

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

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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)		
Processor:	Intel Xeon X5650, 2.66Ghz, 12M Cache,Turbo, HT, 1333MHz Max Mem (317-4052)		
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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)		
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:	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



Date: 9/20/10 8:55:11 AM

Customer Name: UNIV OF MICHIGAN

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

GROUP: 1	QUANTITY: 1	SYSTEM PRICE: \$19,024.72	GROUP TOTAL: \$19,024.72
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Hard Drive:	CARR,HD,2.5,2LED,C6100,MLK (342-1032)		

**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



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)

**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)**

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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**



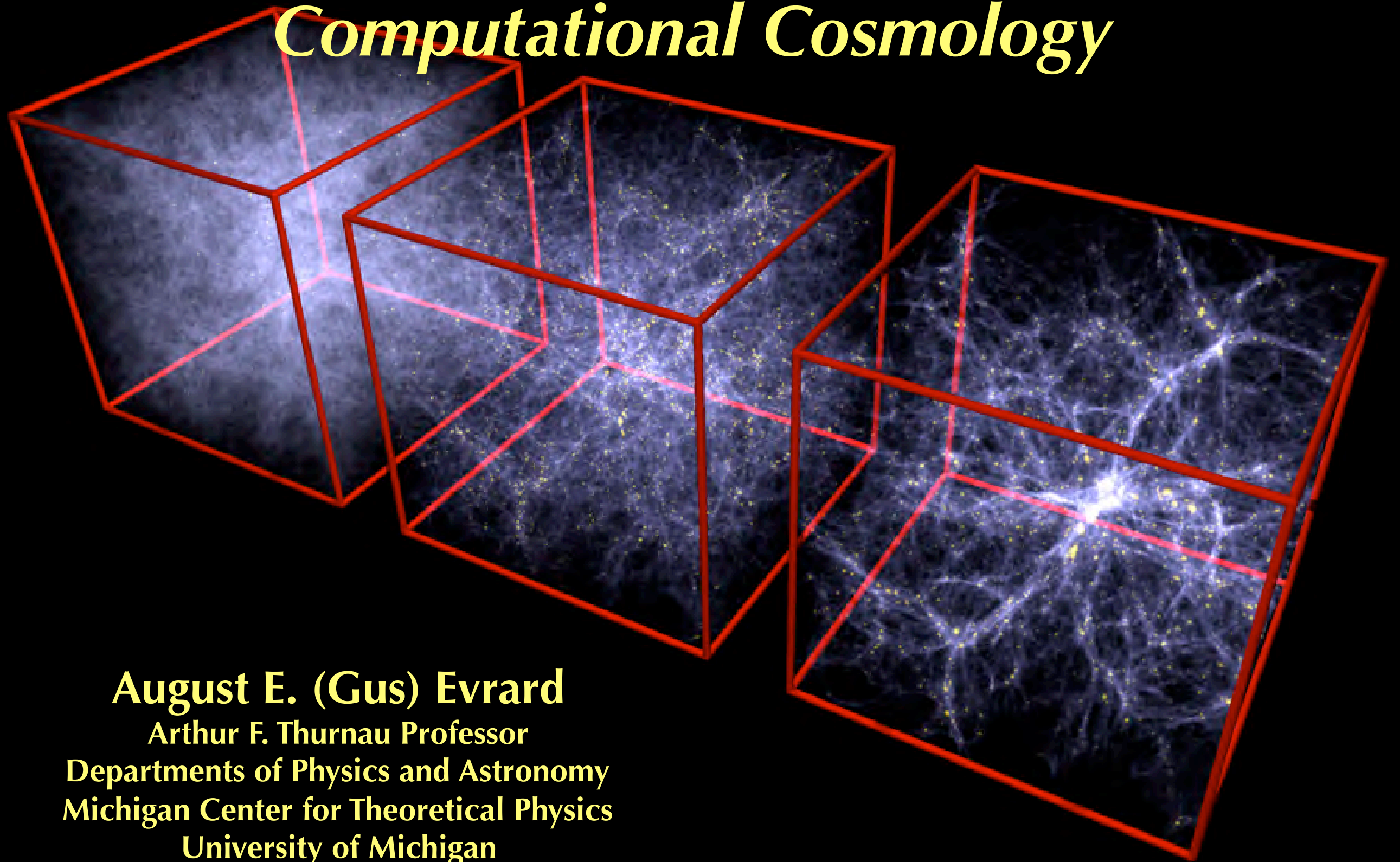
© FAIR USE Larry Smarr, Cyberinfrastructure Days



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

Big Bang plus  
 $10^{-42}$  Seconds

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

quantum effects  
important early  
(Heisenberg)

Big Bang plus  
300,000 Years

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

Light

Gravitational Waves

Now

classical physics  
dominates late  
(Newton)

