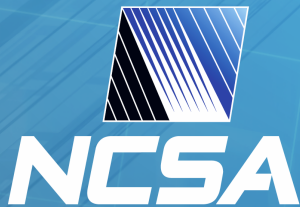


# NCSA Research Fellows 2015 Kick off Presentation

Gabrielle Allen, NCSA Associate Director  
Professor of Astronomy



National Center for Supercomputing Applications  
University of Illinois at Urbana-Champaign

# NCSA 2013



- NCSA: R&D unit of UIUC
  - One of original five NSF-funded supercomputing centers
    - **Mission:** Provide state-of-the-art computing capabilities (hardware, software, hpc expertise) to nation's scientists and engineers
- In total, ~\$1 Billion brought to UIUC since 1985
  - Approximately 200 staff (160+ technical/professional staff), two facilities
  - Operating NSF's most powerful computing system: Blue Waters
    - \$345 Million from NSF
  - Managing NSF's national cyberinfrastructure: XSEDE
    - \$145 Million from NSF
  - Private Sector Program: over 2 dozen partners, ~\$3 Million annual

Source: Thom Dunning



# Petascale Computing Facility: Home to Blue Waters, Research Platform for Nation



- **Blue Waters**

- Funds 50 staff!!
- 13PF, 1500TB, 300PB
- >1PF On real apps
- NAMD, MILC, WRF, PPM, NWChem, etc

- **Modern Data Center**

- 90,000+ ft<sup>2</sup> total
- 30,000 ft<sup>2</sup> raised floor
- 20,000 ft<sup>2</sup> machine room gallery

- **Networking**

- 400 Gbits to outside world

Source: Thom Dunning



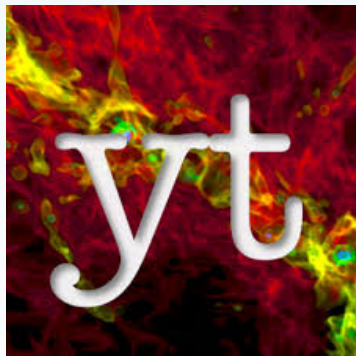
# Example Projects, Centers, Facilities



XSEDE, national cyberinfrastructure



Browndog: Curation for "long tail" unstructured data



Data analysis for large scale simulation data



LSST Data pipeline

- CyberGIS Center for Advanced Digital and Spatial Studies
- I-CHASS Institute for Computing in Humanities, Arts and Social Sciences
- eDream Emerging Digital Research & Education in Arts Media Institute

