

Author(s): August E. Evrard, PhD. 2010

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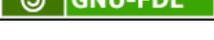
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Cyberscience: Computational Science and the Rise of the Fourth Paradigm

GROUP: 1	QUANTITY: 1	SYSTEM PRICE: \$19,024.72	GROUP TOTAL: \$19,024.72
Base Unit:	PowerEdge C6100 Chassis w/ 4 System Boards and support for 2.5" Hard Drives (224-8427)		
Processor:	Intel Xeon X5650, 2.66Ghz, 12M Cache,Turbo, HT, 1333MHz Max Mem (317-4052)		
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Processor:	Thermal Heatsink (317-3410)		
Processor:	Thermal Heatsink (317-3410)		
Processor:	Dual Processor Option (317-4928)		
Memory:	48GB Memory (12x4GB), 1333MHz Dual Ranked RDIMMs for 2 Processors, Optimized (317-3394)		
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Memory:	48GB Memory (12x4GB), 1333MHz Dual Ranked RDIMMs for 2 Processors, Optimized (317-3394)		
Memory:	Info, Memory for Dual Processor selection (468-7687)		
Hard Drive:	500GB 7.2K RPM SATA 2.5" Hard Drive (342-0974)		
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Hard Drive:	500GB 7.2K RPM SATA 2.5" Hard Drive (342-0974)		
Hard Drive:	500GB 7.2K RPM SATA 2.5" Hard Drive (342-0974)		
Hard Drive:	CARR,HD,2.5,2LED,C6100,MLK (342-1032)		
Hard Drive:	CARR,HD,2.5,2LED,C6100,MLK (342-1032)		
Hard Drive:	CARR,HD,2.5,2LED,C6100,MLK (342-1032)		

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Honors 352, Class #0.14
August E. (Gus) Evrard, PhD

Fall 2010



today

- * lecture: Flux hardware, CI Days highlights, and GRID computing intro
- * **in-class exercise:** consider fundamental requirements for SC design
- * group project updates next Tuesday
- * reading quiz this Sunday

TOTAL QUOTE AMOUNT:		\$19,024.72	
Product Subtotal:	\$19,024.72		
Tax:	\$0.00		
Shipping & Handling:	\$0.00		
Shipping Method:	Ground	Total Number of System Groups:	1

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4-node order
for Flux cluster
from Dell
Computer

2 x hex-core
cpu's per node
= 48 cores

12 x 4Gb memory
per node = 192 Gb
(4 Gb per core)

500 Gb disk drive
per node = 2.0 Tb

4-node order for Flux

40 Gb/s infiniband network port per node

2 x 1100 Watt power supply (two nodes run off one supply)

Hard Drive:	CARR,HD,2.5,2LED,C6100,MLK (342-1032)
Operating System:	No OS, No Utility Partition (420-3323)
Operating System:	No OS, No Utility Partition (420-3323)
Operating System:	No OS, No Utility Partition (420-3323)
Operating System:	No OS, No Utility Partition (420-3323)
NIC:	Mellanox QDR Dual Port 40 Gb/s Infiniband HCA Daughtercard, PE C6100 (317-3413)
NIC:	Mellanox QDR Dual Port 40 Gb/s Infiniband HCA Daughtercard, PE C6100 (317-3413)
NIC:	Mellanox QDR Dual Port 40 Gb/s Infiniband HCA Daughtercard, PE C6100 (317-3413)
NIC:	Mellanox QDR Dual Port 40 Gb/s Infiniband HCA Daughtercard, PE C6100 (317-3413)
Documentation Diskette:	C6100 MLK Documentation (330-8719)
Feature	2.5" Onboard SATA Controller for 1-6 HDs (342-0065)
Feature	Onboard SATA Controller (342-0726)
Feature	2.5" Onboard SATA Controller for 1-6 HDs (342-0065)
Feature	2.5" Onboard SATA Controller for 1-6 HDs (342-0065)
Feature	2.5" Onboard SATA Controller for 1-6 HDs (342-0065)
Feature	Onboard SATA Controller (342-0726)
Feature	Onboard SATA Controller (342-0726)
Feature	Onboard SATA Controller (342-0726)
Feature	C6100 Static Rails, Tool-less (330-8483)
Service:	Basic: Business Hours (5X10) Next Business Day On Site Hardware Warranty Repair 2Year Extended (907-2772)
Service:	Basic: Business Hours (5X10) Next Business Day On Site Hardware Warranty Repair Initial Year (908-3960)
Service:	SATA Hard Drive Ltd Warranty with Basic Support, 2 Year Extended (993-9412)
Service:	SATA Hard Drive Ltd Warranty with Basic Support, Initial Year (994-4500)
Service:	Dell Hardware Limited Warranty Extended Year (907-4098)
Service:	Dell Hardware Limited Warranty Initial Year (907-4207)
Service:	DECLINED CRITICAL BUSINESS SERVER OR STORAGE SOFTWARE SUPPORT PACKAGE-CALL YOUR DELL SALES REP IF UPGRADE NEED (908-7899)
Installation:	On-Site Installation Declined (900-9997)
Misc:	Power Supply,1100W, Redundant Capable (330-8537)
Misc:	Power Supply,1100W, Redundant Capable (330-8537)
Misc:	Label,Regulatory,750/1100W, C6100 (330-8720)
Misc:	Powercord,125Volt,15Amp,10Foot (330-6870)
Misc:	Powercord,125Volt,15Amp,10Foot (330-6870)

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[bit-tech review of westmere chip \(vs.AMD opteron\) 31 March 2010](#)

[QuickPath interconnect \(motherboard network\) \[http://en.wikipedia.org/wiki/Intel_QuickPath_Interconnect\]\(http://en.wikipedia.org/wiki/Intel_QuickPath_Interconnect\)](#)

Cyberinfrastructure Days: highlights from keynote Larry Smarr

**“Set My Data Free: High-Performance CI
for Data-Intensive Research”**

**KeynoteSpeaker
Cyberinfrastructure Days
University of Michigan
Ann Arbor, MI
November 3, 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
Follow me on Twitter: lsmarr**