Big Bang plus  
15 Billion Years

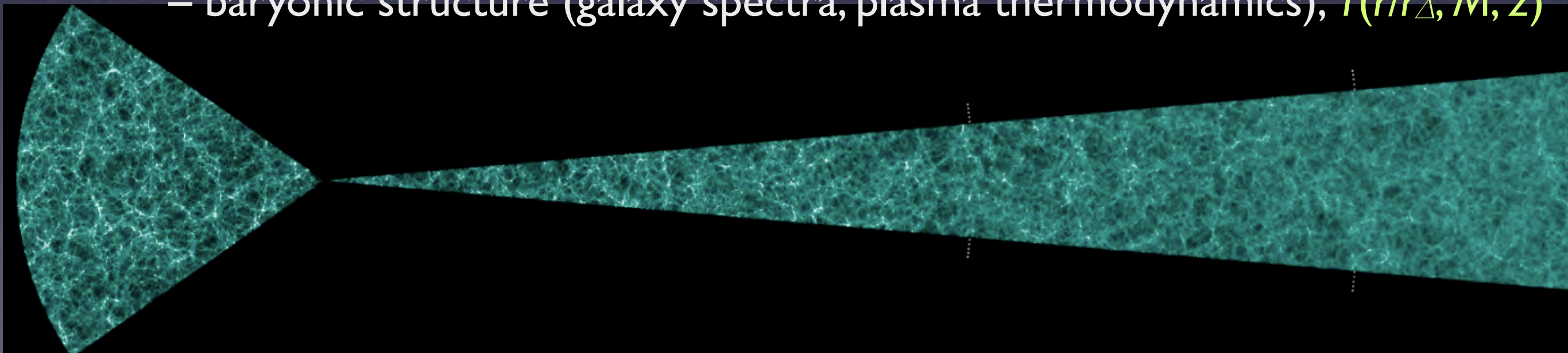
## 2010 paradigm of cosmological **large-scale structure (LSS)**

**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),  $Y(r/r_\Delta, M, z)$





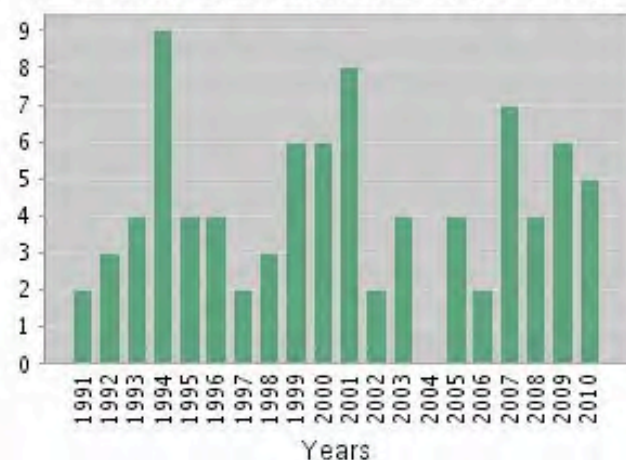
# evrard group research

## Citation Report Author=(evrard, a\*) AND Address=(michigan OR berkeley OR cambridge)

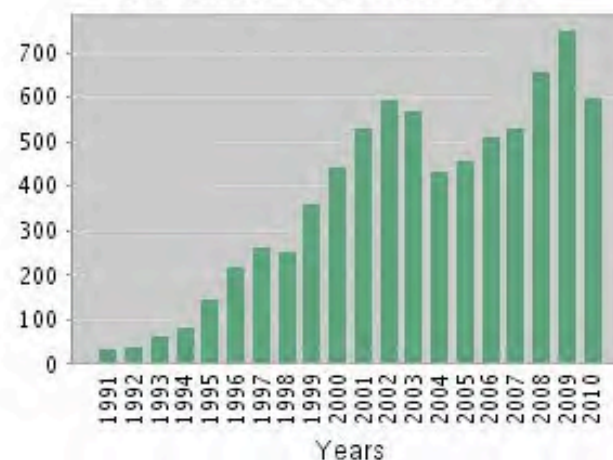
Timespan=All Years. Databases=SCI-EXPANDED, SSCI, A&HCI, CPCI-S, CPCI-SSH.

This report reflects citations to source items indexed within Web of Science. Perform a Cited Reference Search to include citations to items not indexed within Web of Science.

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Results found: 97

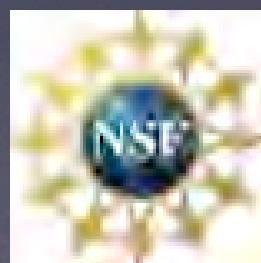
Sum of the Times Cited [?] : 7,606

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Average Citations per Item [?] : 78.41

