“From NCSA to the National Research Platform”

Invited Seminar

National Center for Supercomputing Applications

University of Illinois Urbana-Champaign

May 9, 2024

Dr. Larry Smarr

Founding Director Emeritus, California Institute for Telecommunications and Information Technology;

Distinguished Professor Emeritus, Dept. of Computer Science and Engineering

Jacobs School of Engineering, UCSD

http://lsmarr.calit2.net

NRP NATIONAL RESEARCH PLATFORM

Abstract

The National Research Platform (NRP) currently supports over 4,000 users on 135 campuses, accessing 1300 GPUs, 24,000 CPU cores, and over 10,000 TB of data storage – the largest distributed compute and storage platform supported by the NSF today. In this seminar, I will trace the technological roots of the NRP back to NCSA, the Alliance and I-Wire over 25 years ago. These early NCSA experiences led to my last 22 years of NSF cyberinfrastructure grants, which built the OptIPuter and then the Pacific Research Platform, which has now evolved into the NRP. Applications in Machine Learning as well as diverse applications from neutrino observatories to wildfire prediction are currently empowered by the NRP.

NRP NATIONAL RESEARCH PLATFORM

Documenting The Unmet Supercomputing Needs of A Broad Range of Disciplines Led to the NCSA Proposal to NSF

1982

1983



THE SUPERCOMPUT

Departmen

University of Illinois at Champaign-Urbana

AL

cientific

ercomputing

ILLINOIS

LABOR

CHARTERED 1867

NSF

NATIONAL RESEARCH PLATFORM

40 Years Ago NSF Brought to University Researchers a DOE HPC Center Model

1985/6







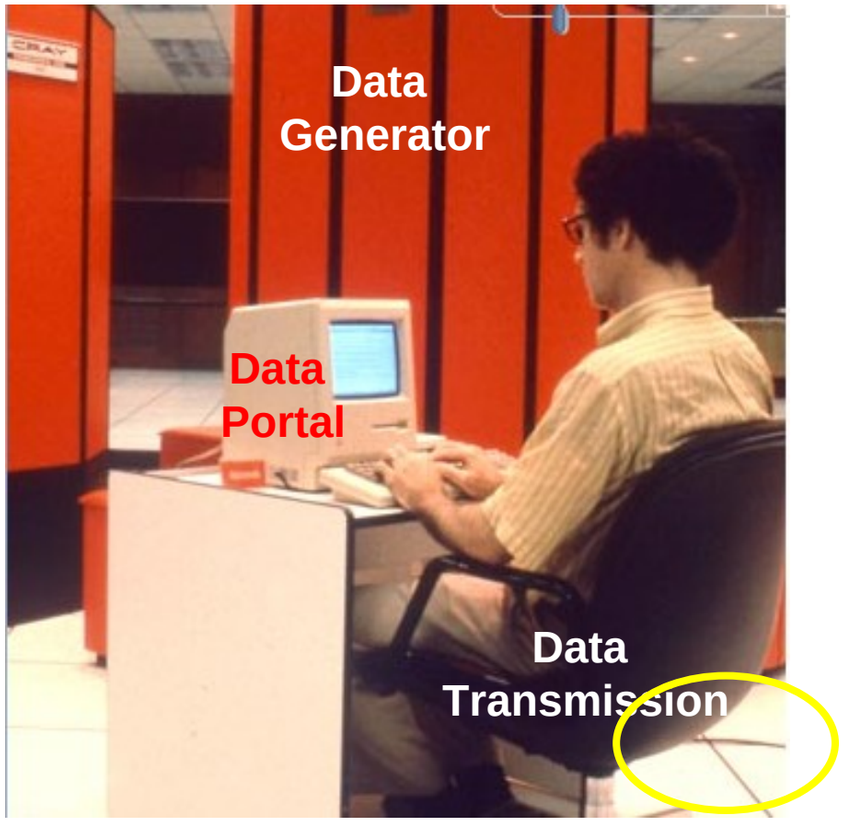
NCSA Was Modeled on LLNL

SDSC Was Modeled on MFEnet

NSF

NRP NATIONAL RESEARCH PLATFORM

NCSA Telnet--“Hide the Cray”
Distributed Computing From the Beginning!



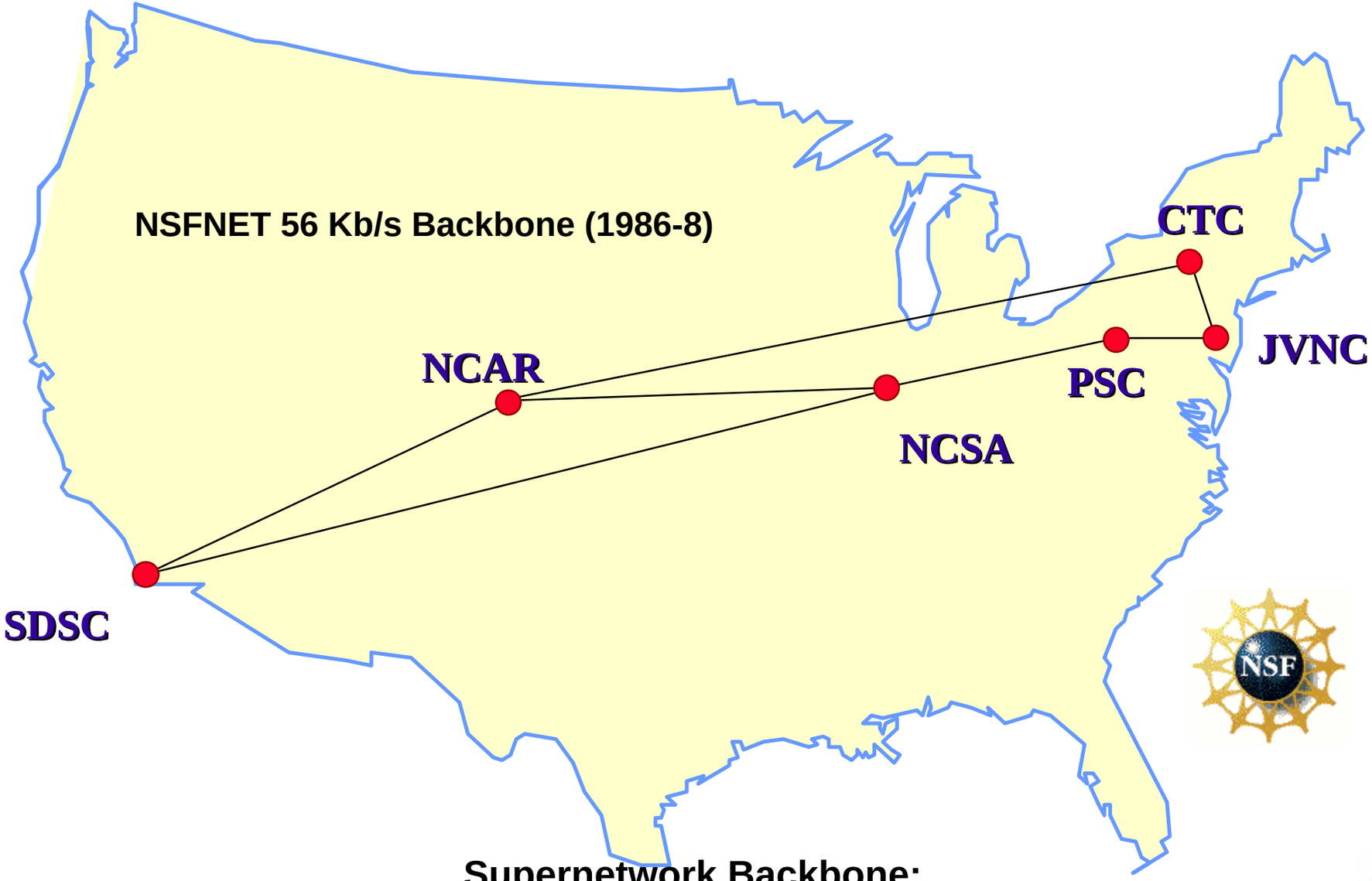
John Kogut Simulating
Quantum Chromodynamics
He Uses a Mac—The Mac Uses the Cray

- **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

NRP NATIONAL RESEARCH PLATFORM

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



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

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Interactive Supercomputing End-to-End Prototype: Using Analog Communications to Prototype the Fiber Optic Future

"What we really have to do is eliminate distance between individuals who want to interact with other people and with other computers."
— Larry Smarr, Director, NCSA

SIGGRAPH 1989

ATT & Sun







**"We're using satellite technology…
to demo what It might be like to have high-speed fiber-optic links between advanced computers
in two different geographic locations."**

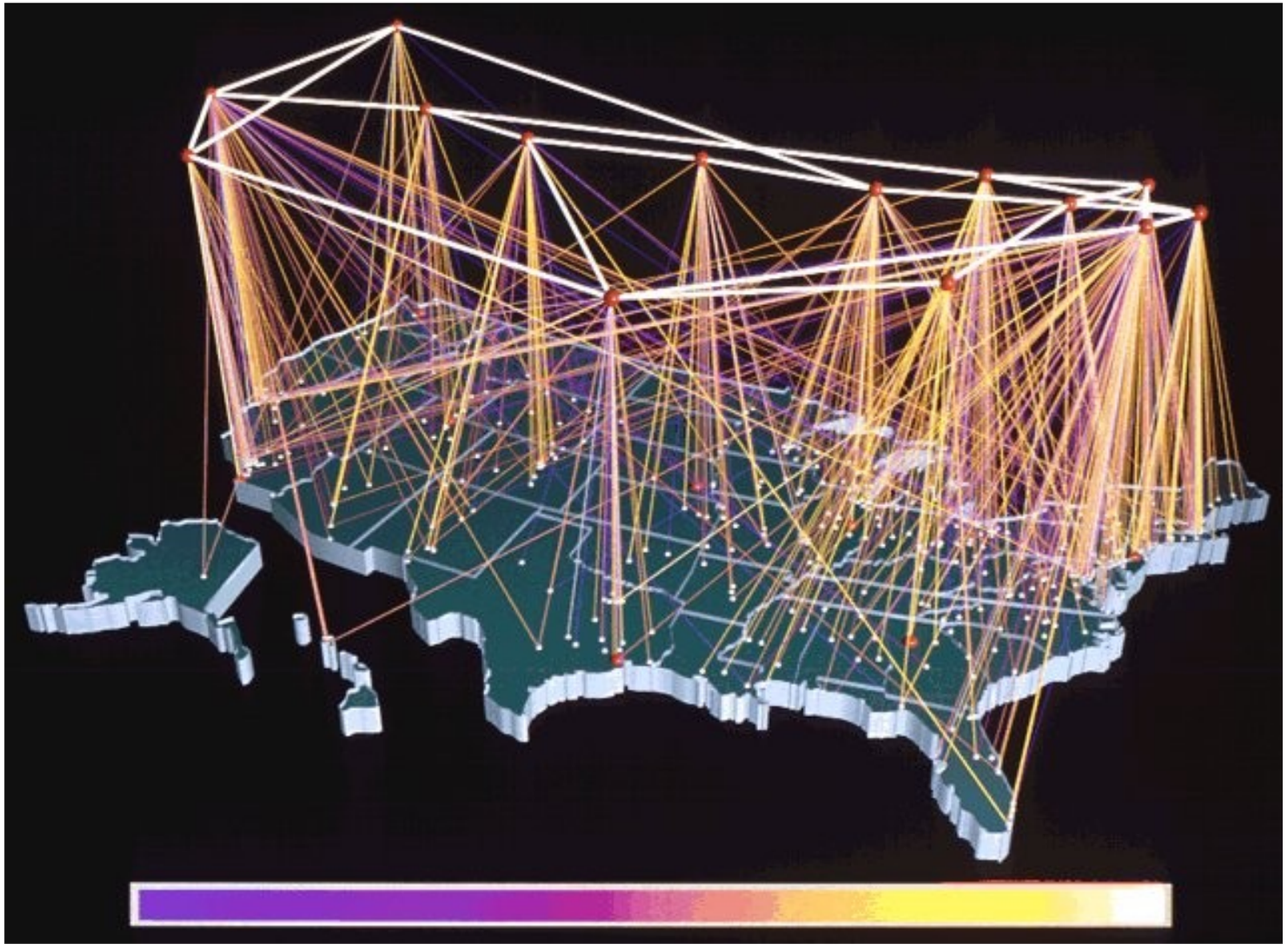
— Al Gore, Senator
Chair, US Senate Subcommittee on Science, Technology and Space

www.youtube.com/watch?v=3eqhFD3S-q4

NCSA

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The Internet Backbone Bandwidth Grew 1000x in Less Than a Decade



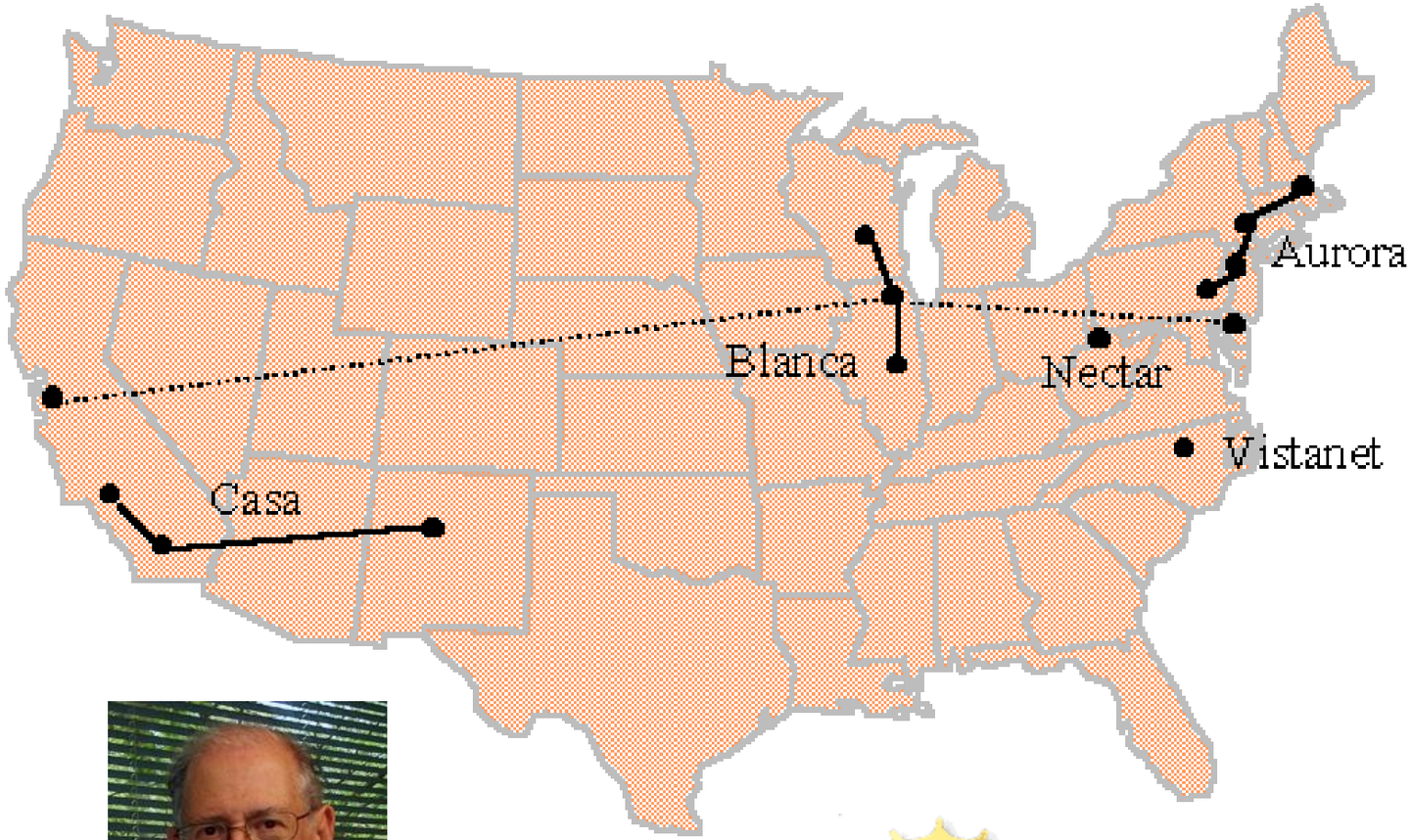
Visualization by NCSA's Donna Cox and Robert Patterson
Traffic on 45 Mbps Backbone December 1994

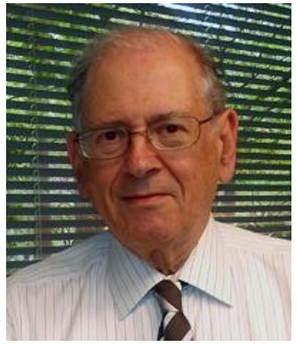
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However, CNRI's Gigabit Testbeds Demonstrated Host I/O Was the Distributed Computing Bottleneck

"Host I/O proved to be *the Achilles' heel* of gigabit networking – whereas LAN and WAN technologies were operated in the gigabit regime, many obstacles impeded achieving gigabit flows into and out of the host computers used in the testbeds."

