Science and Cyberinfrastructure in the Data-Dominated Era

Symposium #1610, How Computational Science Is Tackling the Grand Challenges Facing Science and Society

San Diego, CA

February 22, 2010

Dr. Larry Smarr

Director, California Institute for Telecommunications and Information Technology

Harry E. Gruber Professor,

Dept. of Computer Science and Engineering

Jacobs School of Engineering, UCSD

OptIPuter

it²

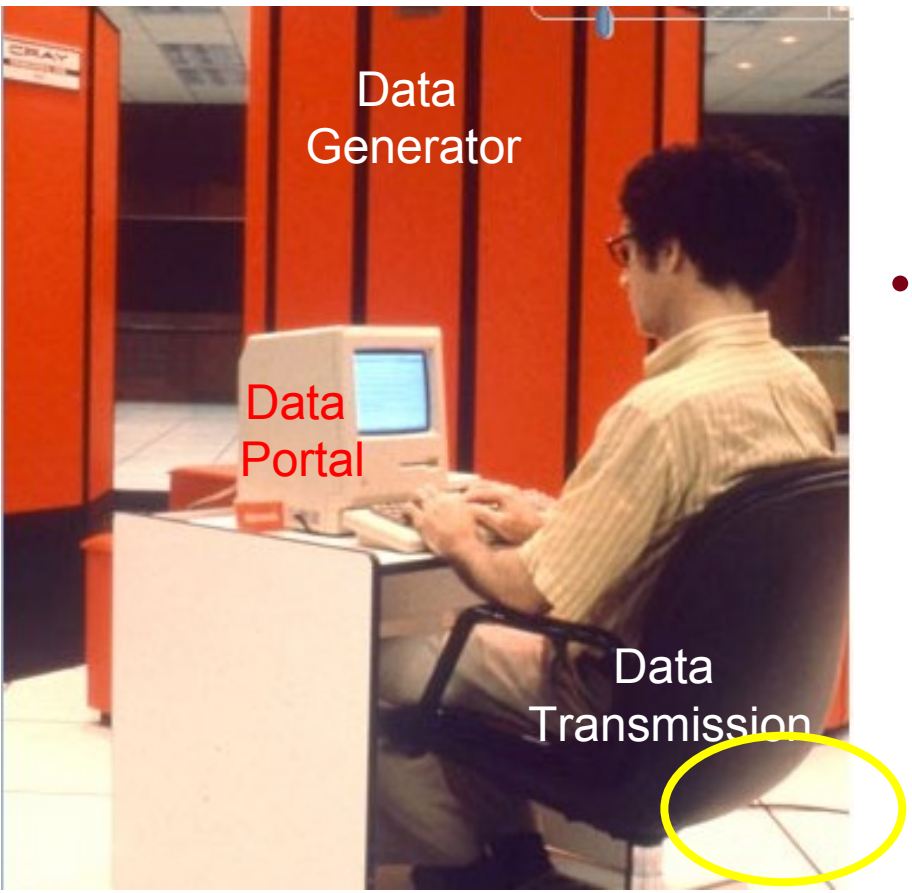
Abstract

The NSF Supercomputer Centers program not only directly stimulated a hundred-fold increase in the number of U.S. university computational scientists and engineers, but it also facilitated the emergence of the Internet, Web, scientific visualization, and synchronous collaboration. I will show how two NSF-funded grand challenges, one in basic scientific research (cosmological evolution) and one in computer science (super high bandwidth optical networks) are interweaving to enable new modes of discovery. Today we are living in a data-dominated world where supercomputers and increasingly distributed scientific instruments generate terabytes to petabytes of data. It was in response to this challenge that the NSF funded the OptIPuter project to research how user-controlled 10Gbps dedicated lightpaths (or "lambdas") could provide direct access to global data repositories, scientific instruments, and computational resources from "OptIPortals," PC clusters which provide scalable visualization, computing, and storage in the user's campus laboratory. The use of dedicated lightpaths over fiber optic cables enables individual researchers to experience "clear channel" 10,000 megabits/sec, 100-1000 times faster than over today's shared Internet—a critical capability for data-intensive science. The seven-year OptIPuter computer science research project is now over, but it stimulated a national and global build-out of dedicated fiber optic networks. U.S. universities now have access to high bandwidth lambdas through the National LambdaRail, Internet2's Dynamic Circuit Services, and the Global Lambda Integrated Facility. A few pioneering campuses are now building on-campus lightpaths to connect the data-intensive researchers, data generators, and vast storage systems to each other on campus, as well as to the national network campus gateways. I will show how this next generation cyberinfrastructure is being used to support cosmological simulations containing 64 billion zones on remote NSF-funded TeraGrid facilities coupled to the end-users laboratory by national fiber networks. I will review how increasingly powerful NSF supercomputers have allowed for more and more realistic cosmological models over the last two decades. The 25 years of innovation in information infrastructure and scientific simulation that NSF has funded has steadily pushed out the frontier of knowledge while transforming our society and economy.