- ISL Innovative Systems Laboratory
- AVL Advanced Visualization Laboratory

# Vice Chancellor for Research

Peter Schiffer

**Executive Associate  
Vice Chancellor**  
*Chief of Staff*  
Melanie Loots

**Administrative  
Aide**  
Juan Chambers

**Associate Vice Chancellor**  
*Humanities, Arts, &  
Related Fields; Research Board*  
Nancy Abelmann

**Associate  
Vice Chancellor**  
*Research Integrity Officer*  
Howard Guenther

**Director of  
Research Information  
Analytics**  
George Chacko

**Director of  
Research  
Communications**  
Melissa Edwards

**Associate  
Vice Chancellor**  
Jennifer Eardley

**Associate Vice Chancellor  
Director,  
Sponsored Programs**  
Dave Richardson

**Associate  
Vice Chancellor**  
*Compliance*  
Jan Novakofski

**Assistant  
Vice Chancellor**  
*HR, Finance, & IT*  
Lauren Stokes

**Associate Vice Chancellor  
Director, Division of  
Animal Resources**  
Lyndon Goodly

**Office of  
Proposal Development**  
Sheryl Goldberg, Director

**OSP**  
Office of  
Sponsored Programs

**Division of  
Research Safety**  
Peter Ashbrook, Director

**I.T. Support Group**  
Michael Brosco,  
Director

**DAR**  
Division of  
Animal Resources

**Beckman Institute for  
Advanced Science  
and Technology**  
Art Kramer, Director

**Institute for  
Genomic Biology**  
Gene Robinson, Director

**Institutional Animal Care &  
Use Committee**  
Phil Solter, Chair

**Human Resources**  
Sue Key,  
Director

**International  
Research Partnerships**  
Kraig Wagenecht, Director

**Prairie Research Institute**  
William Shilts,  
Executive Director

**National Center for  
Supercomputing  
Applications**  
Edward Seidel, Director

**Institutional  
Review Board**  
Anita Balgopal, Director

**Center for  
Advanced Study**  
Leon Dash, Director

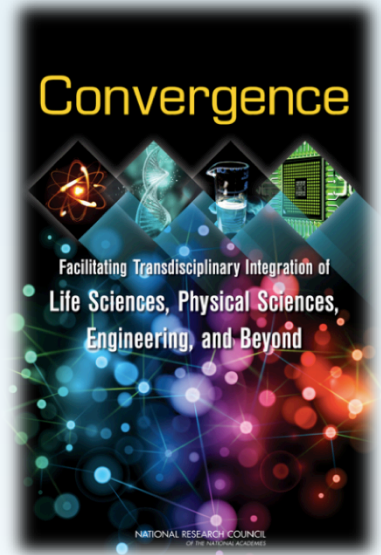
**Institute for  
Sustainability, Energy,  
and the Environment**  
Evan DeLucia, Director

**Interdisciplinary Health  
Sciences Initiative**  
Neal Cohen, Director

**Agricultural Animal Care &  
Use Program**  
Vickie Jarrell, Director

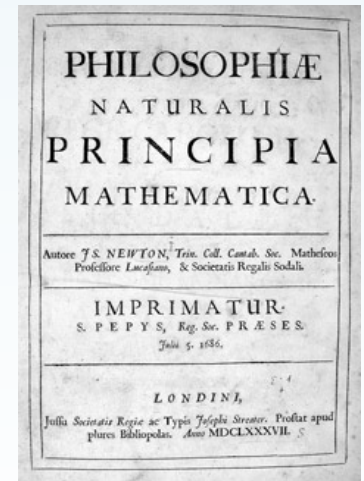
**Carver Biotechnology  
Center**  
Bruce Fouke, Director

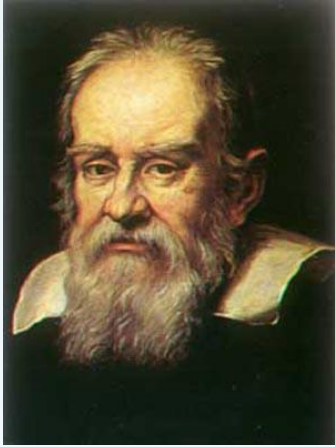
- Research Institutes
- VCR Administration
- Compliance & Research Support Units



21<sup>st</sup> Century Research and Education  
Addressing *Major Challenges for Universities*

# NCSA 2014 AND BEYOND





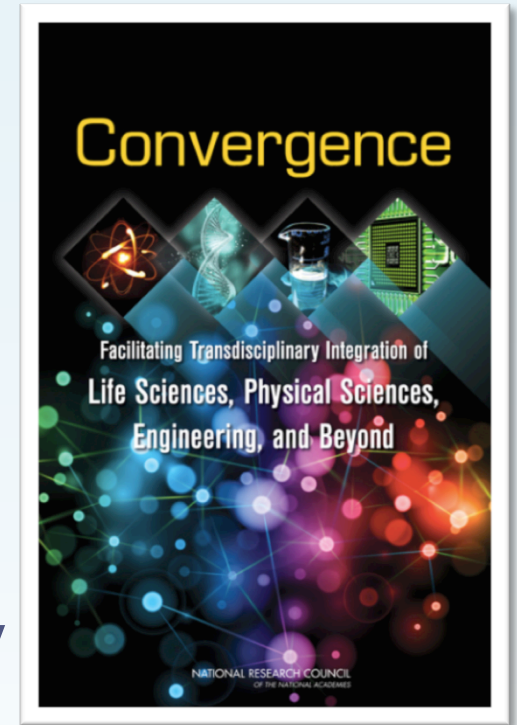
# COLLABORATIONS FOR COMPLEX PROBLEMS



# National Academy Reports...

“*Convergence* [is] a culture shift for academic organizations that are traditionally organized around discipline-based departments....”