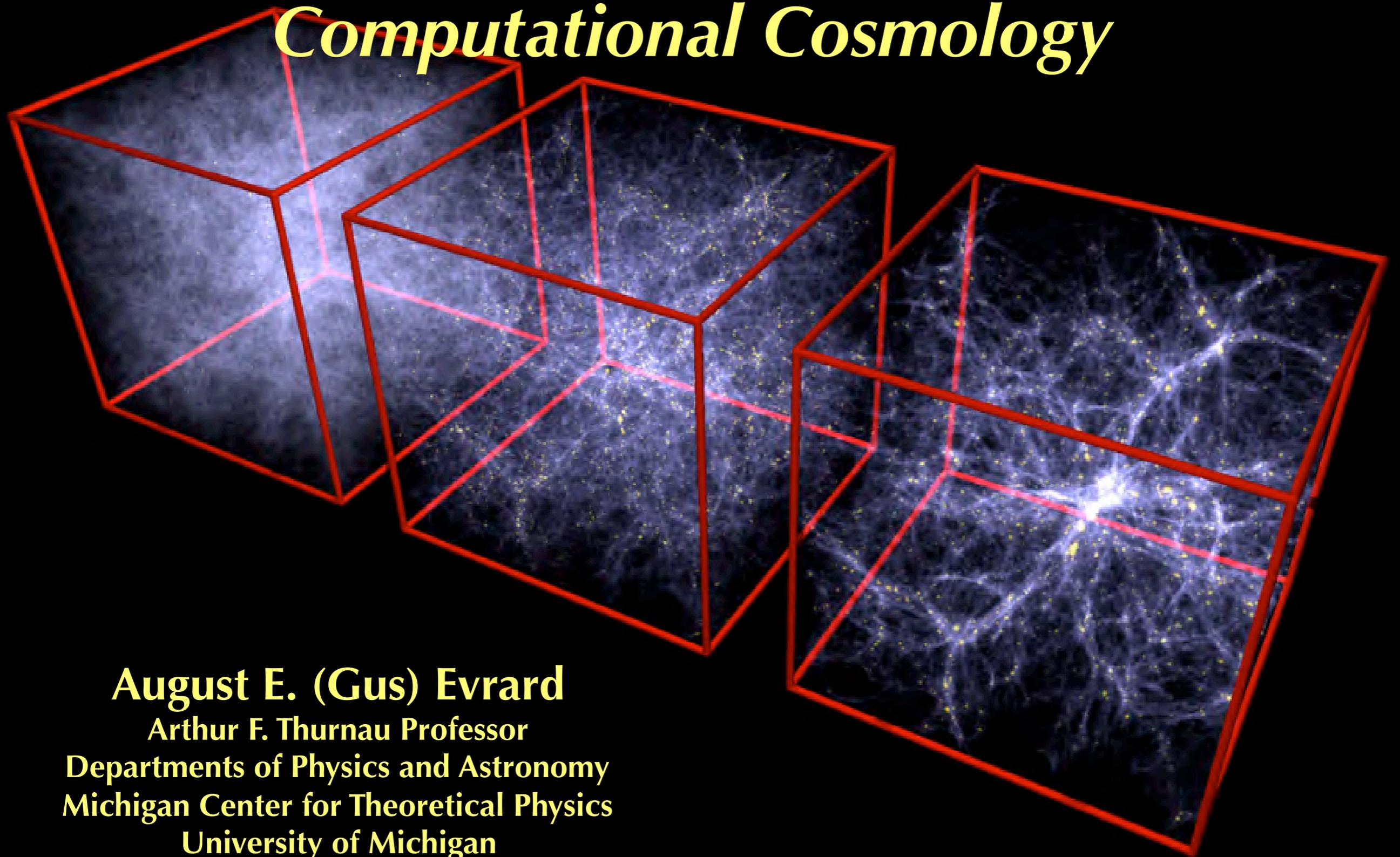


© FAIR USE Larry Smarr, Cyberinfrastructure Days



Please go to the original slide show on this talk at <http://lsmarr.calit2.net/presentations?slideshow=5656616> and reference slides 15, 16, 18, 19, 22, and 23, which have been removed from this presentation.

Computational Cosmology



August E. (Gus) Evrard
Arthur F. Thurnau Professor
Departments of Physics and Astronomy
Michigan Center for Theoretical Physics
University of Michigan

BIG BANG

Gravitational Waves Escape from the Earliest Moments of the Big Bang

WE ARE AMPLIFIED NOISE

Inflation (Big Bang plus 10^{-35} seconds)

Big Bang plus 10^{-42} Seconds

Cosmic microwave background, distorted by seeds of structure and gravitational waves

Big Bang plus 300,000 Years

Light

Gravitational Waves

Now

Big Bang plus 15 Billion Years

quantum effects important early (Heisenberg)

classical physics dominates late (Newton)

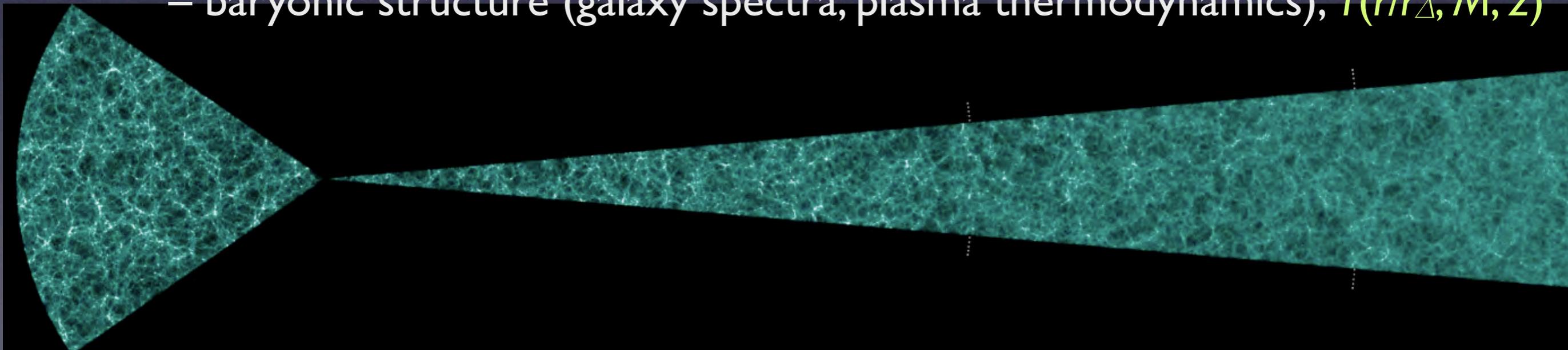
2010 paradigm of cosmological **large-scale structure (LSS)**

LSS: a hierarchical web of quasi-equilibrium bound structures – **halos** – that emerge via gravitational amplification from a noise field imposed by inflation.

Computational Cosmology: model LSS as a multi-fluid, self-gravitating system evolved from known initial conditions.