OptIPuter

it²

NCSA Telnet--"Hide the Cray" Paradigm That We Still Use Today

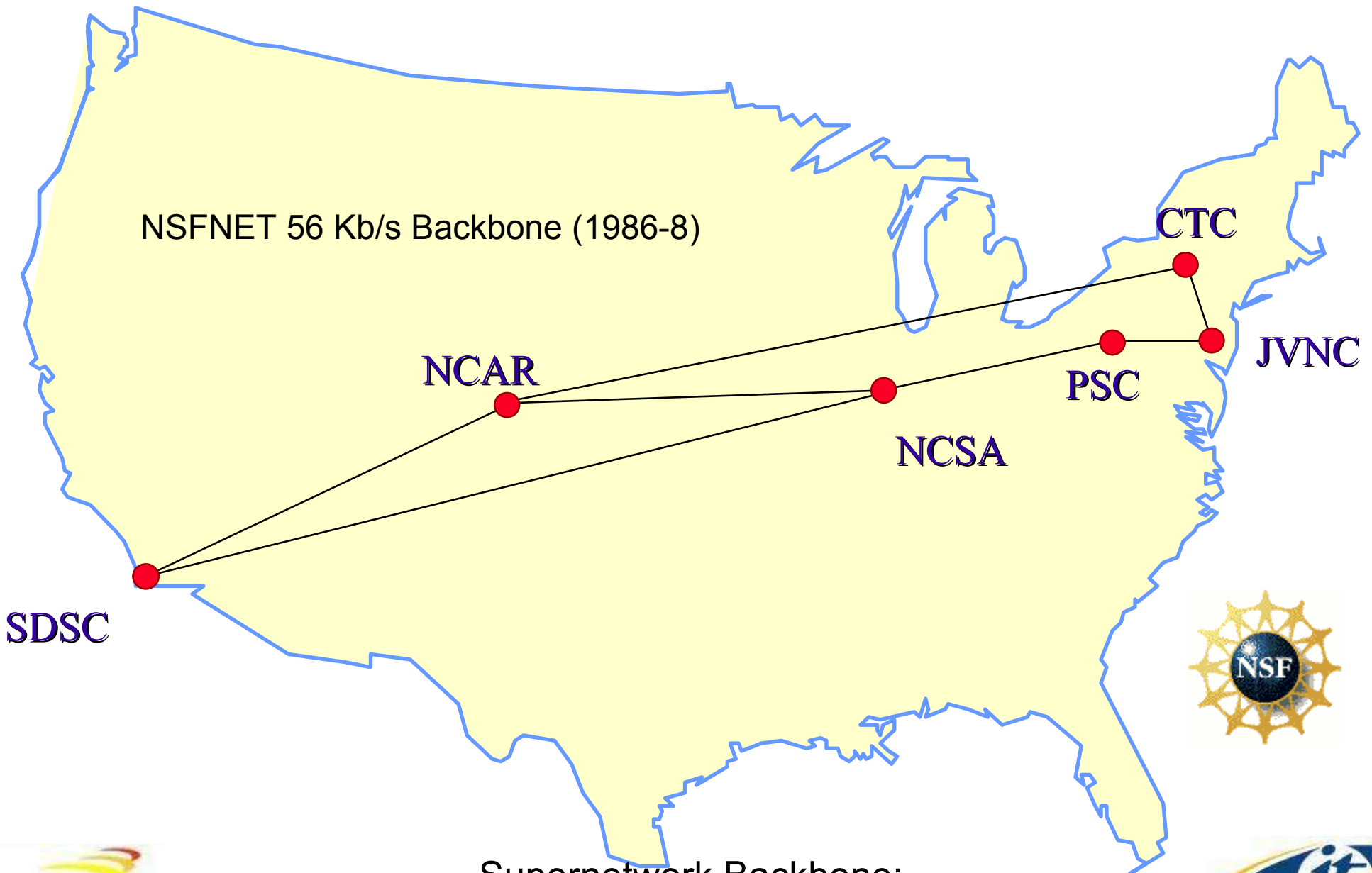


John Kogut Simulating
Quantum Chromodynamics
He Uses a Mac—The Mac Uses the Cray

- **NCSA Telnet -- Interactive Access**
  - **From Macintosh or PC Computer**
  - **To Telnet Hosts on TCP/IP Networks**
- **Allows for Simultaneous Connections**
  - **To Numerous Computers on The Net**
  - **Standard File Transfer Server (FTP)**
  - **Lets You Transfer Files to and from Remote Machines and Other Users**

Source: Larry Smarr 1985

Launching the Nation's Information Infrastructure: NSFnet Supernetwork and the Six NSF Supercomputers

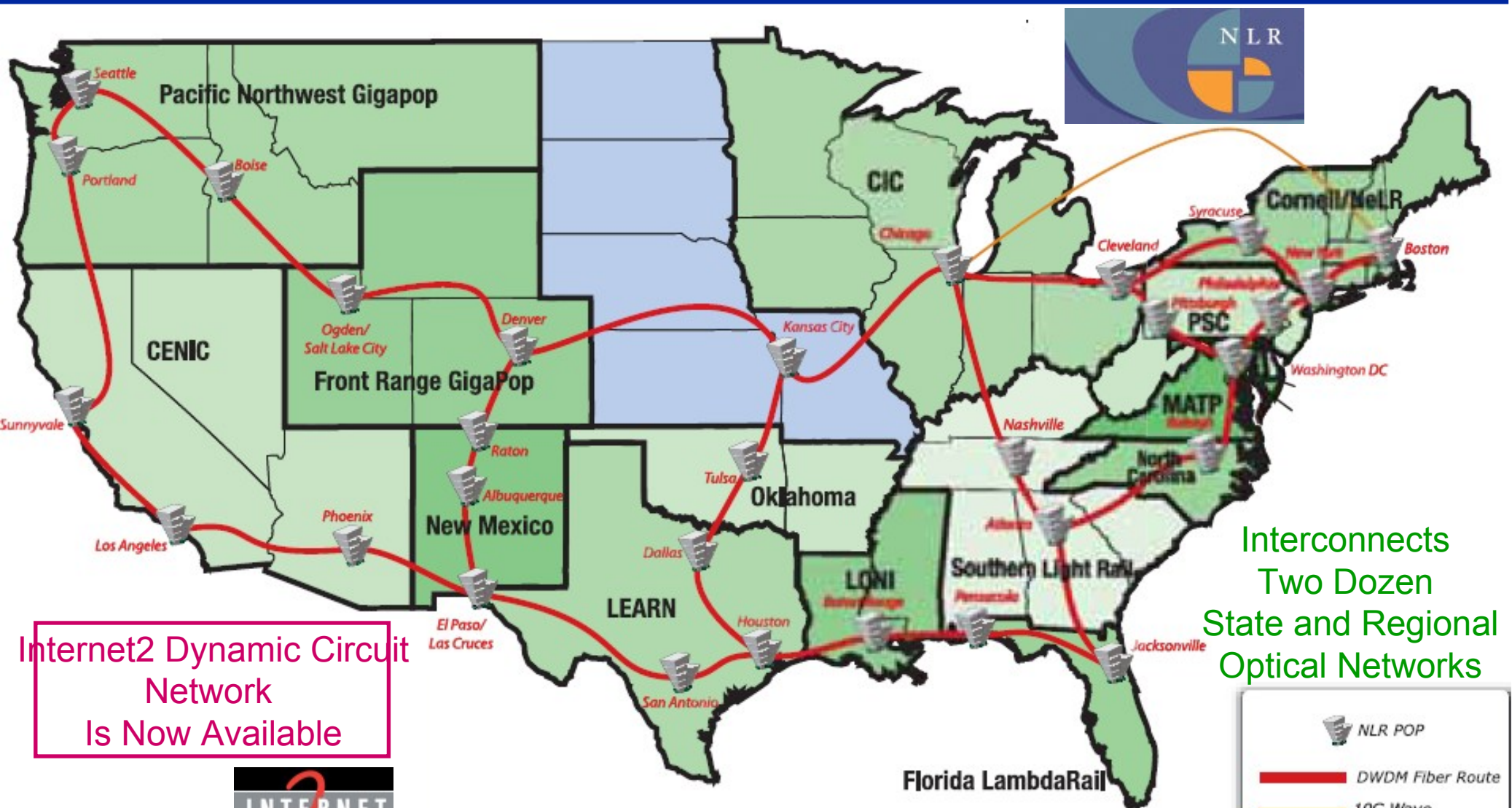


Supernetwork Backbone:
56kbps is 50 Times Faster than 1200 bps PC Modem!