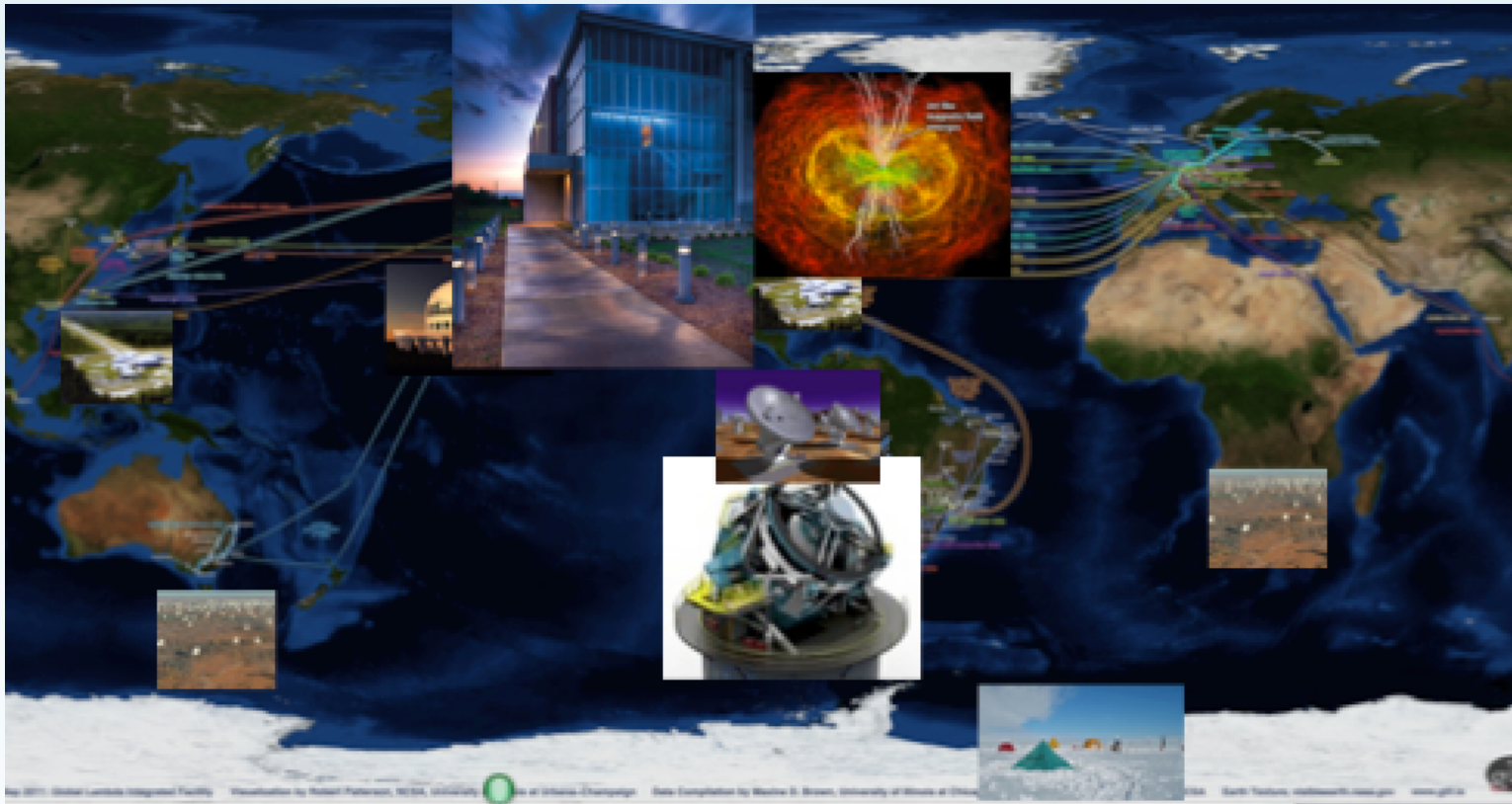
“...most difficult problems do not respect disciplinary boundaries...convergent science, [integrates] insights and approaches from many fields...barriers to convergent science...”



New university infrastructure, education, reward structures:

- Software, networks, data, sharing, computing, etc
- University hiring, promotion and tenure cultures
  - Example: Young Assistant Prof. Candidates...
  - “Publications.” What is a modern publication?





# COMPUTE AND DATA INTENSIVE REVOLUTION



An integral, *integrative* unit of the campus...