Simulations calibrate key enabling ingredients of **Halo Model**

- space density, $n(M, z)$
- spatial N-point correlations (e.g., autocorrelation function), $b(M, z)$
- internal halo structure (kinematics, substructure), $X(r/r_\Delta, M, z)$
- baryonic structure (galaxy spectra, plasma thermodynamics), $Y(r/r_\Delta, M, z)$

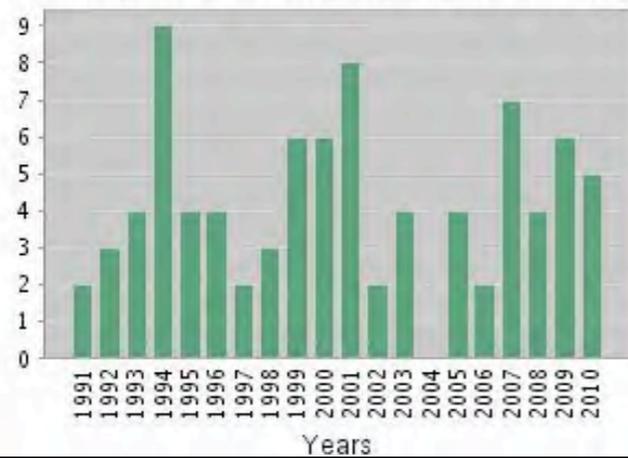


evrard group research

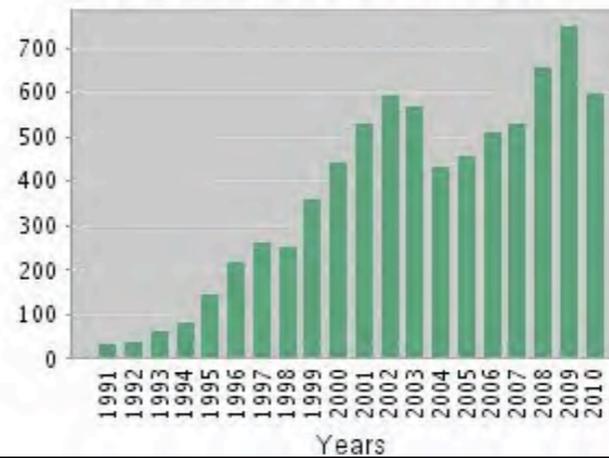
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514 534 660 750 601 7,606

		2006	2007	2008	2009	2010	Total
<input type="checkbox"/>	1. Title: Simulations of the formation, evolution and clustering of galaxies and quasars Author(s): Springel V, White SDM, Jenkins A, et al. Source: NATURE Volume: 435 Issue: 7042 Pages: 629-636 Published: JUN 2 2005	88	133	189	223	170	818
<input type="checkbox"/>	2. Title: The mass function of dark matter haloes Author(s): Jenkins A, Frenk CS, White SDM, et al. Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY Volume: 321 Issue: 2 Pages: 372-384 Published: FEB 21 2001	91	63	67	83	57	734
<input type="checkbox"/>	3. Title: THE BARYON CONTENT OF GALAXY CLUSTERS - A CHALLENGE TO COSMOLOGICAL ORTHODOXY Author(s): WHITE SDM, NAVARRO JF, EVRARD AE, et al. Source: NATURE Volume: 366 Issue: 6454 Pages: 429-433 Published: DEC 2 1993	21	15	18	19	20	688
<input type="checkbox"/>	4. Title: Mass estimates of X-ray clusters Author(s): Evrard AE, Metzler CA, Navarro JF Source: ASTROPHYSICAL JOURNAL Volume: 469 Issue: 2 Pages: 494-507 Part: Part 1 Published: OCT 1 1996	31	31	20	22	12	482
<input type="checkbox"/>	5. Title: Properties of the intracluster medium in an ensemble of nearby galaxy clusters Author(s): Mohr JJ, Mathiesen B, Evrard AE Source: ASTROPHYSICAL JOURNAL Volume: 517 Issue: 2 Pages: 627-649 Part: Part 1 Published: JUN 1 1999	33	16	25	16	8	386
<input type="checkbox"/>	6. Title: The L-X-T relation and intracluster gas fractions of X-ray clusters Author(s): Arnaud M, Evrard AE Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY Volume: 305 Issue: 3 Pages: 631-640 Published: MAY 11 1999	22	26	21	13	11	320
<input type="checkbox"/>	7. Title: FORMATION AND EVOLUTION OF X-RAY-CLUSTERS - A HYDRODYNAMIC SIMULATION OF THE INTRACLUSTER MEDIUM Author(s): EVRARD AE Source: ASTROPHYSICAL JOURNAL Volume: 363 Issue: 2 Pages: 349-366 Part: Part 1 Published: NOV 10 1990	5	4	8	6	9	268
<input type="checkbox"/>	8. Title: EXPECTATIONS FOR X-RAY-CLUSTER OBSERVATIONS BY THE ROSAT SATELLITE Author(s): EVRARD AE, HENRY JP Source: ASTROPHYSICAL JOURNAL Volume: 383 Issue: 1 Pages: 95-103 Part: Part 1 Published: DEC 10 1991	14	13	9	7	7	242
<input type="checkbox"/>	9. Title: The Santa Barbara cluster comparison project: A comparison of cosmological hydrodynamics solutions Author(s): Frenk CS, White SDM, Bode P, et al. Source: ASTROPHYSICAL JOURNAL Volume: 525 Issue: 2 Pages: 554-582 Part: Part 1 Published: NOV 10 1999	20	19	17	22	10	241
<input type="checkbox"/>	10. Title: Galaxy clusters in Hubble volume simulations: Cosmological constraints from sky survey populations Author(s): Evrard AE, MacFarland TJ, Couchman HMP, et al. Source: ASTROPHYSICAL JOURNAL Volume: 573 Issue: 1 Pages: 7-36 Part: Part 1 Published: JUL 1 2002	18	19	22	23	15	201

Sim

Sim

Sim+Data

Sim

Data

Data

Sim

Theory

Sim

Sim

current research and collaborators

Fisher forecasts

Huterer

Cunha

Erickson

LSS simulations

Rasia

Stanek

Nord

Chen

Rudd (IAS)

Pearce (Nottingham)

+ **Virgo Consortium**

grad student

postdoc

faculty



optical + sub-mm surveys

SDSS, **DES** +

South Pole Telescope

McKay

Wechsler (Stanford)

Hao (Fermilab)

Kravtsov (Chicago)

Koester (Chicago)

McMahon

Miller

Ricker (UIUC)

Rozo (Chicago)

Rykoff (UCSB)

Sheldon (BNL)

Johnston (JPL)

Becker (Chicago)

+ **DES Collaboration**

LoCuSS (X-ray)

G. Smith (Birmingham)

+ LoCuSS Collaboration

Evrard Group @ Michigan, August 2009



Anbo Chen - Carlos Cunha - Brandon Erickson - AEE - Greg Green - Rashad Brown - Mitch Adler
Jounghun Lee - Elena Rasia - Rebecca Stanek - Gary Foreman
Brian Nord

Dark Energy Survey is nearing operation

An NSF/DOE-funded study of dark energy using four techniques

- 1) Galaxy cluster surveys (with SPT)
- 2) Galaxy angular power spectrum
- 3) Weak gravitational lensing
- 4) SN Ia distances

