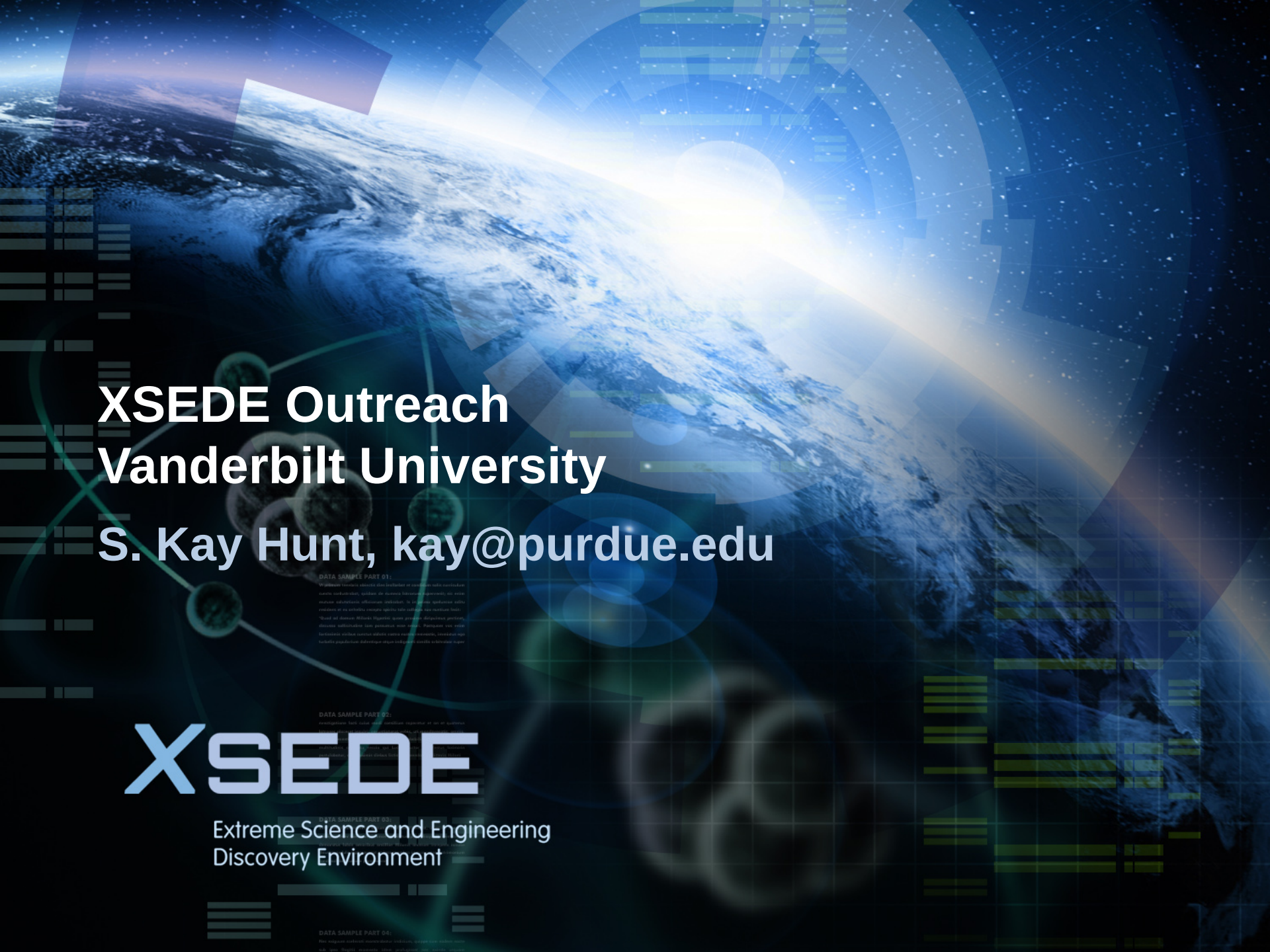
XSEDE Outreach
Vanderbilt University
S. Kay Hunt, kay@purdue.edu
XSEDE
Extreme Science and Engineering
Discovery Environment

