“Toward a National Research Platform to Enable Data-Intensive Open-Source Science Distributed Computing”

Remote Briefing to the
Data & Compute Architecture Study Workshop
September 7, 2022

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

PACIFIC RESEARCH PLATFORM

1985: NSF Adopted a DOE High-Performance Computing Model

NSFNET 56 Kb/s Backbone (1986-8) Adopted TCP/IP







NCSA Was Modeled on LLNL

SDSC Was Modeled on MFEnet

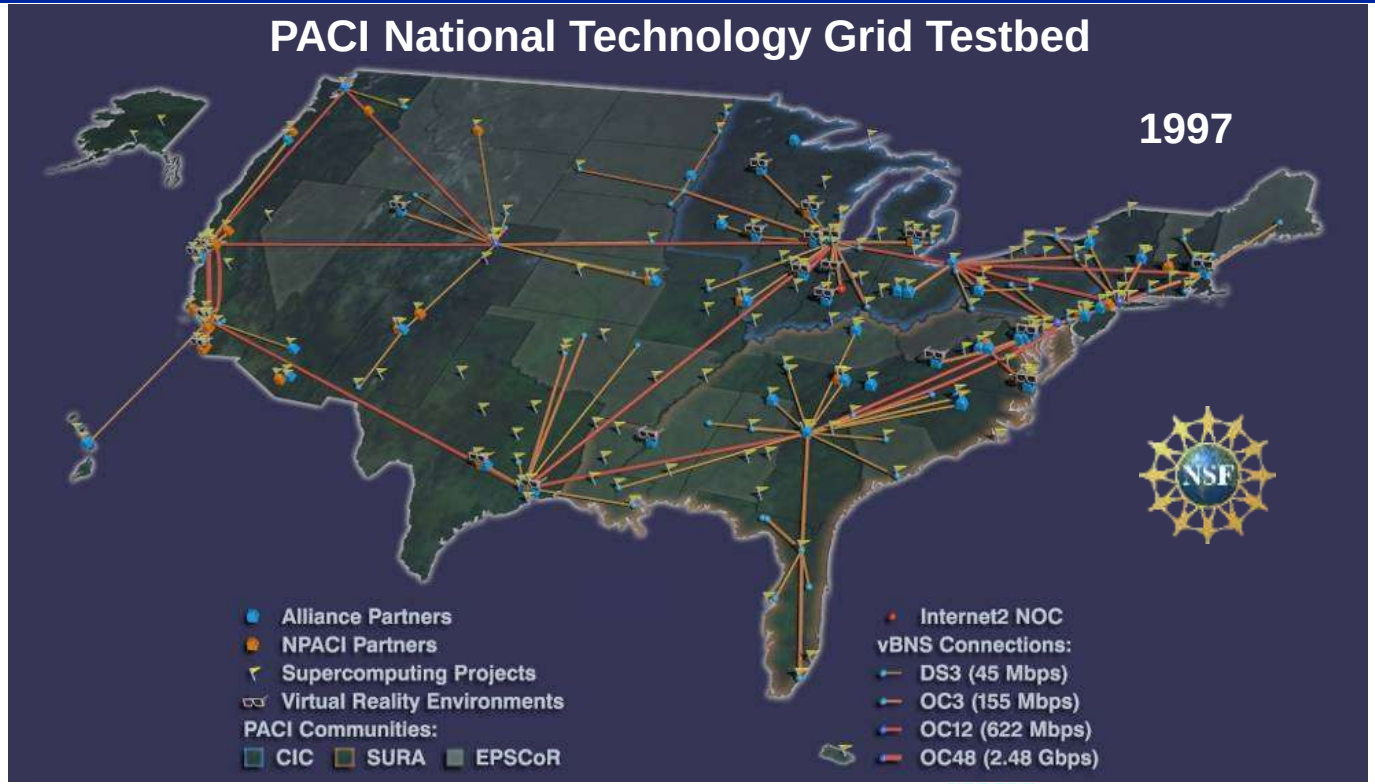
PRP PACIFIC RESEARCH PLATFORM

NCSA

SDSC

1997: NSF's PACI Program was Built on the vBNS to Prototype America's 21st Century Information Infrastructure

Key Role of Miron Livny & Condor



vBNS led to

INTERNET2

PRP PACIFIC RESEARCH PLATFORM

NPACI

National Computational Science ALLIANCE

1999: Dave Bader Created the First Linux 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

Metro & New Mexico

D

UNM To Crank Up $400,000 Supercomputer Today

Machine One of 100 Speediest in World

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

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

PRP PACIFIC RESEARCH PLATFORM

National Computational Science ALLIANCE

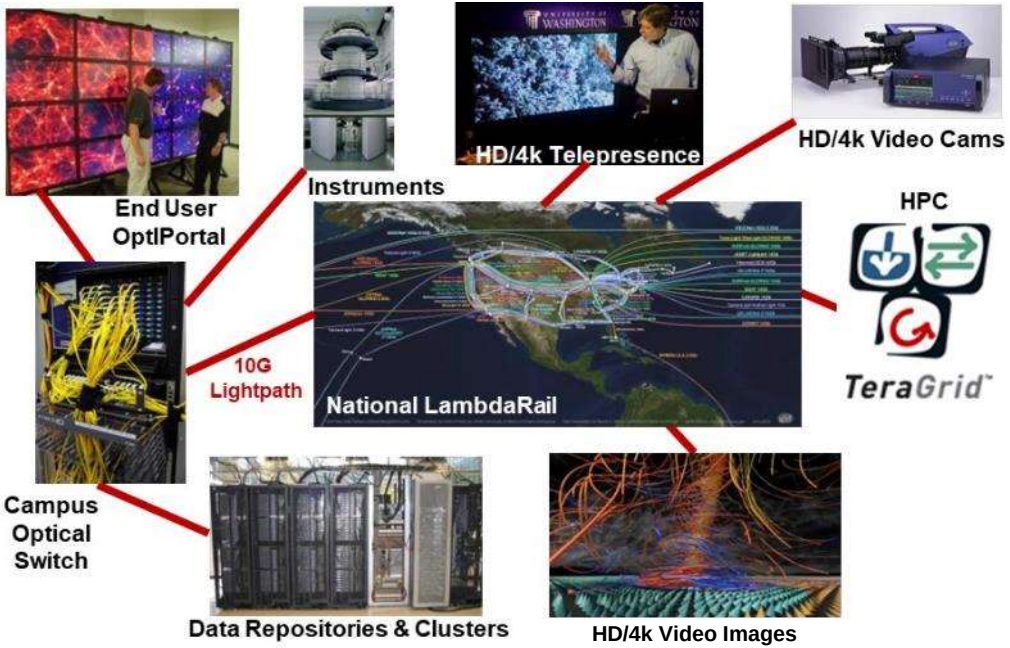
The 25 Years From the National Techology Grid To the National Research Platform

> 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.

PACIFIC RESEARCH PLATFORM

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

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



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

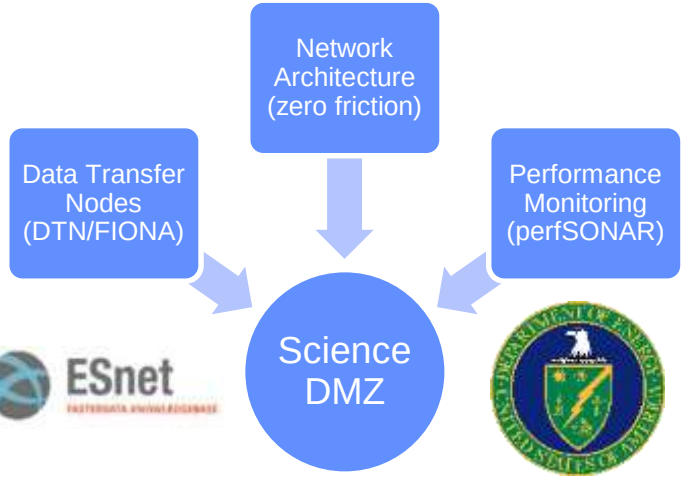
Demonstrating That
Wide-Area Bandwidth
Can Equal
Local Cluster Backplane Speeds

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

PACIFIC RESEARCH PLATFORM

2010-2022:
NSF Adopted a DOE High-Performance Networking Model

ScienceDMZ Coined in 2010 by ESnet



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

Slide Adapted From Inder Monga, ESnet

DOE

NSF

NSF Campus Cyberinfrastructure Program
2012-2022



Has Made Over 340 Awards:
Across 50 States and Territories

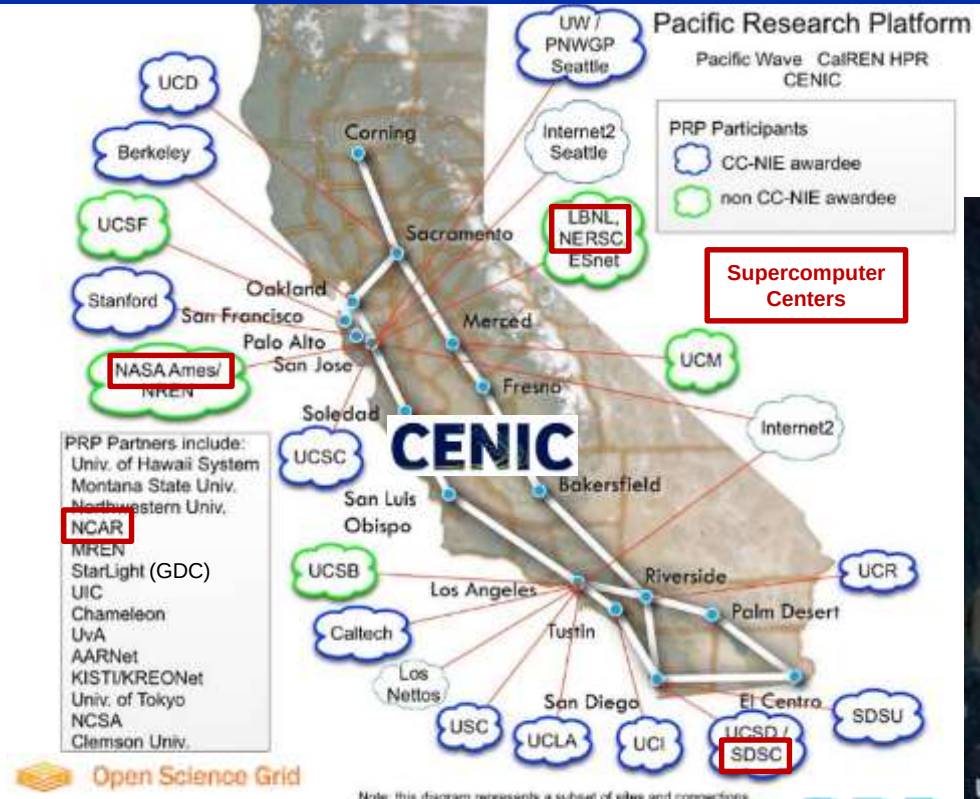
Slide Adapted From Kevin Thompson, NSF

Quartzite

Prism

PACIFIC RESEARCH PLATFORM

2015 Vision: The Pacific Research Platform Will Connect Science DMZs Creating a Regional End-to-End Science-Driven Community Cyberinfrastructure