Two linked, multiband optical surveys

5000 deg² *grizY* colors to ~24th mag

Repeated observations of 40 deg²

Development and schedule

Construction: 2007-2011

New 3 deg² camera (DECam) on Blanco 4m, Cerro Tololo

Data management system at NCSA

Survey Operations: 2012-2016

510 nights of telescope time over 5 years

The Collaboration

 **Fermilab** — The Fermi National Accelerator Laboratory

 **UIUC/NCSA** — The University of Illinois at Urbana-Champaign

 **Chicago** — The University of Chicago

 **LBL** — The Lawrence Berkeley National Laboratory

 **NOAO** — The National Optical Astronomy Observatory

 Spain DES Collaboration

 United Kingdom DES Collaboration

- **IEEC/CSIC** - Instituto de Ciencias del Espacio,
- **IFAE** - Institut de Fisica d'Altes Energies
- **CIEMAT** - Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas

- **UCL** - University College London
- **Cambridge** - University of Cambridge
- **Edinburgh** - University of Edinburgh
- **Portsmouth** - University of Portsmouth
- **Sussex** - University of Sussex
- **Nottingham** - University of Nottingham

 **Michigan** — The University of Michigan

 DES-Brazil Consortium

- **ON** - Observatorio Nacional
- **CBPF** - Centro Brasileiro de Pesquisas Fisicas
- **UFRGS** - Universidade Federal do Rio Grande do Sul

 **Pennsylvania** — The University of Pennsylvania

 **ANL** — Argonne National Laboratory

 **OSU** — The Ohio State University

 Santa Cruz-SLAC-Stanford DES Consortium

- **Santa Cruz** - University of California Santa Cruz
- **SLAC** - SLAC National Accelerator Laboratory
- **Stanford** - Stanford University

 **TAMU** — Texas A&M University

Munich—Universitäts-Sternwarte München

-  **Ludwig-Maximilians Universität**
-  **Excellence Cluster Universe**

 **PD-INEL**

Josh Frieman, Director

Fermilab, U Illinois, U Chicago, LBNL, U Michigan
CTIO/NOAO, Barcelona, UCL, Cambridge, Edinburgh

NSF OCI proposal: distributed workflows to support cosmological survey analysis

NSF Cyberinfrastructure SI2 Proposal

Software Infrastructure for Sustained Innovation

A Cosmic Sky Machine (COSMA) for Astrophysics and Cosmology with Clusters of Galaxies

PI: August Evrard, University of Michigan

co-PI: Andrey Kravtsov, University of Chicago

co-PI: Elena Rasia, University of Michigan

co-PI: Paul Ricker, University of Illinois

co-PI Risa Wechsler, Stanford Univ. & SLAC

Collaborators:

Stefano Borgani, dell'Universita di Trieste & INAF, Italy

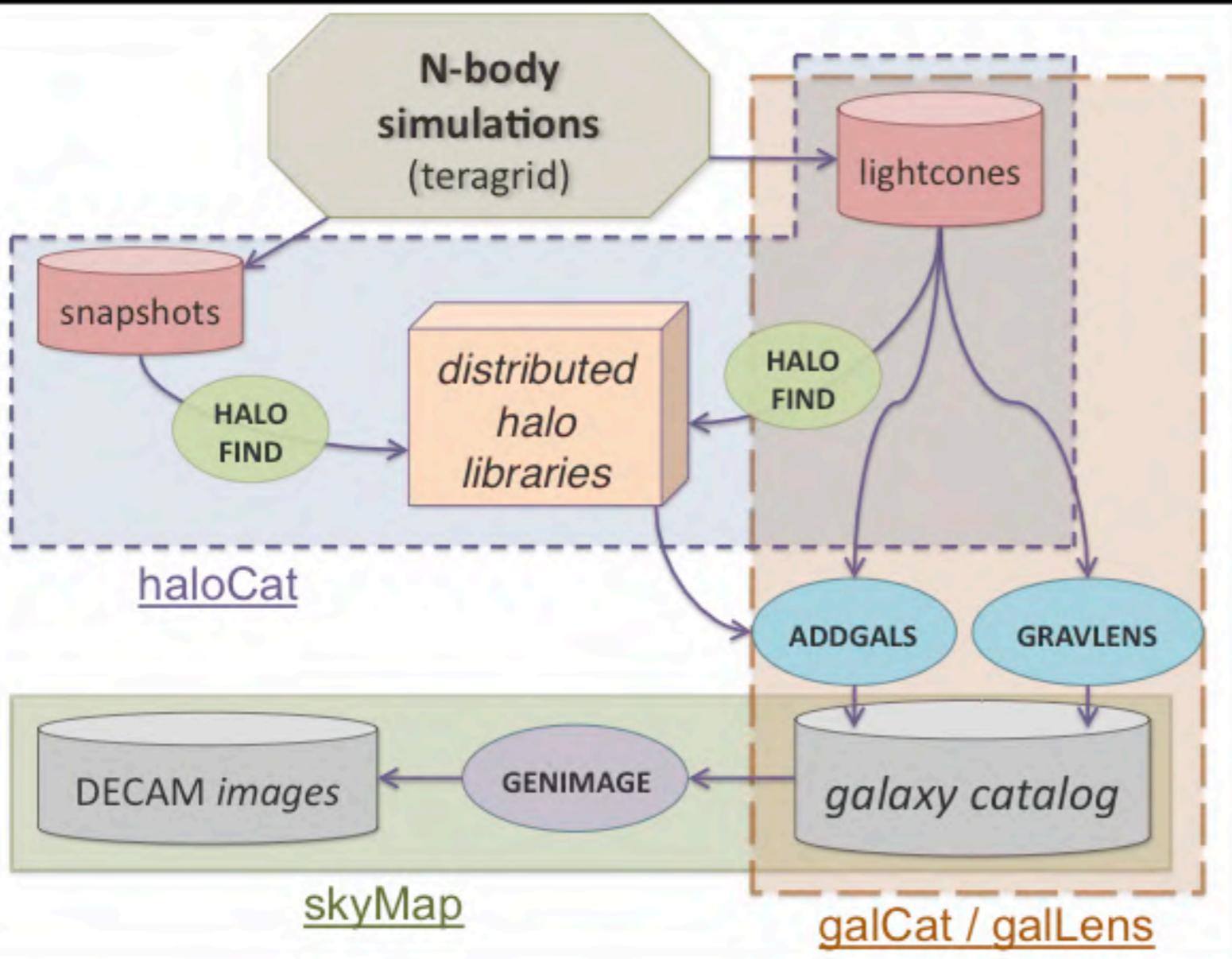
Luiz DaCosta, Observatorio Nacional, Brazil