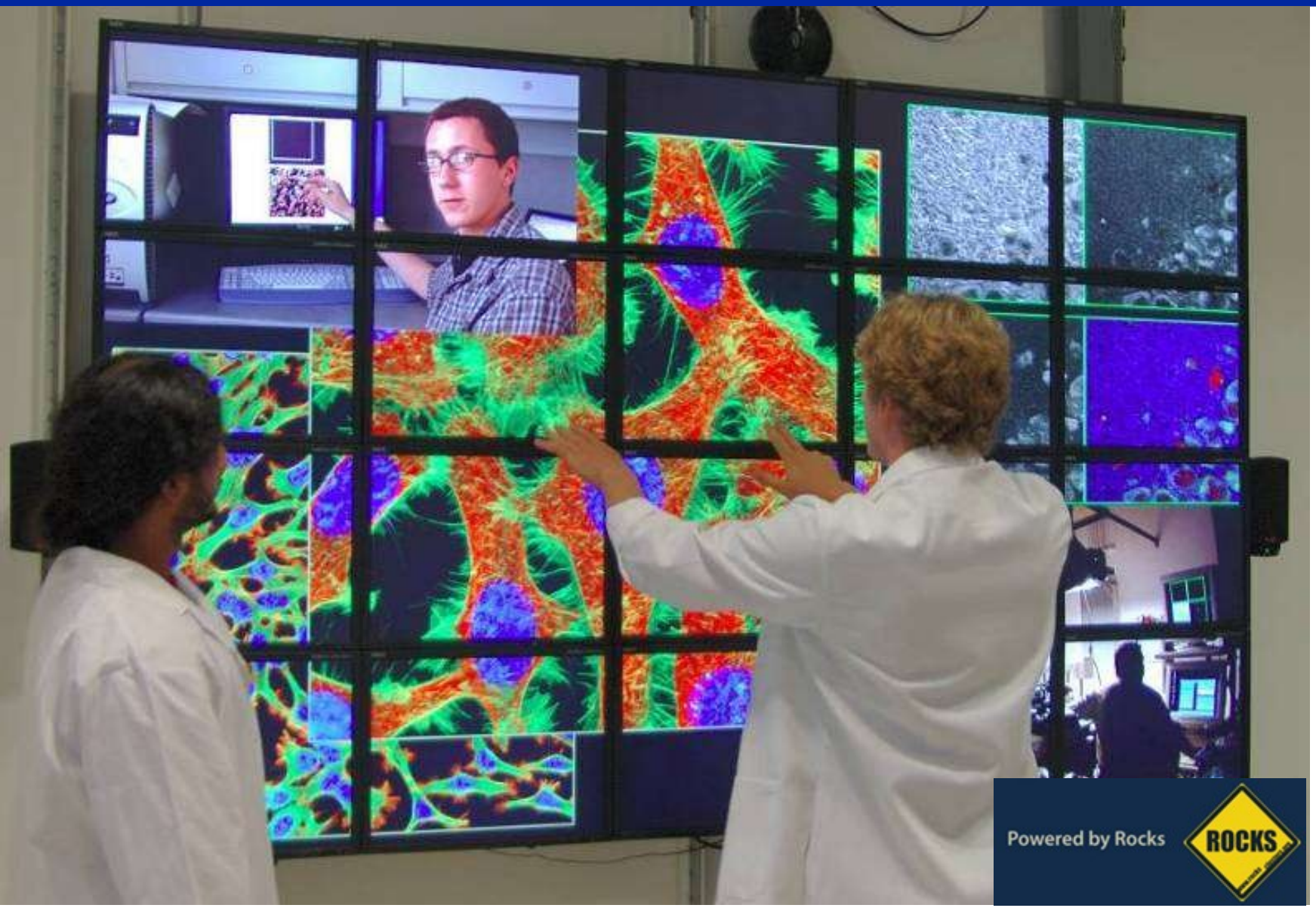
Why Teraflop Supercomputers Matter
For Accurate Science & Engineering Simulations

- FLOating Point OperationS per Spatial Point
  - Ten Variables
  - Hundred Operations Per Updated Variable
  - One Thousand FLOPS per Updated Spatial Point
- One Dimensional Dynamics
  - For 1000 Spatial Points Need MEGAFLOP
- Two Dimensions
  - For 1000x1000 Spatial Points Need GIGAFLOP
- Three Dimensions
  - For 1000x1000x1000 Spatial Points Need TERAFLOP
- Three Dimensions + Adaptive Mesh Refinement
  - Need PETAFLOP

Today Dedicated 10,000Mbps Supernetworks Tie Together State and Regional Fiber Infrastructure



NSF's OptIPuter Project: Using Supernetworks to Meet the Needs of Data-Intensive Researchers



OptIPortal–Termination Device for the OptIPuter Global Backplane

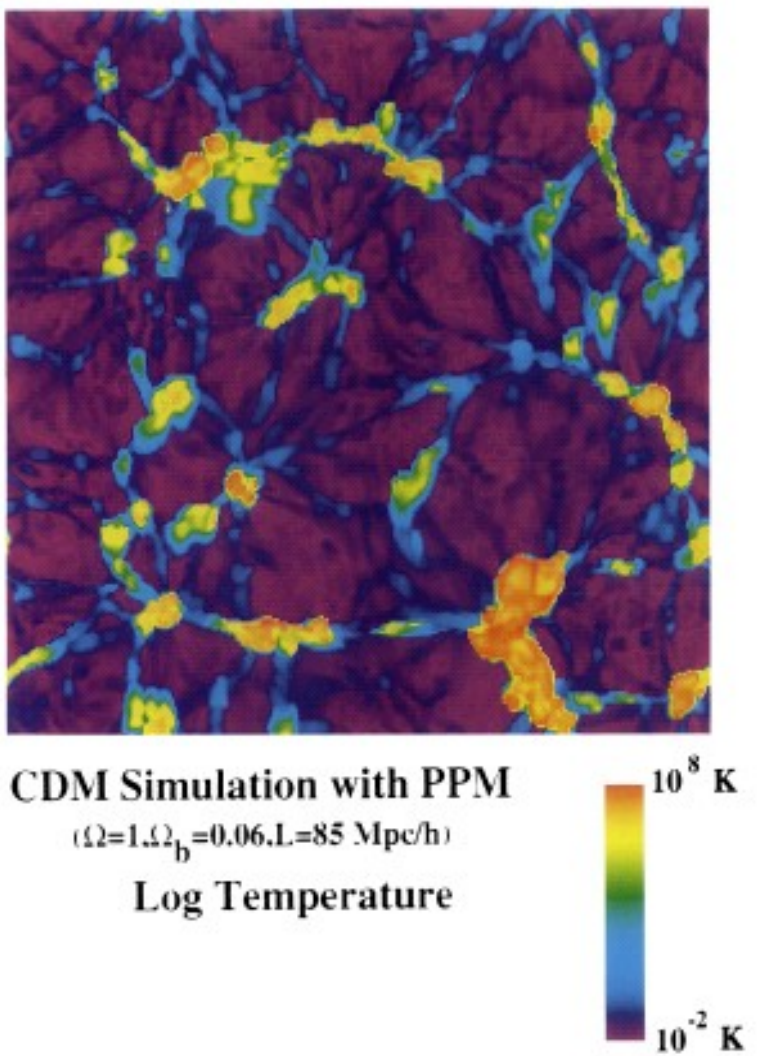
Powered by Rocks

Calit2 (UCSD, UCI), SDSC, and UIC Leads—Larry Smarr PI
Univ. Partners: NCSA, USC, SDSU, NW, TA&M, UvA, SARA, KISTI, AIST
Industry: IBM, Sun, Telcordia, Chiaro, Calient, Glimmerglass, Lucent

Short History of Cosmological Supercomputing: Early Days -1993

- Convex C3880 (8-way SMP) GigaFLOPs
- Simulation of X-ray clusters in a 3D cube 85 Mpc/h on a side and Cartesian grid of size 270^3
- Bryan, Cen, Norman, Ostriker, Stone (1994), ApJ