# NCSA ROLE AT UIUC



# The Three NCSA Pillars

- Big Research and Education Ecosystem
  - Combine best strengths of the cultures of Professional Staff with Faculty, Postdocs, and Students
  - Interdisciplinarity and Innovation
  - Integral to campus: a great environment draws campus *inside* NCSA
- Big Data
  - 21<sup>st</sup> century digital campus, region, nation
  - Instruments, MREFC projects
  - Services, tools, software
  - Research and education
- Big Compute
  - Highest end systems and Applications
  - Tools and software expand to all parts of ecosystem

All with with innovation throughout; PSP and innovation programs

# NCSA Thematic Areas

- Faculty-led research at NCSA organized through a set of thematic areas (faculty, research groups, postdocs, students).
- Address major challenges or opportunities that are complex, multifaceted, and interdisciplinary, going beyond traditional individual/departmental efforts, requiring deep connection to NCSA technologies and expertise.
- Theme characteristics include:
  - Broadly defined with a portfolio of component research projects spanning multiple inter-related activities
  - Contribute to the nation's advanced cyberinfrastructure programs
  - Involve faculty from multiple home departments and colleges.
  - Align with and advance the Illinois Strategic Plan.

# NCSA Thematic Areas

Culture & Society

Donna Cox



Computing & Data Science

Gabrielle Allen



Physics & Astronomy

Athol Kemball



Bioinformatics & Health Sciences

Victor Jongeneel



Earth & Environment

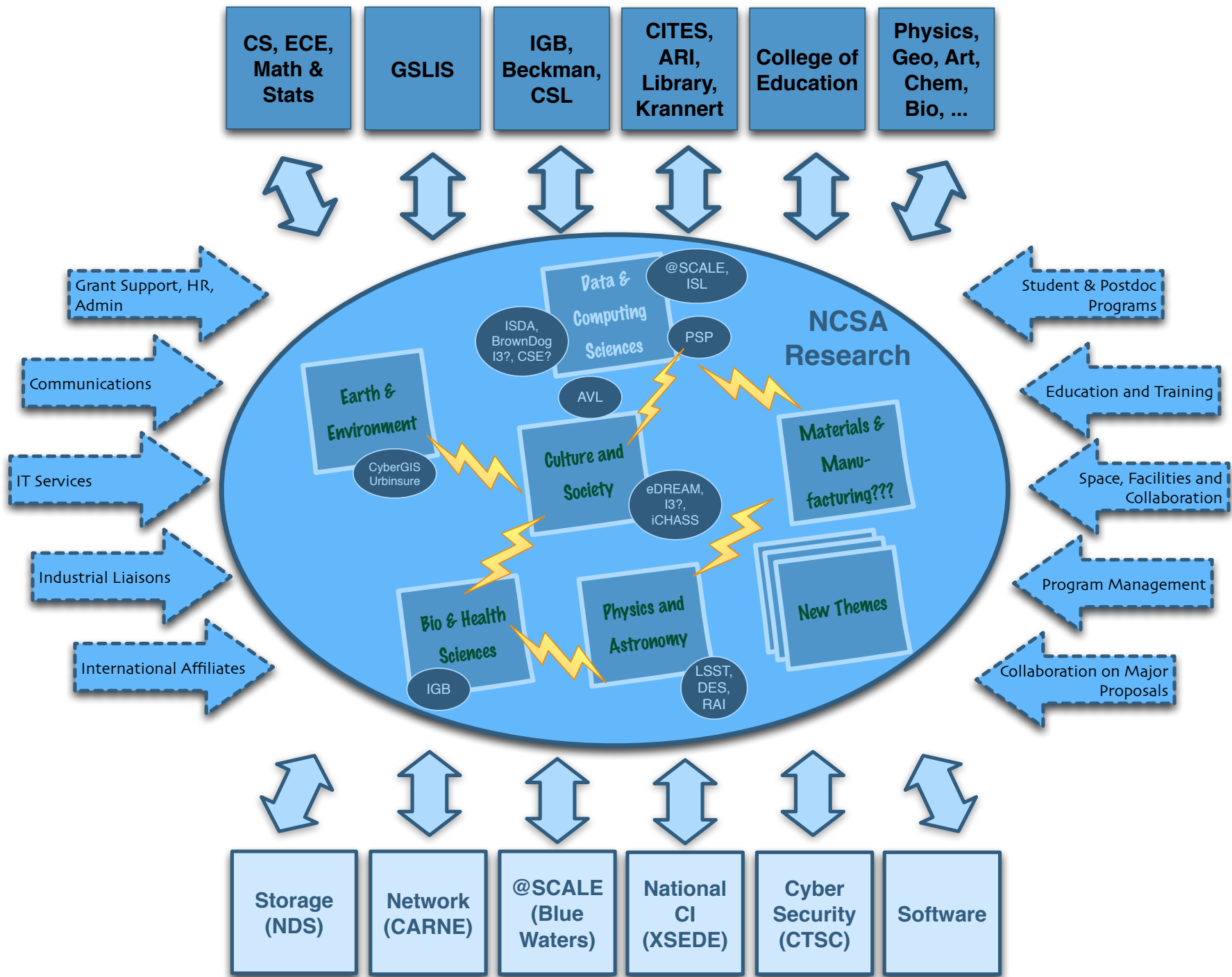
Shaowen Wang



Materials & Manufacturing

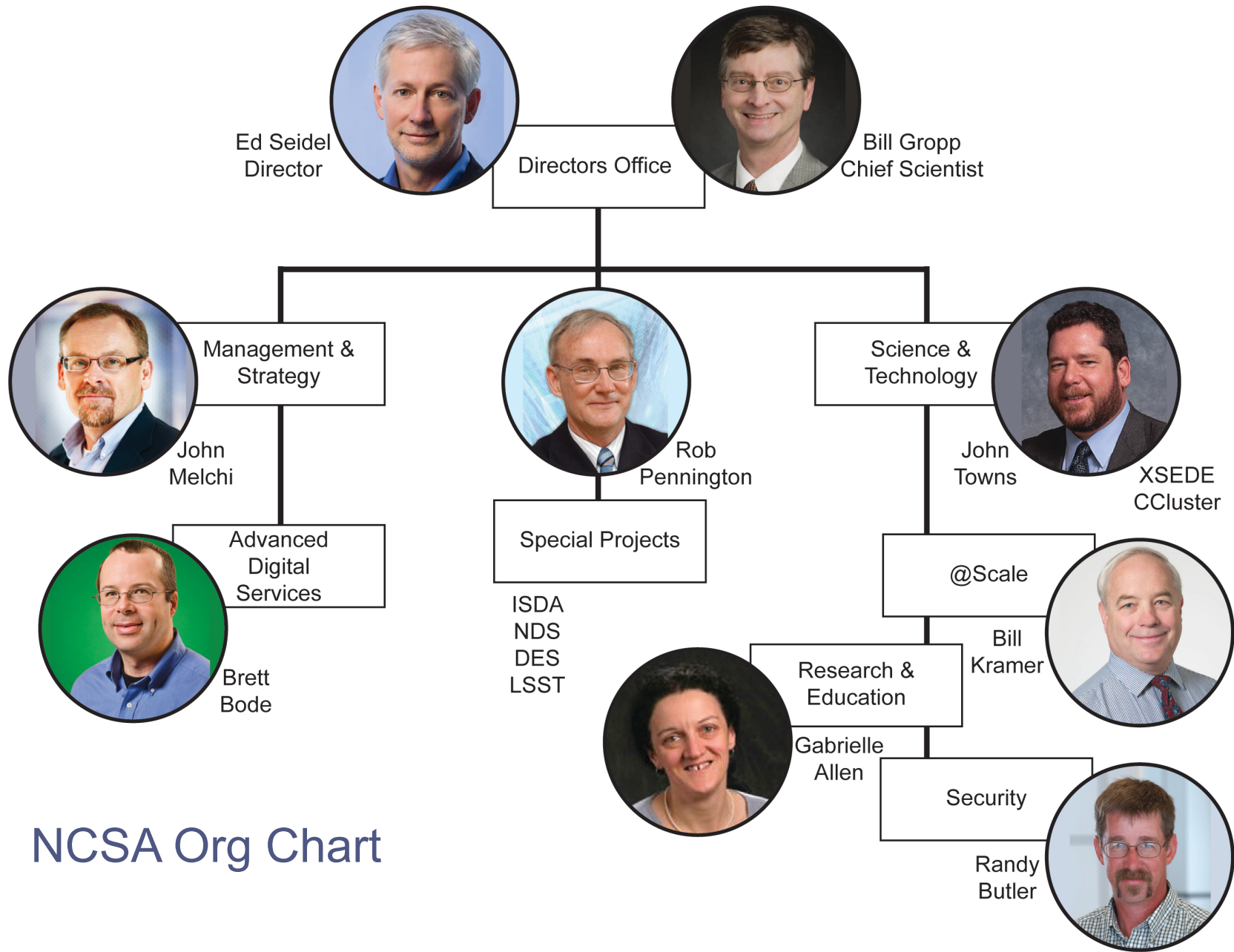
Narayan Aluru





# How NCSA can become an interdisciplinary connecting hub for UIUC

- We are not an academic unit, e.g., as is Physics... but...
- We will have faculty, students, and postdocs...
- What we will have to offer:
  - Compelling intellectual environment that integrates different disciplines, on a foundation of:
    - World class facilities
    - Expert staff
    - ...all in the same building
- NCSA Faculty and Research Fellows important part of helping to plan and implement this vision ...