Klaus Dolag, Max-Planck-Institut fur Astrophysik

Claudio Gheller, CINECA, Italy

Gerard Lemson, Max-Planck-Institut fur Astrophysik

Huan Lin, Fermi National Laboratory, USA



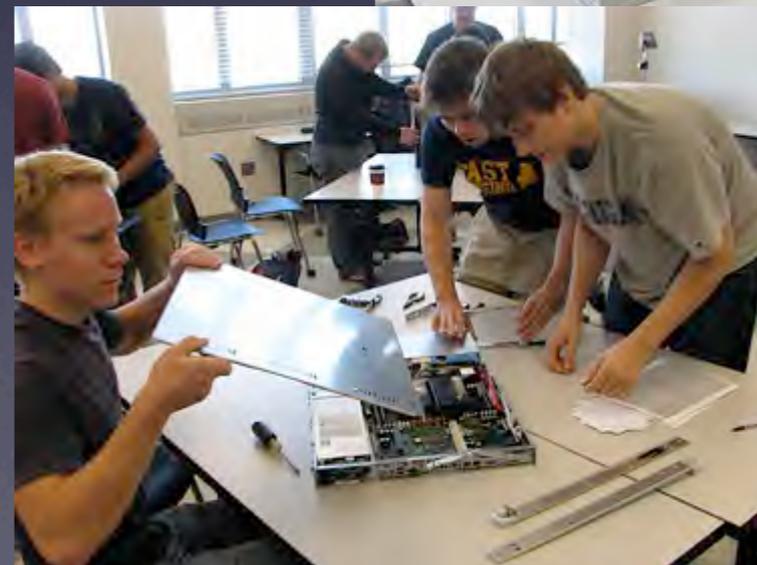
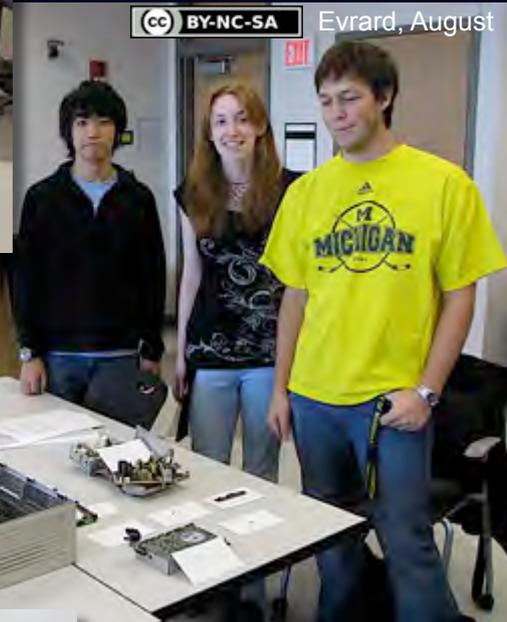
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see Brandon Erickson's poster

there is not an app for this! (yet...)

New course @UM! Honors 352

Cyberscience: Computational Science and the Rise of the Fourth Paradigm



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CC BY-NC-SA Evrard, August

- Course Goals:** Students who have taken this course should:
1. be able to explain what computation means in the context of scientific inquiry, and provide examples of the different roles that computing plays in the sciences;
 2. be aware of the cyberinfrastructure elements that power computational science, including
 - * hardware, software and network components, their historical development and their mutual interactions,
 - * data management processes, including authorization, authentication, and securitization of networked resources, and
 - * institutional roles, including facilities management, governance, and publication of digital assets.
 3. appreciate current challenges to scholarship associated with cyberinfrastructure, such as
 - * the environmental impact of large-scale computing nature of scientific publication, peer review, and career advancement,
 - * costs, benefits and risks to research institutions.

grid computing

* grid reference is by analogy to the power grid

Goal: seamless, 'plug-n-play' access to compute resources and services from a remote device/client/user.

Enable collaborative activities across **virtual organizations**

* required elements

– hardware, software and network infrastructure

Ch 1

– authentication and authorization model (security, billing)

Ch 5

– user interfaces

Ch 2

– job schedulers

– standards bodies

– funding sources (R&D, deployment, maintenance)

(*beowulf*) cluster

* locally networked set of Commercial Off-The-Shelf (COTS) computers

"thirty men's heft of grasp in the gripe of his hand."