Thank You To Our Hosts

- Vanderbilt University

- Will French
- David Ernst
- Kelly Holley-Bockelmann

Agenda

- 2:00-2:30pm Overview of HPC resources at Vanderbilt University – Will French
- 2:30-3:15pm Overview of XSEDE resources and services – Scott Lathrop
-
- **3:15-3:30pm Break**
- 3:30-3:45pm “Building the Black Hole in our own Backyard” - Kelly Holley-Bockelmann
- 3:45-4:15pm XSEDE Collaborative Support Services and Science Success – Jay Alameda
- 4:15-4:30pm Wrap up Questions and Discussion

Presentations for Today

- Posted for your use

XSEDE: An Advanced and Integrated Set of Digital Resources for Science and Engineering

Scott Lathrop, lathrop@illinois.edu

XSEDE

Extreme Science and Engineering Discovery Environment

Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
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Discovery Environment

Extended Collaborative Support Services

Jay Alameda
alameda@illinois.edu

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XSEDE offers huge variety of resources

- Leading-edge distributed memory systems
- Very large shared memory systems
- High throughput systems
- Visualization engines
- Data analytics systems
- Accelerators and co-processors

Many scientific problems have components that call for use of more than one architecture.

Extended Collaborative Support Services Strategic Objective -To Help Users Make More Productive Use of XSEDE Resources

- Support people who understand the discipline as well as the systems (perhaps more than one support person working with a project).
- 37 FTEs, spread over ~80 people at almost a dozen sites.

How do you get Extended Collaborative Support?

- You have to ask for it -it's an allocated resource.
- You can always ask for it, i.e. midstream or even as part of a startup request.
- Lasts up to a year.
- Must have specific goal in mind- can't just say I want additional programming support.

ECSS has 5 support services

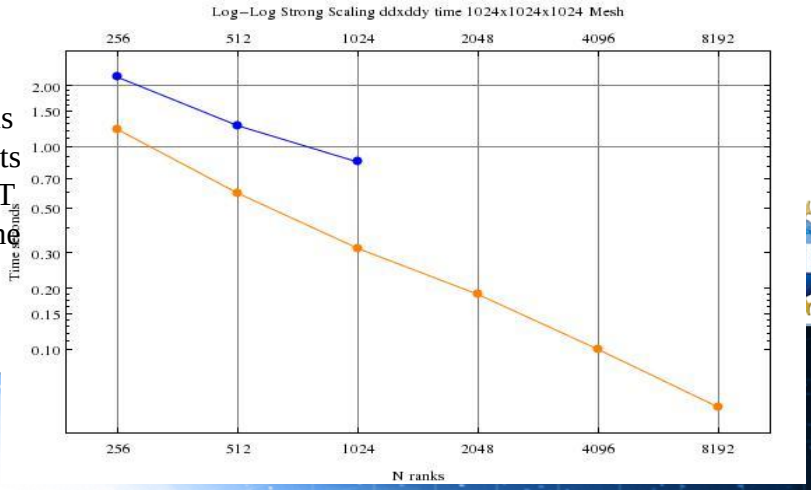
- Support for
  - Research Teams
  - Novel and Innovative Projects
  - Community Capabilities
  - Gateways
  - Training and Outreach

Support for Research Teams
(led by Lonnie Crosby, NICS (U. of Tennessee))

- Optimization
  - Profiling
  - Scaling to higher core count
  - Improving IO
  - Porting to GPUs
  - Finding better solvers (what's better often depends on the degree of parallelization)
- Visualization
- Workflows

Selected Highlight (1)