h-index [?] : 38





							2006	2007	2008	2009	2010	Total
Use the checkboxes to remove individual items from this Citation Report or restrict to items processed between 1900-1914 and 2010 <input type="button" value="Go"/>							514	534	660	750	601	7,606
<input type="checkbox"/>	1.	Title: <a href="#">Simulations of the formation, evolution and clustering of galaxies and quasars</a> Author(s): Springel V, White SDM, Jenkins A, et al. Source: <b>NATURE</b> Volume: <b>435</b> Issue: <b>7042</b> Pages: <b>629-636</b> Published: <b>JUN 2 2005</b>					88	133	189	223	170	818
<input type="checkbox"/>	2.	Title: <a href="#">The mass function of dark matter haloes</a> Author(s): Jenkins A, Frenk CS, White SDM, et al. Source: <b>MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY</b> Volume: <b>321</b> Issue: <b>2</b> Pages: <b>372-384</b> Published: <b>FEB 21 2001</b>					91	63	67	83	57	734
<input type="checkbox"/>	3.	Title: <a href="#">THE BARYON CONTENT OF GALAXY CLUSTERS - A CHALLENGE TO COSMOLOGICAL ORTHODOXY</a> Author(s): WHITE SDM, NAVARRO JF, EVRARD AE, et al. Source: <b>NATURE</b> Volume: <b>366</b> Issue: <b>6454</b> Pages: <b>429-433</b> Published: <b>DEC 2 1993</b>					21	15	18	19	20	688
<input type="checkbox"/>	4.	Title: <a href="#">Mass estimates of X-ray clusters</a> Author(s): Evrard AE, Metzler CA, Navarro JF Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>469</b> Issue: <b>2</b> Pages: <b>494-507</b> Part: <b>Part 1</b> Published: <b>OCT 1 1996</b>					31	31	20	22	12	482
<input type="checkbox"/>	5.	Title: <a href="#">Properties of the intracluster medium in an ensemble of nearby galaxy clusters</a> Author(s): Mohr JJ, Mathiesen B, Evrard AE Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>517</b> Issue: <b>2</b> Pages: <b>627-649</b> Part: <b>Part 1</b> Published: <b>JUN 1 1999</b>					33	16	25	16	8	386
<input type="checkbox"/>	6.	Title: <a href="#">The L-X-T relation and intracluster gas fractions of X-ray clusters</a> Author(s): Arnaud M, Evrard AE Source: <b>MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY</b> Volume: <b>305</b> Issue: <b>3</b> Pages: <b>631-640</b> Published: <b>MAY 11 1999</b>					22	26	21	13	11	320
<input type="checkbox"/>	7.	Title: <a href="#">FORMATION AND EVOLUTION OF X-RAY-CLUSTERS - A HYDRODYNAMIC SIMULATION OF THE INTRACLUSTER MEDIUM</a> Author(s): EVRARD AE Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>363</b> Issue: <b>2</b> Pages: <b>349-366</b> Part: <b>Part 1</b> Published: <b>NOV 10 1990</b>					5	4	8	6	9	268
<input type="checkbox"/>	8.	Title: <a href="#">EXPECTATIONS FOR X-RAY-CLUSTER OBSERVATIONS BY THE ROSAT SATELLITE</a> Author(s): EVRARD AE, HENRY JP Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>383</b> Issue: <b>1</b> Pages: <b>95-103</b> Part: <b>Part 1</b> Published: <b>DEC 10 1991</b>					14	13	9	7	7	242
<input type="checkbox"/>	9.	Title: <a href="#">The Santa Barbara cluster comparison project: A comparison of cosmological hydrodynamics solutions</a> Author(s): Frenk CS, White SDM, Bode P, et al. Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>525</b> Issue: <b>2</b> Pages: <b>554-582</b> Part: <b>Part 1</b> Published: <b>NOV 10 1999</b>					20	19	17	22	10	241
<input type="checkbox"/>	10.	Title: <a href="#">Galaxy clusters in Hubble volume simulations: Cosmological constraints from sky survey populations</a> Author(s): Evrard AE, MacFarland TJ, Couchman HMP, et al. Source: <b>ASTROPHYSICAL JOURNAL</b> Volume: <b>573</b> Issue: <b>1</b> Pages: <b>7-36</b> Part: <b>Part 1</b> Published: <b>JUL 1 2002</b>					18	19	22	23	15	201

Sim

Sim

Sim+Data

Sim

Data

Data

Sim

Theory

Sim

Sim



*Fisher forecasts*

Huterer

Cunha

Erickson

*LSS simulations*

Rasia

Stanek

Nord

Chen

Rudd (IAS)

Pearce (Nottingham)

+ **Virgo Consortium**

grad student

postdoc

faculty

galaxy  
clusters  
as  
massive  
halos

*LoCuSS (X-ray)*

G. Smith (Birmingham)

+ LoCuSS Collaboration

*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**

## 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 deg<sup>2</sup> *grizY* colors to ~24<sup>th</sup> mag

Repeated observations of 40 deg<sup>2</sup>

## Development and schedule

Construction: 2007-2011

New 3 deg<sup>2</sup> 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

 **LBNL** — 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

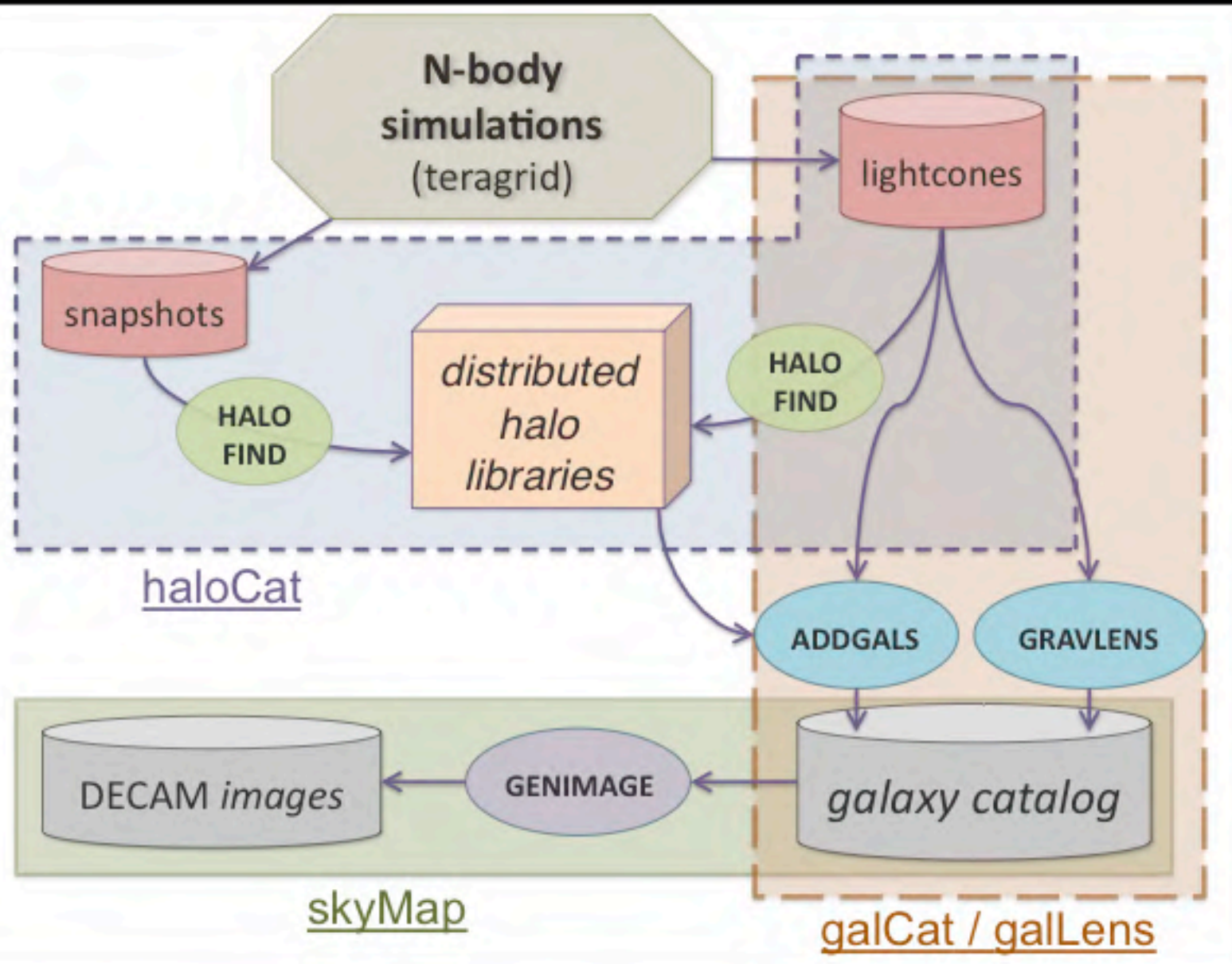
Luiz DaCosta, Observatorio Nacional, Brazil