* benefits

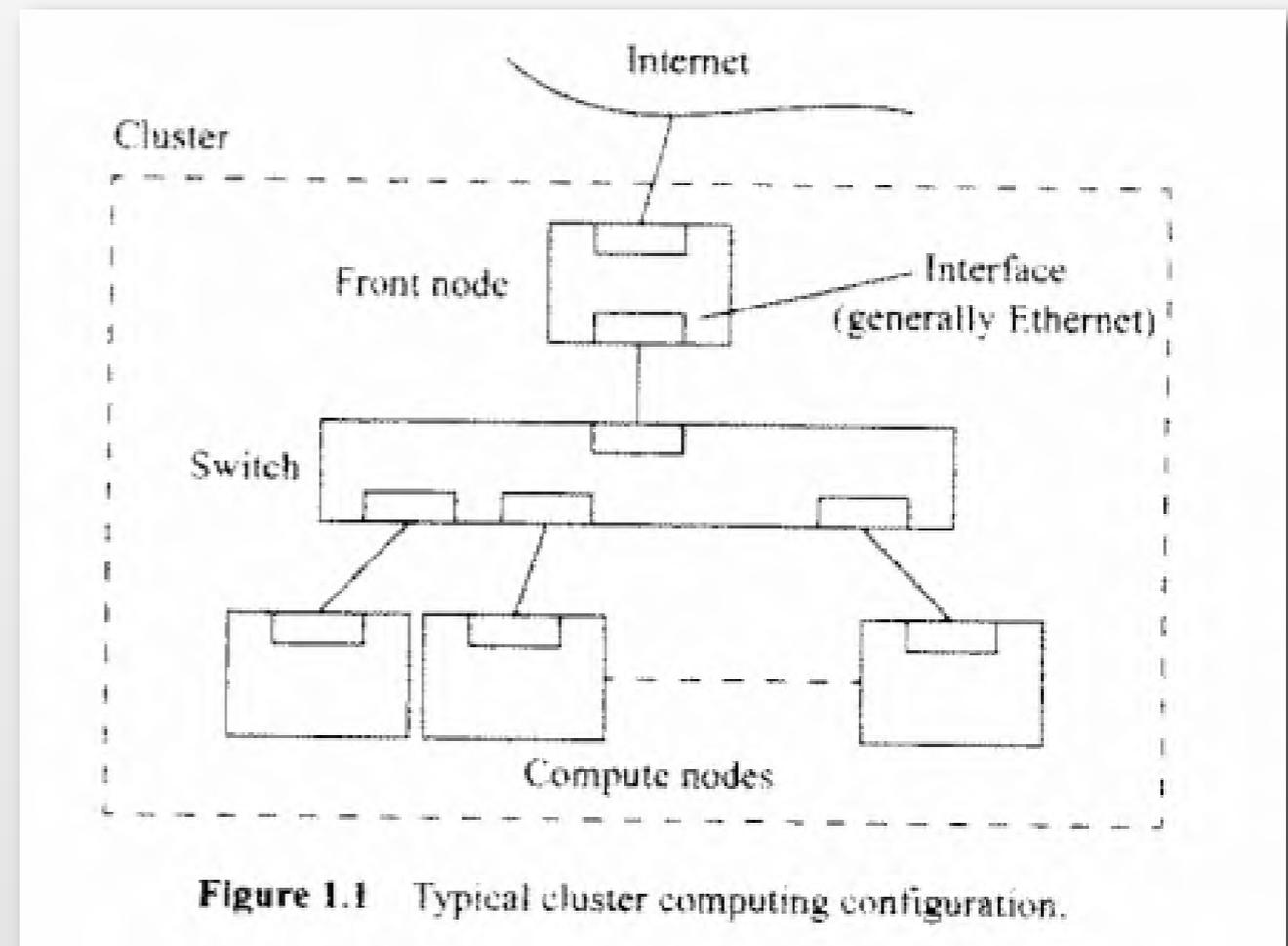
– affordable

– scaleable

* drawbacks

– distributed memory

– difficult to program



Globus toolkit

* offers mechanisms to enable a distributed computing environment, with tools to support

- communication
- resource location
- resource scheduling
- authentication
- data access

* philosophy

- no centralized control
- standard, open protocols
- non-trivial Quality of Service (QoS)

"Together, the various Globus toolkit modules can be thought of as defining a metacomputing virtual machine. The definition of this virtual machine simplifies application development and enhances portability by allowing programmers to think of geographically distributed, heterogeneous collections of resources as unified entities."

© FAIR USE Ian Foster and Carl Kesselman,
"Globus: A Metacomputing Infrastructure Toolkit,"
The International Journal of Supercomputer Applications
and High Performance Computing, 1997.

GLOBUS: A METACOMPUTING INFRASTRUCTURE TOOLKIT

Ian Foster

MATHEMATICS AND COMPUTER SCIENCE DIVISION
ARGONNE NATIONAL LABORATORY
ARGONNE, IL 60439

Carl Kesselman

INFORMATION SCIENCES INSTITUTE
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MARINA DEL REY, CA 90292

Summary

The Globus system is intended to achieve a vertically integrated treatment of application, middleware, and network. A low-level toolkit provides basic mechanisms such as communication, authentication, network information, and data access. These mechanisms are used to construct various higher level metacomputing services, such as parallel programming tools and schedulers. The long-term goal is to build an adaptive wide area resource environment (AWARE), an integrated set of higher level services that enable applications to adapt to heterogeneous and dynamically changing metacomputing environments. Preliminary versions of Globus components were deployed successfully as part of the I-WAY networking experiment.

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history of grid computing concepts