NSF CC*DNI Grant
$6.3M 10/2015-10/2020
Extended - In Year 7 Now



Source: John Hess, CENIC

2015-2022: UCSD Designs PRP Data Transfer Nodes (DTNs) -- Flash I/O Network Appliances (FIONAs)

FIONAs Solved the Disk-to-Disk Data Transfer Problem at Near Full Speed on Best-Effort 10G, 40G and 100G

FIONA

Software Specifications

Installation Instructions

Hardware Specifications

2021 – 2020 – 2019 – 2018 – 2017 – 2016 – 2015

https://pacificresearchplatform.org/fiona/

Today's Roadrunner!



Add Up to 8 Nvidia GPUs Per 2U FIONA
To Add Machine Learning Capability
Up to 240TB Rotating Srorage

PRP PACIFIC RESEARCH PLATFORM

NSF

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

SDSC

QUALCOMM INSTITUTE

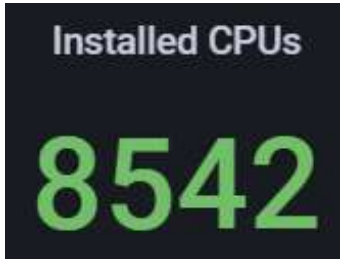
PRP's Nautilus is a Multi-Institution Hypercluster Connected by Optical Networks

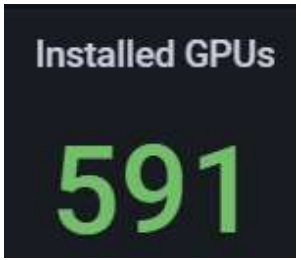
As of Sept 5, 2022

Nautilus

160 GPU & Storage FIONAs on 27 Partner Campuses Networked Together at 10-100Gbps









PRP
PACIFIC RESEARCH PLATFORM

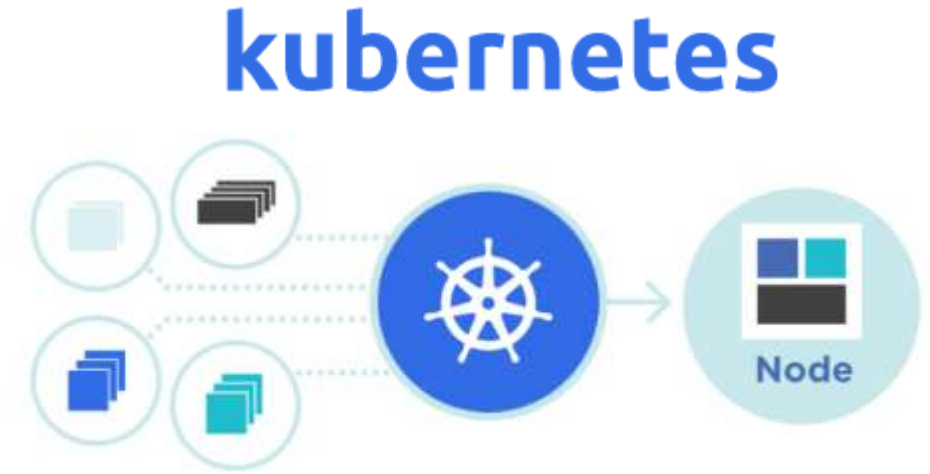
CENIC





2018/2019: PRP Game Changer!
Using Google's Kubernetes to Orchestrate Containers Across the PRP

User Applications



Containers

PRP PACIFIC RESEARCH PLATFORM

Clouds

PRP PACIFIC RESEARCH PLATFORM

CLOUD NATIVE COMPUTING FOUNDATION

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

Nautilus

kubernetes

ROOK

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



Planet Scale

Designed on the same principles that allows Google to run billions of containers a week, Kubernetes can scale without increasing your ops team.

"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

PRP
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The PRP Web Site Provides Widely-Used Open-Source Services For How to Join, Application Research, Development, and Collaboration



Nautilus documentation

Get Access

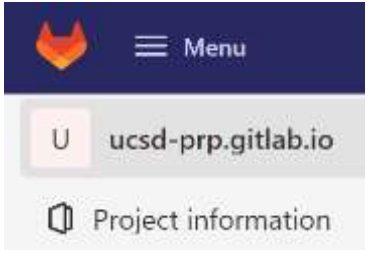
Docker and containers

Basic kubernetes

PRP PACIFIC RESEARCH PLATFORM

[matrix] Chat for Nautilus Users

JupyterLab for Nautilus





Five Major Components of Nautilus Security

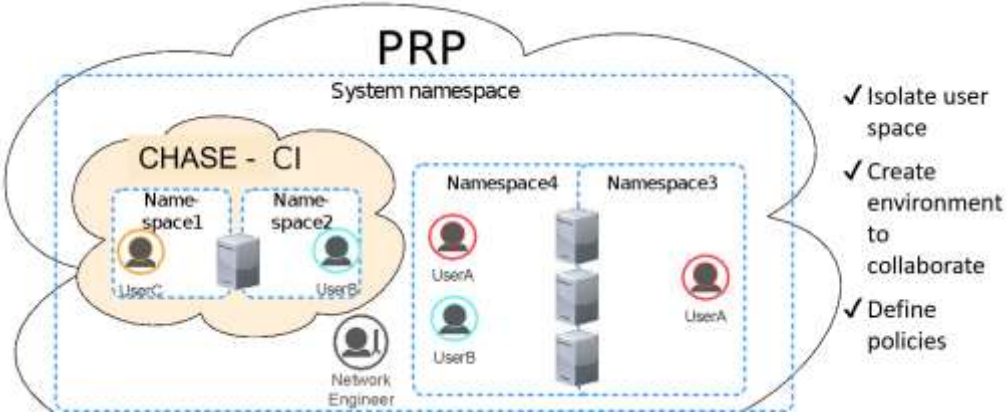
ESnet
ENERGY SCIENCES NETWORK

Science DMZ Security - Firewalls vs. Router ACLs

https://fasterdata.es.net/science-dmz/science-dmz-security/

Nautilus Uses CILogon for Federated Identity
Already Adopted by Most Campuses

CILogon



- ✓ Isolate user space
- ✓ Create environment to collaborate
- ✓ Define policies

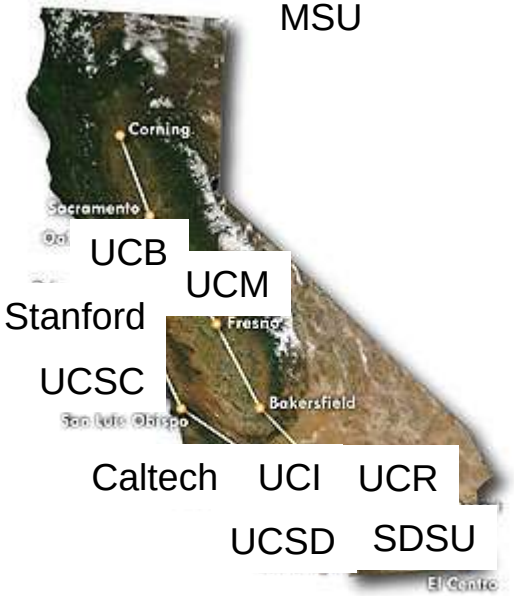
Policy-driven network security



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ElastiFlow
Network Performance and Security Analytics for Open Data Platforms

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 31, 2020

SUBMITTED – January 18, 2017

PI: Larry Smarr, Calit2, UCSD
Co-PIs:

- Tajana Rosing, CSE, UCSD
- Ken Kreutz-Delgado, ECE, UCSD
- Ilkay Altintas, SDSC, UCSD
- Tom DeFanti, QI, UCSD

NSF Has Funded Two Extensions:
CHASE-CI ABR-Smarr PI &
CHASE-CI ENS-DeFanti PI
$2.8M