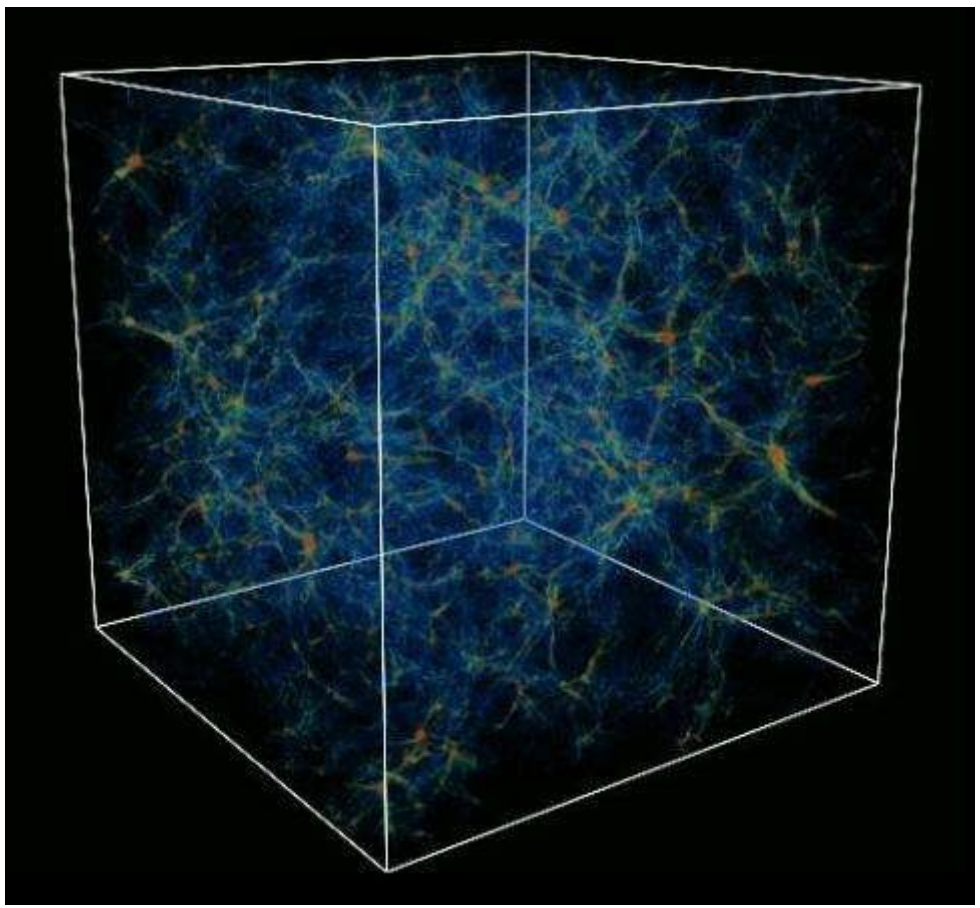
PLATE 2



Source: Michael Norman, SDSC, UCSD

Great Leap Forward-1994

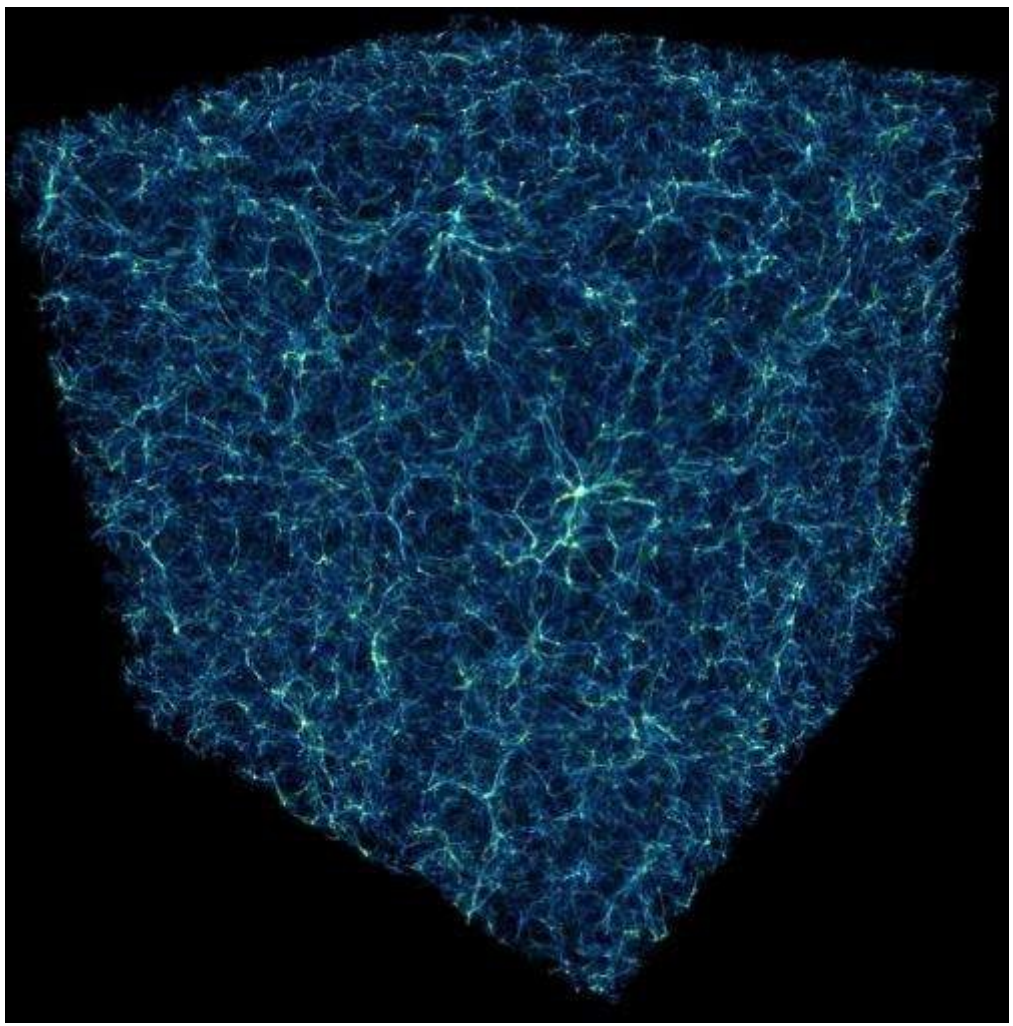
- Thinking Machines CM5 (512-cpu MPP)
- Simulation of X-ray clusters in a 3D cube 170 Mpc/h on a side and Cartesian grid of size 512^3
- Bryan & Norman (1998), ApJ