--Final Report
The Gigabit Testbed Initiative
December 1996
Corporation for
National Research Initiatives (CNRI)





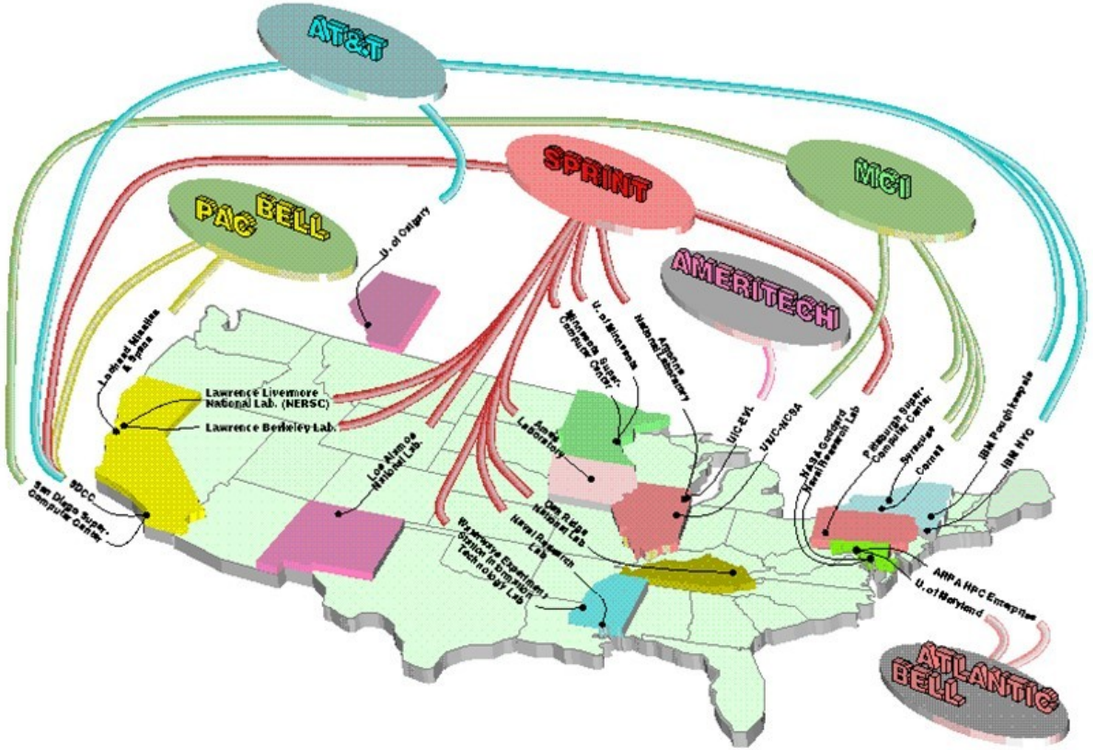
Robert Kahn
CNRI Chairman, CEO & President

NSF DARPA

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I-WAY: Pioneering Distributed Collaborative Computing at Supercomputing ’95

- **The First National 155 Mbps Research Network**
  - **Inter-Connected Telco Networks Via IP/ATM With:**
    - **Supercomputer Centers**
    - **Virtual Reality Research Locations, and**
    - **Applications Development Sites**
  - **Into the San Diego Convention Center**
  - **65 Science Projects**
- **I-Way Featured:**
  - **Networked Visualization Applications**
  - **Large-Scale Immersive Displays**
  - **I-Soft Programming Environment**
    - **Led to the Globus Project**



For details see:
“Overview of the I-WAY: Wide Area Visual Supercomputing”
DeFanti, Foster, Papka, Stevens, Kuhfuss
www.globus.org/sites/default/files/iway_overview.pdf

SC95 Chair Sid Karin
SC95 Program Chair, Larry Smarr

evl electronic visualization laboratory
Argonne NATIONAL LABORATORY
mcs
NCSA™
NRP NATIONAL RESEARCH PLATFORM

Caterpillar / NCSA Demonstrated the Feasibility of Distributed Virtual Reality for Global-Scale Collaborative Prototyping





NCSA™

Real Time Linked Virtual Reality and Audio-Video Between NCSA, Peoria, Houston, and Germany

1996

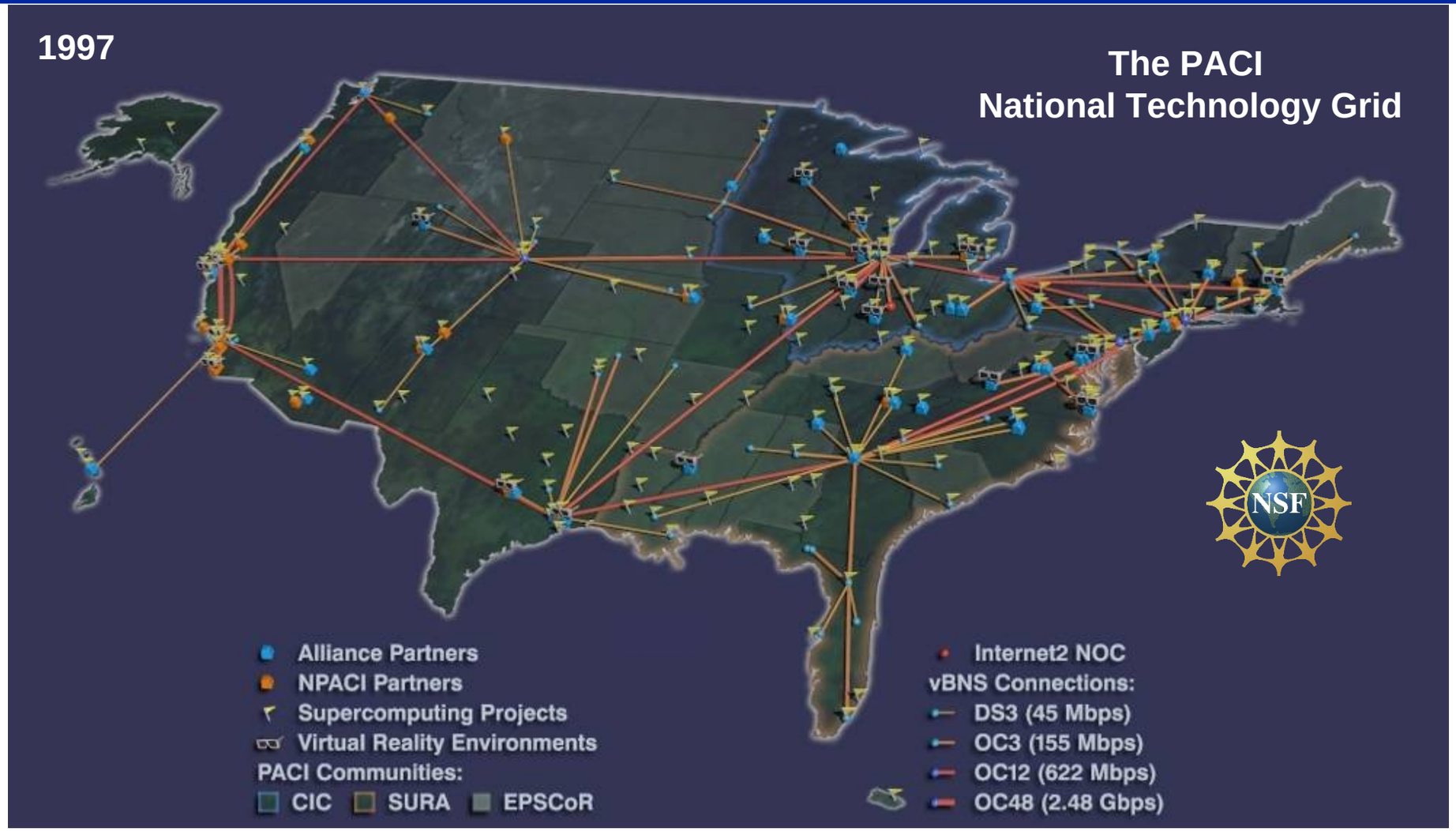
www.sv.vt.edu/future/vt-cave/apps/CatDistVR/DVR.html

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NSF's PACI Program was Built on the vBNS to Prototype America's 21st Century Information Infrastructure

vBNS led to

INTERNET2



Key Role
of Miron Livny
& Condor

NPACI

National Computational Science ALLIANCE

NRP NATIONAL RESEARCH PLATFORM

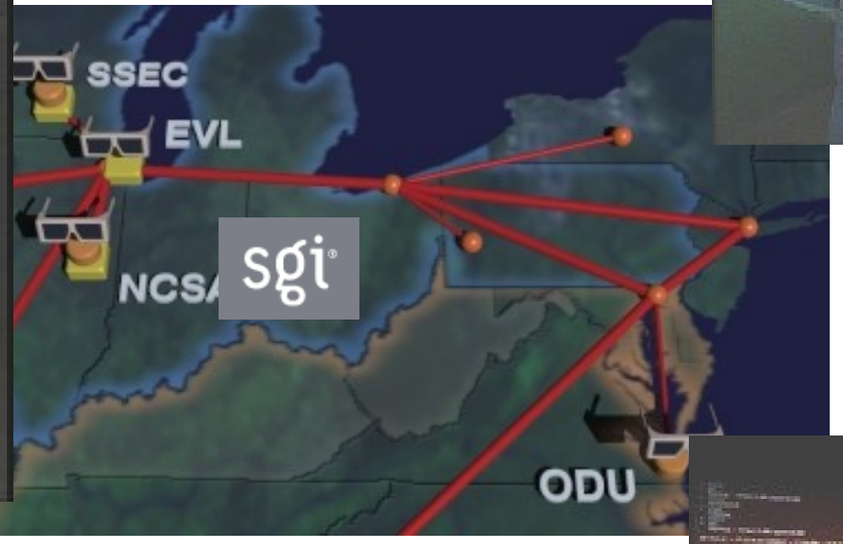
Chesapeake Bay Simulation Collaboratory: vBNS Linked CAVE, ImmersaDesk, Power Wall, and Workstation

Alliance Project: Collaborative Video Production via Tele-Immersion and Virtual Director

Alliance Application Technologies
Environmental Hydrology Team







Alliance 1997





NCSA™ UIC

sgi

ALLIANCE

Donna Cox, Robert Patterson, Stuart Levy, NCSA Virtual Director Team
Glenn Wheless, Old Dominion Univ.

NRP NATIONAL RESEARCH PLATFORM

Dave Bader Created the First Linux COTS PC Supercluster *Roadrunner* on the National Technology Grid, with the Support of NCSA and NSF

ALBUQUERQUE JOURNAL

YOUTH CRIME
Bill would fund state programs that crack down on juvenile offenders
D3

Metro & New Mexico

THURSDAY, APRIL 8, 1999
BUSINESS 4 SECTION
WEATHER 8 D
DEATHS 8

UNM To Crank Up $400,000 Supercomputer Today

Machine One of 100 Speediest in World

BY JOHN FLECK
Journal Staff Writer

A cluster of computers looking like a stack of oversized dorm room refrigerators is about to plug the University of New Mexico into an ambitious new supercomputer "mega-brain" spanning the nation.

Dignitaries from around the country will gather at UNM's Albuquerque High Performance Computing Center today to throw the switch on the "Roadrunner Supercluster."

Fresh out of the box, the Roadrunner is one of the 100 fastest computers in the world.

But its rocket-sled speed is just part of a more ambitious idea — an attempt to give scientists around the country access to a distributed supercomputing "brain" stretching from Boston to Maui, ready to solve their toughest problems.

The Roadrunner Supercluster will be part of what researchers are calling the "National Technology Grid," a collection of supercomputers across the country wired together to help handle scientists' growing demand for computer time.

Sitting at their own desks, the researchers could hook into the grid and begin solving large-scale problems without having to worry about where the computer doing the work is located, explained Larry Smarr, director of the National Computational Science Alliance, the federally funded group that paid for the new machine.

"The goal is to be completely seamless," the University of Illinois-based Smarr said in telephone interview this week.

UNM professor David Bader envisions a day when a researcher studying an ecosystem — Chesapeake Bay, say, or the Rio Grande Valley — can log in and rapidly spin through vast amounts of satellite data on climate and ground cover for their plot of land.

They wouldn't need to be located at a specialized supercomputer research center to do their work, explained Smarr — they could just plug into the grid and let the computers take care of the rest, much as you plug a toaster into the wall without having to worry about which power plant is generating the electricity.



JAIME DISPENZA/JOURNAL

BIG BRAIN: University of New Mexico professor David Bader tests the Roadrunner Supercluster. It will be dedicated today.

"That's the vision," said Bader, who has spent the last week testing the brand new Roadrunner machine in preparation for today's unveiling.

Smarr, one of the leaders of the nation's supercomputer research community, is scheduled to join Sen. Pete Domenici, R-N.M., and others to formally throw the switch turning on the computer at a ceremony this afternoon.

The $400,000 computer, built by Alta Technology Corp., bears the mark of a new breed of moderately priced machines that are making inroads in the high-performance scientific market.

Instead of using specialized high-performance computer chips made especially for supercomputing, it's built around 128 top-of-the-line Intel Pentiums, the same breed of computer chips used in desktop computers.

Programmers split up a large problem into smaller pieces, farming them out so that each of the 128 chips can work on a portion of the problem and then share results.

"You get to profit from the collapse of PC prices," explained Victor Yodaiken, a computer scientist at the New Mexico Institute of Mining and Technology who does research on a similar "cluster" machine at Tech.

Similar machines also have been built at Sandia and Los Alamos national labs for nuclear weapons and physics research, and the experience of the New Mexico research community is one reason UNM was chosen to host the new machine, Smarr said.

UNM is one of six "supernodes" on the National Technology Grid. In addition to the Roadrunner Cluster, the grid will be connected to UNM's Maui High Performance Computing Center, an Air Force-funded research complex in Hawaii run by the university for the military.