NCSA Org Chart



# NCSA Research Fellows Program

- With different names, has been running since 1999
- Around 8 fellows a year, modest funds (~\$25K per award) for faculty to collaborate with NCSA, aim to lead to future externally funded activities
- Current aim:
  - Research fellows integrated with NCSA, projects more aligned to build on existing investments, and contribute to our strategic plans to build up thematic areas – want long lasting partnerships, deep connections to campus units
  - Fellows are made affiliate members of NCSA, access to programs and resources

# Current Fellows

- **Taras Pogorelov**, Chemical Sciences: *An Open Environment for Automation of Molecular Dynamics Simulations of Membrane-Active Host Defense Peptides*
- **Scott Althaus**, Political Science and Communications: *Building a Non-Consumptive Global News Observatory for Data Science Research*
- **David LeBauer**, Institute for Genomic Biology: *Coupling meteorology, plant biology, and economic engineering models within a CyberGIS framework*
- **Rosa M. Espinosa-Marzal**, Civil and Environmental Engineering : *Critical Molecular Interactions Underlying Biomineralization*
- **Matthew Hudson**, Crop Sciences : *Sequencing and Bioinformatics Pipeline for Rapid Detection of Structural Variations in Crop Genomes*
- **Daniel Work**, Civil and Environmental Engineering : *Improving the Efficiency of Taxi Systems through Real-time Seek Time Prediction*
- **John Toenjes**, Dance: LAIT: *Laboratory for Audience Interactive Technologies*
- **Iwona Jasiuk**, Mechanical Science and Engineering: *Multiscale Modeling of Bone Fracture and Strength*
- **Narayana Aluru**, Mechanical Science and Engineering : *Nanopore Genome*

# NCSA Fellow Program

- An opportunity for faculty and researchers at the UIUC to catalyze and develop long-term research collaborations between Illinois departments, research units, and the NCSA.
- Competitive program provides seed funding for demonstration, start-up projects, workshops, and/or other activities with the potential to lead to longer-term collaborations around research, development & education.
- **Jan. 23, 2015:** NCSA Fellowships kickoff: solicitation goals and focus, help potential applicants understand its scope, answer questions
- **Jan. 30, 2015: NCSA Fellowships Ideas Accelerator. 1-3 pm, NCSA Auditorium. Speed match-making event between potential applicants and NCSA staff and researchers.**
- **Feb. 22, 2015:** Deadline to submit to the NCSA Fellowships Program
- **April 1, 2015:** Target date for decisions



# Alignment with NCSA

- Projects are encouraged that build on existing NCSA activities, including the center's six thematic areas:
  - Bioinformatics and Health Sciences (Contact: C. Victor Jongeneel)
  - Computing and Data Sciences (Contact: Gabrielle Allen)
  - Culture and Society (Contact: Donna Cox)
  - Earth and Environment (Contact: Shaowen Wang)
  - Materials and Manufacturing (Contact: Narayana Aluru)
  - Physics and Astronomy (Athol Kemball)
- and major projects and programs, including:
  - Blue Waters (Contact: Greg Bauer)
  - XSEDE (Contact: Jay Alameda)
  - Innovative Systems Laboratory (Contact: Volodymyr Kindratenko)
  - Advanced Visualization Laboratory (Contact: Donna Cox)
  - Cybersecurity (Contact: Randy Butler)
  - National Data Service (Contact: Ray Plante)
  - Innovative Software and Data Analysis (Contact: Kenton McHenry)
  - Private Sector Program (Contact: Merle Giles).