Klaus Dolag, Max-Planck-Institut fur Astrophysik

Claudio Gheller, CINECA, Italy

Gerard Lemson, Max-Planck-Institut fur Astrophysik

Huan Lin, Fermi National Laboratory, USA



Source Undetermined

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

Course Goals: Students who have taken this course should:

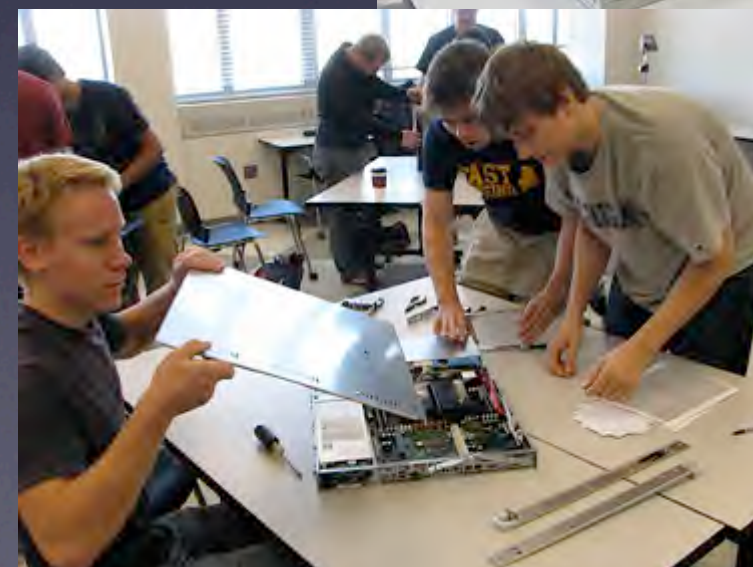
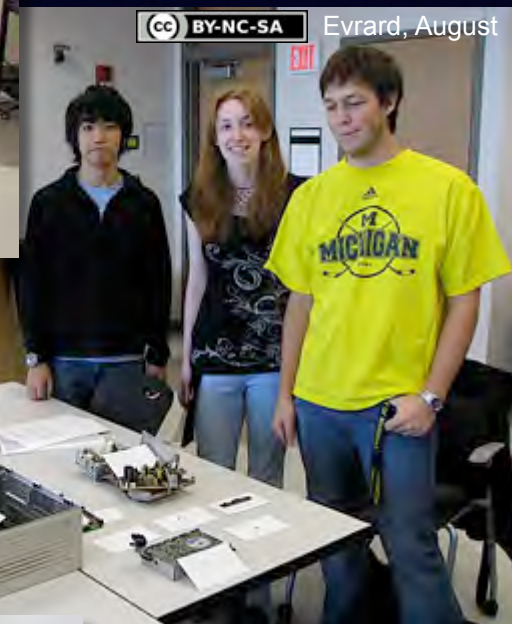
1. be able to explain what computation means in the context of scientific inquiry, and provide examples of the different roles that computing plays in the sciences;