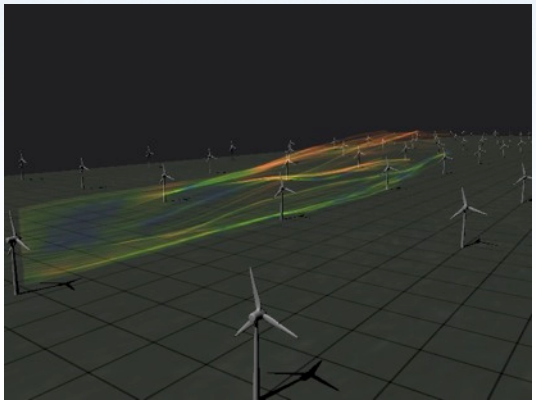
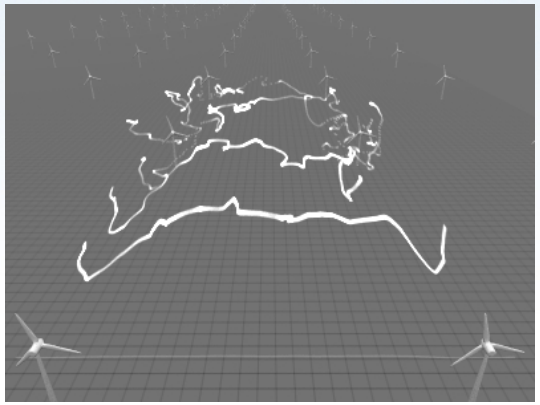
- ***Large eddy simulations of extended wind farms, and direct numerical simulations of turbulent channel***
  - PI: Meneveau, Johns Hopkins
  - ECSS Project Team: Darren Adams and David Bock (NCSA)
- Interaction between large wind farms with multiple wind-turbines and the atmospheric boundary layer flow
- The ECSS goals were to provide assistance implementing two dimensional domain decomposition and parallel FFT as well as 3D visualization representations to assist in simulations and analysis of large wind farms.
- The work plan was modified part way through to abandon an approach that included developing a stand-alone MPI transpose and custom 2D FFT. Instead, the team modified the existing P3DFFT library to completely skip the FFT and transpose operations on the 3rd array index.



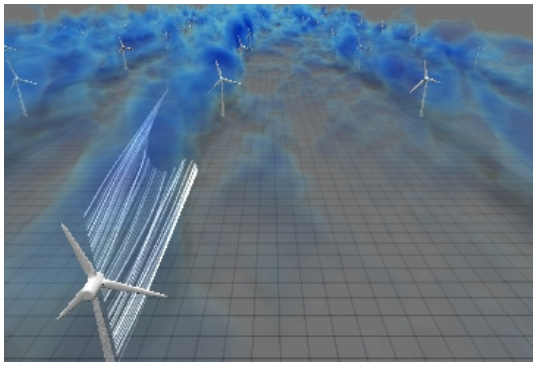
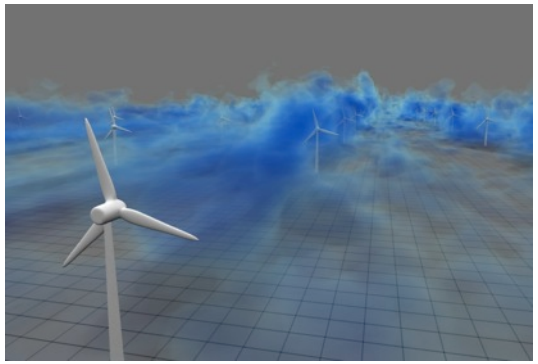
Performance of the 2D FFT in calculation the x and y derivatives. This was obtained from runs on the NICS Kraken system. The figure presents scaling of a $1{,}024^3$ mesh. The blue points are from the original 2D FFT implemented with 1D domain decomposition. The orange points are the new 2D MPI FFT scaled out to 8,192 processors.

Selected Highlight (2)

- Visualization representations
  - designing and developing a myriad of different techniques visualizing the changing vector field over time. Work focused specifically on various particle advection, tracing, and streamline

  - development of high quality scenes integrating new particle visualization methods developed above with earlier existing volume rendering techniques to show multiple variables in a single representation.

