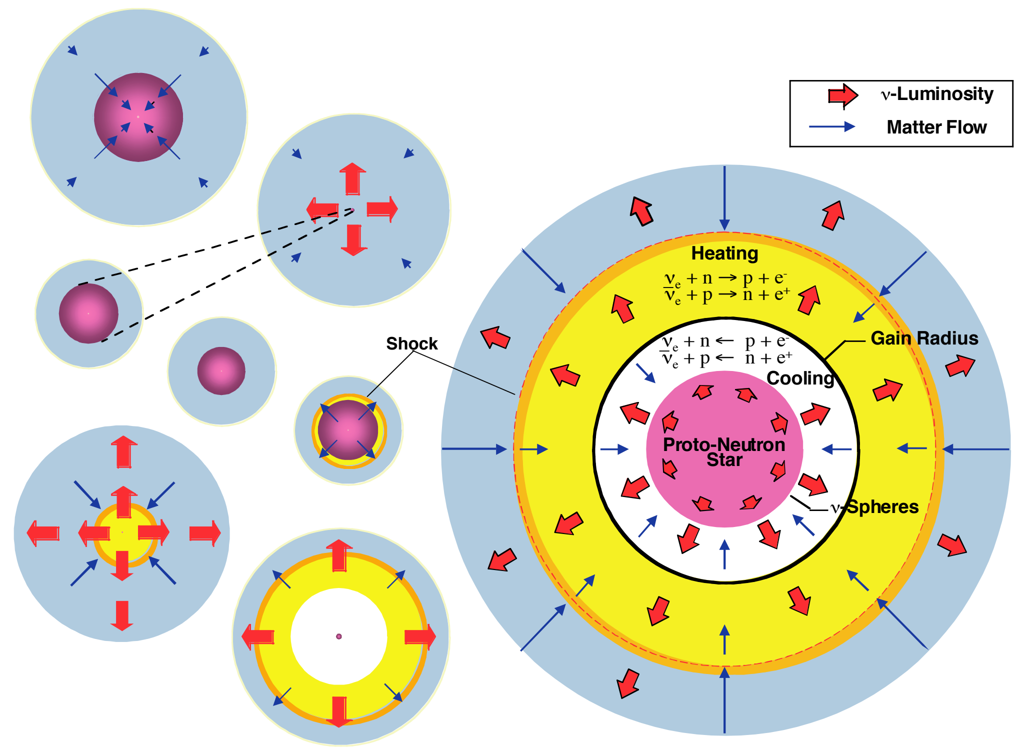
Supernova Core-Collapse Phenomena

- Shortly after reaching a central density of 109 g/cm^3, unable to support itself against its own gravity, the core collapses.
- When the inner core reaches 2-3 times the density of nuclear matter, it rebounds as a unit, sending pressure waves outward. These pressure waves steepen to form a shock at a radius of some tens of kilometers. This shock begins to propagate outward, heating and dissociating material as it moves to larger radii.
- But!!!! In most simulations, the shock stalls at a radius of ~200 km.
  - Dissociation losses as nuclei pass through the shock and are converted to free nucleons and helium
  - Electron capture on the resulting free protons, producing neutrinos that are able to escape the core.
- The simulations undertaken by this LCF project are designed to ultimately answer how the supernova shock wave is revived.



Proposed Computations

- 3D Hydrodynamics-only simulations to understand the role of a newly discovered supernova shock wave instability -The Stationary Accretion Shock Instability (SASI)
- 3D "ray-by-ray" neutrino transport, in which transport is restricted to radial rays and lateral transport is suppressed.
- 2D simulations with 2D multi-frequency neutrino transport.



Summary

- **National Center for Computational Sciences provides an unparalleled environment for enabling new discoveries that will dramatically impact the nation's ability to produce a secure energy economy and increase mankind's understanding of our world.**
  - Astrophysics
  - Climate and carbon research
  - Computational biology
  - Fusion simulation
  - Industrial innovation
  - Materials research
  - Nanomaterials theory

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