Source: Michael Norman, SDSC, UCSD

The Power of Adaptive Mesh Refinement-2006

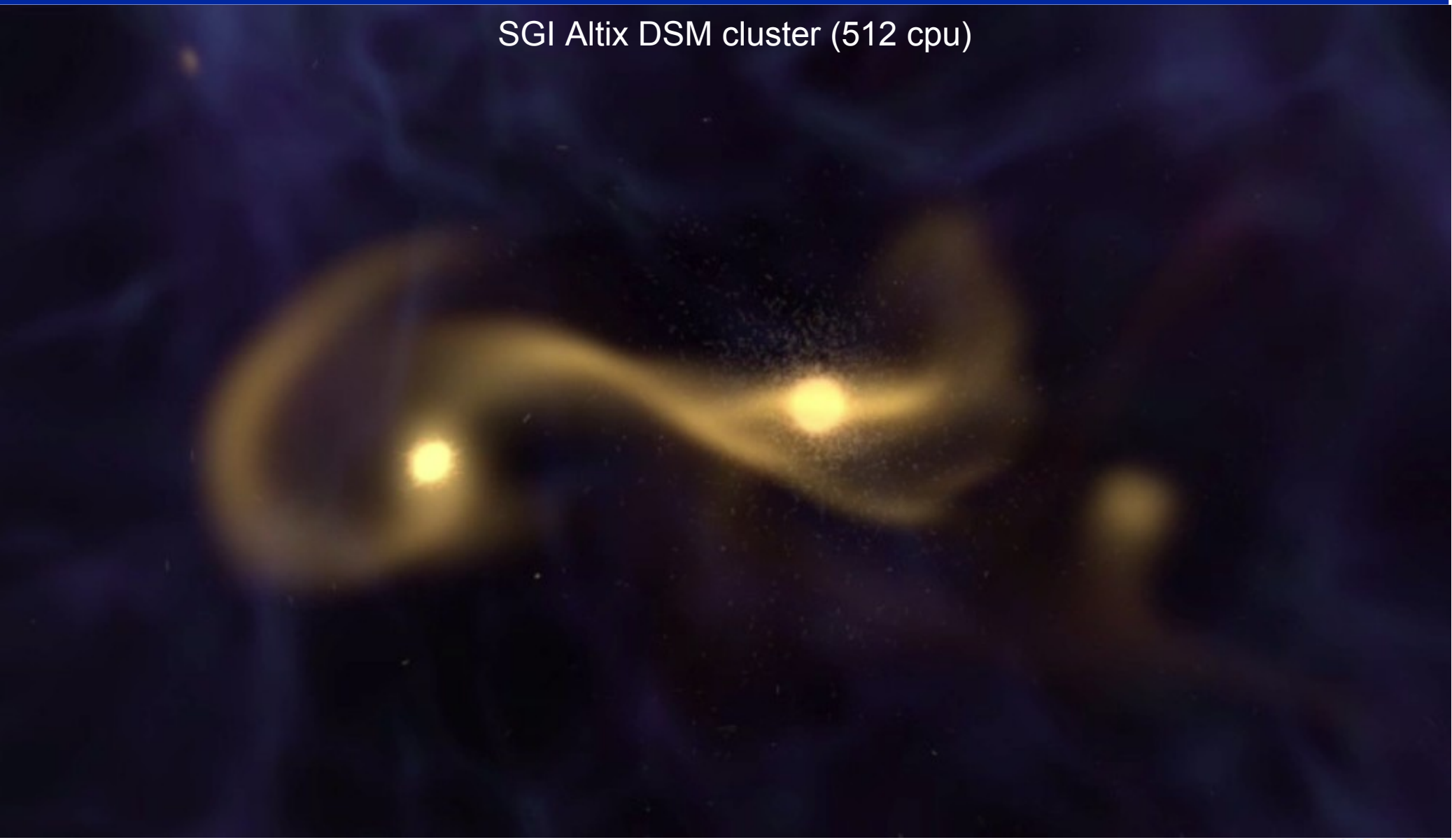
- IBM Power4 cluster (64 node, 8-way SMP)
- Simulation of X-ray clusters in a 3D cube 512 Mpc/h on a side with 7-level AMR for an effective resolution of $65{,}562^3$
- Norman et al. (2007)



Source: Michael Norman, SDSC, UCSD

Adaptive Grids Resolve Individual Galaxy Collisions as Clusters Form in 15 Million Light Year Volume

SGI Altix DSM cluster (512 cpu)

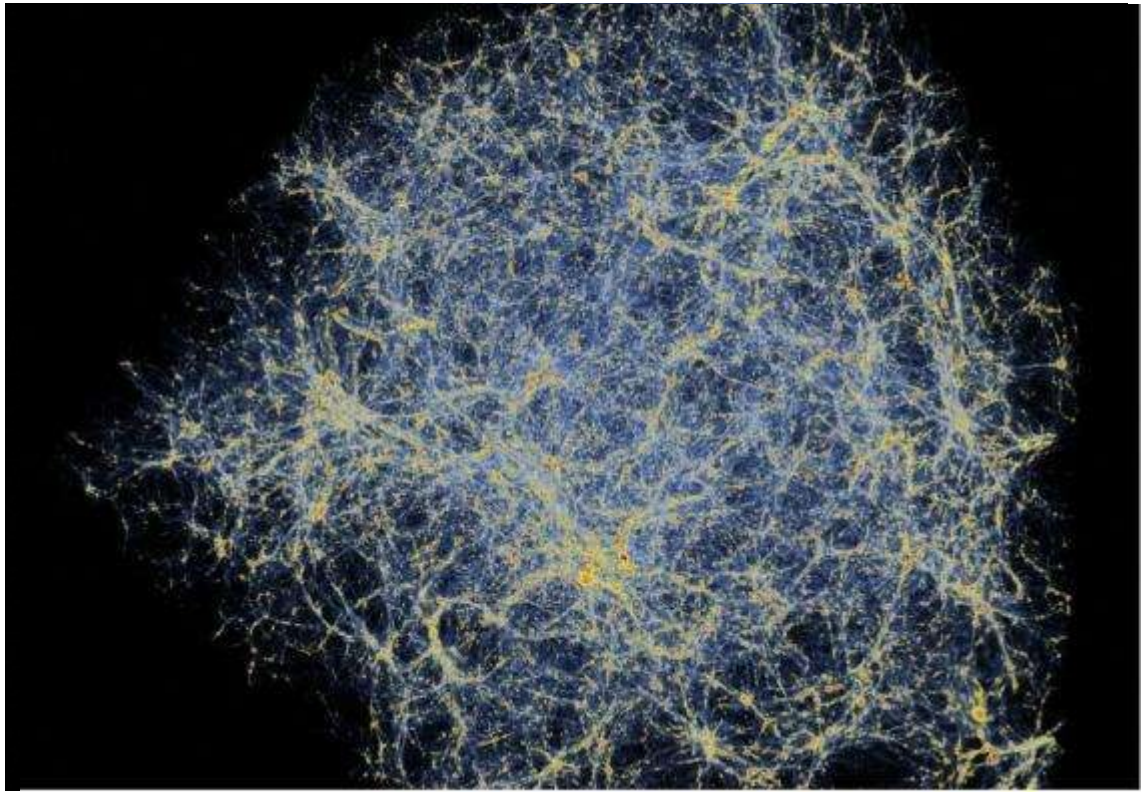


Source: Simulation: Mike Norman and Brian O'Shea; Animation: Donna Cox, Robert Patterson, Matthew Hall, Stuart Levy, Jeff Carpenter, Lorne Leonard-NCSA