NCSA Director Larry Smarr (left), UNM President William Gordon, and U.S. Sen. Pete Domenici turn on the Roadrunner Supercomputer in April 1999



David Bader Selected to Receive the 2021 IEEE Computer Society Sidney Fernbach Award

National Computational Science ALLIANCE

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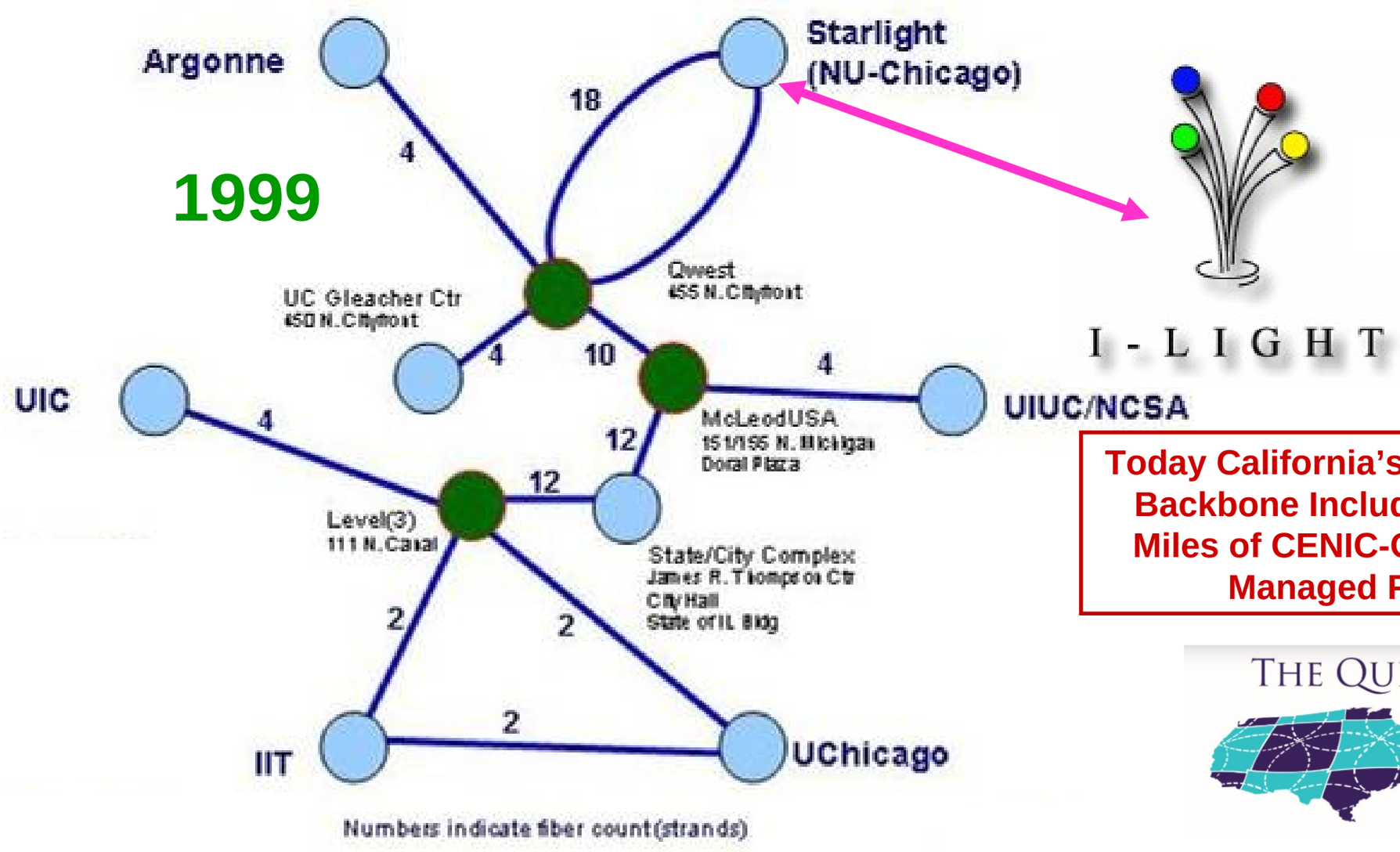
The 25 Years From the National Techology Grid To the National Research Platform

> The goal is a powerful, persistent, distributed U.S. national resource as usable in the future as the NSF Supercomputer Center standalone machines were in the 1980s and 1990s.

From *I-WAY to the National Technology Grid*, CACM, 40, 51 (1997)
Rick Stevens, Paul Woodward, Tom DeFanti, and Charlie Catlett

NRP NATIONAL RESEARCH PLATFORM

Illinois's I-WIRE and Indiana's I-LIGHT Dark Fiber Networks Inspired Many Other State and Regional Optical



I - L I G H T

Today California's CENIC R&E Backbone Includes ~ 8,000 Miles of CENIC-Owned and Managed Fiber

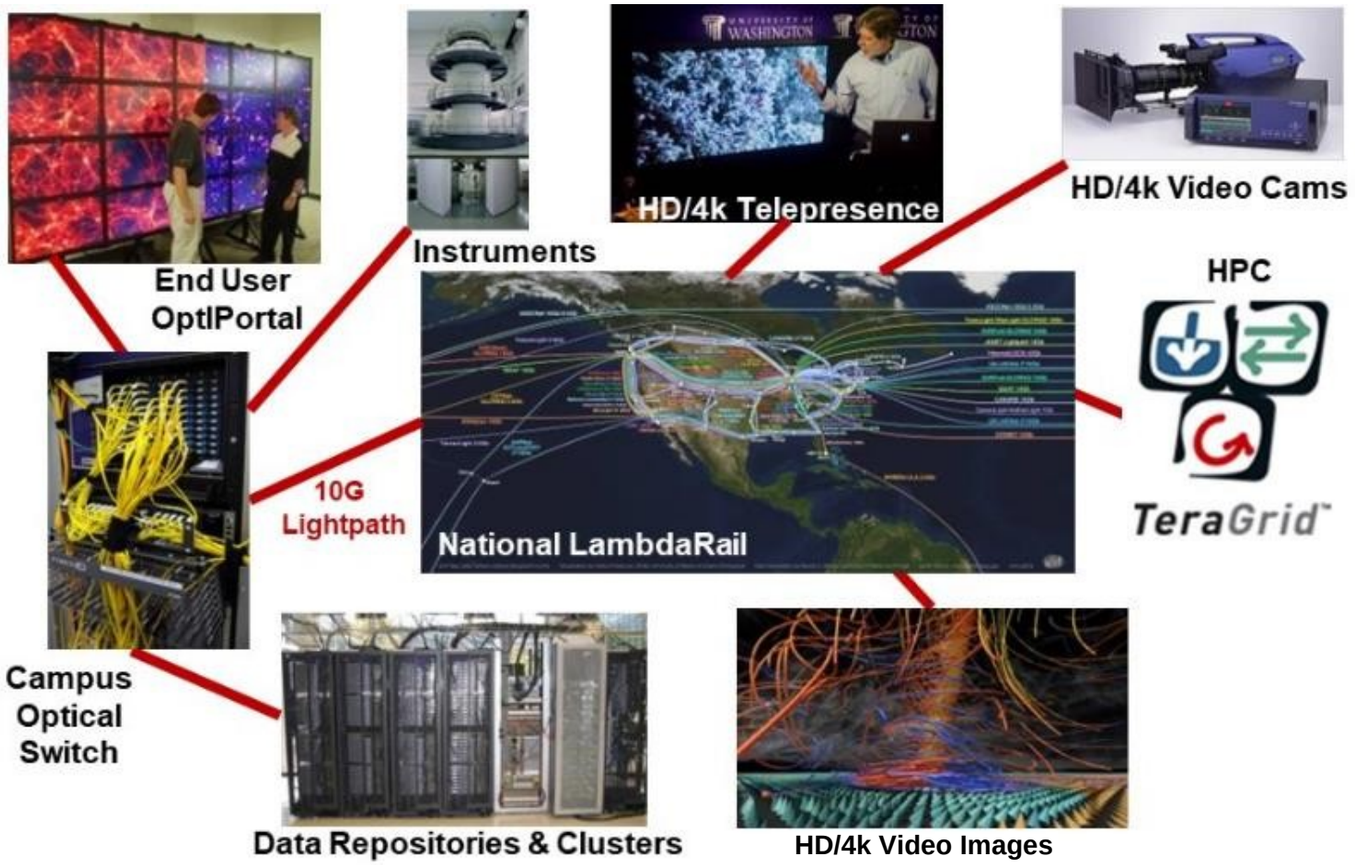
THE QUILT



Source: Larry Smarr, Rick Stevens, Tom DeFanti, Charlie Catlett

NRP NATIONAL RESEARCH PLATFORM

2002-2009: The NSF-Funded OptIPuter Grant
Developed a Uniform Bandwidth Optical Fiber Connected Distributed System



The OptIPuter
Exploits a New World
in Which
the Central Architectural Element
is Optical Networking,
Not Computers.

Demonstrating That
Wide-Area Bandwidth
Can Equal
Local Cluster Backplane Speeds

OptIPuter
$13.5M
PI Smarr,
Co-PIs DeFanti, Papadopoulos, Ellisman, UCSD
Project Manager Maxine Brown, EVL
2002-2009

So Why Don't We Have a National Big Data Cyberinfrastructure?

"Research is being stalled by 'information overload,' Mr. Bement said, because data from digital instruments are piling up far faster than researchers can study. In particular, he said, campus networks need to be improved. High-speed data lines crossing the nation are the equivalent of six-lane superhighways, he said. But networks at colleges and universities are not so capable. "Those massive conduits are reduced to two-lane roads at most college and university campuses," he said. Improving cyberinfrastructure, he said, "will transform the capabilities of campus-based scientists."

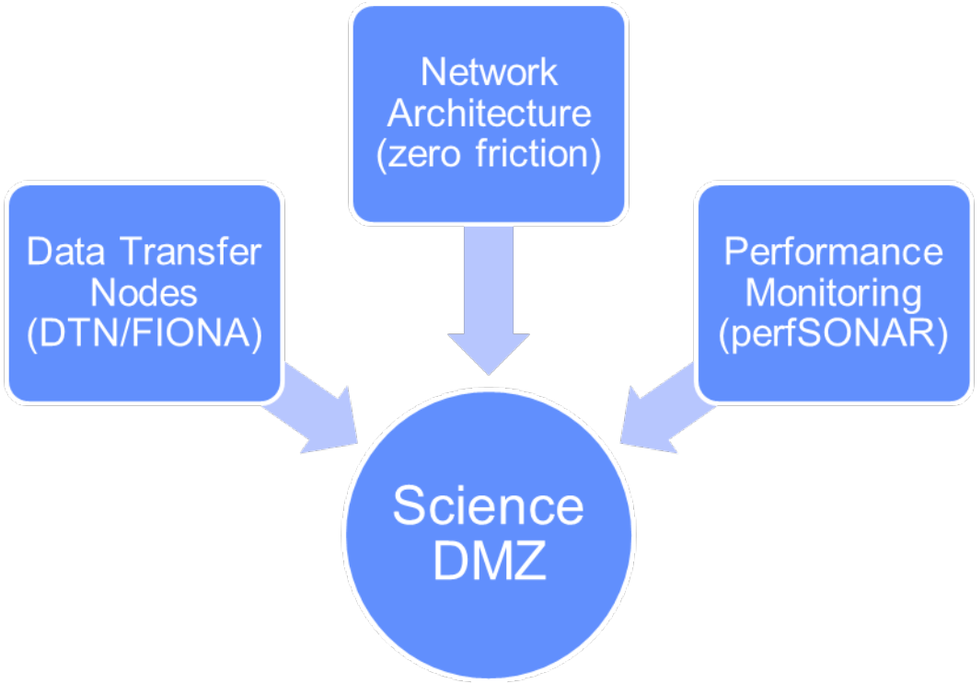
-- Arden Bement, the director of the National Science Foundation May 2005



NRP NATIONAL RESEARCH PLATFORM

Thirty Years After NSF Adopts DOE Supercomputer Center Model
NSF Adopts DOE ESnet's Science DMZ to Allow Campuses to Terminate Supernetworks

ScienceDMZ Coined in 2010 by ESnet-Basis of PRP Architecture and Design

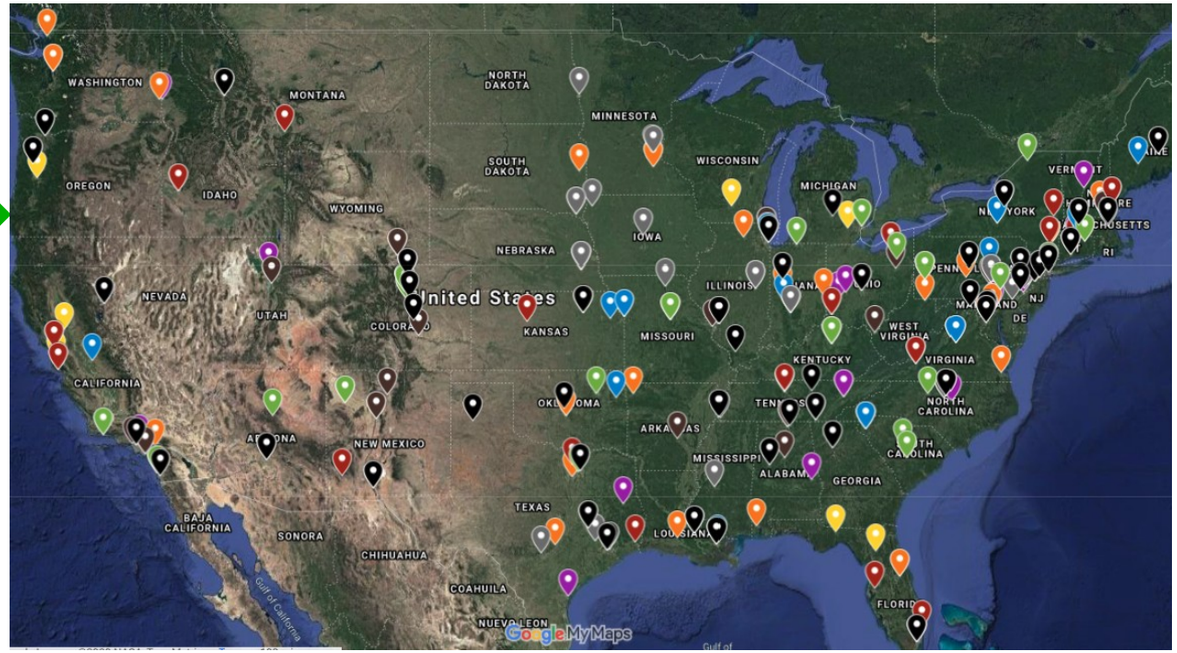


http://fasterdata.es.net/science-dmz/

NSF Campus Cyberinfrastructure Program Has Made Over 385 Awards Totaling Over $100M Since 2012

DOE

NSF



Source: Kevin Thompson, NSF

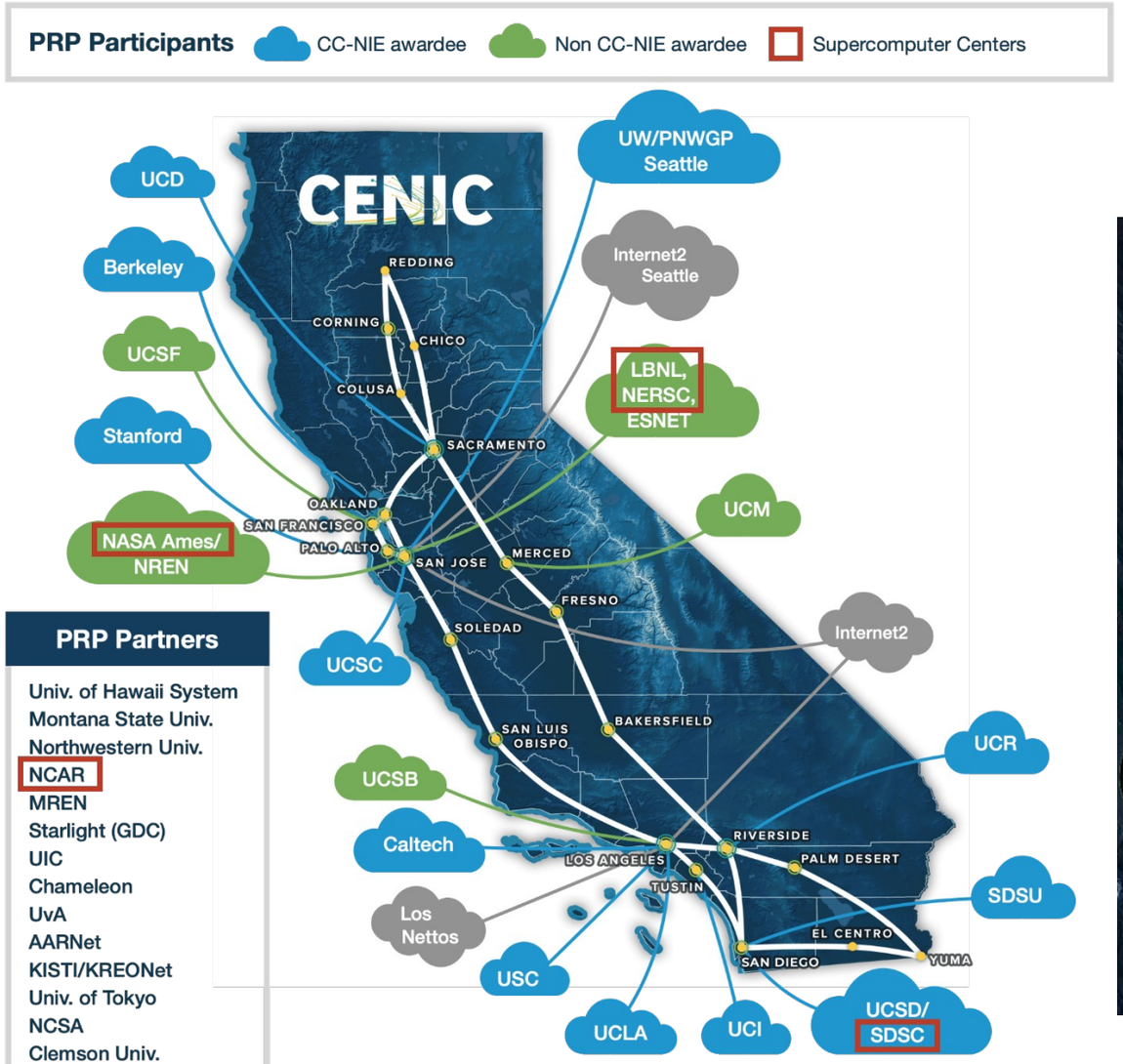
ESnet
FASTERDATA KNOWLEDGEBASE

Slide Adapted From Inder Monga, ESnet

NSF

NRP NATIONAL RESEARCH PLATFORM

2015 Vision: The Pacific Research Platform Will Build on CENIC to Connect Science DMZs Creating a Regional Community Cyberinfrastructure



Source: John Hess, & Hunter Hadaway, CENIC

NSF CC*DNI Grant
$6.3M 10/2015-10/2020
Extended – Ended Year 7 in Oct 2022



NRP NATIONAL RESEARCH PLATFORM

2015-2021: UCSD Customized Science DMZ Optical Fiber Termination DTNs: COTS PCs Optimized for Big Data Transfers

Flash I/O Network Appliances (FIONAs)
Solved the 1996 Gigabit Testbed Disk-to-Disk Data Transfer Problem
at Near Full Speed on Best-Effort 10G, 40G and 100G

Today's Roadrunner!