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

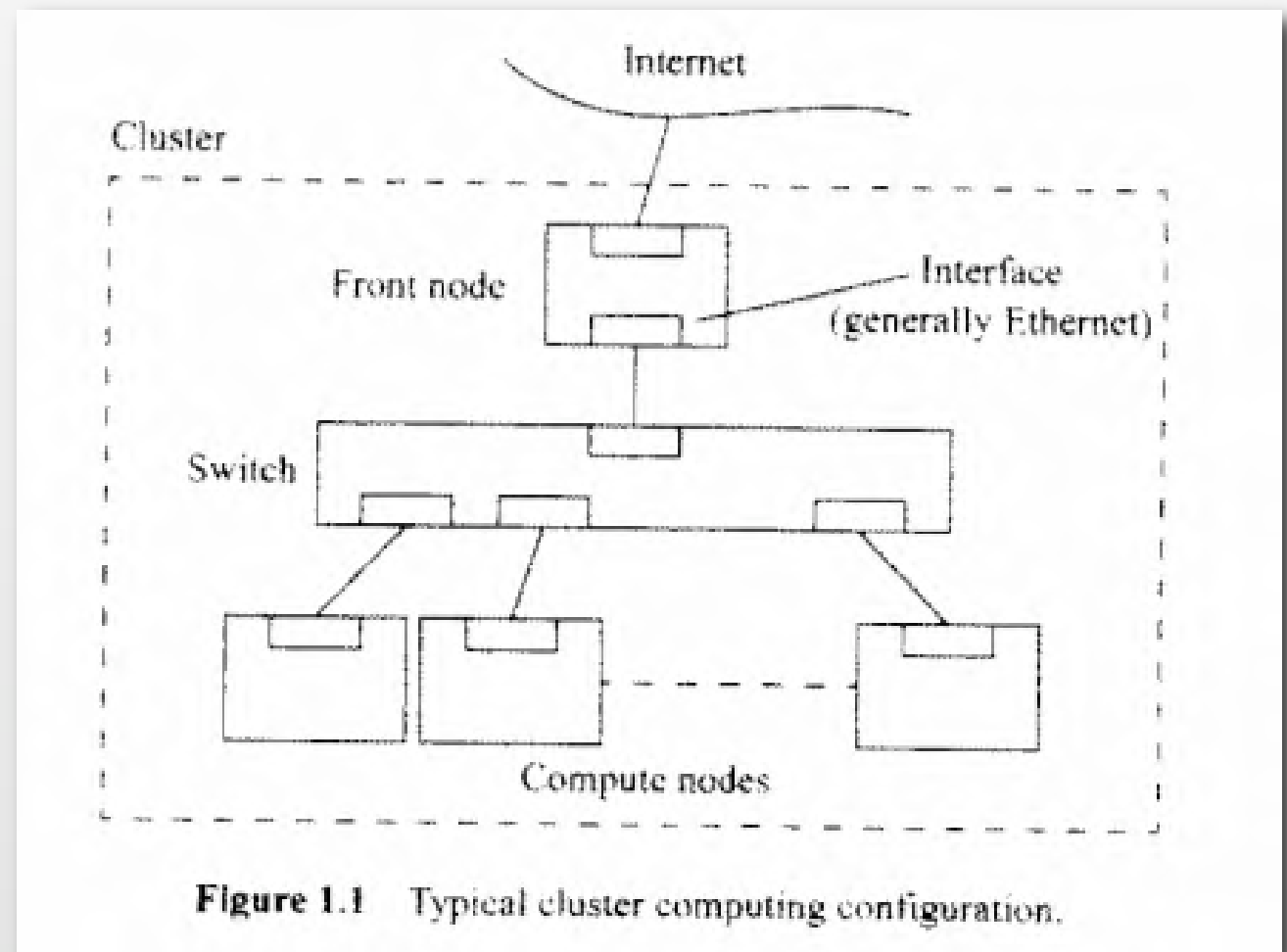
"thirty men's heft of grasp in the gripe of his hand."

- \* 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  
UNIVERSITY OF SOUTHERN CALIFORNIA  
MARINA DEL REY, CA 90292