Exploring Cosmology With Supercomputers, Supernetworks, and Supervisualization

Source: Mike Norman, SDSC

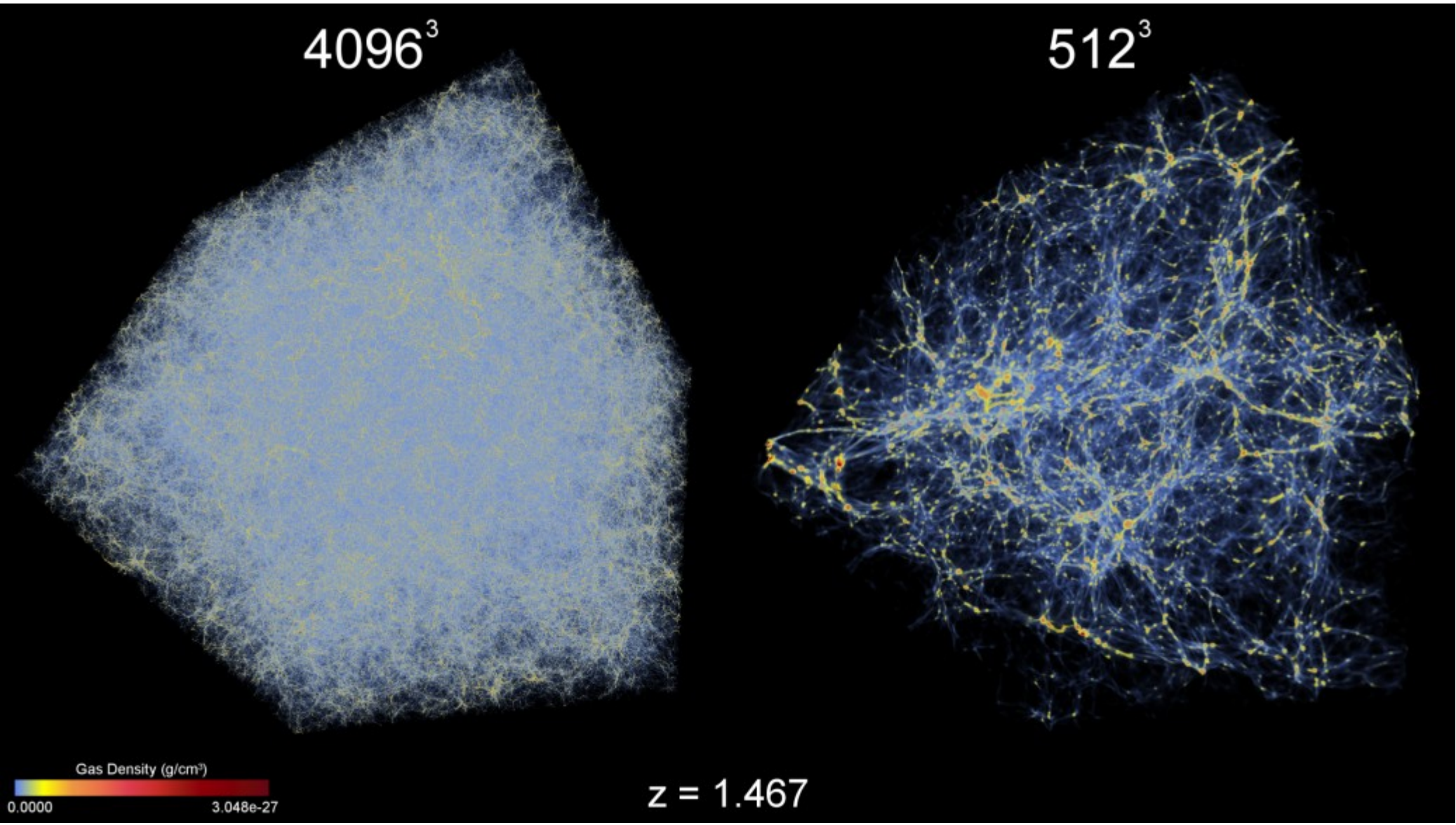
Intergalactic Medium on 2 GLyr Scale



Science: Norman, Harkness,Paschos SDSC
Visualization: Insley, ANL; Wagner SDSC

- **4096^3 Particle/Cell Hydrodynamic Cosmology Simulation**
- **NICS Kraken (XT5)**
  - **16,384 cores**
- **Output**
  - **148 TB Movie Output (0.25 TB/file)**
  - **80 TB Diagnostic Dumps (8 TB/file)**

Enormous Detail in Simulation: Full Simulation with Blowup of a 1/512 Subcube



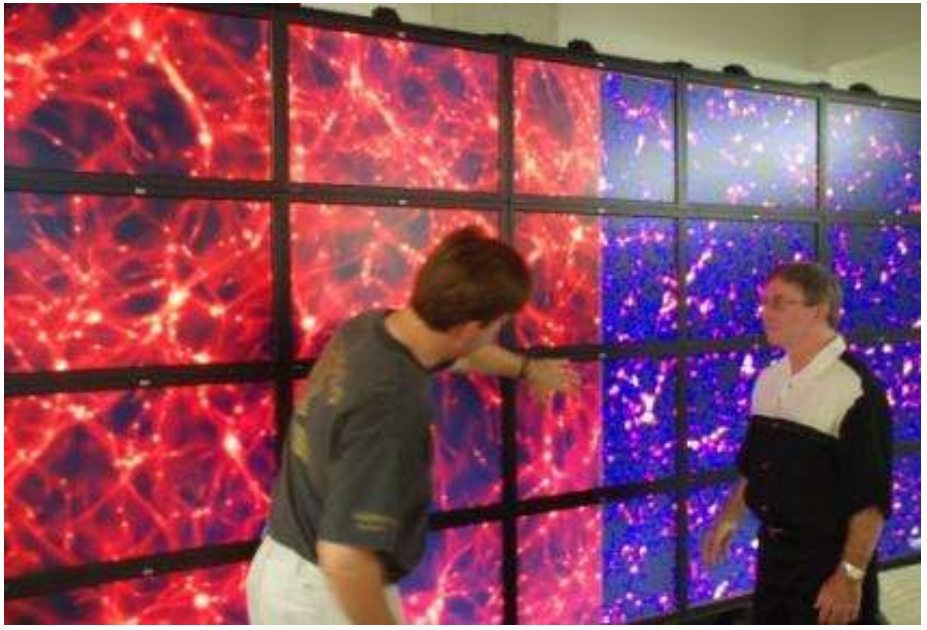
OptIPuter

it²

Project StarGate Goals: Combining Supercomputers and Supernetworks

- **Create an "End-to-End" 10Gbps Workflow**
- **Explore Use of OptIPortals as Petascale Supercomputer "Scalable Workstations"**
- **Exploit Dynamic 10Gbps Circuits on ESnet**
- **Connect Hardware Resources at ORNL, ANL, SDSC**
- **Show that Data Need Not be Trapped by the Network "Event Horizon"**

OptIPortal@SDSC



Rick Wagner Mike Norman

Source: Michael Norman, SDSC, UCSD

- ANL * Calit2 * LBNL * NICS * ORNL * SDSC

Using Supernetworks to Couple End User's OptIPortal to Remote Supercomputers and Visualization Servers

Source: Mike Norman, SDSC



From 1985 to
Project StarGate

Argonne NL

DOE Eureka
100 Dual Quad Core Xeon Servers
200 NVIDIA Quadro FX GPUs in 50
Quadro Plex S4 1U enclosures
3.2 TB RAM



ESnet
10 Gb/s fiber optic network

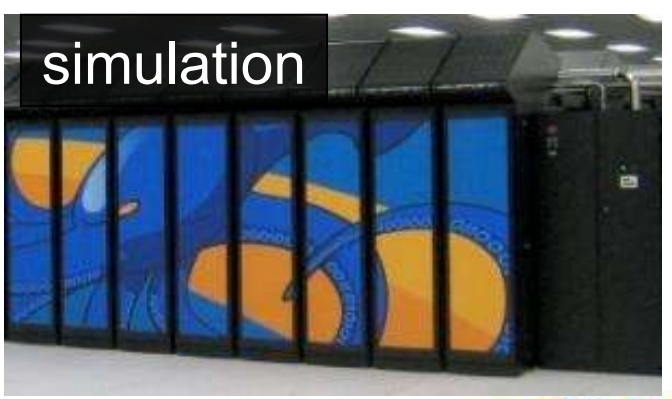
SDSC



Calit2/SDSC OptIPortal1
20 30" (2560 x 1600 pixel) LCD panels
10 NVIDIA Quadro FX 4600 graphics
cards > 80 megapixels
10 Gb/s network throughout

NICS
ORNL

NSF TeraGrid Kraken
Cray XT5
8,256 Compute Nodes
99,072 Compute Cores
129 TB RAM



OptIPuter

*ANL * Calit2 * LBNL * NICS * ORNL *
SDSC

it²

Project StarGate Credits

Argonne National Laboratory

Network/Systems

- Linda Winkler
- Loren Jan Wilson

Visualization

- Joseph Insley
- Eric Olsen
- Mark Hereld
- Michael Papka

Lawrence Berkeley National Laboratory (ESnet)

- **Eli Dart**

National Institute for Computational Sciences

- Nathaniel Mendoza

Oak Ridge National Laboratory

- Susan Hicks

Calit2@UCSD

- Larry Smarr (Overall Concept)
- Brian Dunne (Networking)
- Joe Keefe (OptIPortal)
- Kai Doerr, Falko Kuester (CGLX)