48-Core CPU
Add Up to 8 Nvidia GPUs Per 2U FIONA
To Add Machine Learning Capability
TBs of SSD/Up to 256TB Storage



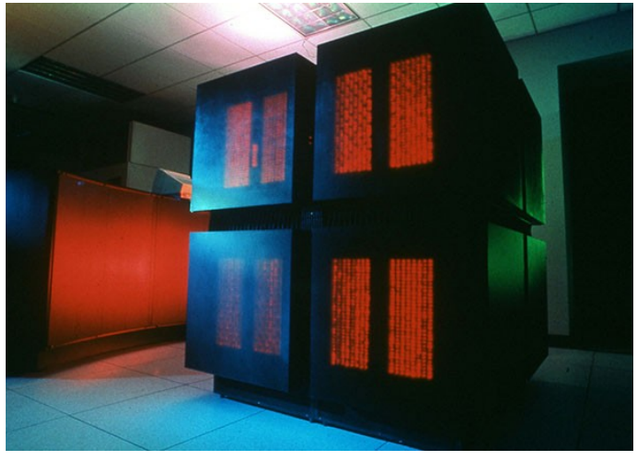
FIONAs Are Rack Mounted

FIONAs Designed by UCSD's Phil Papadopoulos, John Graham, Joe Keefe, and Tom DeFanti

QUALCOMM INSTITUTE SDSC NRP NATIONAL RESEARCH PLATFORM

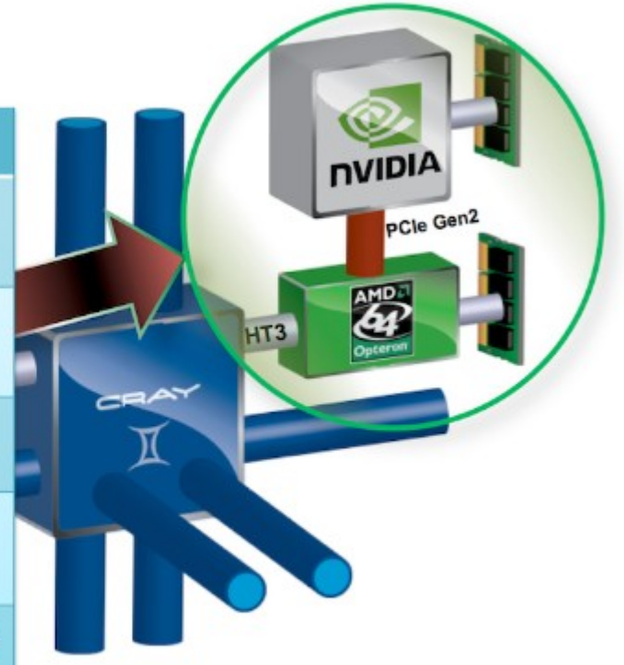
DTN and Supercomputer Architectures Remain Shared Memory CPU Plus SIMD Co-Processor

Supercomputer Architectures Remain von Neumann Shared Memory CPU Plus SIMD Co-Processor





XK7 Compute Node Characteristics	
Host Processor	AMD Series 6200 (Interlagos)
Host Processor Performance	156.8 Gflops
Kepler Peak (DP floating point)	1.32 Tflops
Host Memory	32GB 51 GB/sec
Kepler Memory	6GB GDDR5 capacity > 180 GB/sec



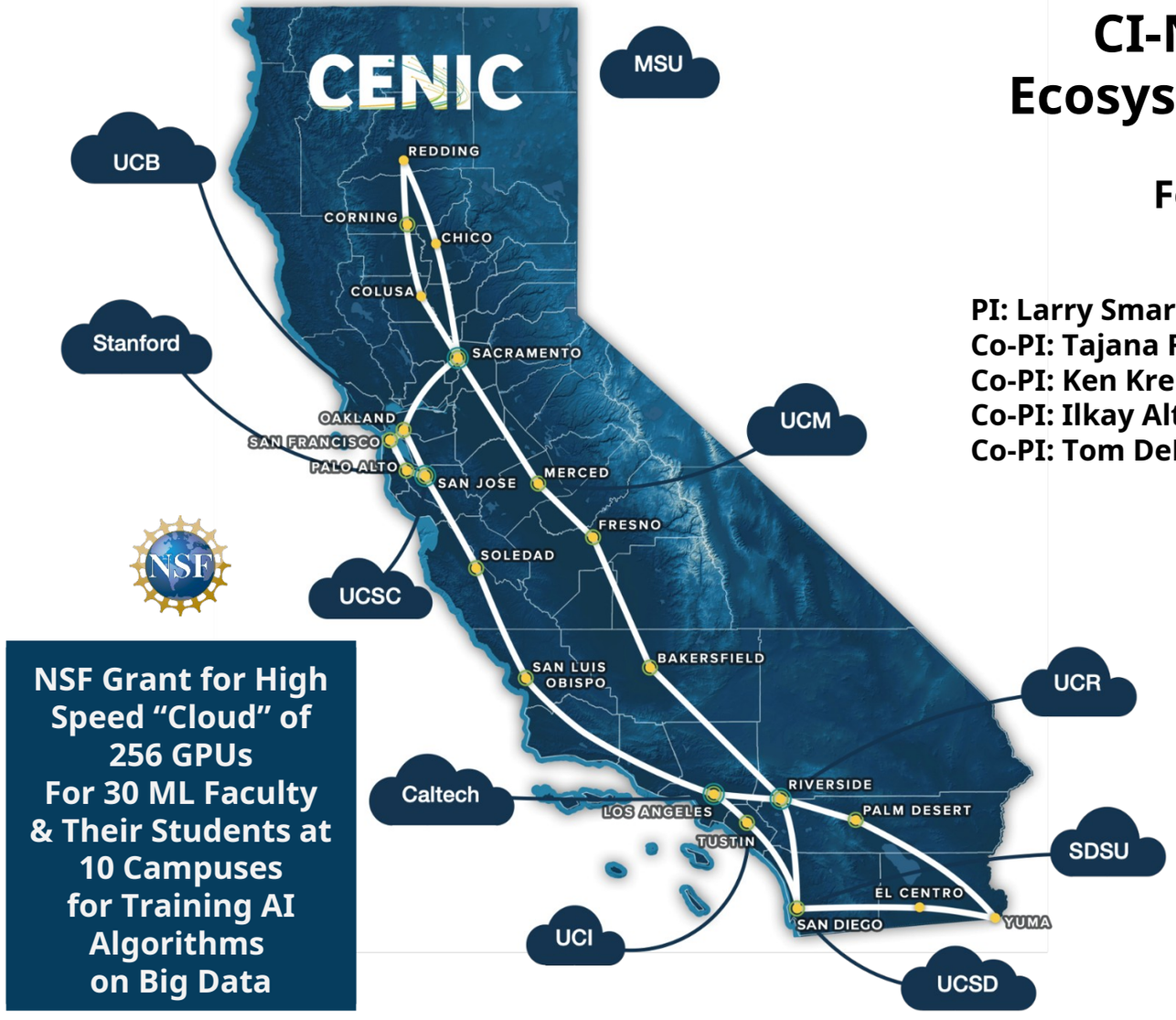
Blue Waters System Overview

NCSA 1988

NCSA 2016

NRP NATIONAL RESEARCH PLATFORM

2017-2020: NSF CHASE-CI Grant Adds a Machine Learning Layer Built on Top of the Pacific Research Platform



NSF Grant for High Speed "Cloud" of 256 GPUs For 30 ML Faculty & Their Students at 10 Campuses for Training AI Algorithms on Big Data

CI-New: Cognitive Hardware and Software Ecosystem Community Infrastructure (CHASE-CI)

For the Period September 1, 2017 – August 21, 2020

PI: Larry Smarr, Professor of Computer Science and Engineering, Director Calit2, UCSD
Co-PI: Tajana Rosing, Professor of Computer Science and Engineering, UCSD
Co-PI: Ken Kreutz-Delgado, Professor of Electrical and Computer Engineering, UCSD
Co-PI: Ilkay Altintas, Chief Data Science Officer, San Diego Supercomputer Center, UCSD
Co-PI: Tom DeFanti, Research Scientist, Calit2, UCSD

Defining Researcher's Unmet AI/ML GPU Needs – Same Methodology as in the 1985 NCSA Black Proposal

JACOBS SCHOOL OF ENGINEERING
SDSC UC San Diego QUALCOMM INSTITUTE

NRP NATIONAL RESEARCH PLATFORM

Installing Community Shared
FIONA CPU/GPU/Storage Systems on CENIC-Connected Campuses









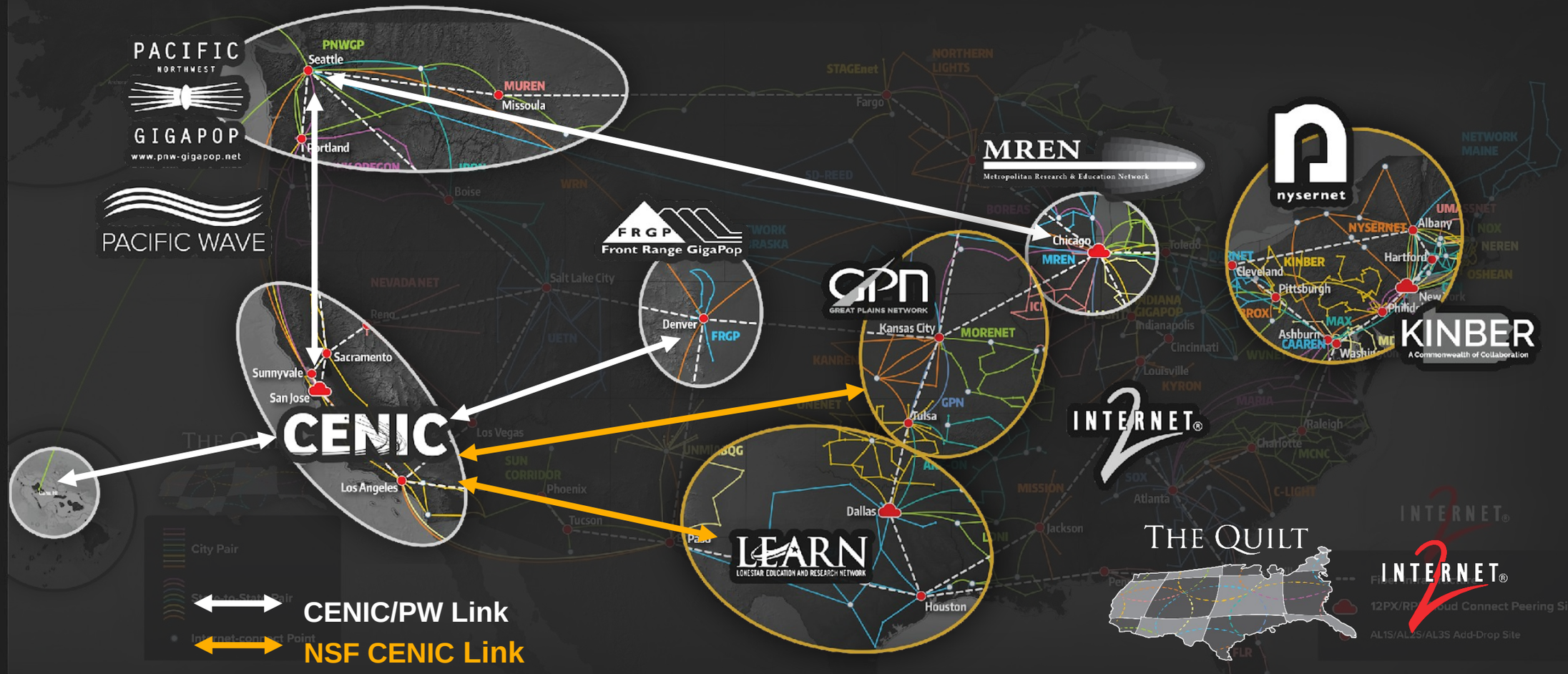




2018-2021: Toward the National Research Platform (NRP) - Using CENIC & Internet2 to Connect Quilt Regional R&E Networks

"Towards The NRP"
3-Year Grant
Funded By
NSF $2.5M
October 2018

PI Smarr
Co-PIs Altintas
Papadopoulos
Wuerthwein
Rosing
DeFanti



SDSC

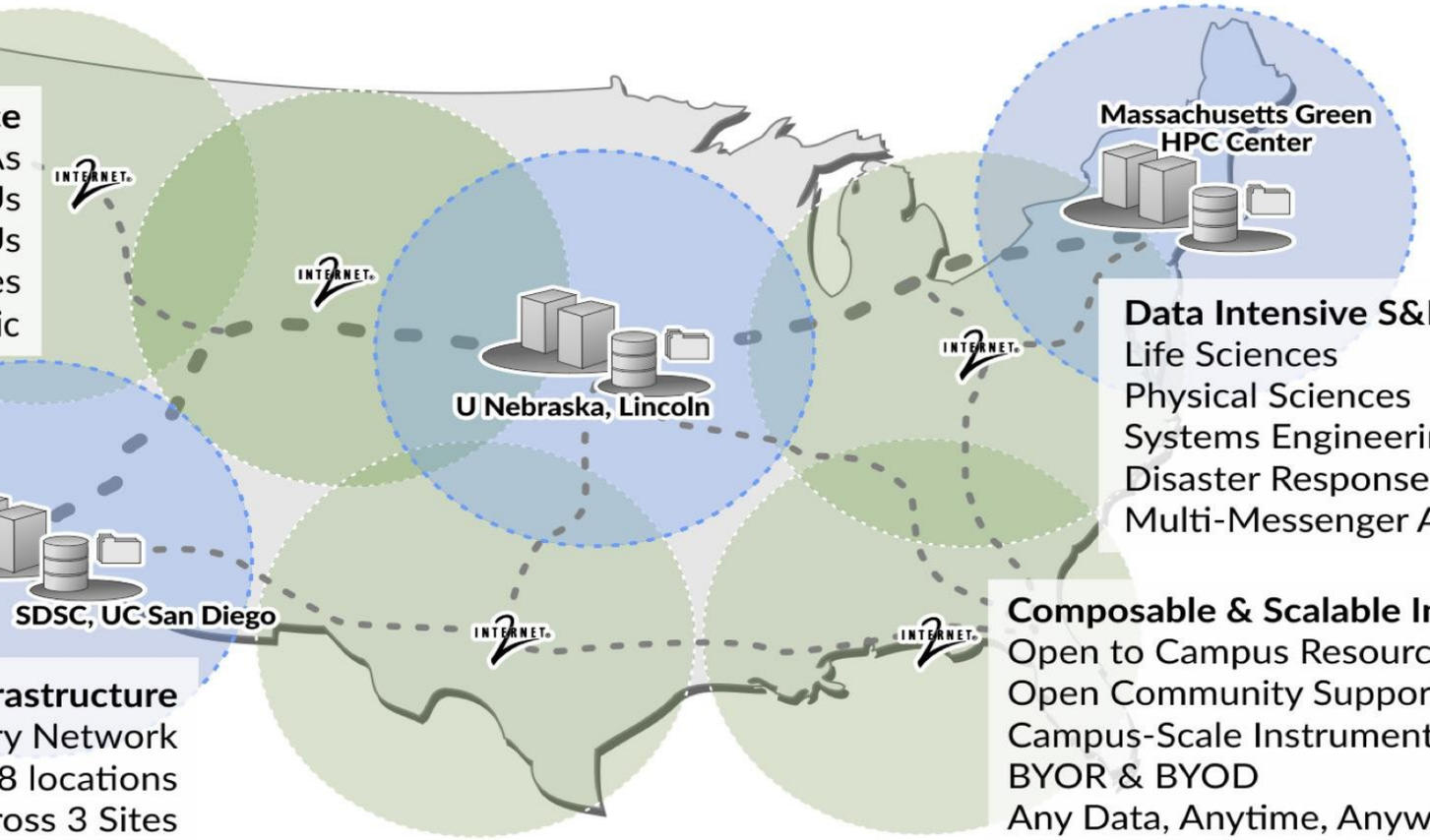
NRP NATIONAL RESEARCH PLATFORM

NRP Nautilus

2021-2026: PRP Federates with NSF-Funded *Prototype National Research Platform*

SDSC

HPC/HTC Resource
32 ALVEO FPGAs
288 NVIDIA FP32 GPUs
48 NVIDIA FP64 GPUs
Tbps WAN IO Capabilities
Configurable Low Latency HPC Fabric