### Summary

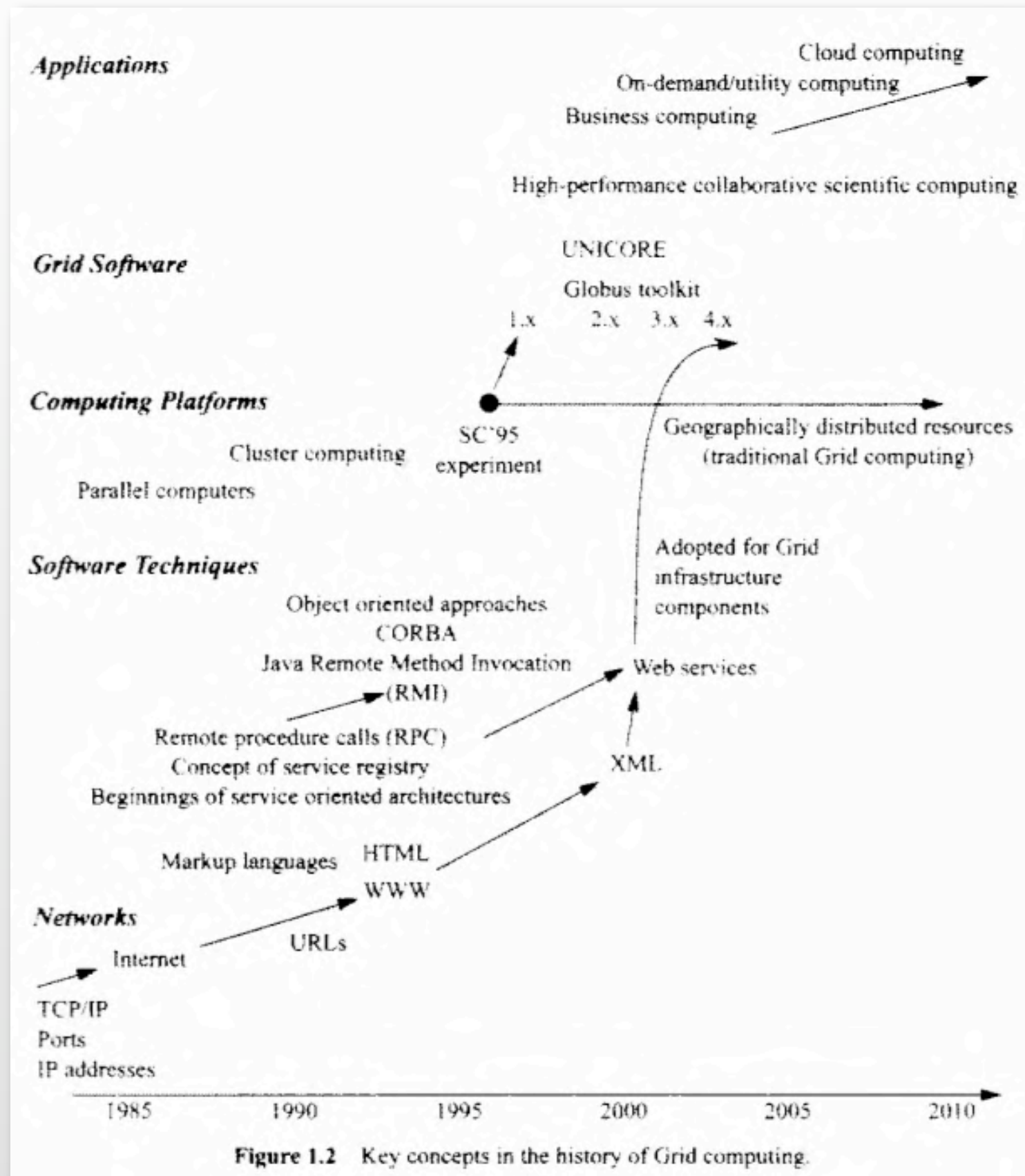
The Globus system is intended to achieve a vertically integrated treatment of application, middleware, and network. A low-level toolkit provides basic mechanisms such as communication, authentication, network information, and data access. These mechanisms are used to construct various higher level metacomputing 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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*The International Journal of Supercomputer Applications and High Performance Computing*  
Volume 11, No. 2, Summer 1997, pp. 115-128  
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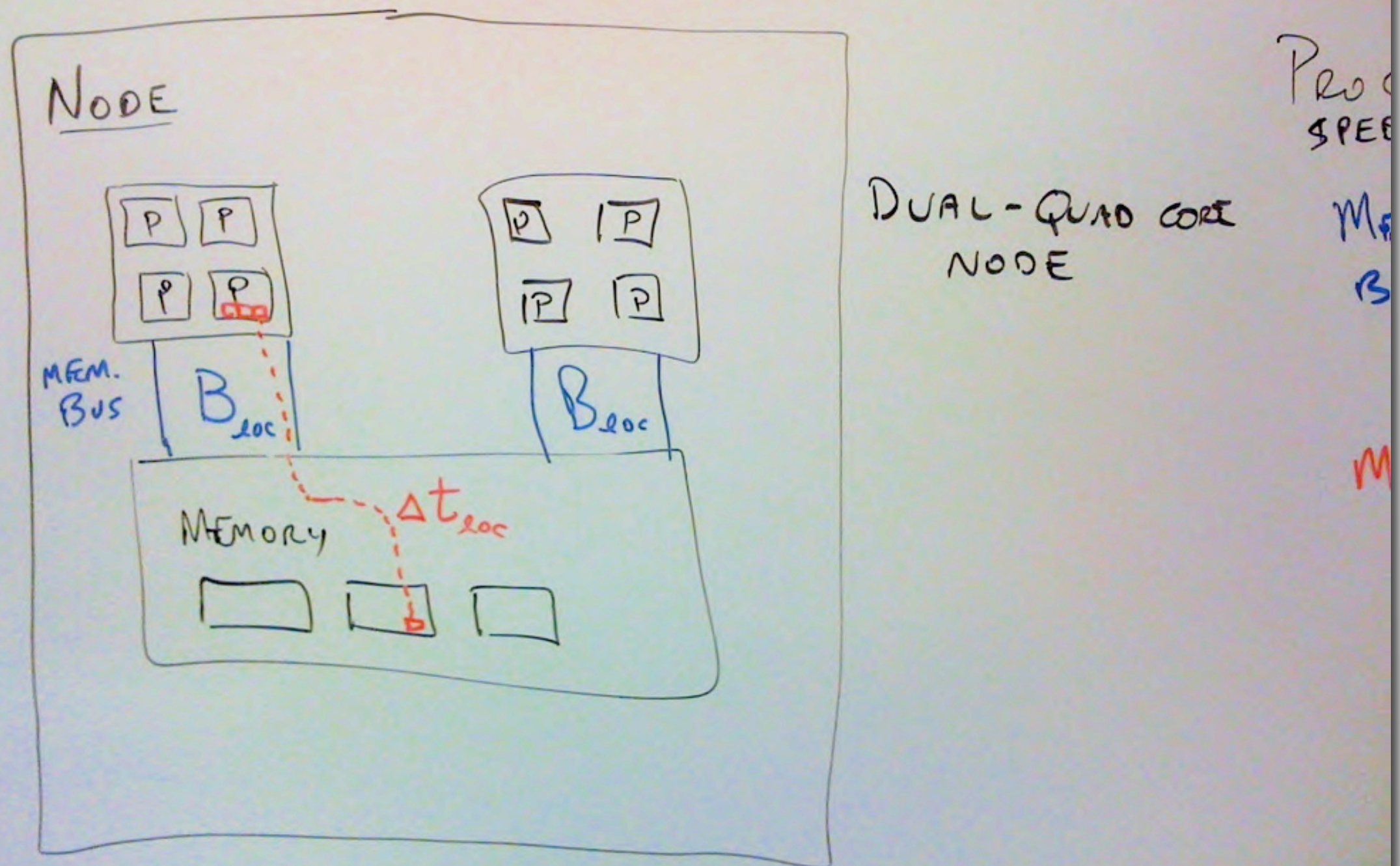