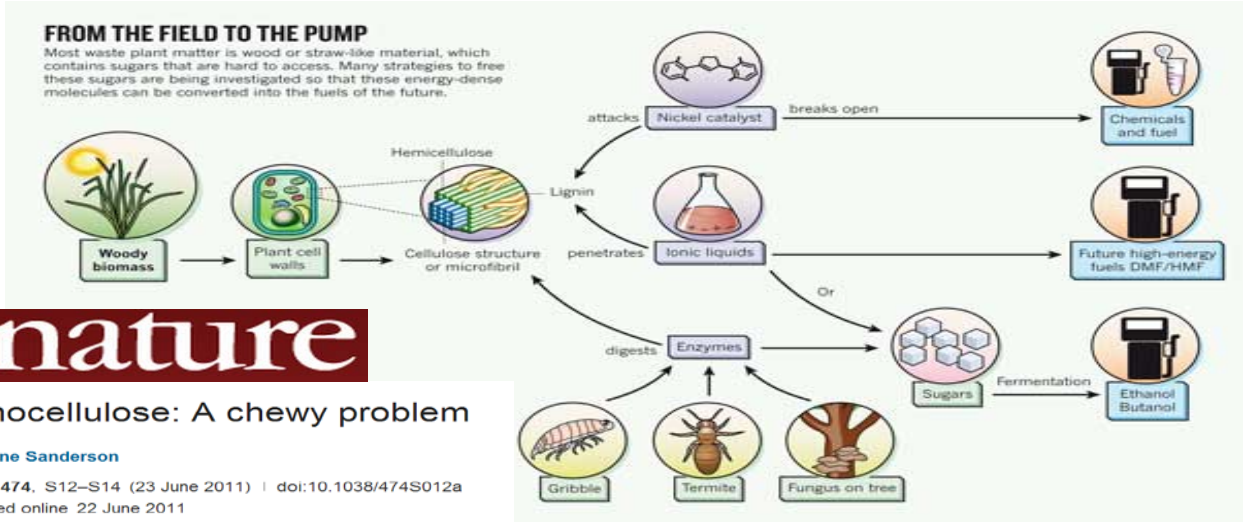
Support for Novel and Innovative Projects
(led by Sergiu Sanielevici, Pittsburgh Supercomputing Center)

- Pro-actively reaching out to communities new to advanced computing, e.g.
  - social science
  - social network analysis
  - language processing
  - genomics
  - digital humanities (occasioned recent temporary hire)
  - economics
  - library science
  - public health
- Look for pioneers, work with them to craft the project, and then help them begin to execute it.

Large Genome Assemblies

- ECSS Staff working with leading researchers and code developers
- Largest ever metagenome assembly, using 3.5 TB RAM on PSC Blacklight

"I wouldn't have been able to do anything on Blacklight without ECSS staff… (consultant) took a real interest and solved a lot of things that were hard for me. He found bugs in the software and got them resolved with the software authors. I'd worked for months and not made that progress. Without his expertise, I might have given up…"



nature

Lignocellulose: A chewy problem

Katharine Sanderson

Nature **474**, S12–S14 (23 June 2011) | doi:10.1038/474S012a
Published online 22 June 2011

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Support for Community Codes
(led by John Cazes, Texas Advanced Computing Center)

Community codes – applications, tools, and libraries used by multiple research groups

- Deploying, hardening, and optimizing useful software systems
- Assisting users with community codes and tools
- Establishing relationships between XSEDE and developer communities
- Extending XSEDE documentation to cover community code implementations