San Diego Supercomputer Center

Science application

- **Michael Norman**
- **Rick Wagner (coordinator)**

Network

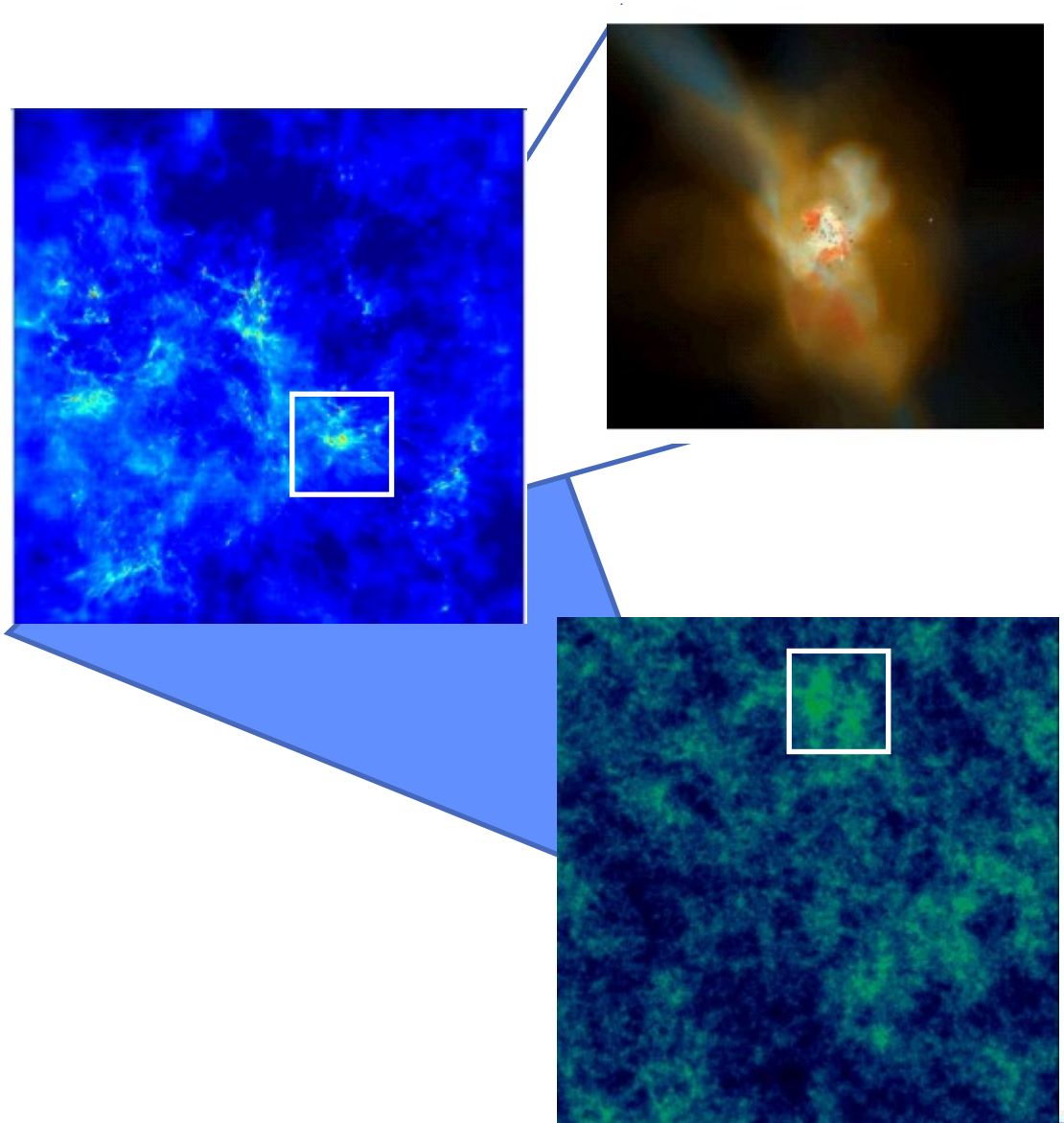
- **Tom Hutton**

OptIPuter

- ANL * Calit2 * LBNL * NICS * ORNL * SDSC

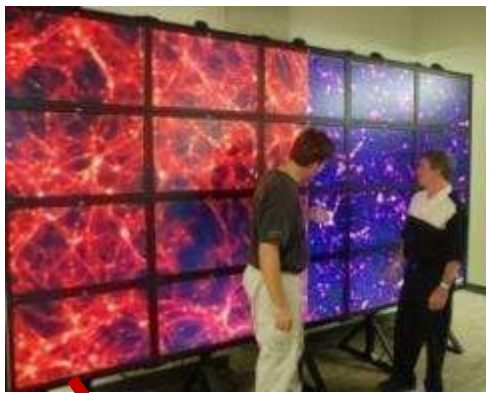
Blue Waters is a Sustained PetaFLOPs Supercomputer One Million Times the Convex 3880 of 1993!

- Planned for 2011-2012
- Science
  - Self-consistent simulation of the formation of the first galaxies and cosmic ionization
- Scale of Simulations
  - AMR: 1536^3 base grid, 10 levels of refinement
  - Cartesian: 6400^3 with radiation transport



Source: Michael Norman, SDSC, UCSD

Academic Research "OptIPlatform" Cyberinfrastructure: A 10Gbps "End-to-End" Lightpath Cloud