Data Intensive S&E
Life Sciences
Physical Sciences
Systems Engineering
Disaster Response
Multi-Messenger Astrophysics

Distributed Data Infrastructure
National Scale Content Delivery Network
50TB 100Gbps NVMe Caches in 8 locations
4.5PB Distributed Data Origin across 3 Sites

Composable & Scalable Innovation
Open to Campus Resource Integration
Open Community Support Model
Campus-Scale Instrument integration
BYOR & BYOD
Any Data, Anytime, Anywhere

NSF Award OAC #2112167 (June 2021) [$5M Over 5 Years]
PI Frank Wuerthwein (UCSD, SDSC)
Co-PIs Tajana Rosing (UCSD), Thomas DeFanti (UCSD),
Mahidhar Tatineni (SDSC), Derek Weitzel (UNL)

NRP NATIONAL RESEARCH PLATFORM

2023 - The National Research Platform Emerges As a Unification of 22 Years of NSF Cyberinfrastructure Grants

NRP NATIONAL RESEARCH PLATFORM

NEWS GRANTS TECHNOLOGY COMMUNITY JOIN / CONTACT



Professor Frank Würthwein

- Director - SDSC
- Distributed High-Throughput Computing Lead - SDSC

Designed for Growth and Inclusion

The National Research Platform (NRP) is a partnership of more than 50 institutions, led by researchers and cyberinfrastructure professionals at UC San Diego, supported in part by awards from the National Science Foundation.

https://

Nautilus is NRP's Multi-Institution Hypercluster Which Creates a Community Owned and Operated "AI Resource"

May 9, 2024

~200 FIONAs on 27 Partner Campuses Networked Together at 10-100Gbps

Installed GPUs	Installed CPU Cores	Rotating Storage
1314	23416	7000 TB

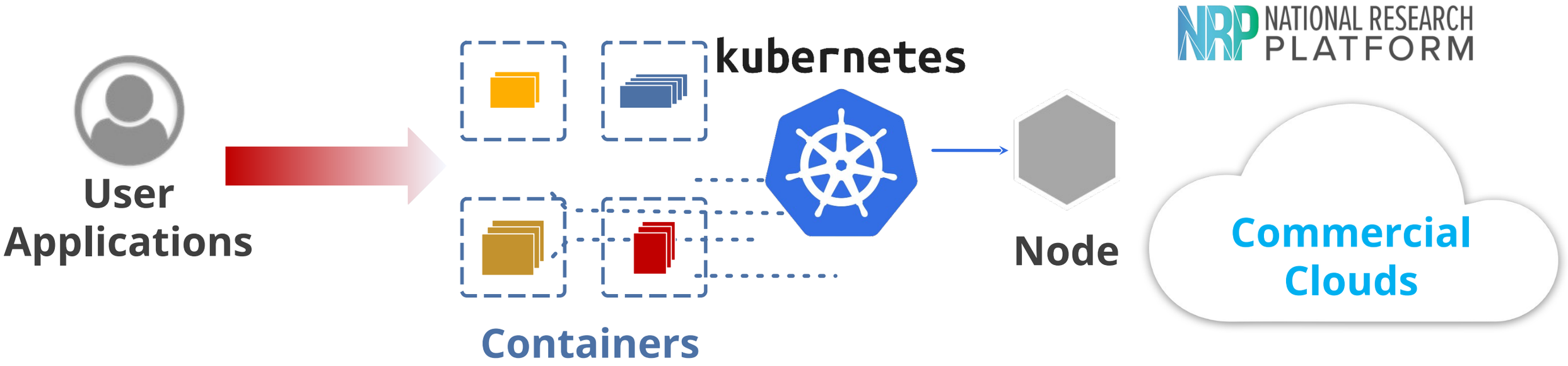


NRP NATIONAL RESEARCH PLATFORM

Nautilus Users Can Execute Their Containerized Applications in the NRP or in Commercial Clouds

Nautilus Containerized Applications Are "Cloud Ready"

Nautilus



NRP NATIONAL RESEARCH PLATFORM

NRP's *Nautilus* Hypercluster Adopted Open-Source Kubernetes and Rook to Orchestrate Software Containers and Manage Distributed Storage

Nautilus

Production-Grade Container Orchestration



kubernetes

ROOK

ceph

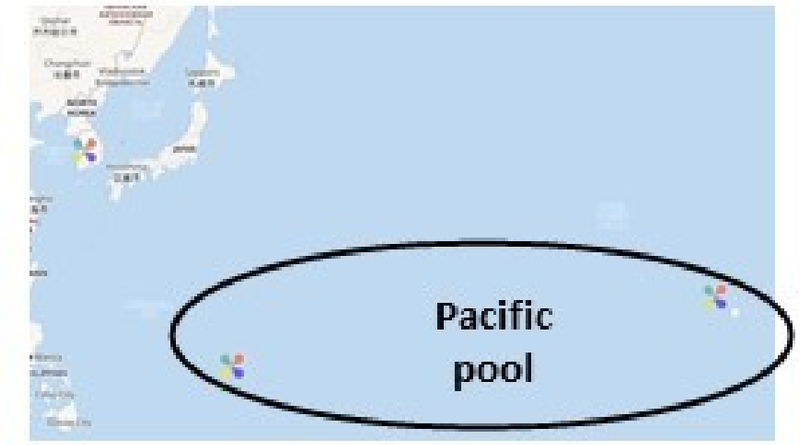
Open source file, block & object storage for your cloud-native environment

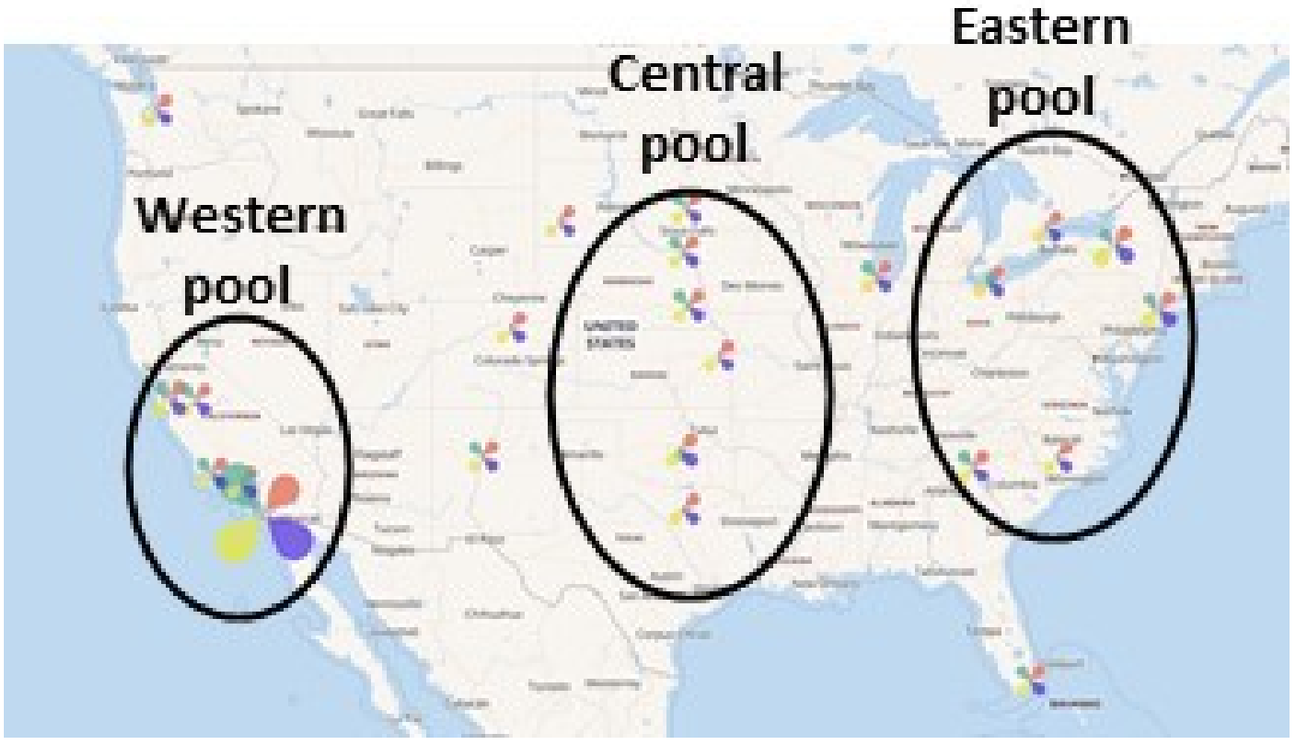
"Kubernetes with Rook/Ceph Allows Us to Manage Petabytes of Distributed Storage and GPUs for Data Science, While We Measure and Monitor Network Use."

--John Graham, UC San Diego

NRP NATIONAL RESEARCH PLATFORM

Nautilus Has Established a Distributed Set of Ceph Storage Pools Managed by Rook/Kubernetes





NRP Forms Optimal-Scale Ceph Pools With Best Performance and Lowest Latency

Allows Users to Select the Placement for Compute Jobs Relative to the Storage Pools

NRP NATIONAL RESEARCH PLATFORM

PRP Provides Widely-Used Kubernetes Services For Application Research, Development and Collaboration





NRP NATIONAL RESEARCH PLATFORM

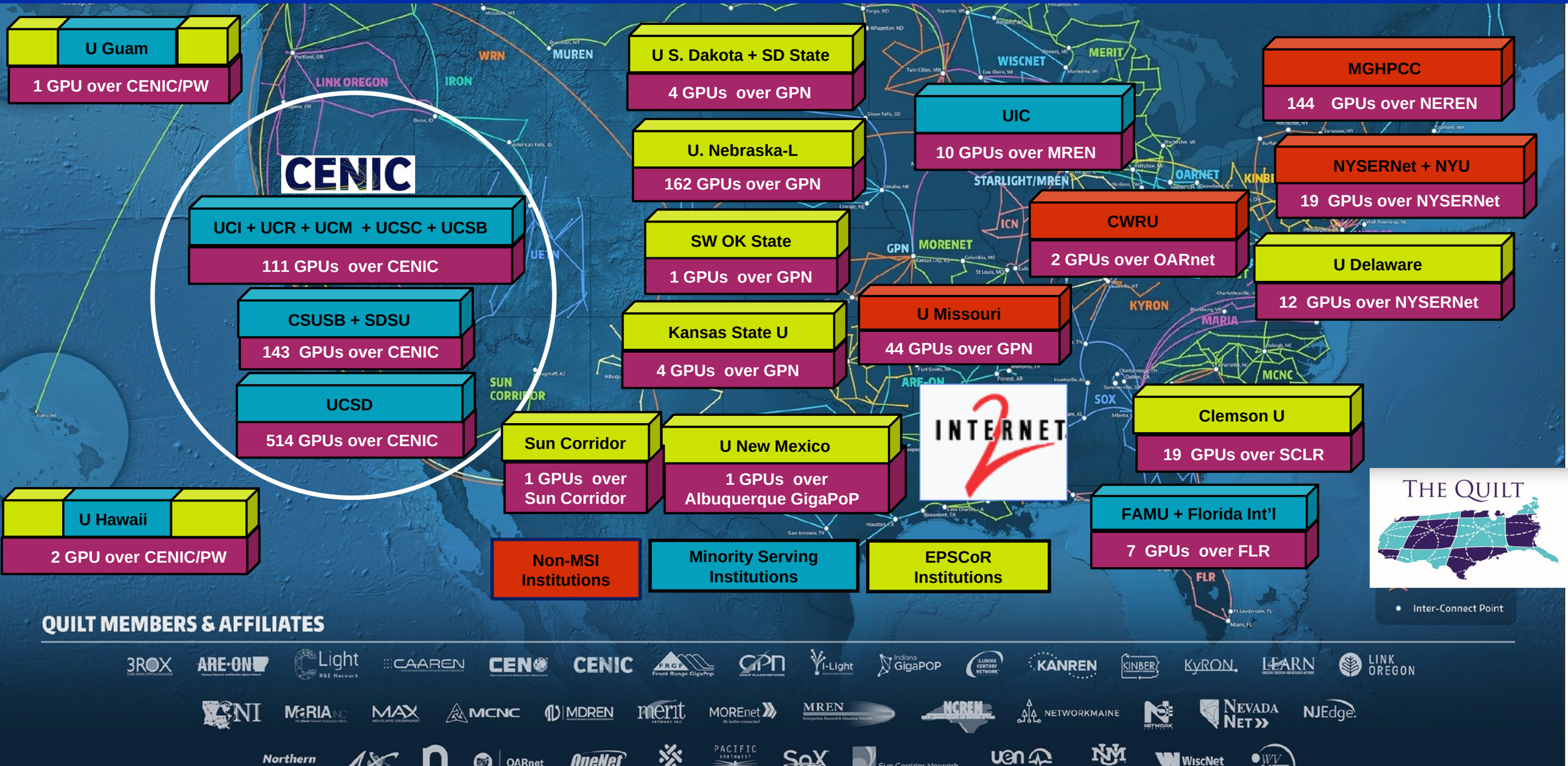
The Majority of *Nautilus* GPUs Reside in the CENIC AI Resource (CENIC-AIR): Hosted by and Available to CENIC Members



Graphics by Hunter Hadaway, CENIC; Data by Tom DeFanti, UCSD

NRP NATIONAL RESEARCH PLATFORM

The Users of the CENIC-Connected AI Resource Can Burst into NRP's Nautilus Hypercluster Outside of California



NRP Applications:
Disciplinary Plus The Rapid Rise of AI/ML Computing

NRP NATIONAL RESEARCH PLATFORM

2023: The New Pacific Research Platform Video Shown at 4NRP Highlighted 3 Disciplinary Applications, But Made No Mention of AI/ML



Pacific Research Platform Video:
https://nationalresearchplatform.org/media/pacific-research-platform-video/