Selected Highlight

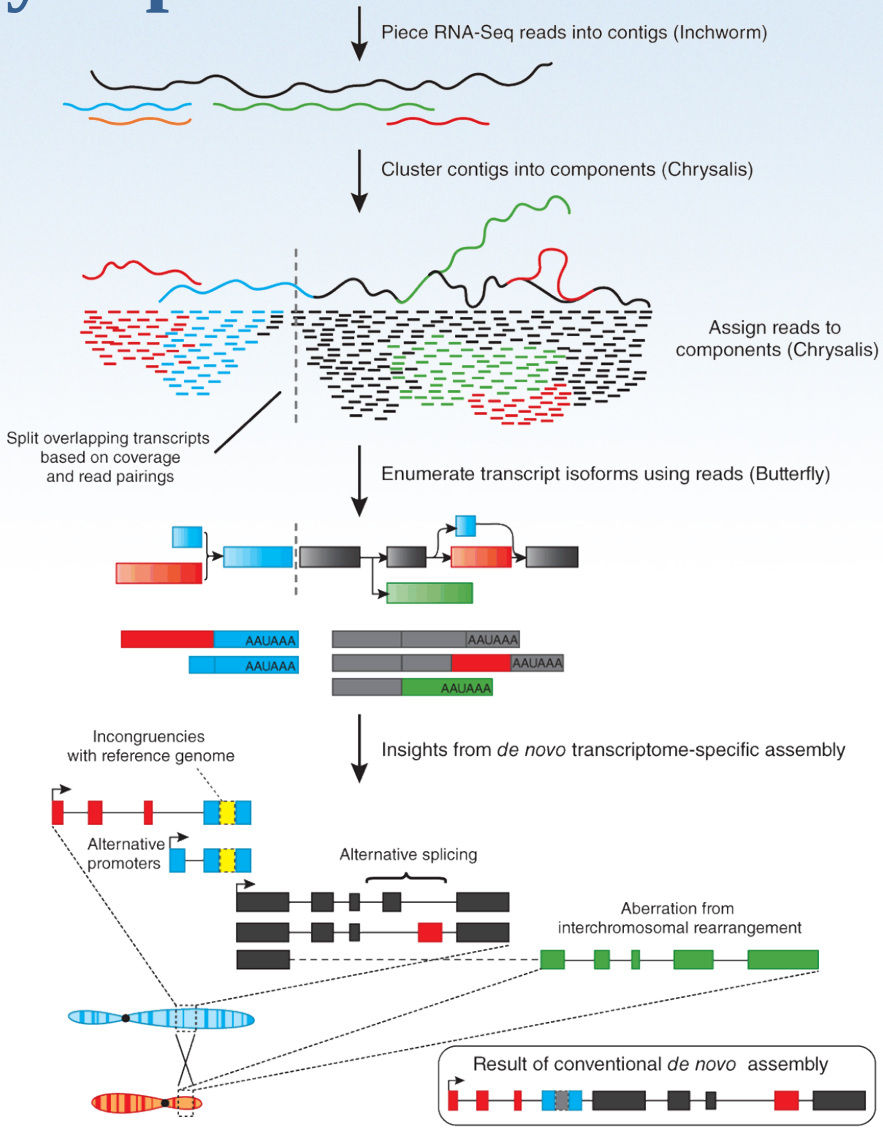
- ***Collaboration with the Broad Institute: Genomics Community Capabilities***
- Internal project to provide support to over 15 research groups
- Goal: Port and optimize the widely used genomics applications, Trinity and ALLPATHS-LG, to Blacklight and other XSEDE resources
- Challenges: Neither was designed for a parallel architecture
- Solution:
  - Adjusted the workflow to work with parallel filesystems
  - Collaborated with the Broad Institute and the National Center for Genome Analysis to include parallel optimizations in the code base
- Success: Enabled the largest Trinity job ever
  - 20 assemblies with 1.5 billion reads each