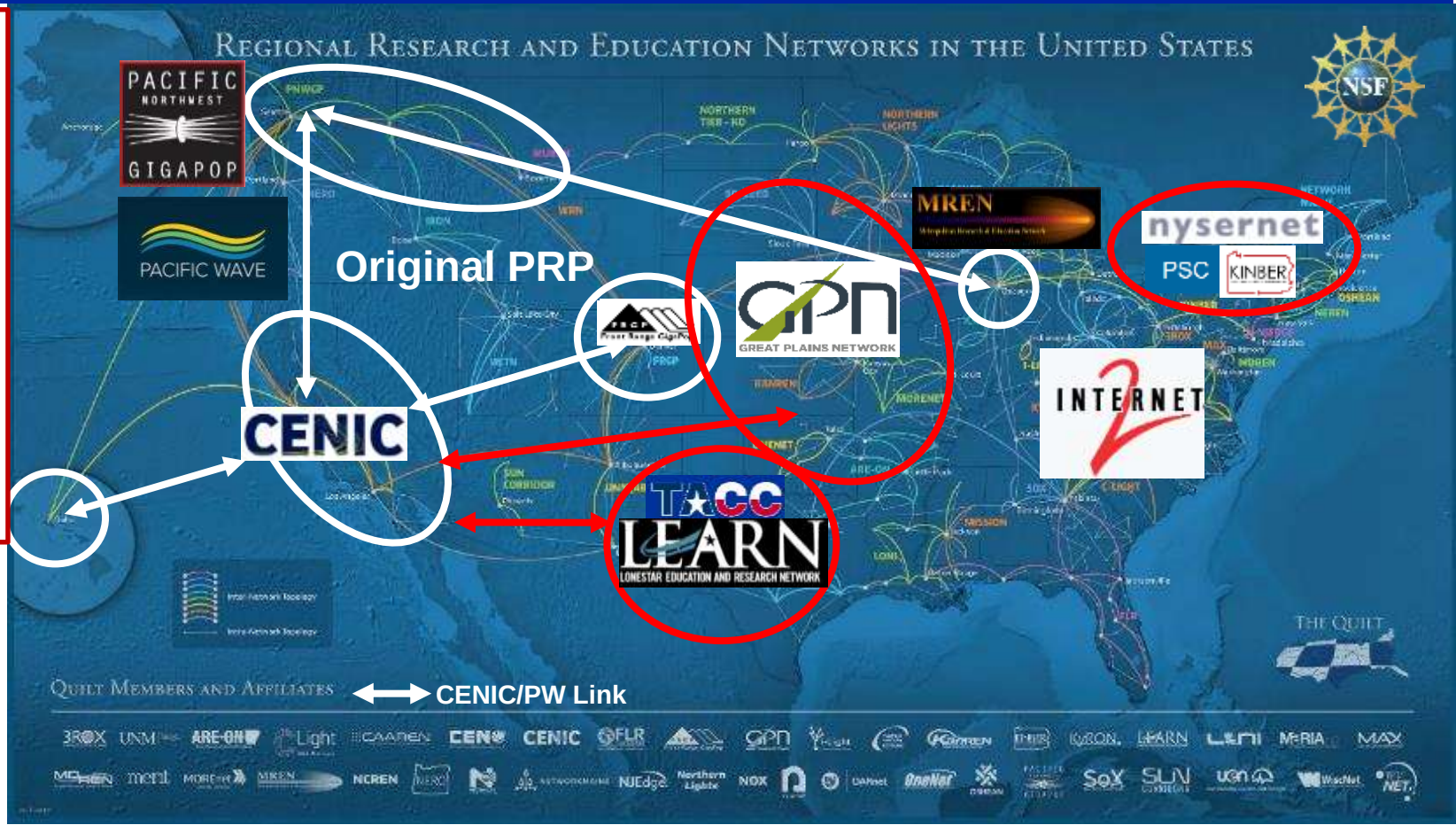
PACIFIC RESEARCH PLATFORM

JACOBS SCHOOL OF ENGINEERING
SDSC UC San Diego QUALCOMM INSTITUTE

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

"Towards The NRP"
3-Year Grant Funded by NSF
$2.5M
October 2018
Award #1826967

PI Smarr
Co-PIs Altintas
Papadopoulos
Wuerthwein
Rosing
DeFanti

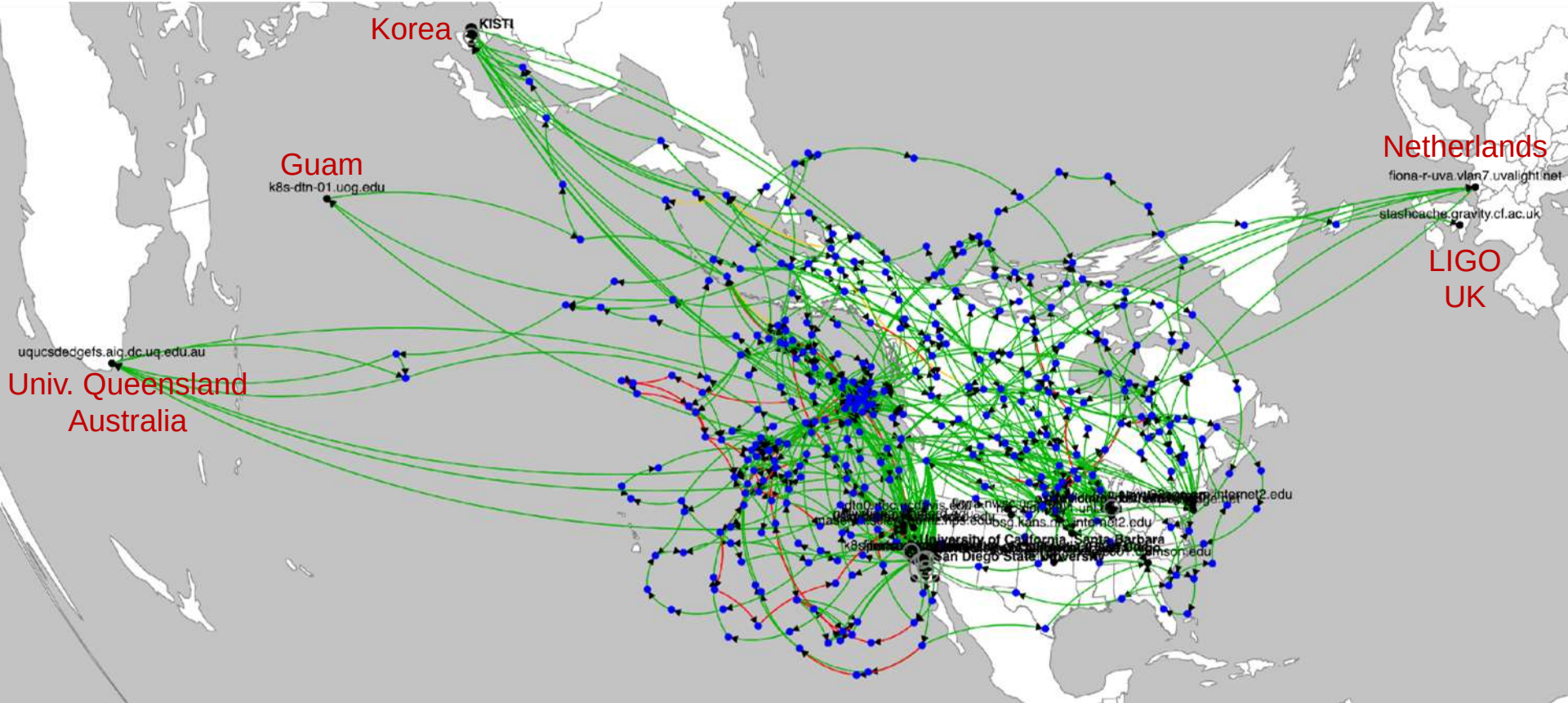


PACIFIC RESEARCH PLATFORM

Operational Metrics: Containerized Trace Route Tool Allows Realtime Visualization of Status of PRP Network Links on a National and Global Scale

9/16/2019

Source: Dima Mishin, SDSC



Some Examples of PRP Namespace GPU Usage for Earth Sciences Applications Oct 1, 2021 to June 30, 2022

- ***digits:*** Deep learning model for real-time wildland fire smoke detection
  - **UCSD [17,855 GPU-hrs]**
- ***wifire-quicfire:*** *Computation of Firemap from environmental datasets*
  - ***UCSD [15,306 GPU-hrs]***
- ***udel-ambari***: Studies on the Delaware coastal water
  - **UDel [5,736 GPU-hrs]**
- ***environmental-analytics-group-usra*:** Machine learning applied to wildfire, air quality, earthquake, floods, datasets
  - **USRA [503 GPU-hrs]**
- ***ai-os***: Train and evaluate deep learning models on MODIS and VIIRS sea surface temperature, ECCO ocean model outputs, & PODAAC sea surface height
  - **UCSC [293 GPU-hrs]**
- ***udel-erddap*:** Analysis of NOAA ERDDAP coast watch data
  - **UDel [107 GPU-hrs]**

PRP PACIFIC RESEARCH PLATFORM

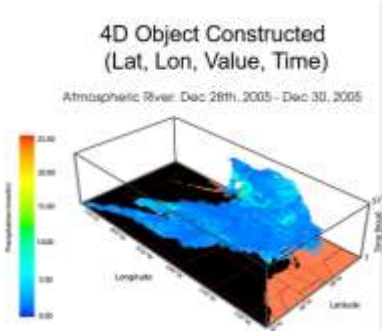
https://portal.nrp-nautilus.io/namespaces-g

Nautilus

PRP Accelerates by 532x *Atmospheric Water* Data-Intensive ML Workflow Between NASA's GES DISC MERRA V2 Archive Data Portal, UCI & UCSD









Director:
Soroosh Sorooshian



Scott Sellers, PhD CHRS; Postdoc CW3E 2016-2019

Big Data Collaboration with:



Director:
F. Martin Ralph

Complete Workflow Time:
19.2 days→52 Minutes!