# history of grid computing concepts



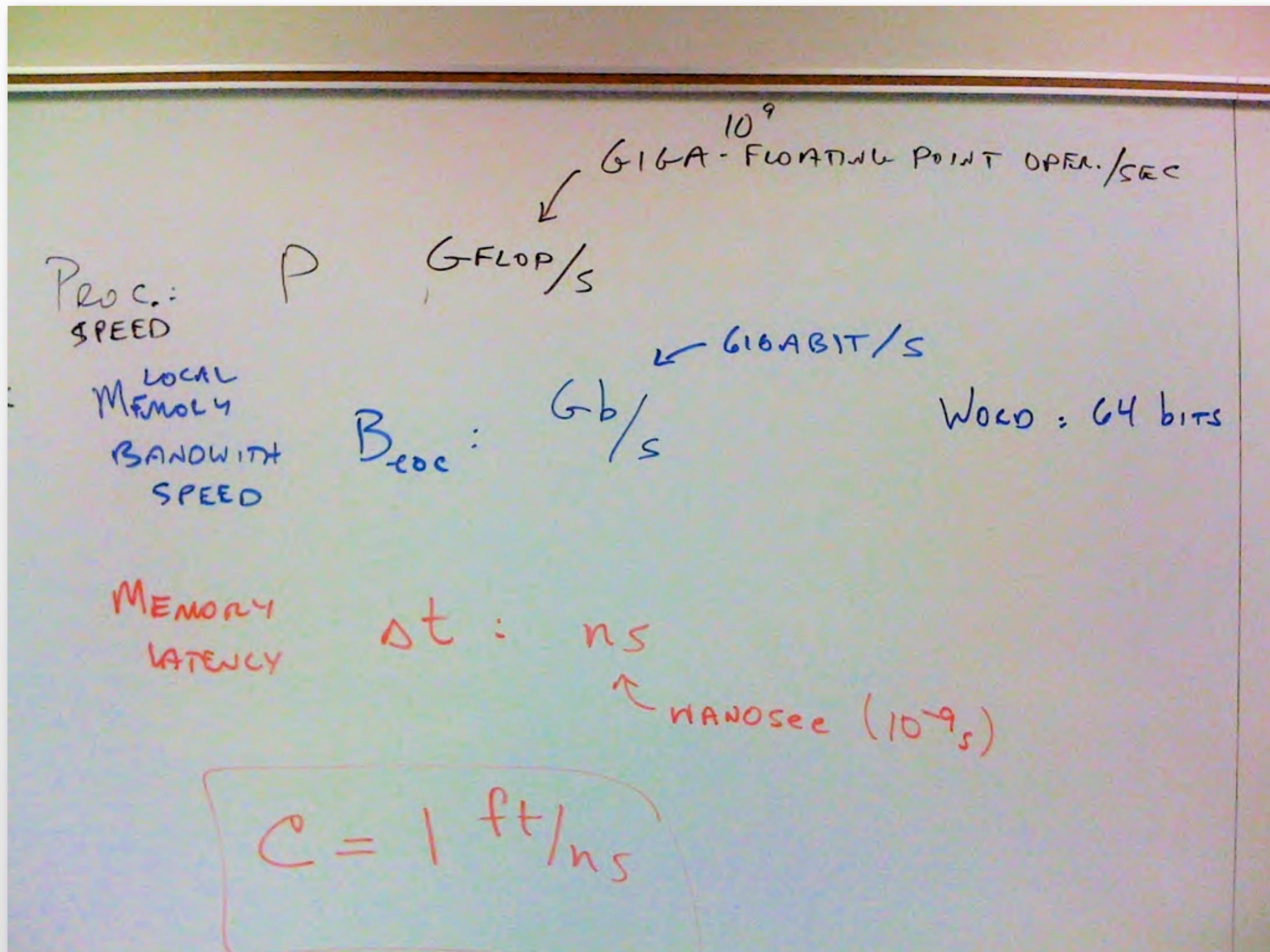
# exercise: board 1

WHAT IS A SUPERCOMPUTER?