Trinity Pipeline

Inchworm
64 cores ~100 hours

Chrysalis
128 cores ~400 hours

Butterfly
64 cores ~50 hours



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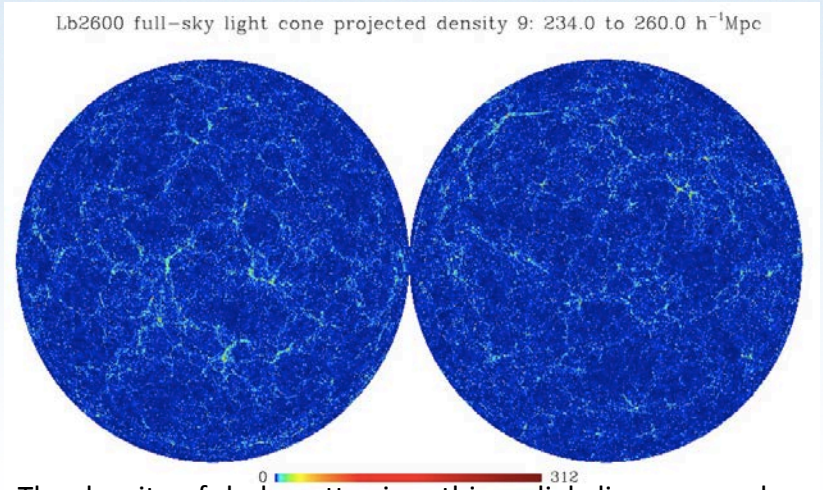
Support for Science Gateways
(led by Marlon Pierce, Indiana U)

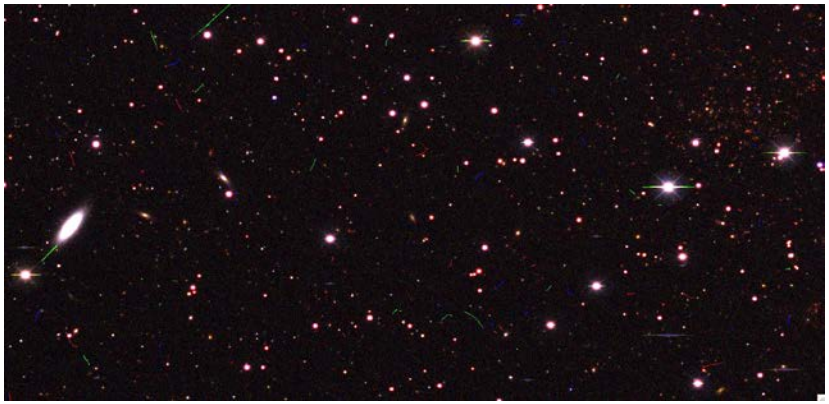
- Science Gateways enable communities of users associated with a common discipline to use computational resources through a familiar and simpler interface e.g. a web interface.
- Examples of ECSS Science Gateway Support
  - Assist with job submission and data movement to XSEDE
  - Automation of scientific processes through workflows
  - Integration of XSEDE resources into a portal/gateway
  - Support with grid security and community accounts

Realizing the Universe for the Dark Energy Survey (DES)

PI's: August Evrard (UM) and Andrew Kravtsov (UC)



The density of dark matter in a thin radial slice as seen by a synthetic observer located in the 8 billion light-year computational volume. Courtesy: Matthew Becker, University of Chicago.



A synthetic 2x3 arcmin DES sky image showing galaxies, stars, and observational artifacts. Courtesy Huan Lin, FNAL.

- ECSS provided support to the Dark Energy Survey Simulation Working Group in developing large, multi-staged computations (workflows) to develop Blind Cosmology Challenge (BCC) catalogs.
- These executions Catalog a variety of sky realizations in different cosmologies are analyzed, in a blind manner, by science teams generate expectations for galaxy yields in various cosmologies.
- Analysis of these simulated catalogs offers a quality assurance capability for cosmological and astrophysical analysis of upcoming DES telescope data.

Support for Training, Education, and Outreach

(led by Jay Alameda, NCSA)

- Collaboration with XSEDE Training, Education, and Outreach Services
- Training support
  - On-line course development and update
  - Synchronous training (live, web, …)
  - Collaboratively identify new training areas
- Education
  - Online course support
- Outreach
  - Conferences, speakers bureau, campus visits

Education: Applications of Parallel Computers

- Adapted from Jim Demmel's CS267 Course
  - Video, Slides in Cornell's Virtual Workshop
  - Quizzes in every class
- 3 Homework (programming) problems
  - ECSS staff helped port to XSEDE resources
  - ECSS staff part of support team for students
  - Autograding by Berkeley team
- Capped enrollment at 300 students
  - Limit reached in < 3 days
- Evolved into a Small Private Online Course (SPOC), in collaboration with a number of campuses.

Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
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Questions and Discussion

- Thank you for your presence