NRP CITRIS AND THE BANATAO INSTITUTE

The Open Science Grid (OSG) Has Been Integrated With the PRP

Source: Frank Würthwein,
OSG Exec Director; PRP co-PI; UCSD/SDSC

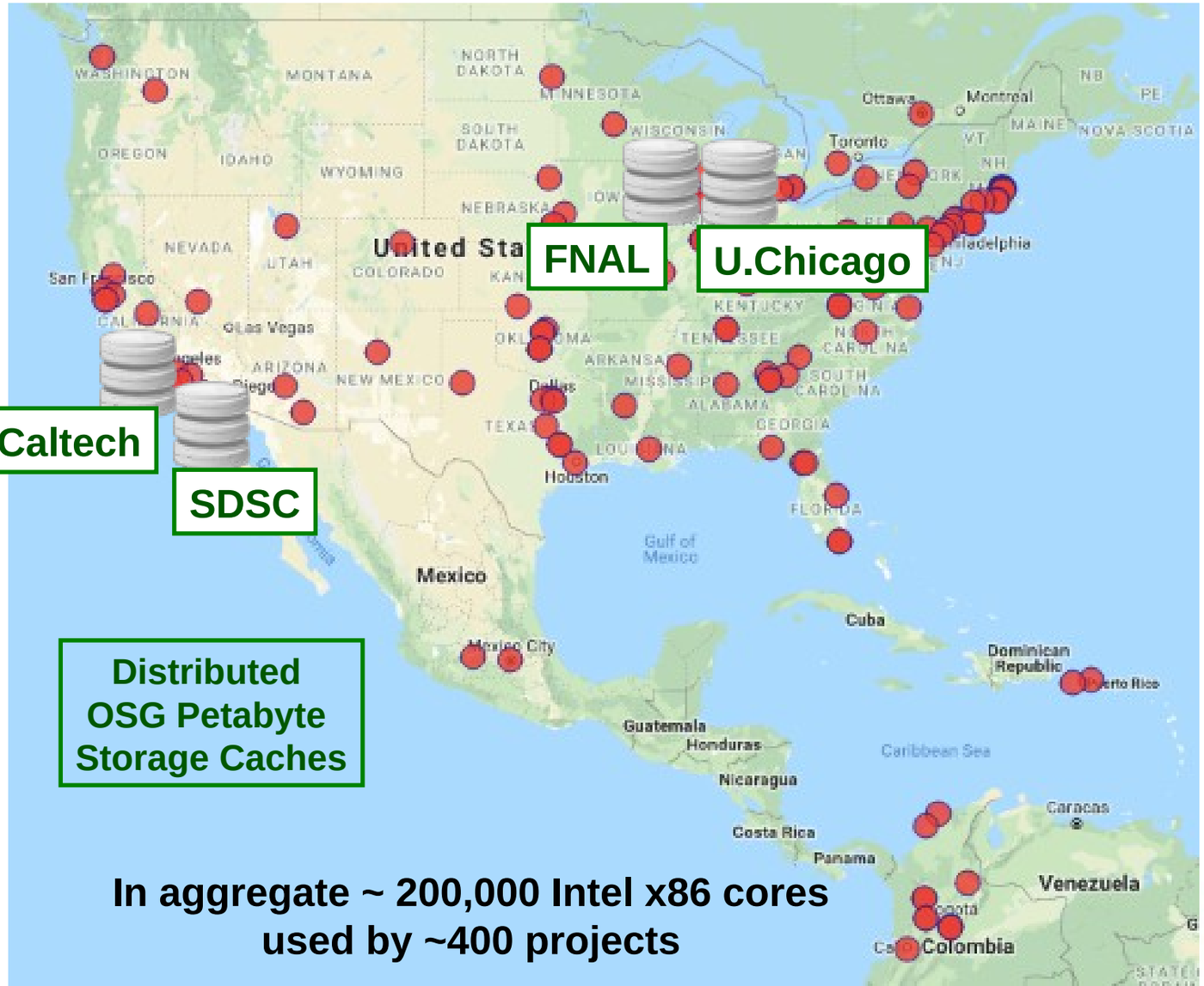
OSG Federates ~100 Clusters Worldwide

All OSG User Communities Use HTCondor for Resource Orchestration

HTCondor
High Throughput Computing

NSF

Open Science Grid

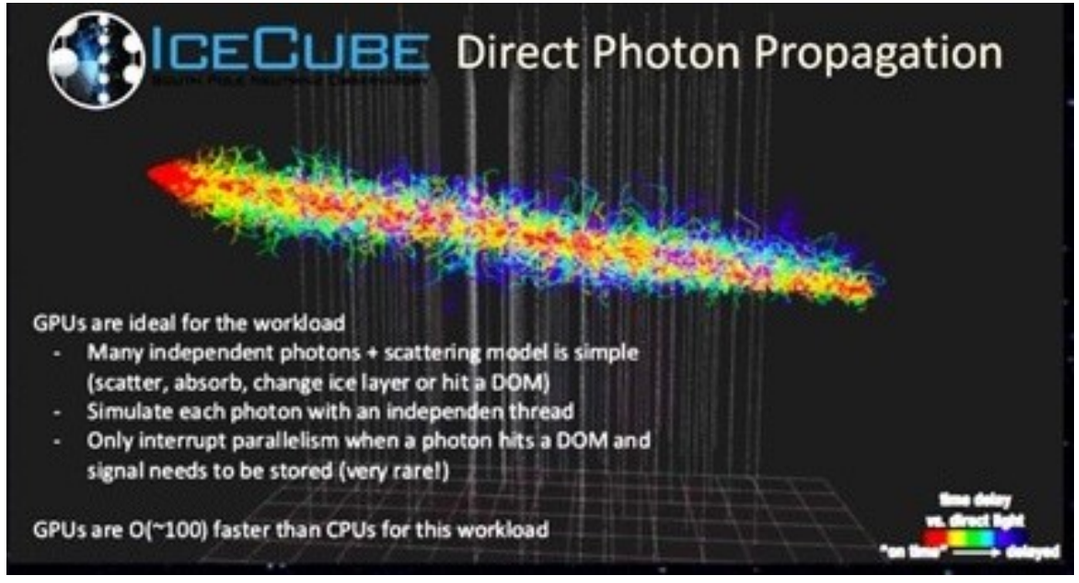


In aggregate ~ 200,000 Intel x86 cores used by ~400 projects

NRP NATIONAL RESEARCH PLATFORM

NSF Large-Scale Observatories Are Using PRP and OSG as a Cohesive, Federated, National-Scale Research Data Infrastructure





GPU Simulations Needed *to Improve Ice Model*.
=> Results in *Significant Improvement*
in Pointing Resolution for Multi-Messenger Astrophysics

WISCONSIN
UNIVERSITY OF WISCONSIN-MADISON
WIPAC
Wisconsin IceCube Particle Astrophysics Center
NSF

IceCube Peaked at 560 GPUs in 2022!

> 1M PRP GPU-Hours Used via OSG Integration Within the Last 2 Years

NSF's IceCube & LIGO Both See Nautilus as Just Another OSG Resource

Open Science Grid

2017: PRP 20Gbps Connection of UCSD SunCAVE and UCM WAVE Over CENIC
2018-2019: Added Their 90 GPUs to PRP for Machine Learning Computations



UC Merced WAVE (20 Screens, 20 GPUs)

CENIC



UCSD SunCAVE (70 Screens, 70 GPUs)

See These VR Facilities in Action in the PRP Video

Leveraging UCM Campus Funds and NSF CNS-1456638 & CNS-1730158 at UCSD

NRP NATIONAL RESEARCH PLATFORM

NSF-Funded WIFIRE Uses PRP/CENIC to Couple Wireless Edge Sensors With Supercomputers, Enabling Fire Modeling Workflows

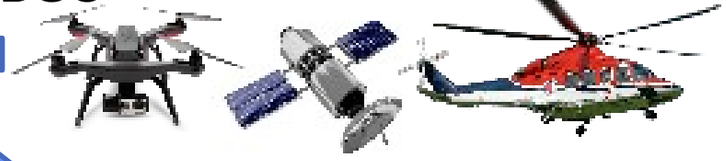


Real-Time Meteorological Sensors

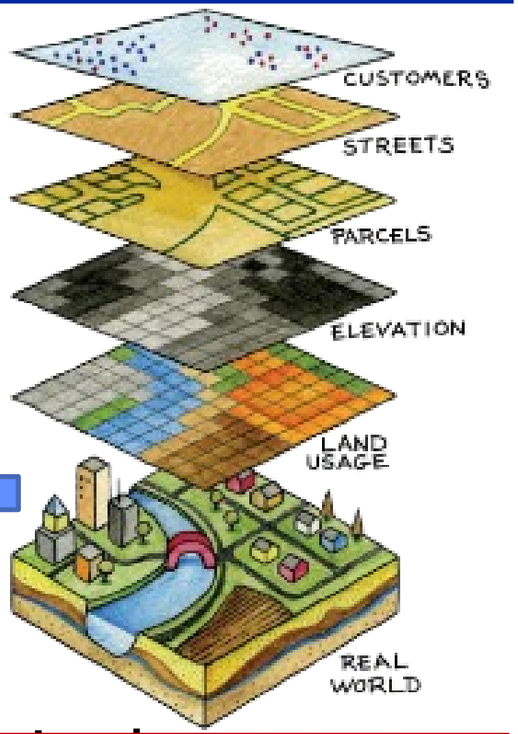
HPWREN



Source: Ilkay Altintas, SDSC



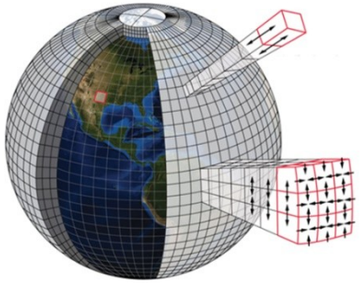
WIFIRE

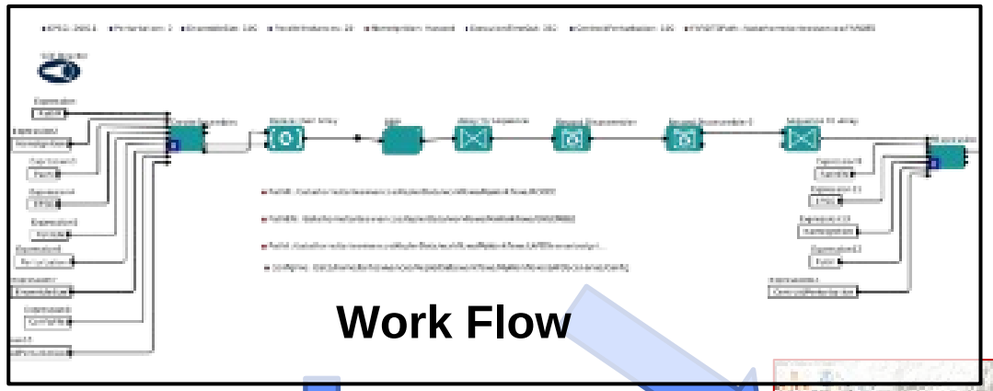


PRP

CENIC

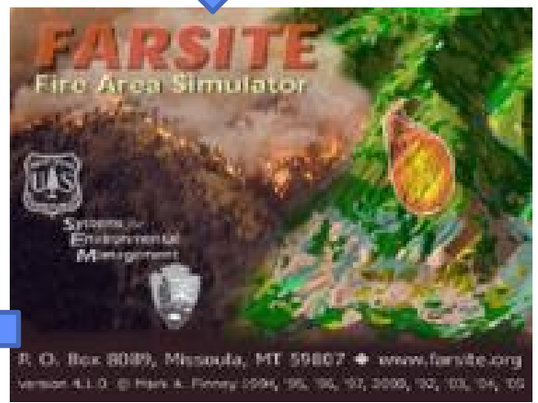
Weather Forecasts

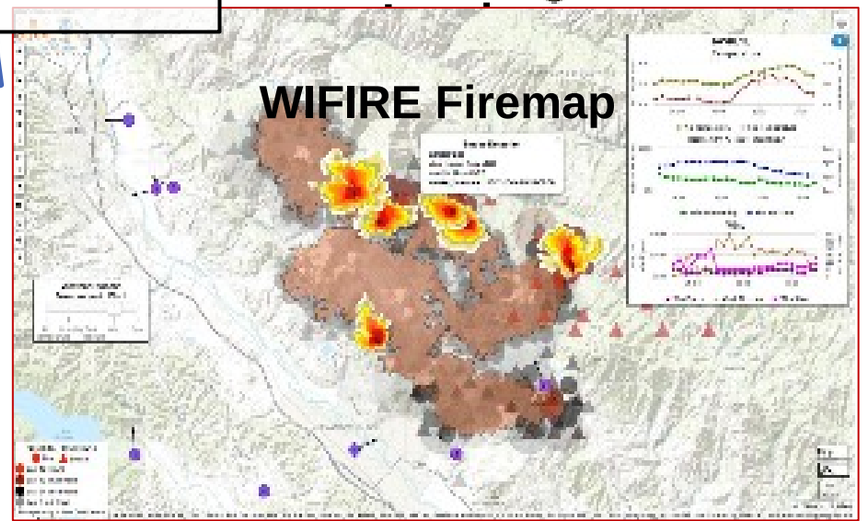




Work Flow







NSF

OpenForceField Uses OPEN Software, OPEN Data, OPEN Science and NRP to Generate Quantum Chemistry Datasets for Druglike Molecules



OPEN SOFTWARE

Automated infrastructure enables rapid experimentation with minimum human intervention



OPEN DATA

Access to large, high quality experimental and quantum chemical data facilities easy curation of balanced train / test sets



OPEN SCIENCE

Exploring new force field science:

hypothesis –

build software –

train - test - iterate

is now almost routine

open forcefield

OFF Open-Source Models are Used in Drug Discovery, Including in the COVID-19 Computing on Folding@Home.

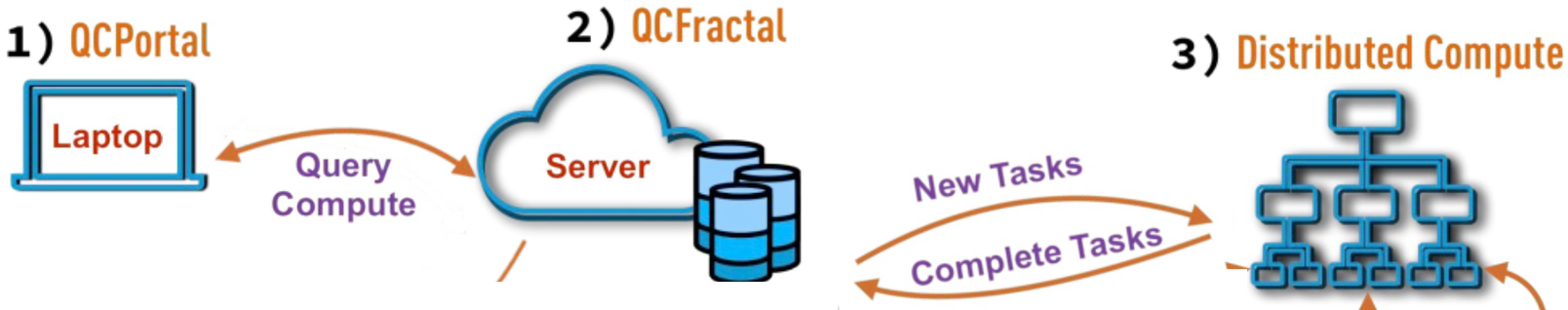
www.openforcefield.org

NRP NATIONAL RESEARCH PLATFORM

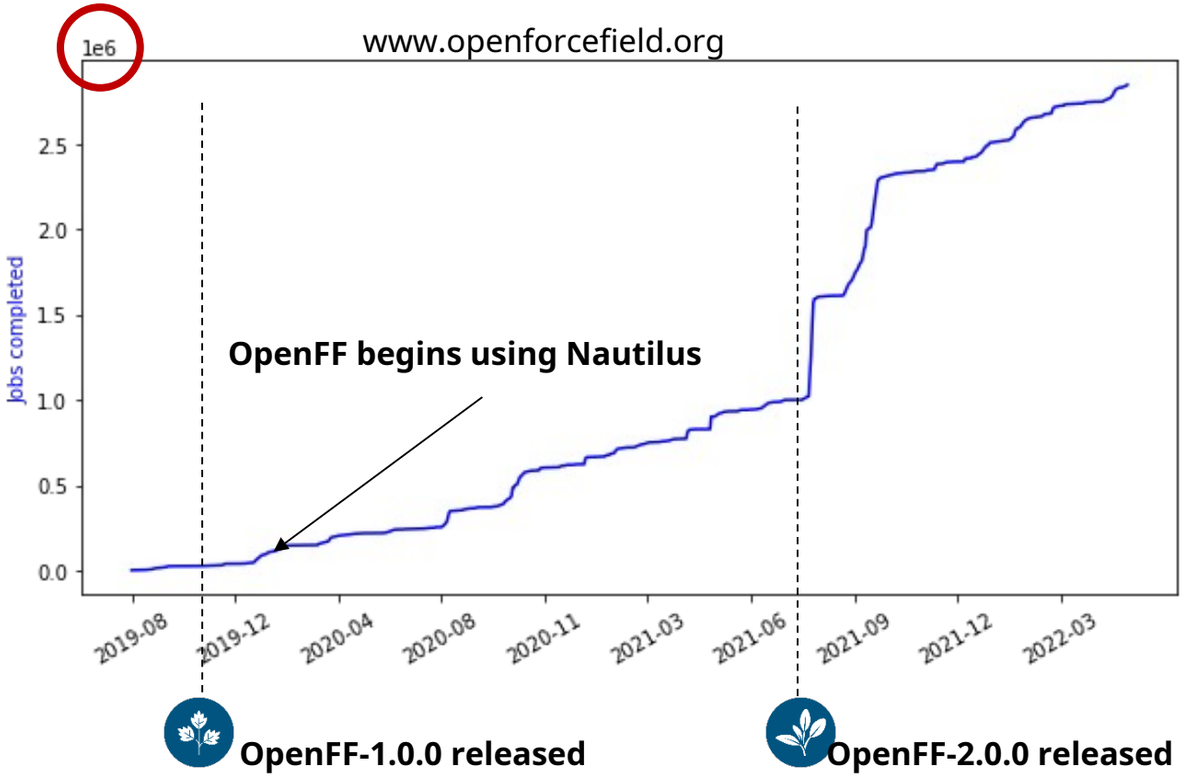
OpenForceField Running on PRP is Capable of Running Millions of Quantum Chemistry Workloads