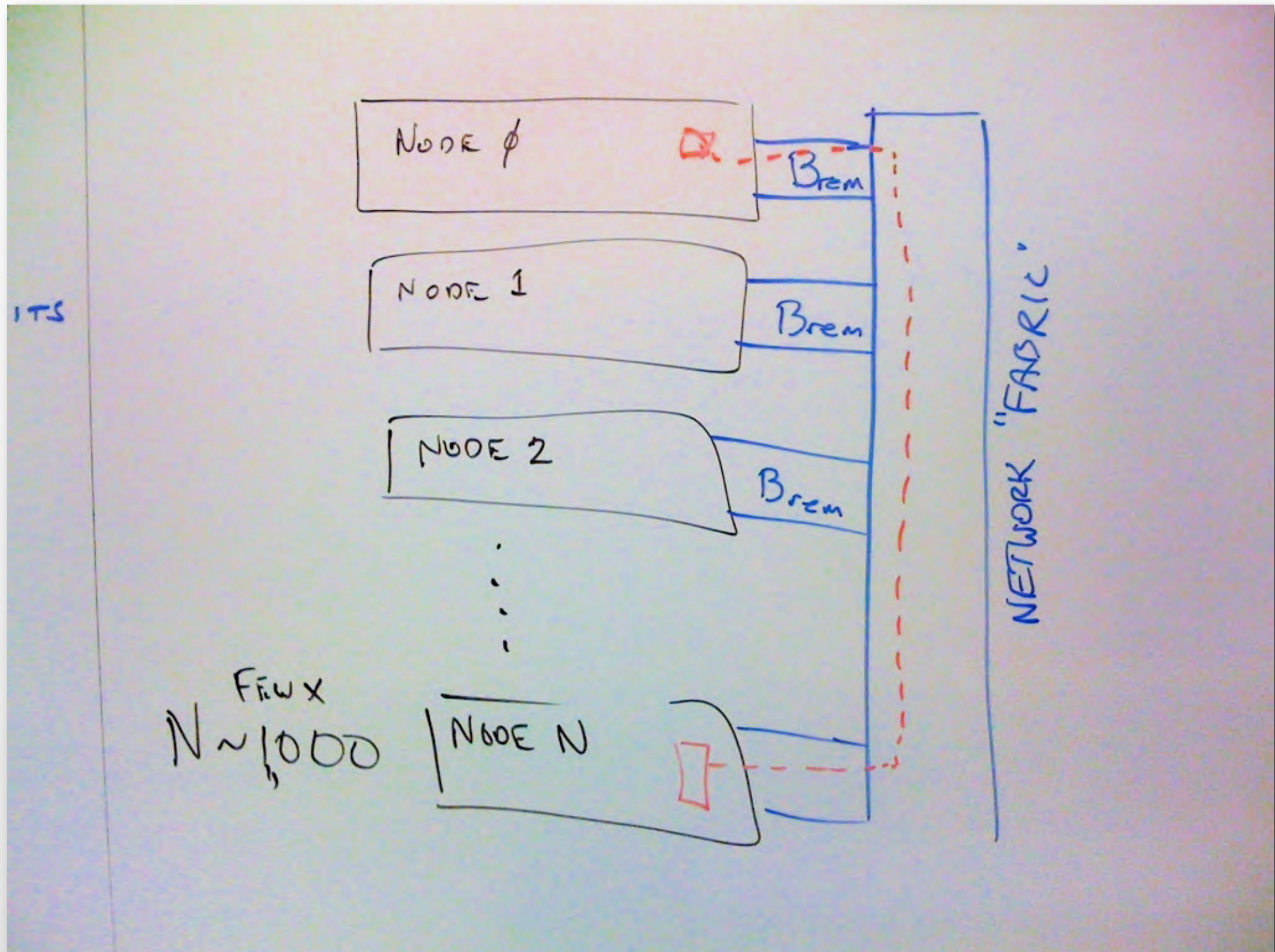


# exercise: board 2





# exercise: board 3



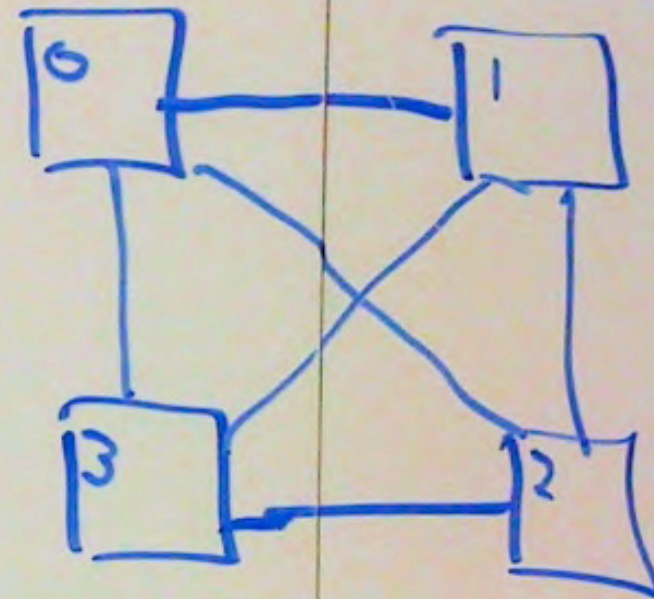
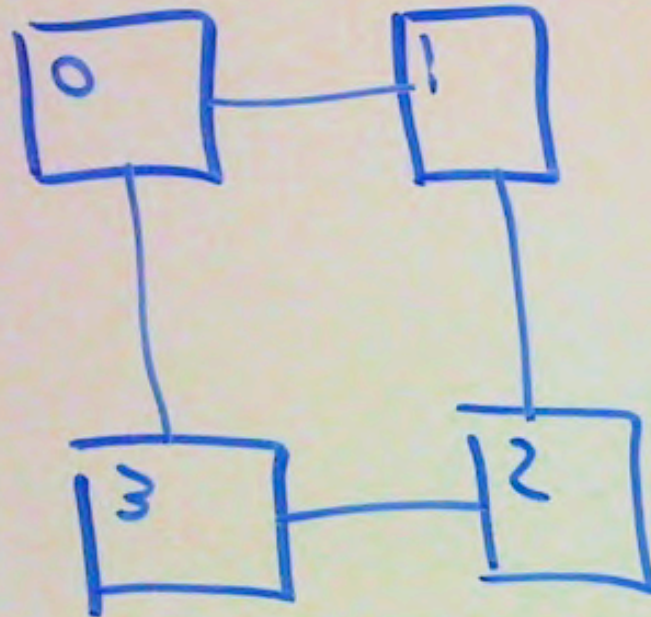


# exercise: board 4

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

Few x  
 $N \sim 100$

## 4-NODE TOPOLOGIES



OR OTHERS



# exercise: board 5

REMOTE  
BANDWIDTH

$B_{rem}$

REMOTE  
LATENCY

$\Delta t_{rem}$

## 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  $P$ ,  $B_{loc}$ ,  $\Delta t_{loc}$ ,  $B_{rem}$ ,  $\Delta t_{rem}$

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](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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Slide 22: A. E. Evrard, University of Michigan

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