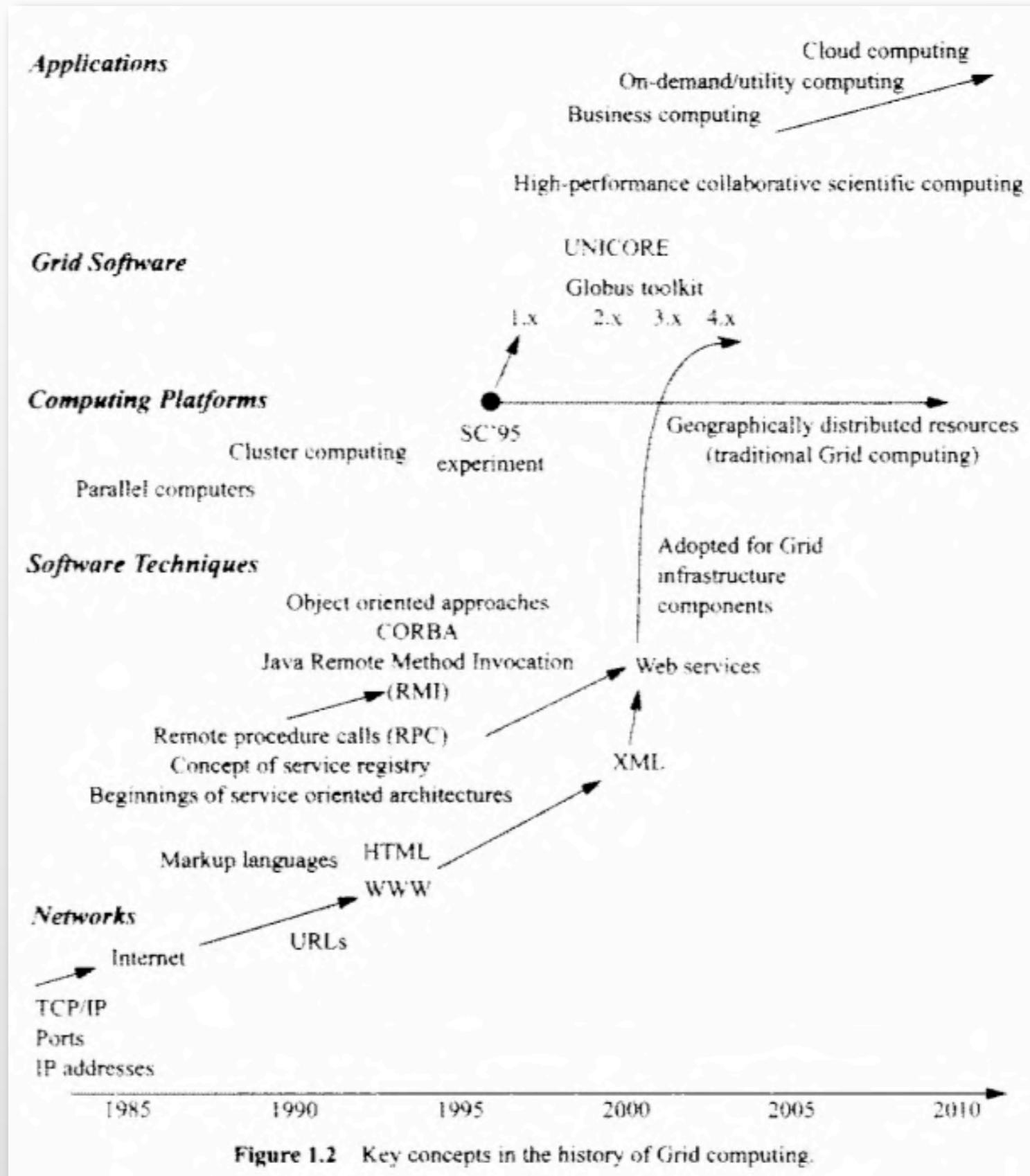
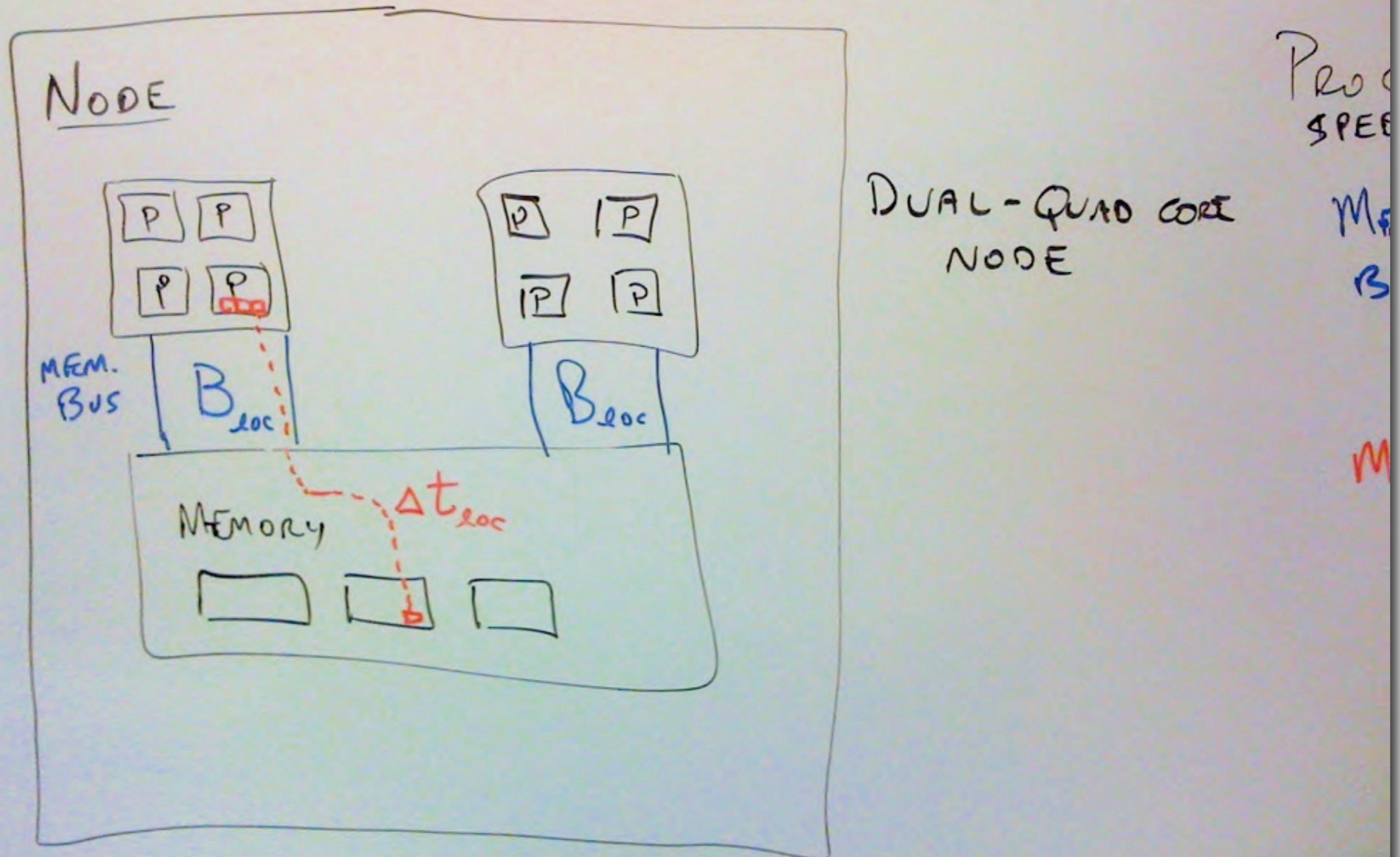


Figure 1.2 Key concepts in the history of Grid computing.

exercise: board 1

WHAT IS A SUPERCOMPUTER?