QC Archive
A MolSSI Project
VIRGINIA TECH

50% of OFF compute is run on Nautilus.



www.openforcefield.org

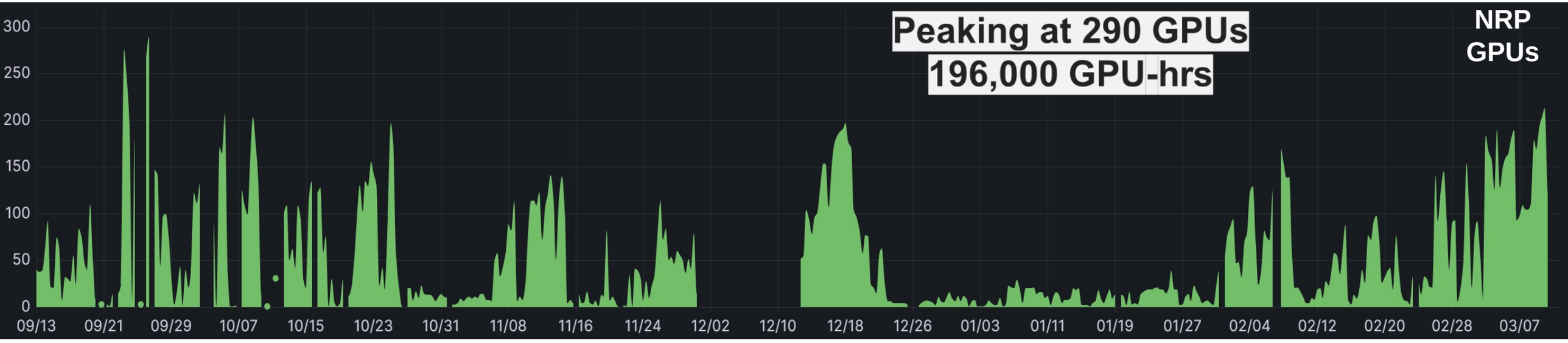


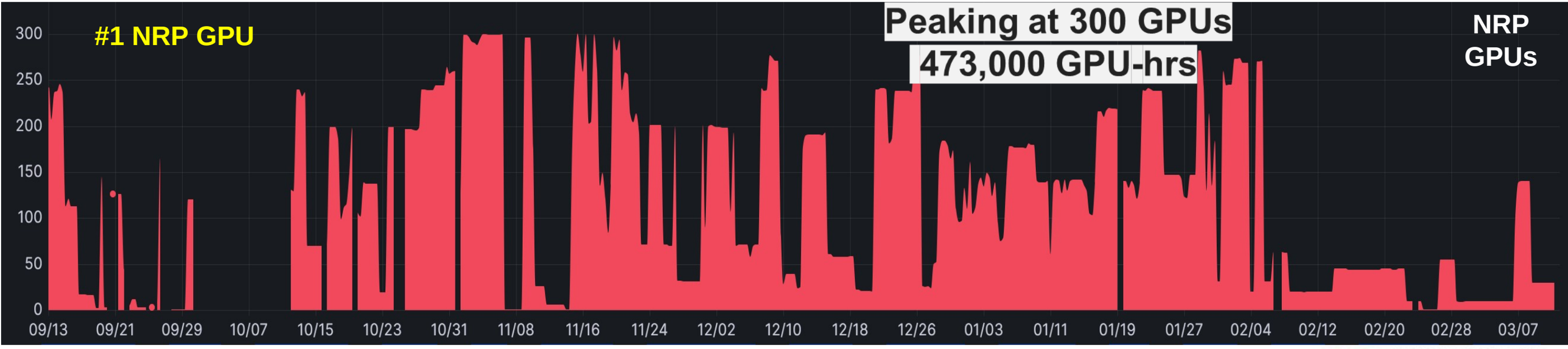
We run "workers" that pull down QC jobs for computation from a central project queue. These jobs require between minutes and hours, and results are uploaded to the central, public QCArchive server.Workers are deployed from Docker images, which are very easy to schedule on PRP's Kubernetes system. Due to the short job duration, these deployments can still be effective if interrupted every few hours.

PRP PACIFIC RESEARCH PLATFORM

NRP NATIONAL PL open forcefield

Namespace *openforcefield* Surpasses Namespace *osg-icecube* in NRP GPU Usage Over Last 6 Months



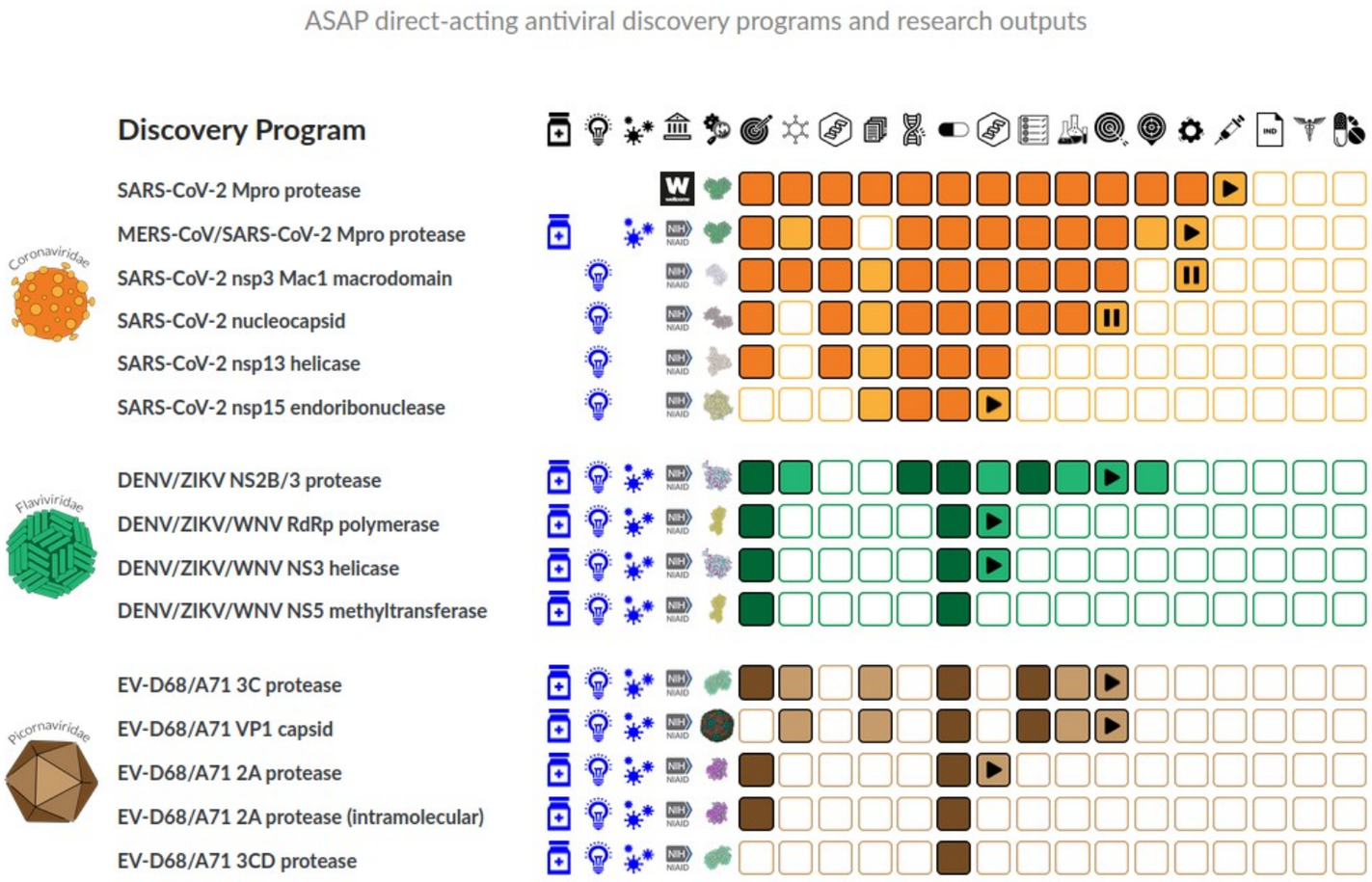


Namespaces osg-icecube, openforcefield

NRP NATIONAL RESEARCH PLATFORM

But OpenForceField's NRP GPU Use is Then Used by an AI-Driven Structure-Enabled Antiviral Platform (ASAP) That Builds on OFF

$68M NIH-Funded Open Science Drug Discovery Effort



ASAP uses AI/ML and computational chemistry to accelerate structure-based, open science antiviral drug discovery and deliver oral antivirals for pandemics with the goal of global, equitable, and affordable access.

Peaking at 242 GPUs
94,000 GPU-hrs

ASAP
Accessible Antivirals to Prevent Pandemics

https://asapdiscovery.org/

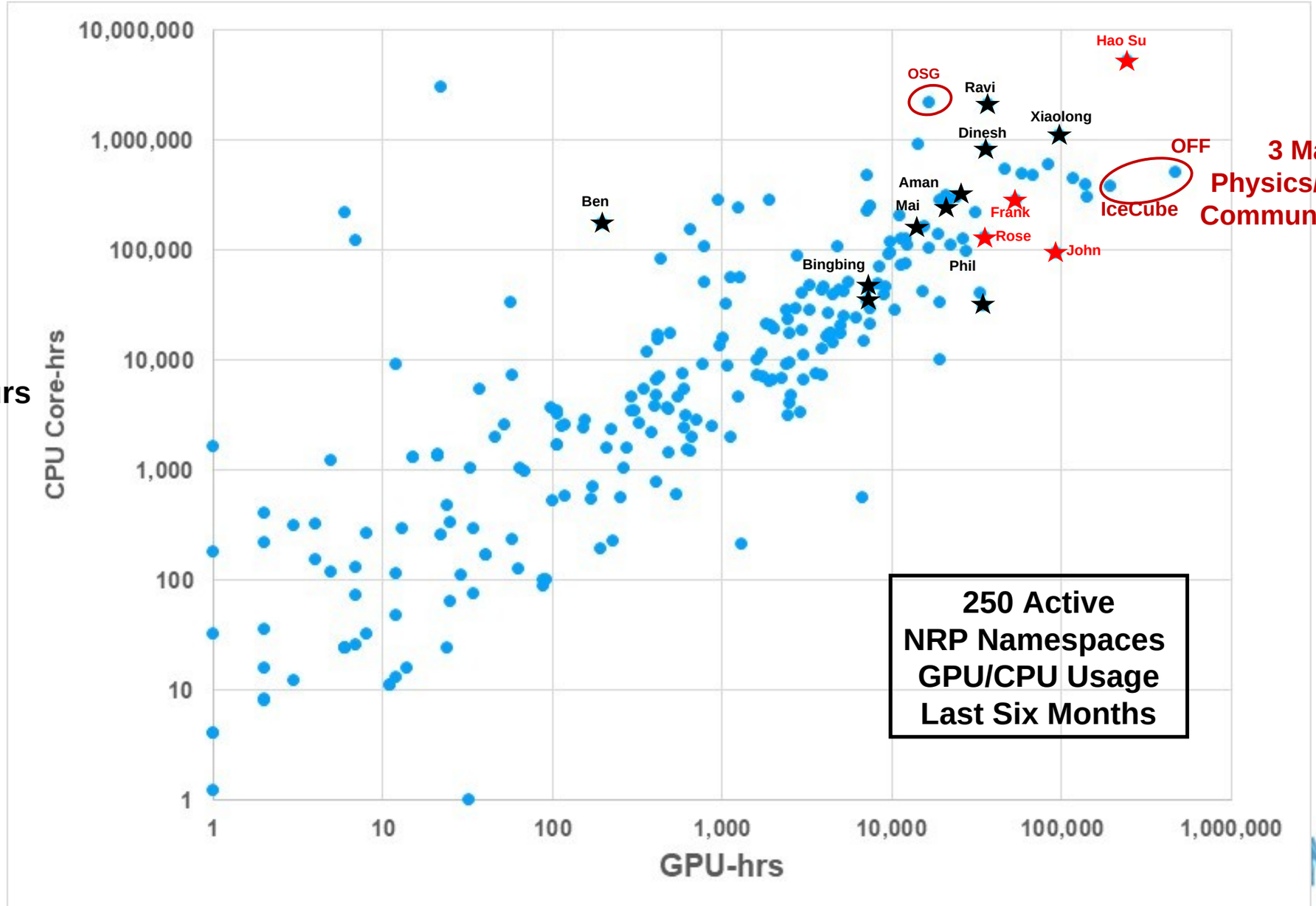
John Chodera, Memorial Sloan-Kettering Cancer Center
Namespace choderalab

NRP NATIONAL RESEARCH PLATFORM

2024: By 5NRP
Almost All NRP Namespaces Use AI/ML

5NRP Speakers:

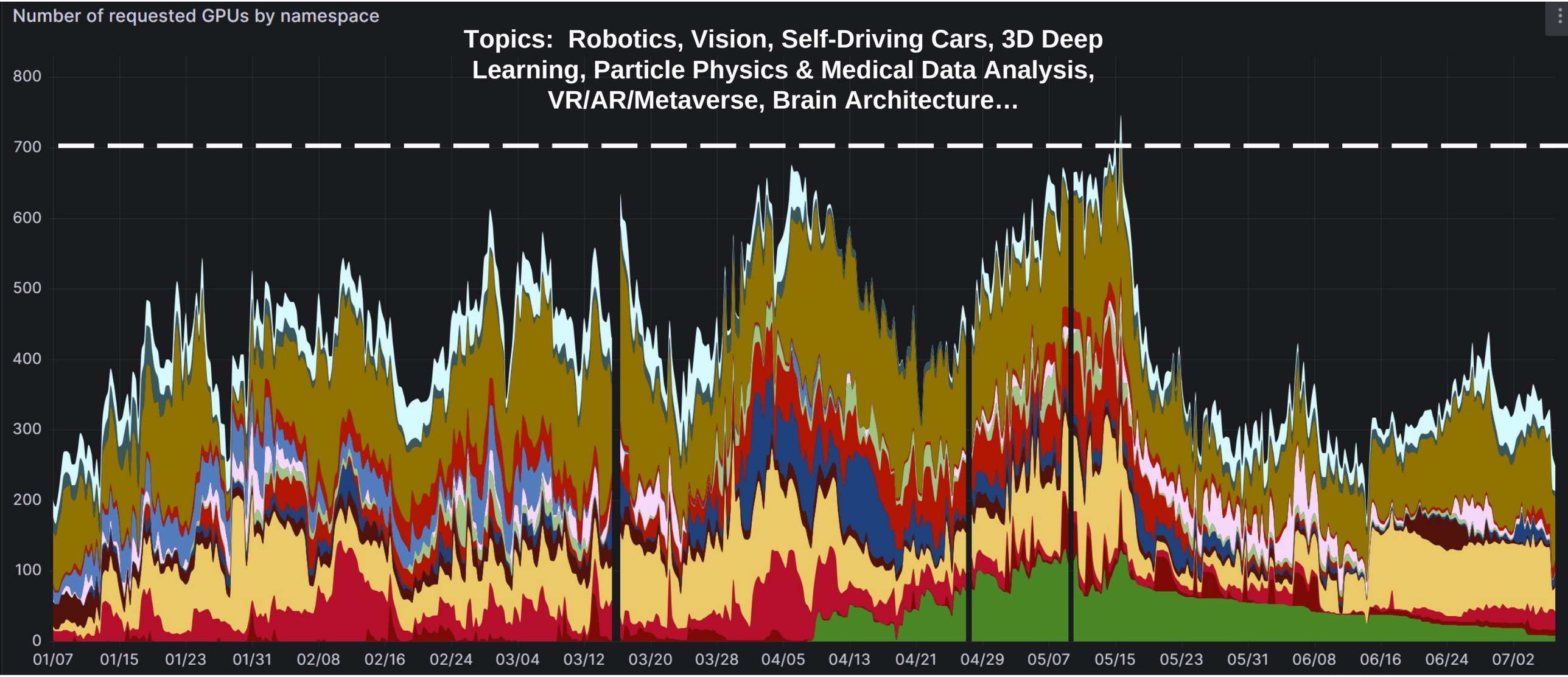
- ★ Weds/Thurs
- ★ My Talk



3 Massive Physics/Chemistry Community Projects

NRP NATIONAL RESEARCH PLATFORM

Top 15 GPU-Consuming ML/AI NRP Research Projects In Six Months-Peaking at Over 700 GPUs!