PRP Namespace *connect*

See Paper by Sellars, et al., IEEE eScience (2019)
http://lsmarr.calit2.net/sellars_accelerating_image_segmentation.pdf

PRP
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PRP Portal to CASPER Open Source Tools/Libraries Developed by PRP's John Graham, UCSD

CASPER: Collaboration for Radio Astronomy Signal Processing and Electronics Research

Dan Werthimer, Matt Dexter, Jonathan Kocz, Wei Liu, David MacMahon
University of California, Berkeley; and ~1000 collaborators

Open Source Hardware, Gateware, GPUware, Software
Libraries, Tools, Reference Designs, Lab Tutorials, Videos
Astronomy, Physics, Electrical and Mechanical Engineering, Medical Research

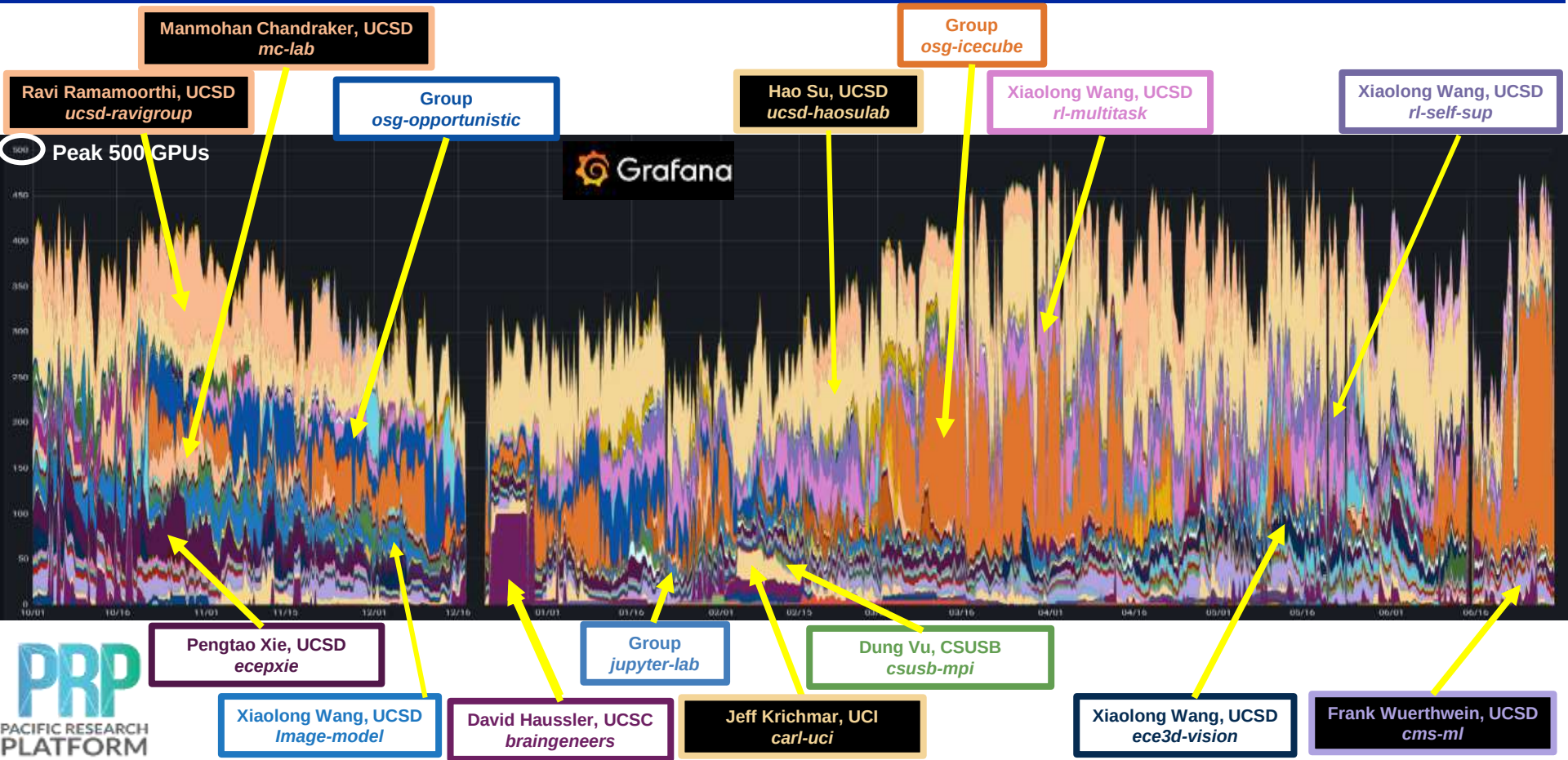


Source: Dan Werthimer, UC Berkeley

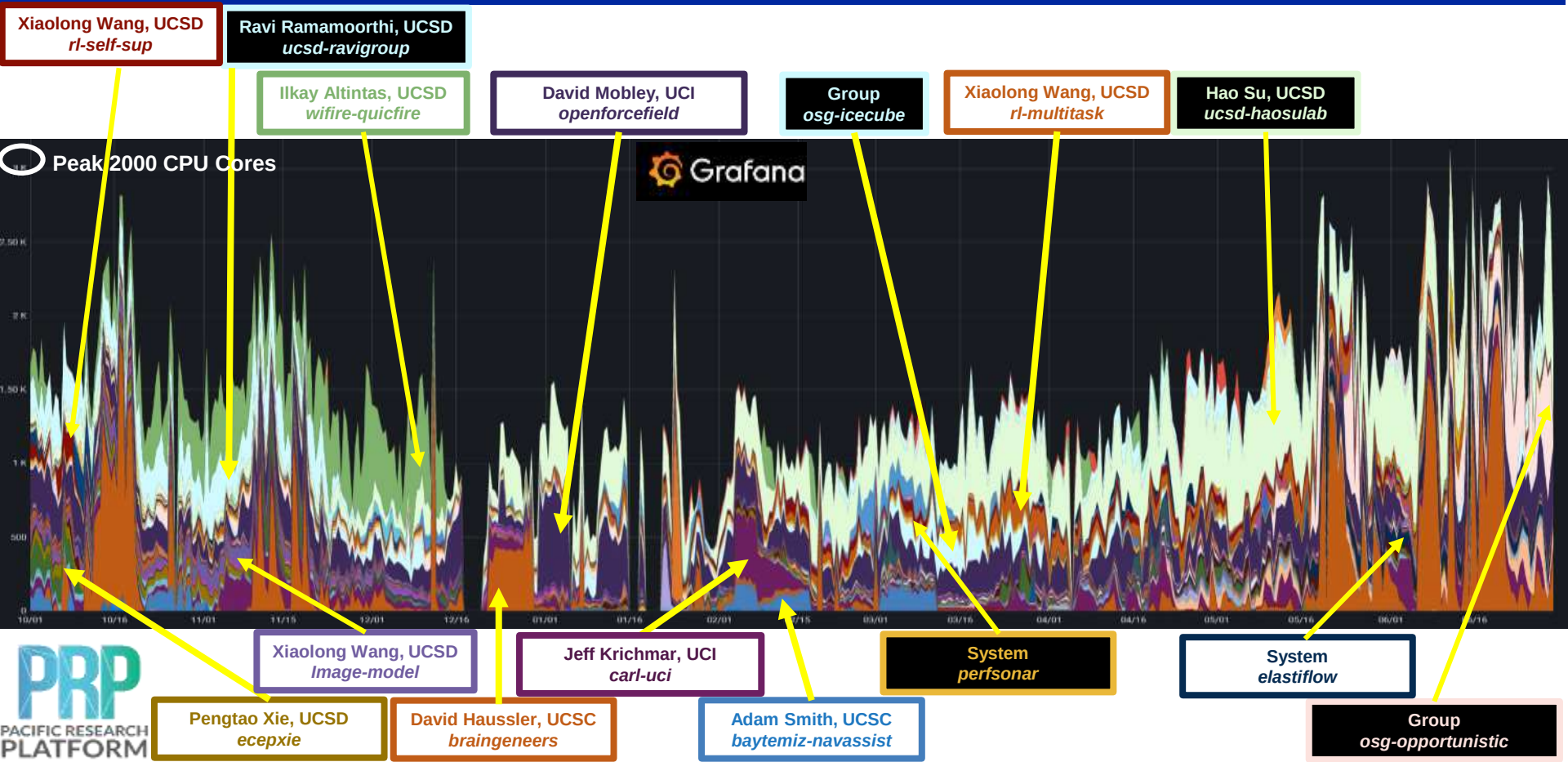
https://casper.berkeley.edu/

CASPER
The Collaboration for Astronomy Signal Processing and Electronics Research

Top 15 (Out of ~700) Nautilus Namespace GPU Users (>32 GPU-months) Oct 1, 2021 to June 30, 2022: A Mix of LHC, IceCube, ML/AI Projects



Top 15 (Out of ~700) Nautilus Namespace CPU Users (>110,000 CPU core-hrs) Oct 1, 2021 to June 30, 2022: A Mix of Wildfire, COVID, IceCube, ML/AI Projects



PACIFIC RESEARCH PLATFORM

The New Pacific Research Platform Video Highlights 3 Different Applications Out of 700 Nautilus Namespace Projects



Pacific Research Platform Video:
www.thequilt.net/campus-cyberinfrastructure-program-resource/
www.pacificresearchplatform.org