End User OptIPortal



Instruments



HD/4k Telepresence



HD/4k Video Cams

HPC



10G Lightpath

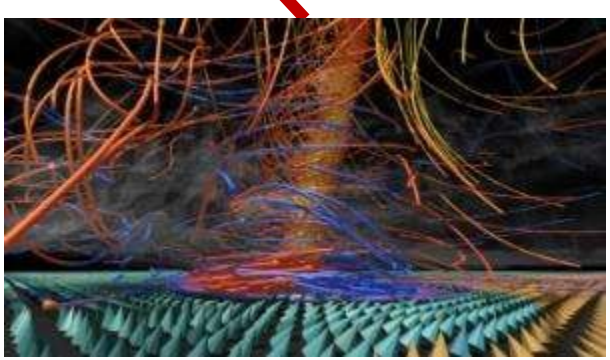


TeraGrid

Campus Optical Switch



Data Repositories & Clusters

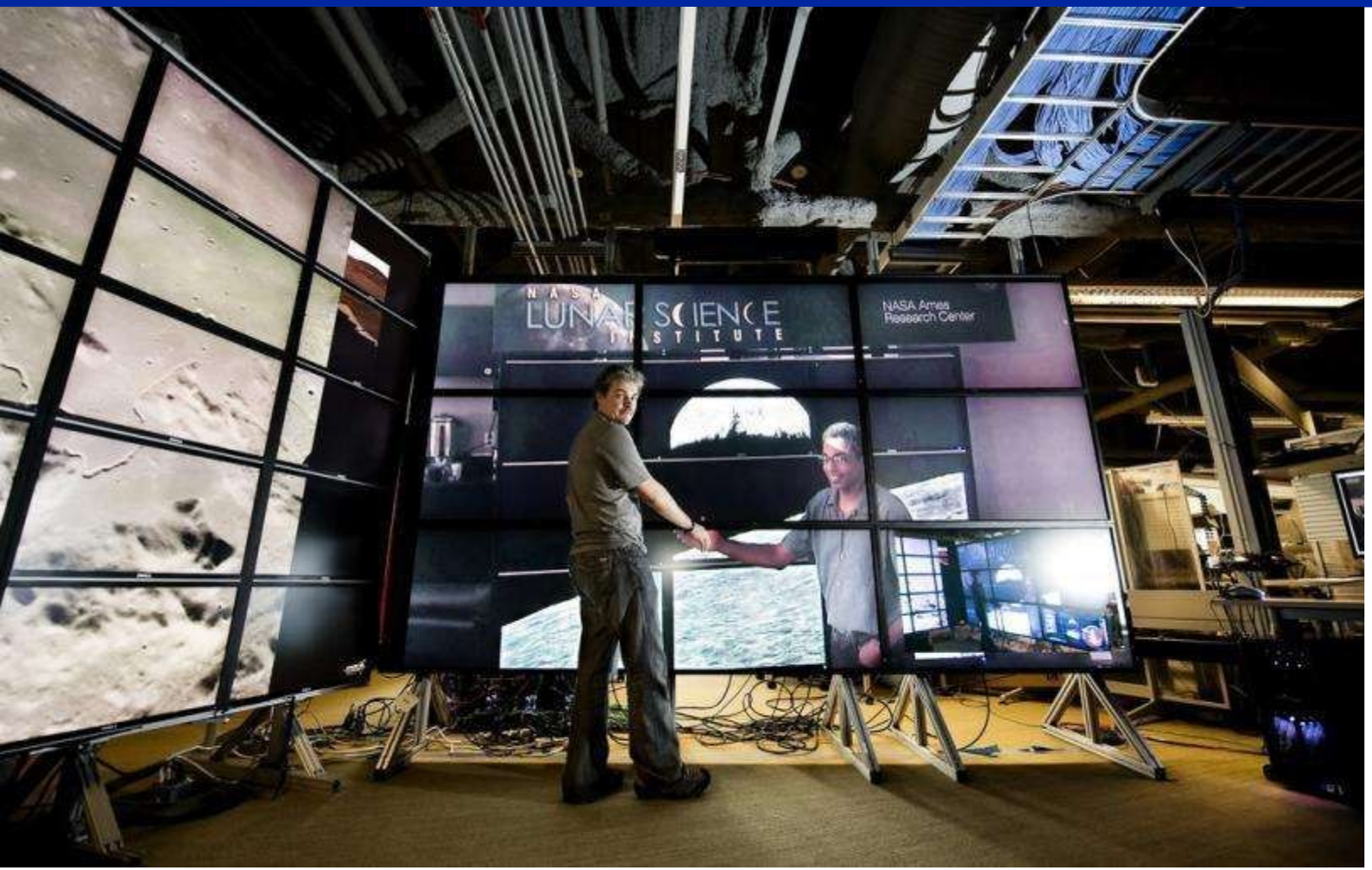


HD/4k Video Images

OptIPuter

it²

High Definition Video Connected OptIPortals: Virtual Working Spaces for Data Intensive Research



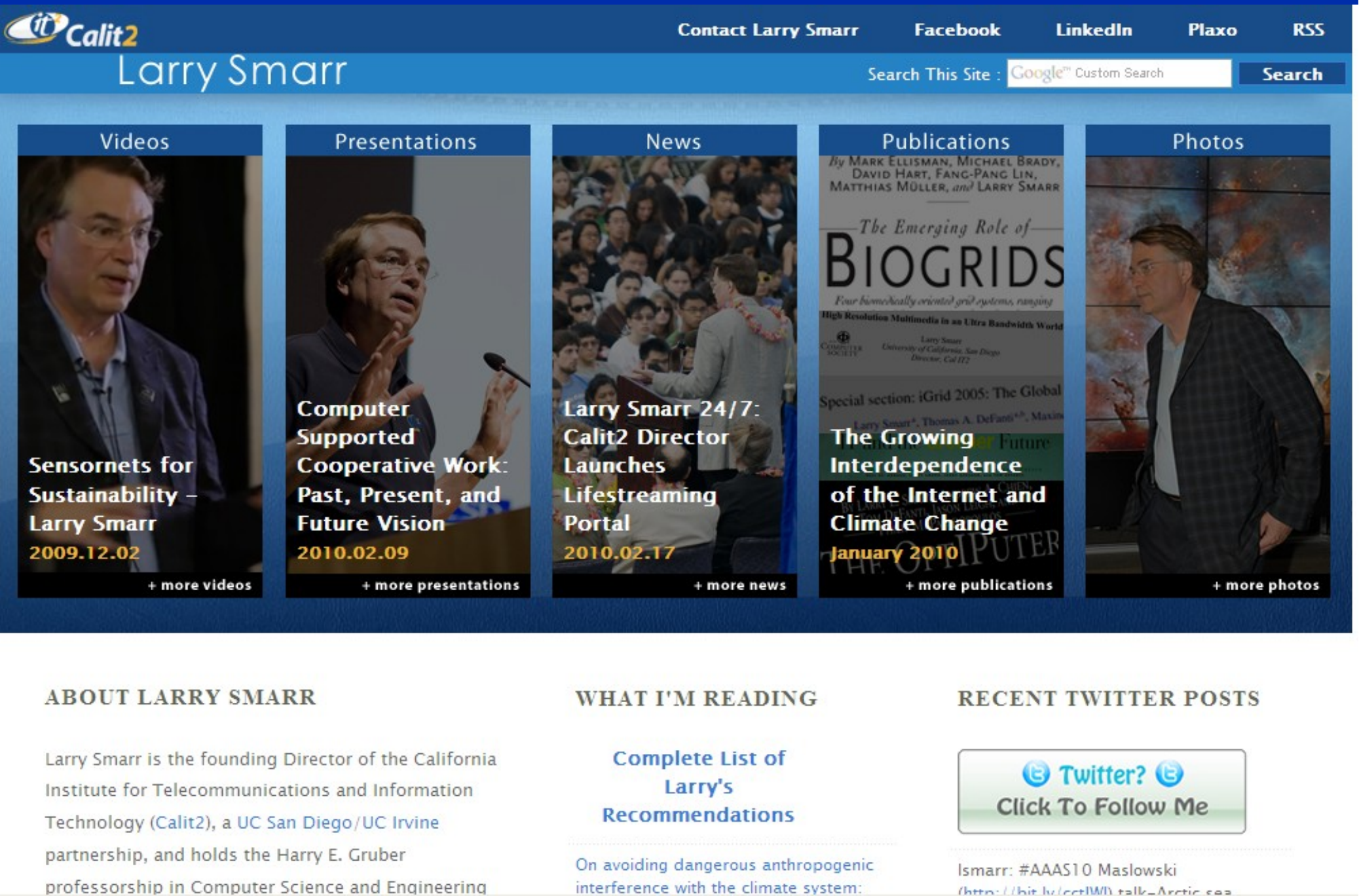
LifeSize HD

NASA Ames
Lunar Science Institute
Mountain View, CA

NASA Interest
in Supporting
Virtual Institutes

Source: Falko Kuester, Kai Doerr Calit2; Michael Sims, NASA

You Can Download This Presentation at lsmarr.calit2.net



ABOUT LARRY SMARR

Larry Smarr is the founding Director of the California Institute for Telecommunications and Information Technology (Calit2), a UC San Diego/UC Irvine partnership, and holds the Harry E. Gruber professorship in Computer Science and Engineering

WHAT I'M READING

Complete List of Larry's Recommendations

On avoiding dangerous anthropogenic interference with the climate system:

RECENT TWITTER POSTS

Twitter? Click To Follow Me

lsmarr: #AAAS10 Maslowski