exercise: board 2

Proc.: P GFLOP/S

LOCAL MEMORY BANDWIDTH SPEED

MEMORY LATENCY

$\Delta t : ns$

Word : 64 bits

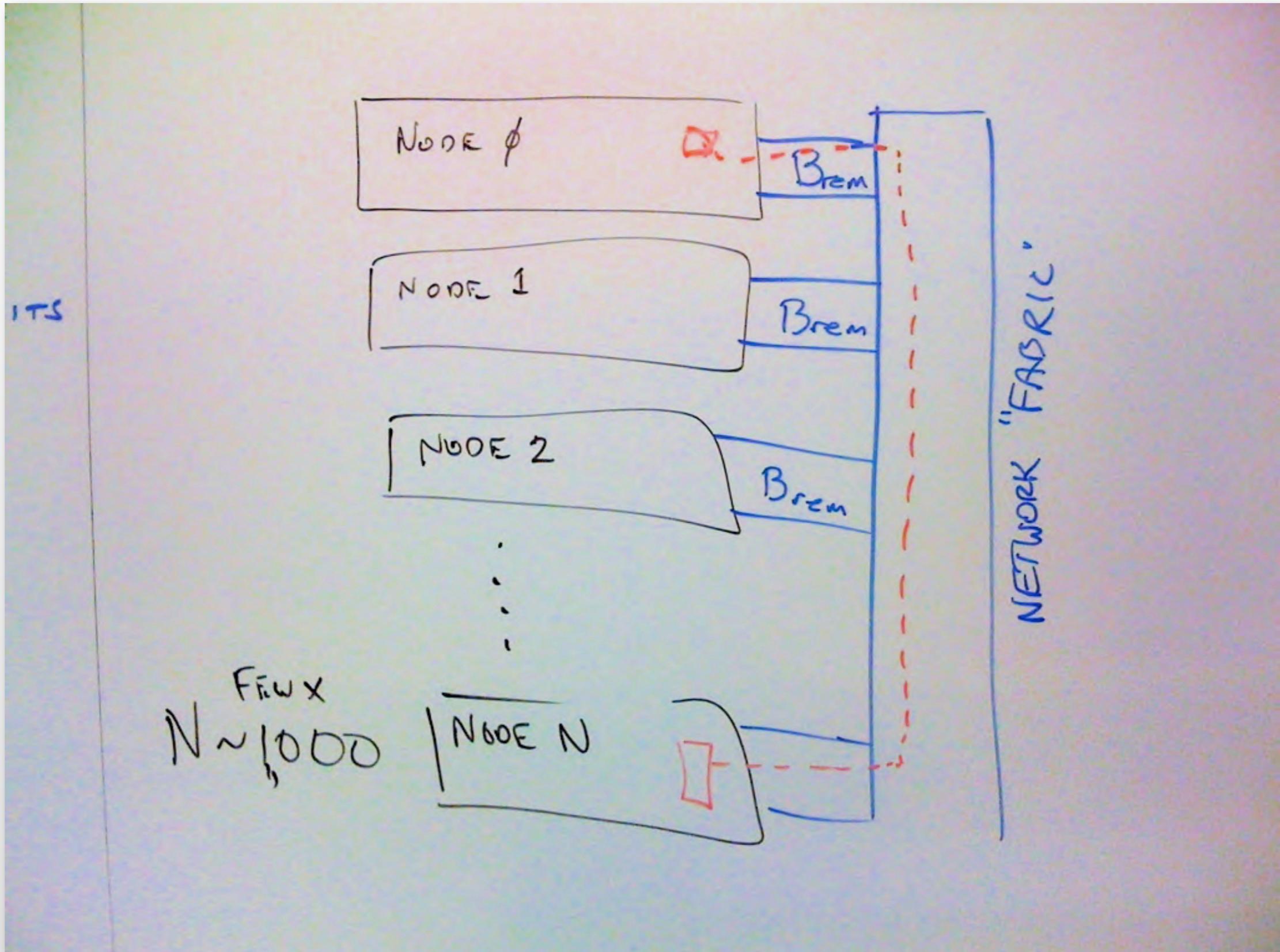
$C = 1 \text{ ft/ns}$

10^9 GIGA-FLOATING POINT OPER./SEC

GIGABIT/S

↑ NANOSEC ($10^{-9}s$)

exercise: board 3

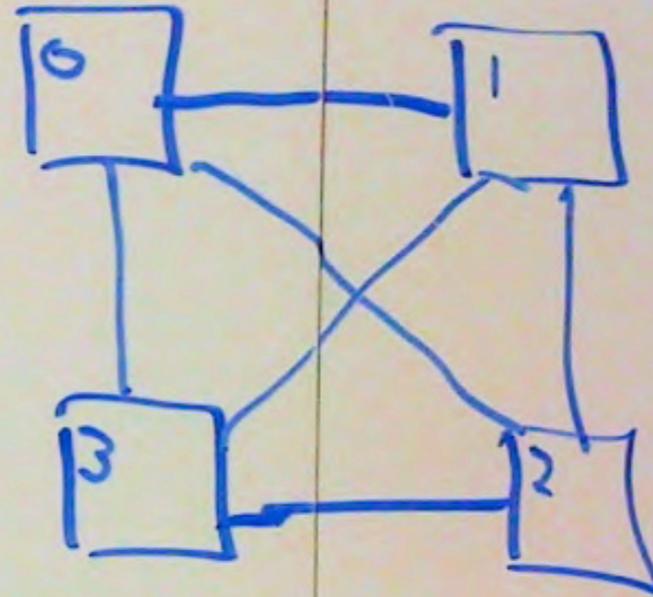
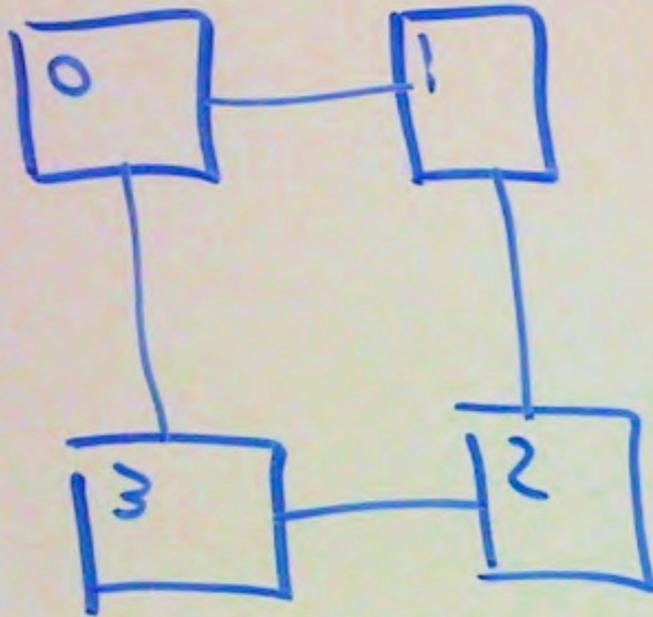


exercise: board 4

see ($10^{-9}s$)

Few x
 $N \sim 100$

4-NODE TOPOLOGIES



OR OTHERS

exercise: board 5

REMOTE
BANDWIDTH

B_{rem}

REMOTE
LATENCY

Δt_{rem}

APPLICATIONS

- ① SORT VERY
LARGE ARRAY
 $x(i+1) > x(i)$
- ② VECTOR
MULTIPLY
 $c(i) = a(i) * b(i)$

EXERCISE:

- ① DISCUSS DESIGN REQUIREMENTS IN TERMS OF P , B_{loc} , Δt_{loc} , B_{rem} , Δt_{rem}
- ② HOW IMPORTANT IS THE NETWORK "FABRIC"?

Additional Source Information

for more information see: <http://open.umich.edu/wiki/CitationPolicy>

Slide 3: Source Undetermined

Slide 5: Source Undetermined

Slide 6: Source Undetermined

Slide 7: Larry Smarr, "Set My Data Free: High-Performance CI for Data-Intensive Research," Cyberinfrastructure Days, <http://ismarr.calit2.net/presentations?slideshow=5656616>.

Slide 8: Volker Springel, Max-Planck-Institute for Astrophysics.

Slide 9: United States Federal Government, <http://science.nasa.gov/media/medialibrary/2010/03/31/BigBang2b.jpg>

Slide 10: Gus Evrard and Andrzej Kudlicki, Max-Planck-Institute for Astrophysics.

Slide 11, Image 1 (top): <http://apps.isiknowledge.com>

Slide 11, Image 2 (bottom, left): United States Federal Government, National Science Foundation

Slide 11, Image 3 (Bottom, right): United States Federal Government, NASA

Slide 12: Screenshot of search results from <http://apps.isiknowledge.com>.

Slide 13: A. E. Evrard, University of Michigan

Slide 14: A. E. Evrard, University of Michigan

Slide 15: David Walker, "4m-Victor M. Blanco Telescope," Wikimedia Commons, http://en.wikipedia.org/wiki/File:4m-Victor_M._Blanco_Telescope.jpg, CC: BY-SA 3.0, <http://creativecommons.org/licenses/by-sa/3.0/>

Slide 16: Source Undetermined

Slide 17 (all images): A. E. Evrard, University of Michigan

Slide 19: Source Undetermined

Slide 20: Foster and Kesselman, The International Journal of Supercomputer Applications and High Performance Computing, 1997, 11:2, 115-128.

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