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

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

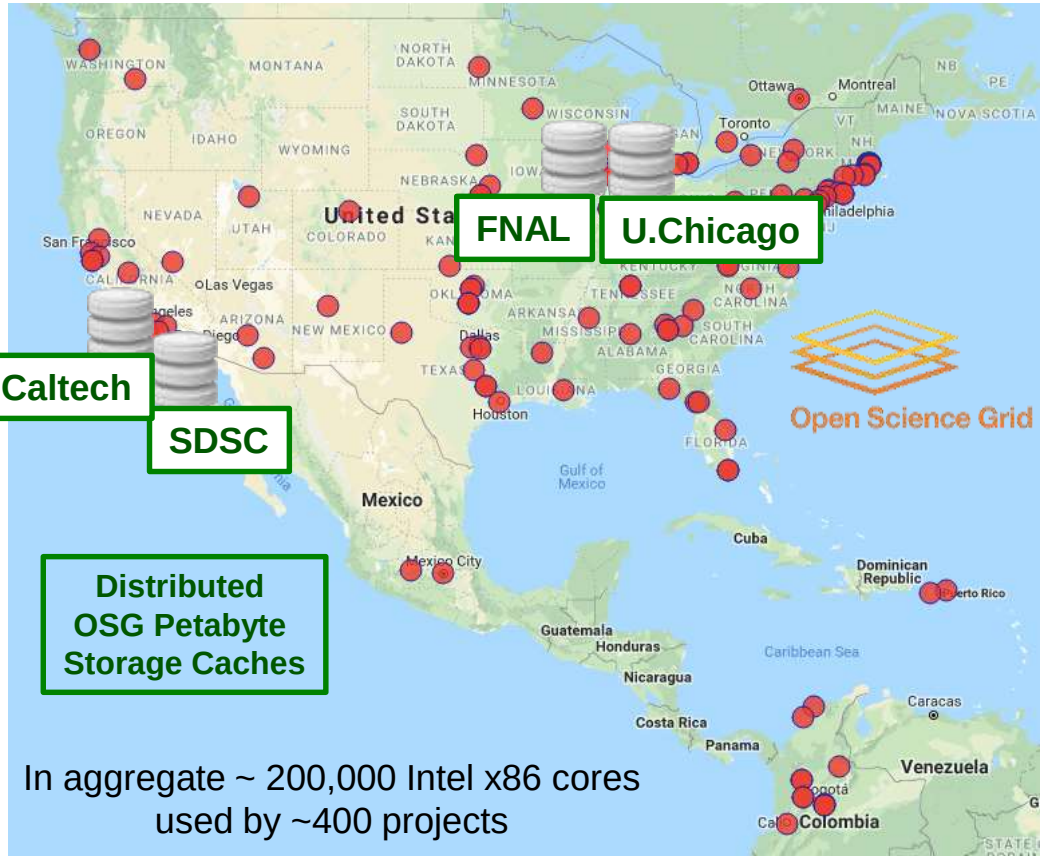
All OSG User Communities
Use HTCondor for Resource Orchestration

HTCondor
High Throughput Computing

NSF

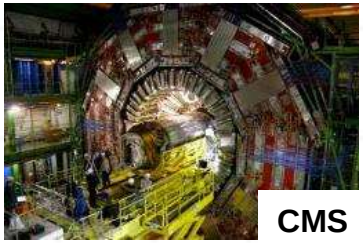
PRP
PACIFIC RESEARCH PLATFORM

OSG Federates ~100 Clusters Worldwide



The Open Science Grid Delivers to Over 50 Fields of Science
2.4 Billion Core-Hours Per Year of Distributed High Throughput Computing

NCSA Delivered ~35,000 Core-Hours Per Year in 1990



CMS



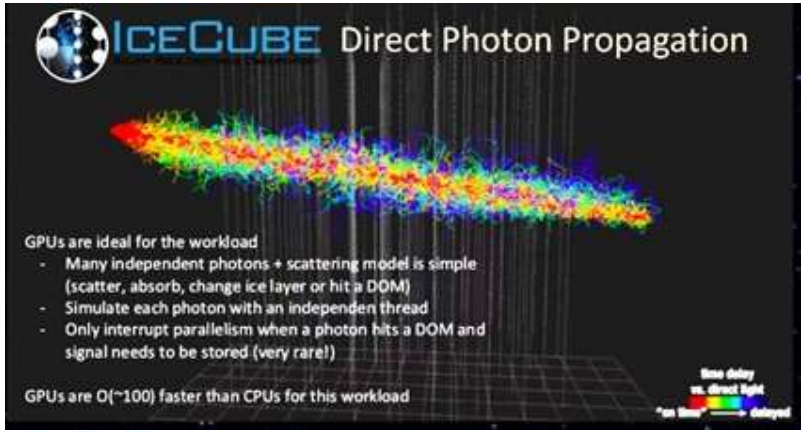
ATLAS

More Than 1 Million GPU-Hours on PRP Used via OSG Integration Within the Last 2 Years

https://gracc.opensciencegrid.org/dashboard/db/gracc-home

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 WIPAC Wisconsin IceCube Particle Astrophysics Center NSF

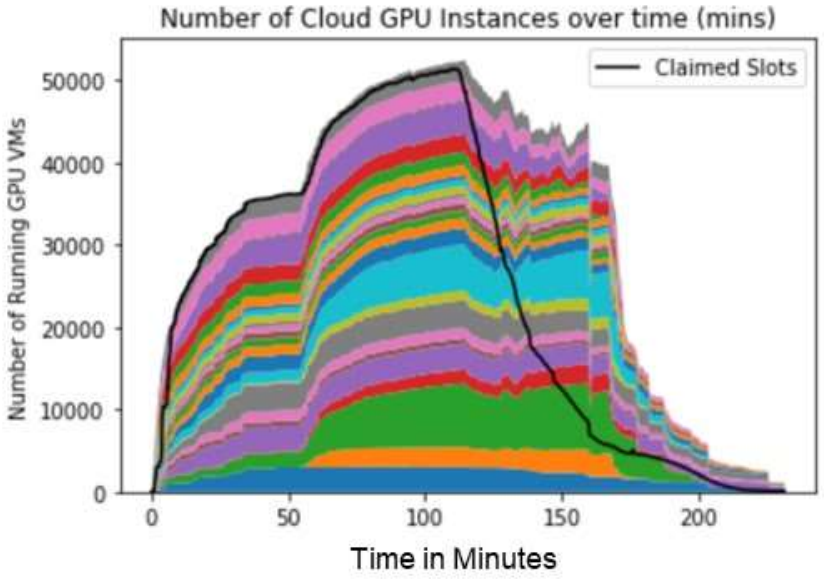
IceCube Used Up to 300 of PRP's 500 GPUs in 2021!

PRP Pacific Research Platform

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

Open Science Grid

Running a 51k GPU Burst for Multi-Messenger Astrophysics with IceCube Across All Available GPUs in AWS, Azure, and Google Clouds



Each color is a Different
Cloud Region in US, EU, or Asia.

Total of 28 Regions in Use

This Demo Used Just the Standard HTCondor Tools
8 Generations of NVIDIA GPUs Used

Peaked at 51,500 GPUs

~380 Petaflops of fp32

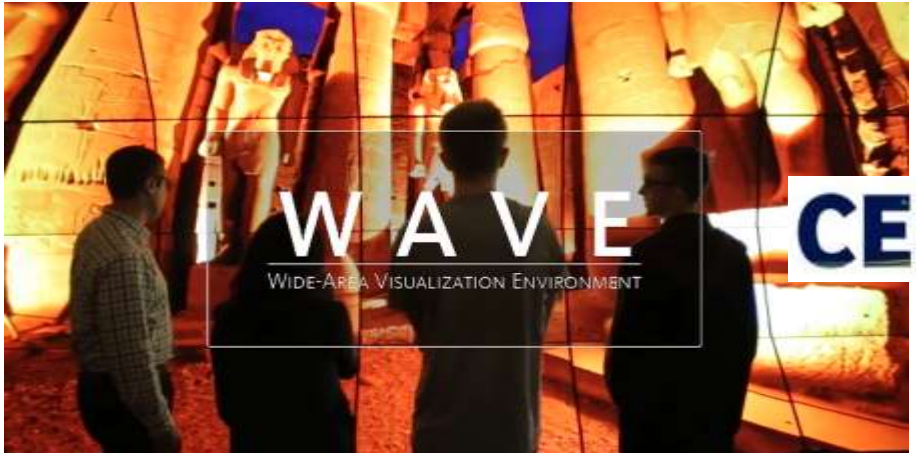
Demonstrating a Pre-Exascale, Cost-Effective Multi-Cloud Environment for Scientific Computing: Producing a fp32 ExaFLOP hour worth of IceCube simulation data in a single workday

Authors: Igor Sfiligoi, David Schultz, Benedikt Riedel, Frank Wuerthwein, Steve Barnet, Vladimir Brik
Authors Info & Claims

PEARC '20: Practice and Experience in Advanced Research Computing • July 2020 • Pages 85–90 • https://doi.org/10.1145/3311790.3396625

PACIFIC RESEARCH PLATFORM

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

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

HPWREN: 15 Years of NSF-Funded Real-Time Network Cameras and Meteorological Sensors on Top of San Diego Mountains for Environmental Observations

- **PRP Uses CENIC 100G Optical Fiber to Link UCSD, SDSU & UCI HPWREN Servers**
  - **Data Redundancy**
  - **Disaster Recovery**
  - **High Availability**
  - **Kubernetes Handles Software Containers and Data**



https://hpwren.ucsd.edu/

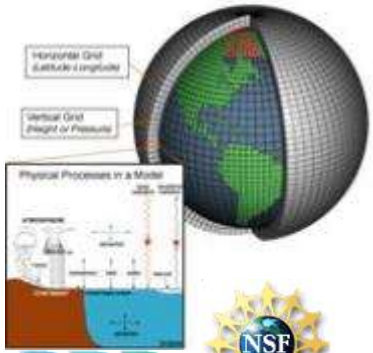
Hans Werner Braun, Frank Vernon
HPWREN PIs

NSF-Funded WIFIRE Uses PRP to Couple Wireless Edge Sensors to Supercomputers to Enable to Fire Modeling Workflows