Computing &  
Data Science



Gabrielle  
Allen

Physics &  
Astronomy



Athol  
Kembell

Culture &  
Society



Donna  
Cox

Bioinformatics &  
Health Sciences



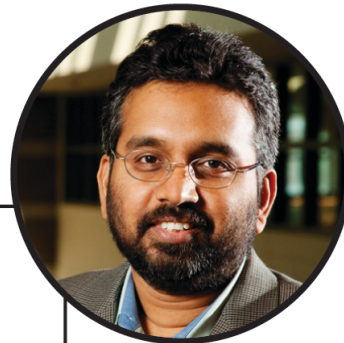
Victor  
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Narayan  
Aluru

Blue Waters

Greg Bauer



Advanced Visualization Lab

Donna Cox



XSEDE

Jay Alameda



Volodymyr Kindratenko



Inovative Systems Lab

Cybersecurity



Randy Butler

Ray Plante

National Data Service



Kenton McHenry

Innovative Software & Data Analysis



Merle Giles

Private Sector Program

# Fellows at NCSA

- Fellows are provided a zero-percent NCSA appointment and are responsible for contributing to the center's academic core, play a significant role in advising on center strategy, contribute to and take part in large collaborative funding efforts, and act as liaisons with their home departments.
- Fellows are provided with office space at NCSA as appropriate and have direct access to NCSA research scientists, staff, and services. Where possible, NCSA will provide access to compute, data, and other cyberinfrastructure, including software licenses, needed for fellowship projects.

# Applying

- Easychair used for proposal submission
- Competitive proposals: individual or multiple faculty, well defined activity, need for close collaboration with NCSA, new collaborations with clear outcomes that contribute to our strategic plan and lead to new funding
- Successful proposals will:
  - Advance the development of existing or new thematic areas at NCSA
  - Leverage and build on major NCSA projects and investments
  - Demonstrate a compelling need for NCSA funding and involvement
  - Outline a clear plan for activities to contribute to the NCSA environment (e.g. students working at NCSA)
  - Include NCSA staff as integral contributors to the project (strongly encouraged)



## Collaboration with NCSA Staff

- Fellows are strongly encouraged to have an active, close collaboration with NCSA staff for the duration of the fellowship, and **applicants should discuss these collaborations in detail with the NCSA staff involved before submitting proposals.**
- Proposals should describe the nature of the collaboration, anticipated staff time commitment staff, source of support for staff involvement.
- Support for NCSA staff can come from existing project or grant funds or can be requested as part of the proposal from the NCSA Director's Office\*.

\*requests of one month effort or less are the most likely to be supported, should discuss their plans with their supervisor

# Proposal Format

- Proposals should be *no more than six pages*, consisting of:
  - Project summary (suggested length: 1/2 page)
  - Problem statement and potential impact (suggested length: 1 page)
  - Approach (suggested length: 1 page)
  - Need for collaboration and advanced cyberinfrastructure (suggested length: 1 page)
  - Plans for continuation of activity (e.g., submit proposals, other funding) (suggested length: 1/2 page)
  - Description of project team, location of activities, mechanisms of collaboration, and required compute/data (or other) infrastructure (suggested length: 1 page)
  - Milestones and/or assessment (suggested length: 1/2 page)
- Proposals should also include a budget and budget justification and may include references, short (2- or 3-page NSF/DOE or NIH style) resumes for all project participants, and may include references; these materials are not included in the six-page limit.

# Letters of Commitment

- Because we have had some issues in past with people not realizing they were part of proposals.
- Short letters of commitment should be included for all co-PI's and NCSA staff collaborating in fellowship proposals
- Template on web page: confirm involvement, NCSA staff includes confirmation they have discussed with supervisor and source of funding.

# Budgets

Note meant to limit projects, discuss with Jay Roloff if you have questions.

- Up to \$25,000 over 12 months (starting July 1, 2015). Follow-on funding for previously funded fellowships will be considered only in cases where additional funding is required to complete or develop a proposal for an active or imminent RFP.
- Fellowship funds can be used for the following purposes:
  - Adjustment of teaching responsibilities, to be negotiated with department heads
  - Research assistant support (GRA, postdoc, etc.)
  - Travel support—maximum of \$1,500 for conference travel or travel to other sites
  - Faculty summer salary
- **Project activities are strongly encouraged to take place in the NCSA Building where they will contribute to a collaborative, interdisciplinary research environment.**
- Project budgets do not need to include benefits, tuition remission, or overheads.

# Review Process

- NSF-style: 3-4 reviews for each proposal, reviewers from campus and NCSA. Panel to make recommendations on highly competitive, competitive, non-competitive.
- Awards made based on panel recommendation, match to strategic goals, leveraging of NCSA resources

# Questions/Comments??