For More Details on Nautilus Applications, Including ML/AI Namespaces Like the Ones Above See my 4NRP Talk: www.youtube.com/watch?v=1yUz0BwObGs&list=PLbbCsk7MUIGdHZzgZqNbZkV7KGVZ7gn1g&index=19

NRP NATIONAL RESEARCH PLATFORM

NRP's Nautilus Cyberinfrastructure Supports a Wide Array of AI/ML Algorithms

Nautilus was Designed to Support Research in 6 Broadly Defined Families of Information Extraction and Pattern Recognition Algorithms that are Commonly Used in AI/ML Research:

1) **Deep Neural Network (DNN) and Recurrent Neural Network (RNN) Algorithms Including Layered Networks:**
   - **Convolutional layers (CNNs),**
   - **Generative adversarial networks (GANs), &**
   - **Transformer Neural Networks (e.g., LLMs)**
2) **Reinforcement Learning (RL) and Inverse-RL Algorithms & Related Markov Decision Process (MDP) Algorithms**
3) **Variational Autoencoder (VAE) and Markov Chain Monte Carlo (MCMC) Stochastic Sampling**
4) **Support Vector Machine (SVM) Algorithms and Various Ensemble ML Algorithms**
5) **Sparse Signal Processing (SSP) Algorithms, Including Sparse Bayesian Learning (SBL)**
6) **Latent Variable (LVA) Algorithms for Source Separation**

Source: CHASE-CI Proposal

NRP NATIONAL RESEARCH PLATFORM

Today's Over 1000 Nautilus Namespaces Have Utilized Many of These Algorithms

The Great Majority of Nautilus AI/ML Namespaces are Using Some Form of NNs or RL

- **For NNs PyTorch, TensorFlow, and Keras are the Preferred (in that order) Open-Source Deep Learning (DL) Frameworks Used on Nautilus.**
- **Our AI/ML Researchers Use Different Subtypes of DNNs, Including:**
  - **Deep Belief Networks (DBN),**
  - **Quantum NNs (QNN),**
  - **Graph NNs (GNNs) and**
  - **Long Short-Term Memory (LSTM) RNNs-Specifically Designed to Handle Sequential Data, such as Time Series, Speech, and Text**
- **Nautilus Namespaces Use RL and Inverse-RL Algorithms in Many Areas of Dynamic Decision-Making, Robotics, and Human/Robotic Transfer Learning**

Nautilus Namespaces with Descriptions:
https://portal.nrp-nautilus.io/namespaces-g

NRP NATIONAL RESEARCH PLATFORM

NRP's Largest GPU-Consuming AI/ML Researchers Point to the Rapid Growth of Transformer NNs

Transformer NNs Have Become the Default Architecture for Applications Involving Images, Sound, or Text

- **A Growing Number of NRP Namespaces are Using Transformer-Based Large Language Models (LLMs), Such as GPT, LLaMa, and BERT in Natural Language Processing (NLP), or Vision Language Models, Such as CLIP and ViT, for Image Understanding Research**

- **Also Popular are Generative models, Such as GANs and Diffusion Models, Which are Prevalent in Data Synthesis, Such as For Text to Image Generation, Like Stable Diffusion**

- **Finally, We See Many Namespaces Working in Fields Such as Learning for Dynamics and Control (L4DC), Computer Vision (CV), and Trustworthy ML**

NRP NATIONAL RESEARCH PLATFORM

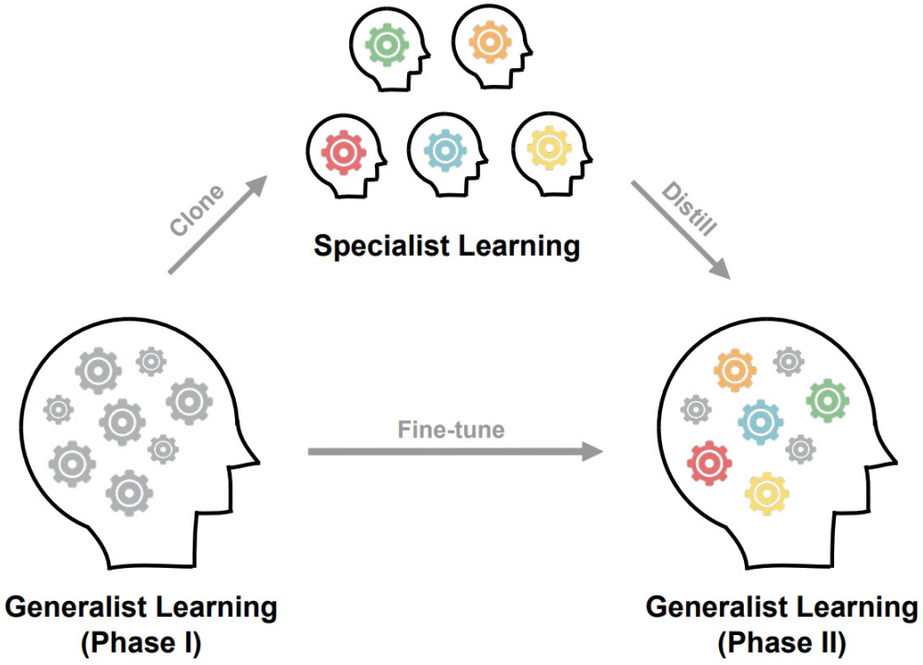
A Major Project in UCSD's Hao Su Lab is Large-Scale Robot Learning

- **We Build A Digital Twin of The Real World in Virtual Reality (VR) For Object Manipulation**
- **Agents Evolve In VR**
  - **Specialists (Neural Nets) Learn Specific Skills by Trial and Error**
  - **Generalists (Neural Nets) Distill Knowledge to Solve Arbitrary Tasks**

Peaking at 219 GPUs
245,000 GPU-hrs

NRP

- On **Nautilus**:
  - *Hundreds* of specialists have been trained
  - Each specialist is trained in *millions* of environment variants
  - ~10,000 GPU hours per run



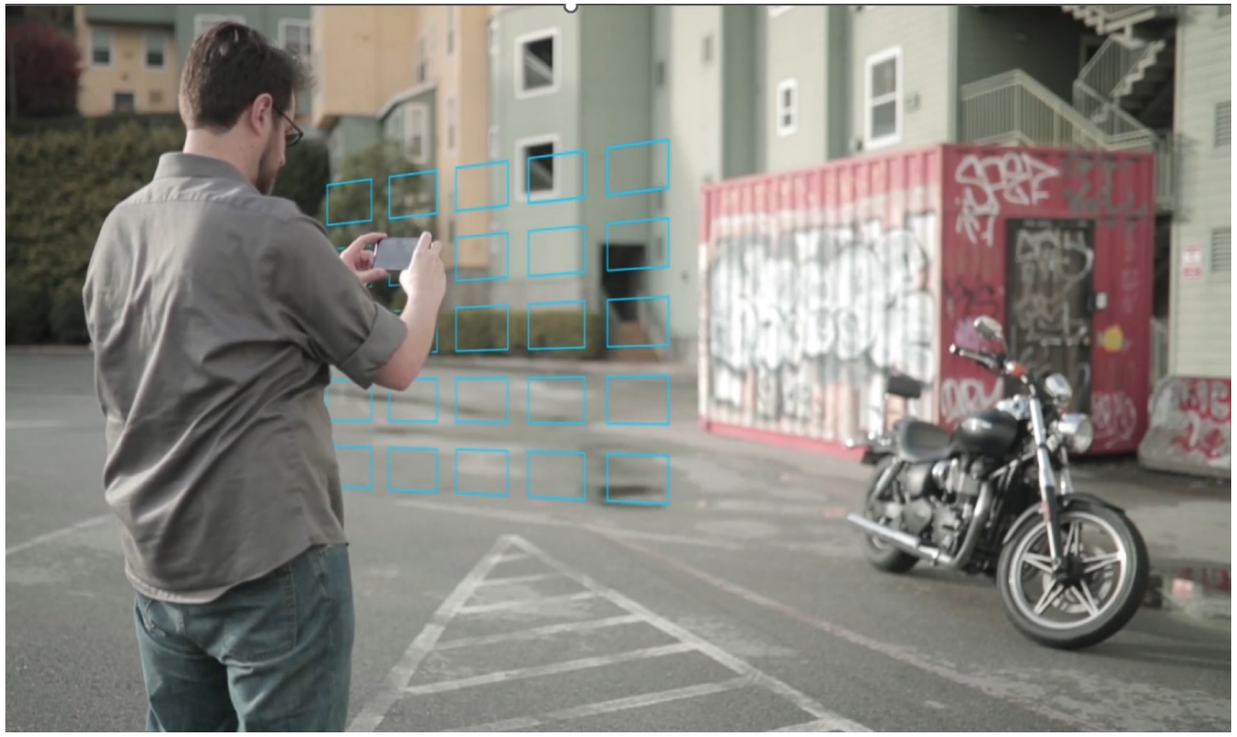
Source: Prof. Hao Su, UCSD

NRP NATIONAL RESEARCH PLATFORM

UCSD's Ravi Group: How to Create Visually Realistic 3D Objects or Dynamic Scenes in VR or the Metaverse

ML Computing Transforms a Series of 2D Images Into a 3D View Synthesis

Peaking at 122 GPUs
200,000 GPU-Hours





Source: Prof. Ravi Ramamoorthi, UCSD

NRP NATIONAL RESEARCH PLATFORM

Machine Learning-Based
Neural Radiance Fields for View Synthesis (NeRFs) Are Transformational!

Meta Is Investing in NeRF for 3D Object Scanning

https://youtu.be/hvfV-iGwYX8

The New York Times | T R&D

Spatial Journalism

Creating Workflows for NeRF Portraiture

September 27, 2022

← THE BEST INVENTIONS OF 2022

TIME

Automated 3D Rendering

NVIDIA Instant NeRF

BY JARED LINDZON
NOVEMBER 10, 2022

A neural radiance field (NeRF) is a fully-connected neural network that can generate novel views of complex 3D scenes, based on a partial set of 2D images.

https://datagen.tech/guides/synthetic-data/neural-radiance-field-nerf/

Source: Prof. Ravi Ramamoorthi, UCSD

NRP NATIONAL RESEARCH PLATFORM

Community Building Through Large-Scale Workshops
From Alliance Chautauquas to the NRP Workshops









2GRP Workshop
September 20-24, 2021

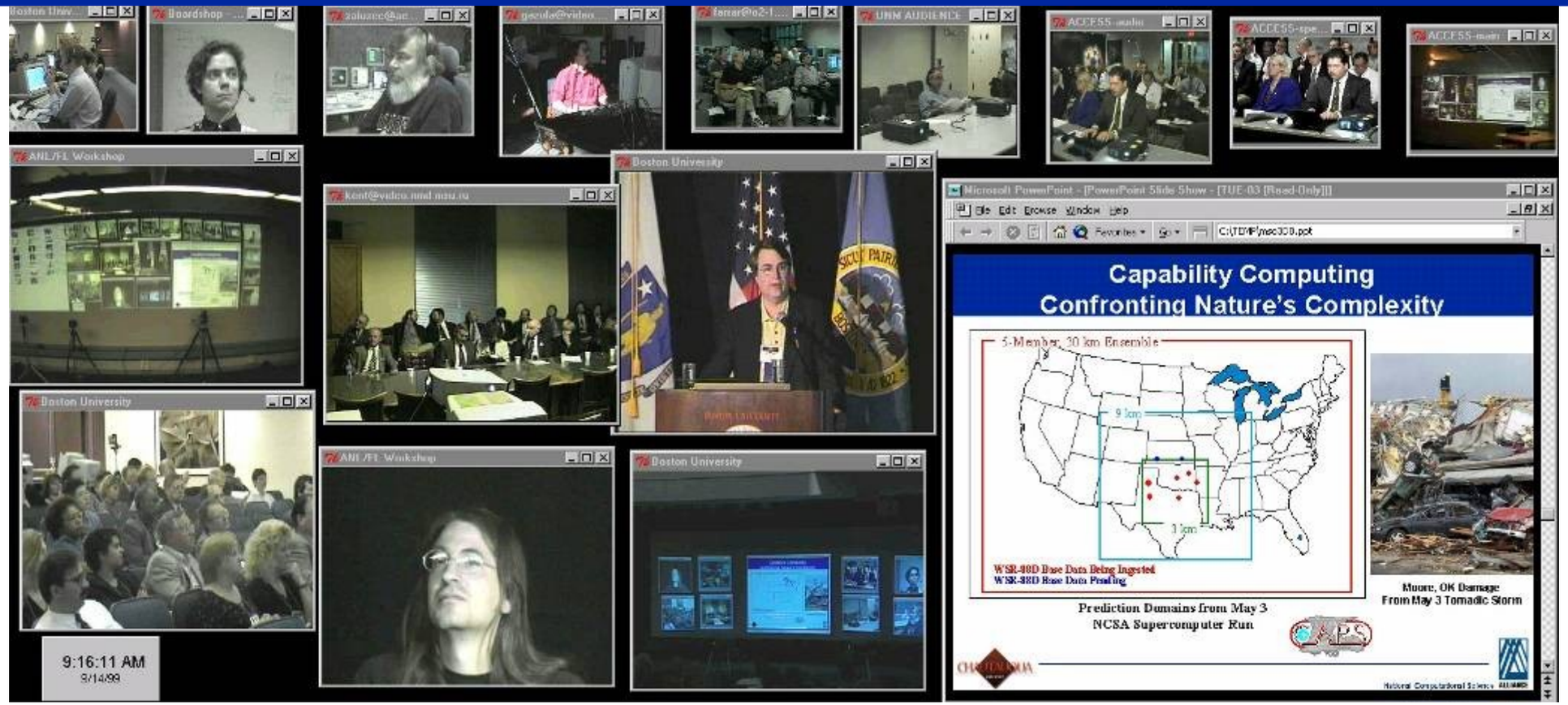
3GRP Workshop
October 10-11, 2022

4NRP Workshop
February 8-10, 2023

5NRP Workshop
March 19-22, 2024

NRP NATIONAL RESEARCH PLATFORM

From Telephone Conference Calls to Access Grid Engineering Meetings Using IP Multicast



1999

CHAUTAUQUA ALLIANCE

National Computational Science ALLIANCE

Access Grid Lead-Argonne
NSF STARTAP Lead-UIC's Elec. Vis. Lab

NRP NATIONAL RESEARCH PLATFORM

To the NRP Weekly Engineering Zoom Meeting
25 Years Later!



NRP NATIONAL RESEARCH PLATFORM