Real-Time Meteorological Sensors

Weather Forecast

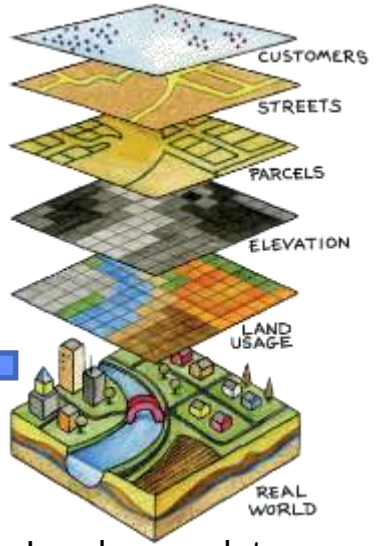




Source: Ilkay Altintas, SDSC

WIFIRE

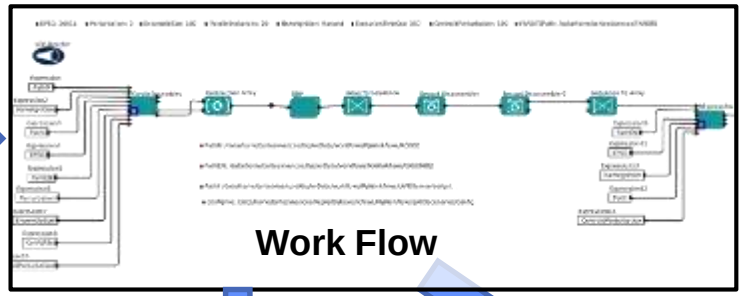




Landscape data

PRP







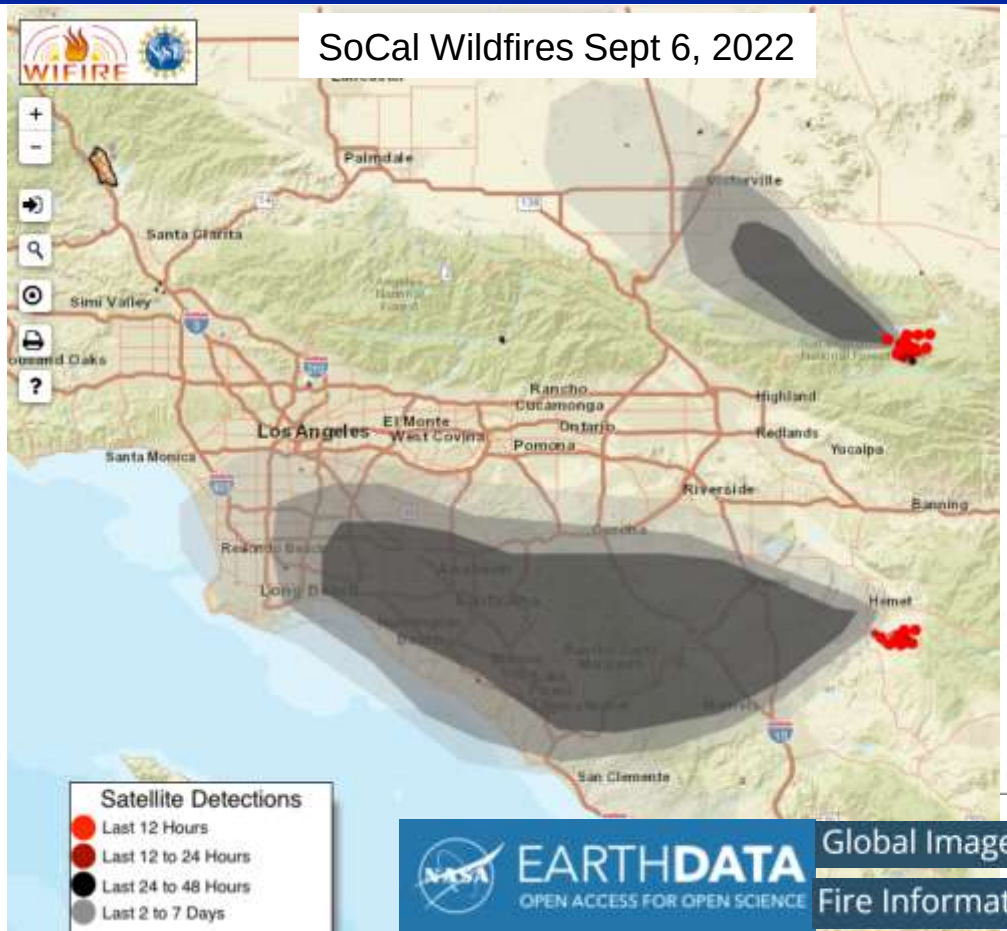


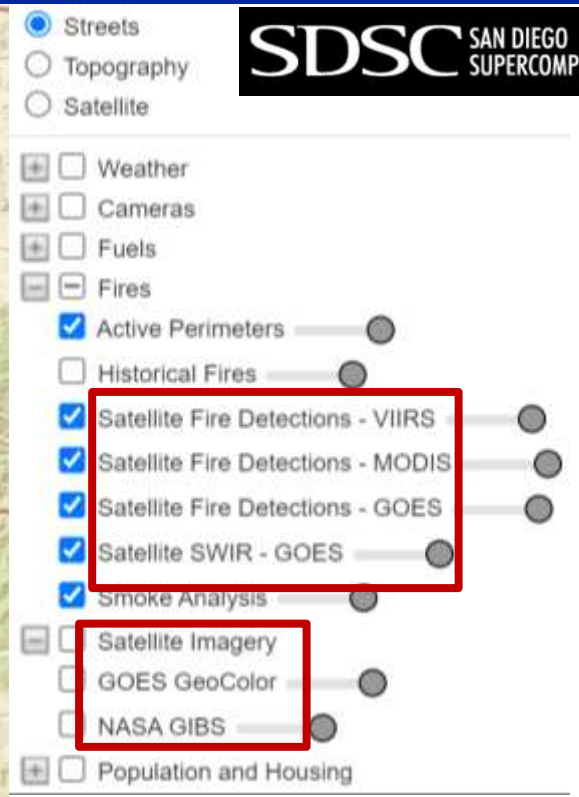


NSF

PRP
PACIFIC RESEARCH PLATFORM

WIFIRE's Firemap Provides Public Website Combining Satellite Fire Detections with GIS





SDSC SAN DIEGO SUPERCOMPUTER CENTER

PRP PACIFIC RESEARCH PLATFORM

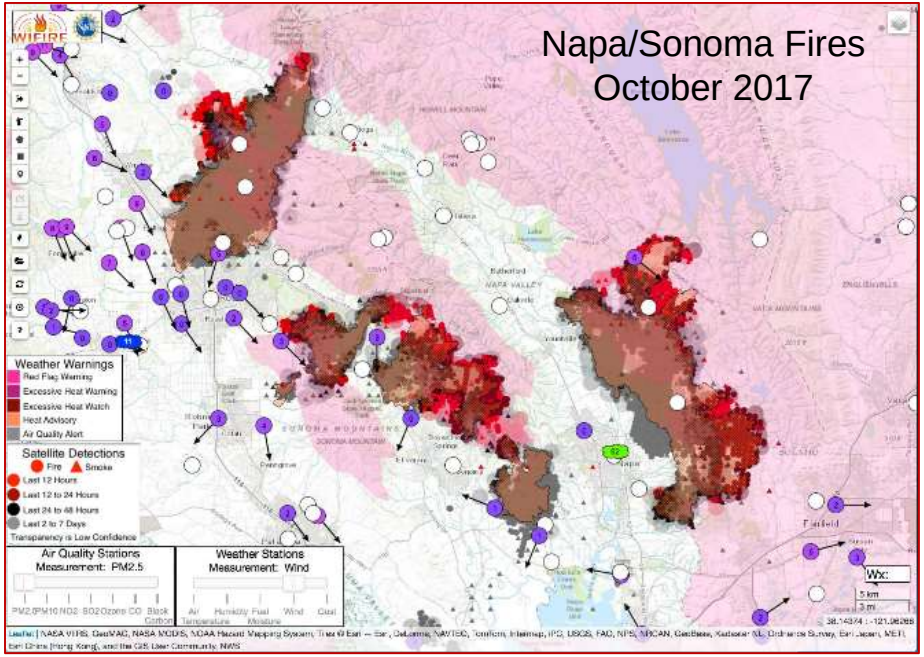
EARTHDATA OPEN ACCESS FOR OPEN SCIENCE

Global Imagery Browse Services (GIBS)

Fire Information for Resource Management System (FIRMS)

WIFIRE's Firemap Was Heavily Used by Public For California Wildfires October 2017 through December 2017

800K+ unique visitors and 8M+ hits





PACIFIC RESEARCH PLATFORM

http://firemap.sdsc.edu

WIFIRE

NSF

SDSC SAN DIEGO SUPERCOMPUTER CENTER

PRP is Building on NSF-Funded SAGE Technology to Bring ML/AI to the Edge For Smoke Plume Detection

Source: Ilkay Altinas, SDSC, HDSI



Training Data: Archive of
25,000 Labeled Wireless Camera Images
of Wildland Fires

FlgLib & SmokeyNet: Dataset and Deep Learning Model for Real-Time Wildland Fire Smoke Detection

by Anshuman Dewangan [1], Yash Pande [1], Hans-Werner Braun [2], Frank Vernon [3], Ismael Perez [2], Ilkay Altintas [2], Garrison W. Cottrell [1] and Mai H. Nguyen [2,*]

www.mdpi.com/2072-4292/14/4/1007

PRP namespace *digits*

PRP PACIFIC RESEARCH PLATFORM

Nautilus SDSC HPWREN EXPANSE ALERT Wildfire



Sage

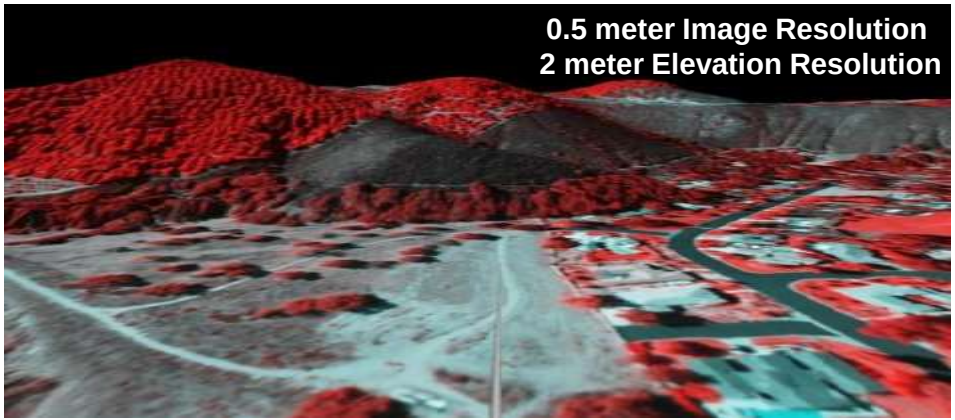
Building atop standard community software:

TensorFlow TensorRT PYTORCH TensorFlow Lite OpenCV

docker NVIDIA CUDA K3S ROS

Source: Charlie Catlett, Pete Beckman, Argonne National Lab

Interactive Virtual Reality Viewing of San Diego County "Digital Twin" Includes Live Feeds From 200 Meteorological Stations





Chief Porter was appointed Director, California Department of Forestry and Fire Protection by Governor Gavin Newsom on January 8, 2019



PACIFIC RESEARCH PLATFORM

Source: Jessica Block, Calit2

Community Building
Through Large-Scale Workshops









PRP
PACIFIC RESEARCH PLATFORM

2GRP Workshop
September 20-24, 2021

3GRP Workshop
October 10-11, 2022

4NRP Workshop
February 8-10, 2023

Community Building Though Inclusion and Diversity

- **Grants**
  - 3 Female co-PIs
  - 1 Hispanic co-PI
- **Campuses**
  - 16 Minority-Serving Institutions (MSIs) Using PRP
  - 20 EPSCoR States Have Campuses Using PRP
- **Workshops**
  - NRP2 Workshop Steering Committee 80% Female
  - Multiple MSI, EPSCoR Focused Workshops















2NRP Montana State University MSI Workshop

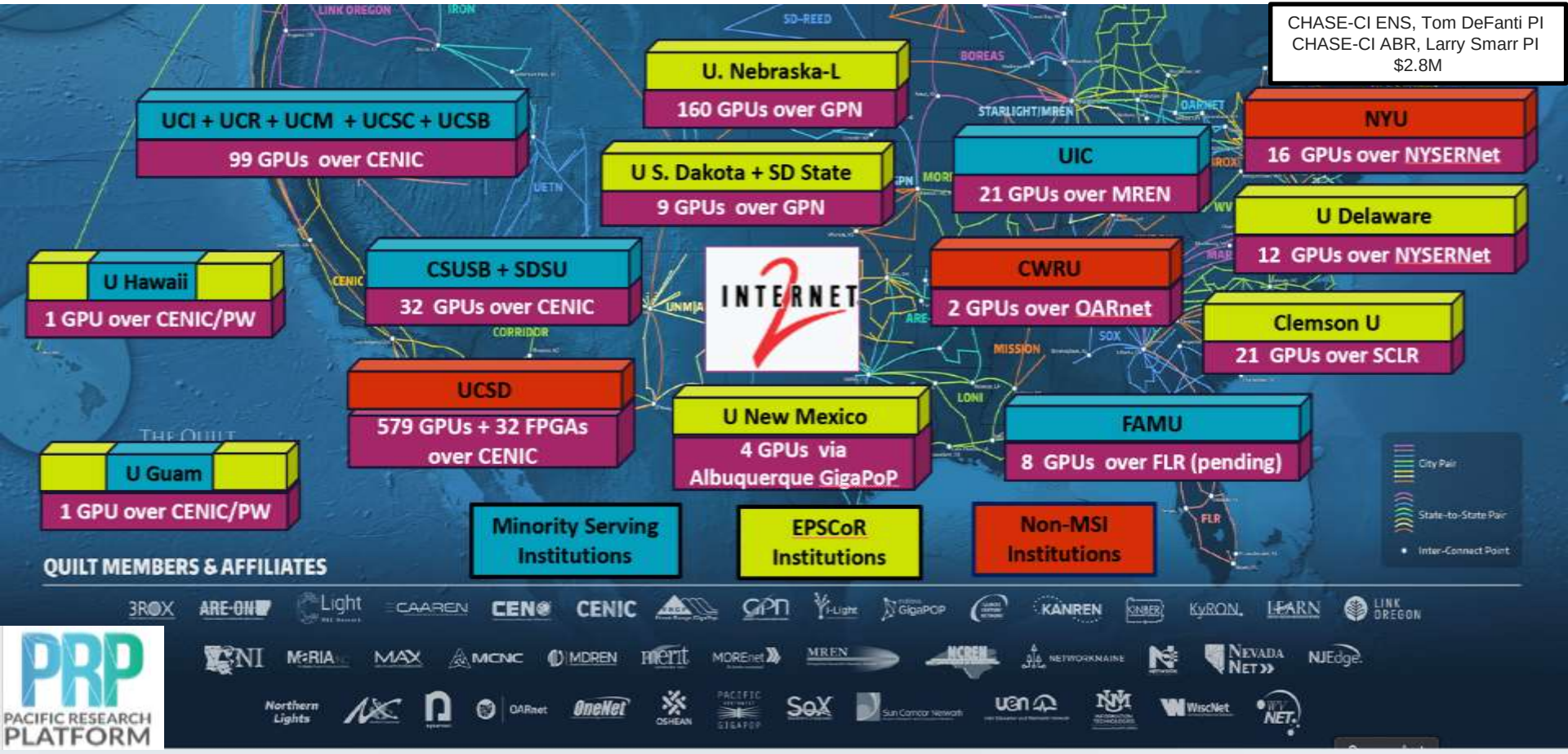
Presenting FIONettes

PRP PACIFIC RESEARCH PLATFORM

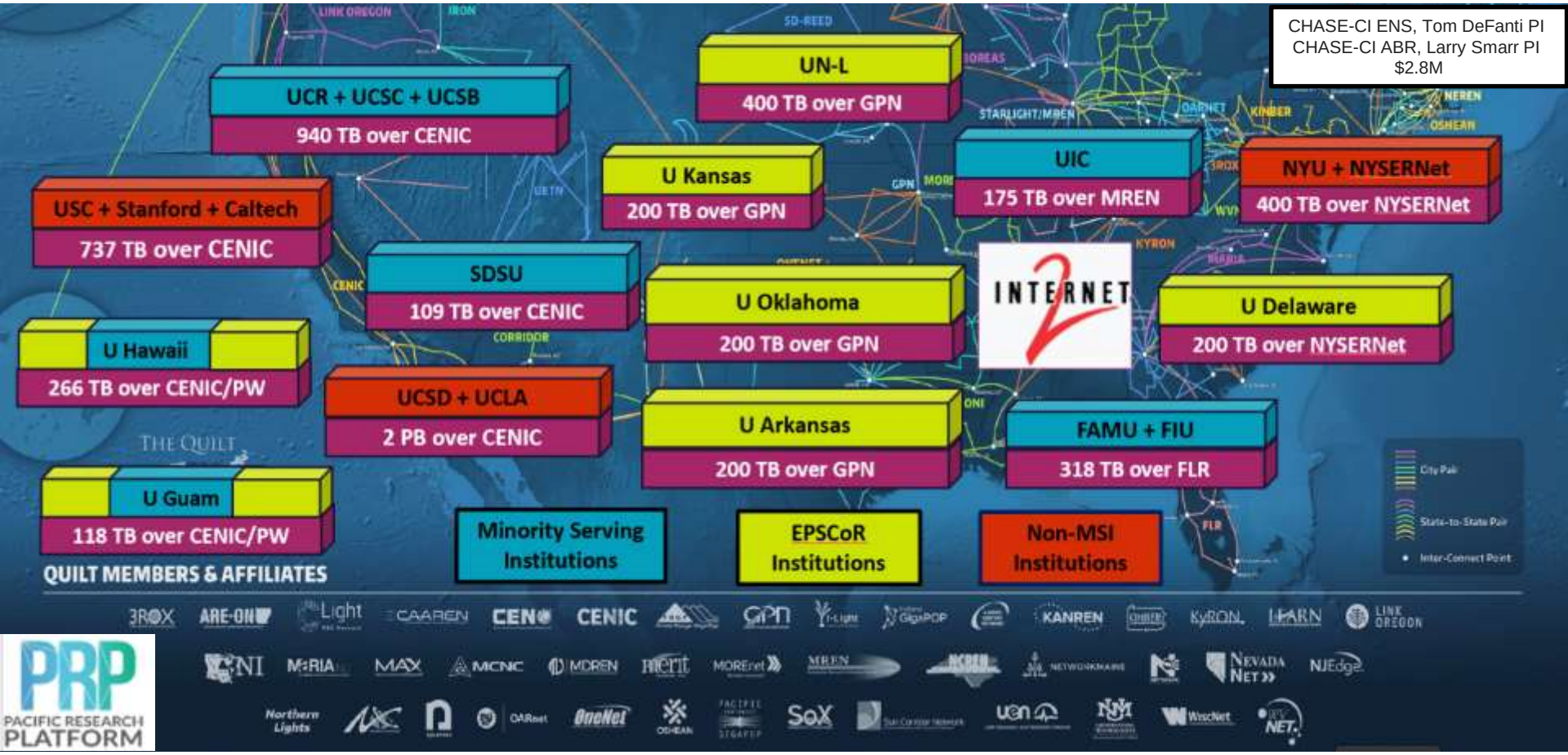
The Next Four Phases
Of the Creation of a National Research Platform

PACIFIC RESEARCH PLATFORM

2021-2024 NRP Future I: Funded Extension of Nautilus
1000 GPUs and ~10,000 CPU Cores Distributed over Networks—2022



2021-2024 NRP Future I: Funded Extension of Nautilus
~6 PB Nautilus Ceph Storage Over Networks—2022



2021-2026 NRP Future II: PRP Federates with SDSC's EXPANSE Using CHASE-CI Developed Composable Systems

EXPANSE

COMPUTING WITHOUT BOUNDARIES
5 PETAFLOP/S HPC and DATA RESOURCE

SDSC

XSEDE

HPC RESOURCE
13 Scalable Compute Units
728 Standard Compute Nodes
52 GPU Nodes: 208 GPUs
4 Large Memory Nodes

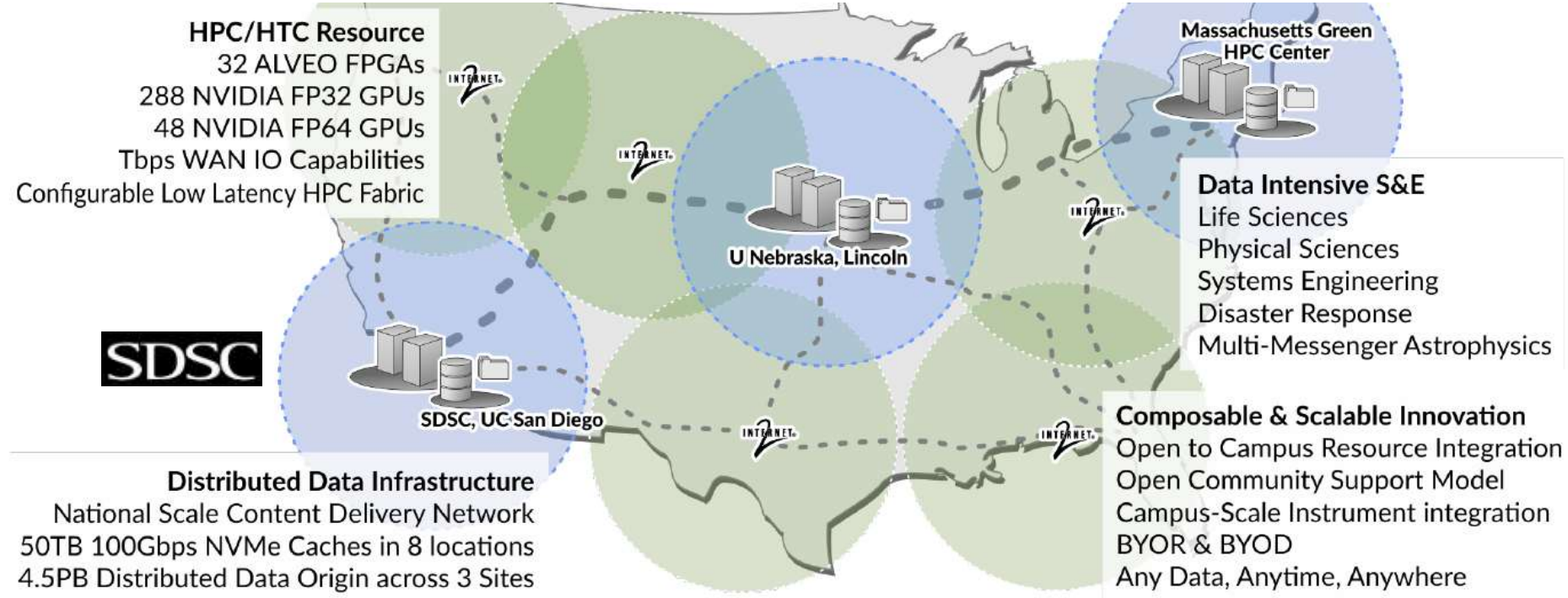
DATA CENTRIC ARCHITECTURE
12PB Perf. Storage: 140GB/s, 200k IOPS
Fast I/O Node-Local NVMe Storage
7PB Ceph Object Storage
High-Performance R&E Networking



LONG-TAIL SCIENCE
Multi-Messenger Astronomy
Genomics
Earth Science
Social Science

INNOVATIVE OPERATIONS
Composable Systems
High-Throughput Computing
Science Gateways
Interactive Computing
Containerized Computing
Cloud Bursting

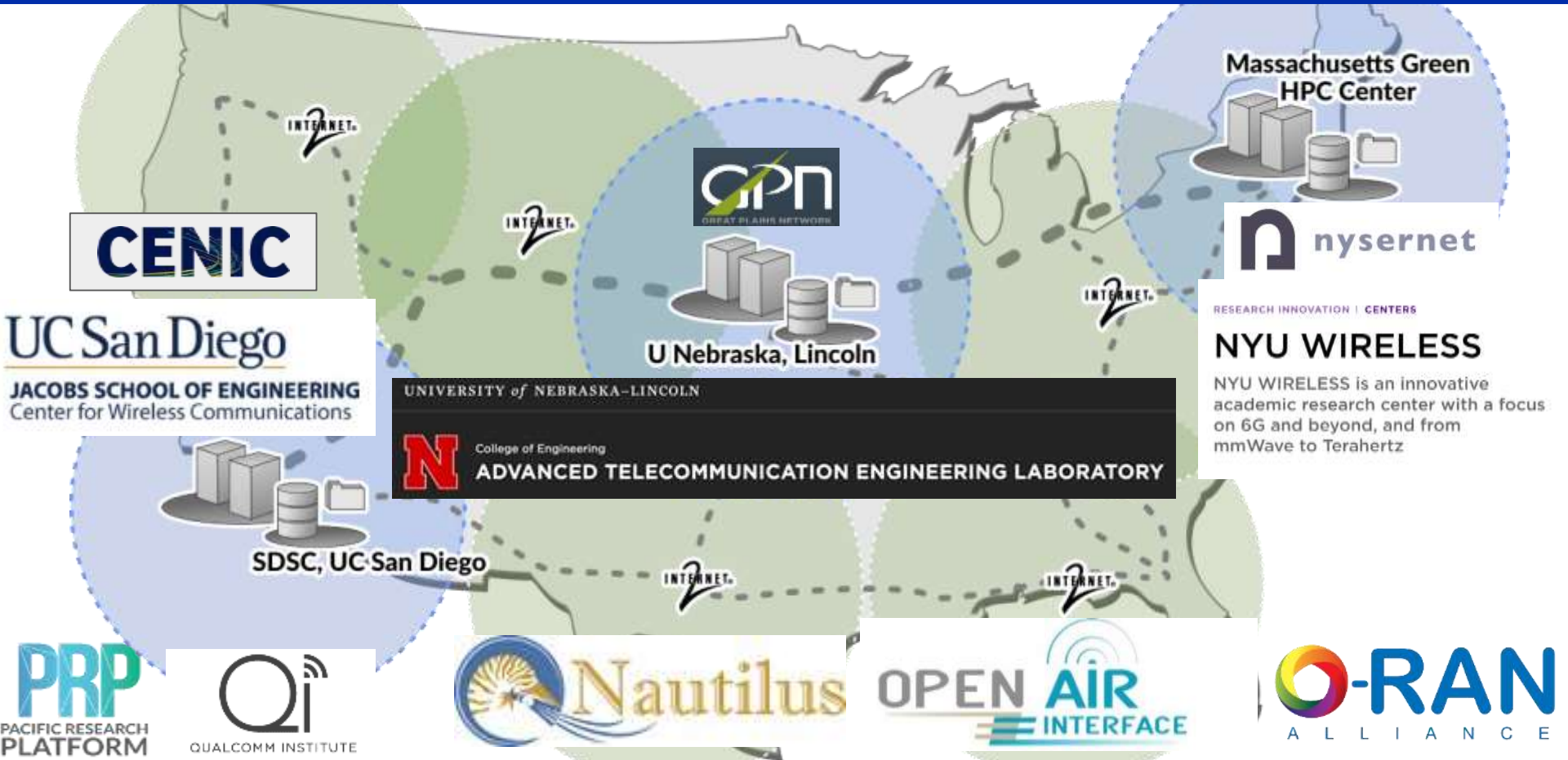
2021-2026 NRP Future III: PRP Federates with NSF-Funded *Prototype National Research Platform*



PRP PACIFIC RESEARCH PLATFORM

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)

2022-2027: NRP Future IV – Open Wireless 5G/6G End-to-End National-Scale Optical Fiber / "Future Wireless" Testbed



NASA Open Science Program with PRP Team Guidance Could:

- Present a Talk at UCSD Feb 2023 4NRP Conference on NASA Open Science
- Set up a PRP ML-Enabled Workflow for Selected Earth Satellite Datasets
  - Build on Scott Sellars Experience with MERRA V2
- Develop Jupiter PRP-Enabled Notebooks for NASA Open Science Algorithms
  - Use Existing JupyterLab Namespace to Get Started
- Create a PRP Gateway to NASA Open Science Software Tools
  - Build on John Graham CASPER Gateway
- Chose a NASA HEC System and Federate with PRP/NRP
  - Build on PRP/Expanse Federation Experience
- Identify Current NASA Researchers Using OSG CPUs for Data Analysis
  - Extend to PRP GPUs and FPGAs for ML/AI Analysis
- Join Forces with PRP on Selected MSI Campuses
  - Build on 15 Years of Calit2/SDSC & PRP Experience

PRP
PACIFIC RESEARCH PLATFORM

PRP's Support and Community:



- National Science Foundation (NSF) awards to UCSD:
  - CNS (1456638, 1730158, 2120019, 2100237), ACI (1540112, 1541349), OAC(1826967, 2112167)
- Department of Defense DURIP to UCSD
- UCSD: Calit2 & its Qualcomm Institute; and UCSD's Research IT and Instructional IT
- UCB CITRIS and the Banatao Institute
- UC Office of the President
- Partner Campuses: UCB, UCSC, UCI, UCR, UCLA, UCD, UCM, UCSB, USC, Caltech, Stanford, NU, UWash, UChicago, UIC, UHM, UWM, IU, NPS, CSUSB, CSUS, SDSU, SJSU, UMC, UMo, UArk, MSU, NYU, UNL, UNM, SDakSU, Uok, UNC, UTA, WSU, FAMU, FIU, Clemson, UDel, UGuam, JCU, KISTI, UVA, AIST, NTU, UQ, UTokyo
- Computing Partners: San Diego Supercomputer Center, LBNL/NERSC, NCAR/UCAR & Wyoming Supercomputing Center, NASA NAS/USRA, Texas Advanced Computing Center, MGHPCC, NSCC, Open Science Grid, Chameleon Cloud, SLATE, AWS, Google Cloud, Microsoft, Cisco, Juniper, Arista
- Network Partners: CENIC, Pacific Wave/PNWGP, FRGP, StarLight/MREN, HPWREN, The Quilt, Great Plains Network, KINBER, LEARN, NYSERNet, OARnet, FLR, Internet2, DOE Esnet, AMPATH, AARNet, CESnet, KREOnet, PIREN, SURFnet, SCLR, SingAREN

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