“NRP Application Drivers”

Presentation
4th National Research Platform (4NRP) Workshop
February 9, 2023

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

Nautilus

2023: NRP's Nautilus is a Multi-Institution National to Global Scale Hypercluster Connected by Optical Networks

Nautilus

Feb 9, 2023

~200 FIONAs on 25 Partner Campuses Networked Together at 10-100Gbps

NSF

Installed GPUs	Installed CPUs	Rotating Storage
1324	19302	4000 TB

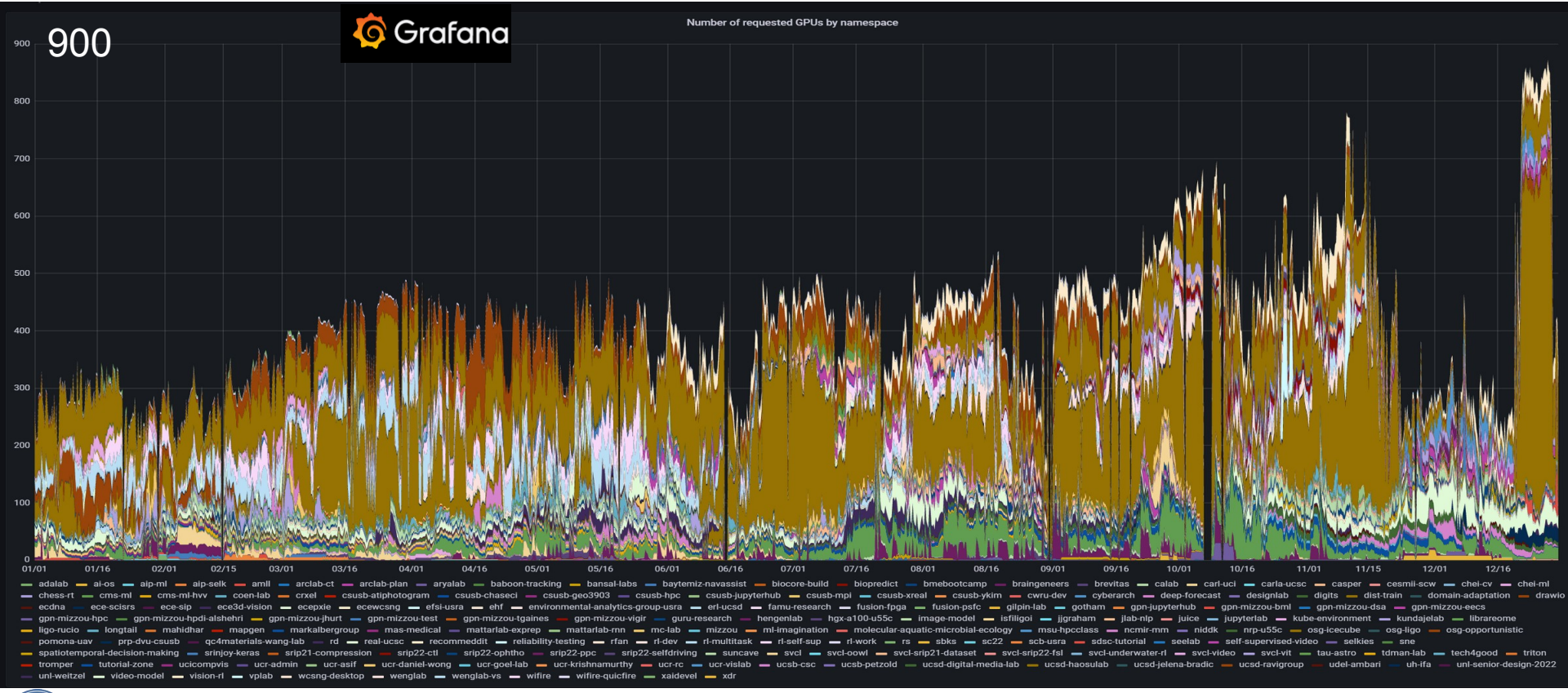
CENIC

THE QUILT

INTERNET 2

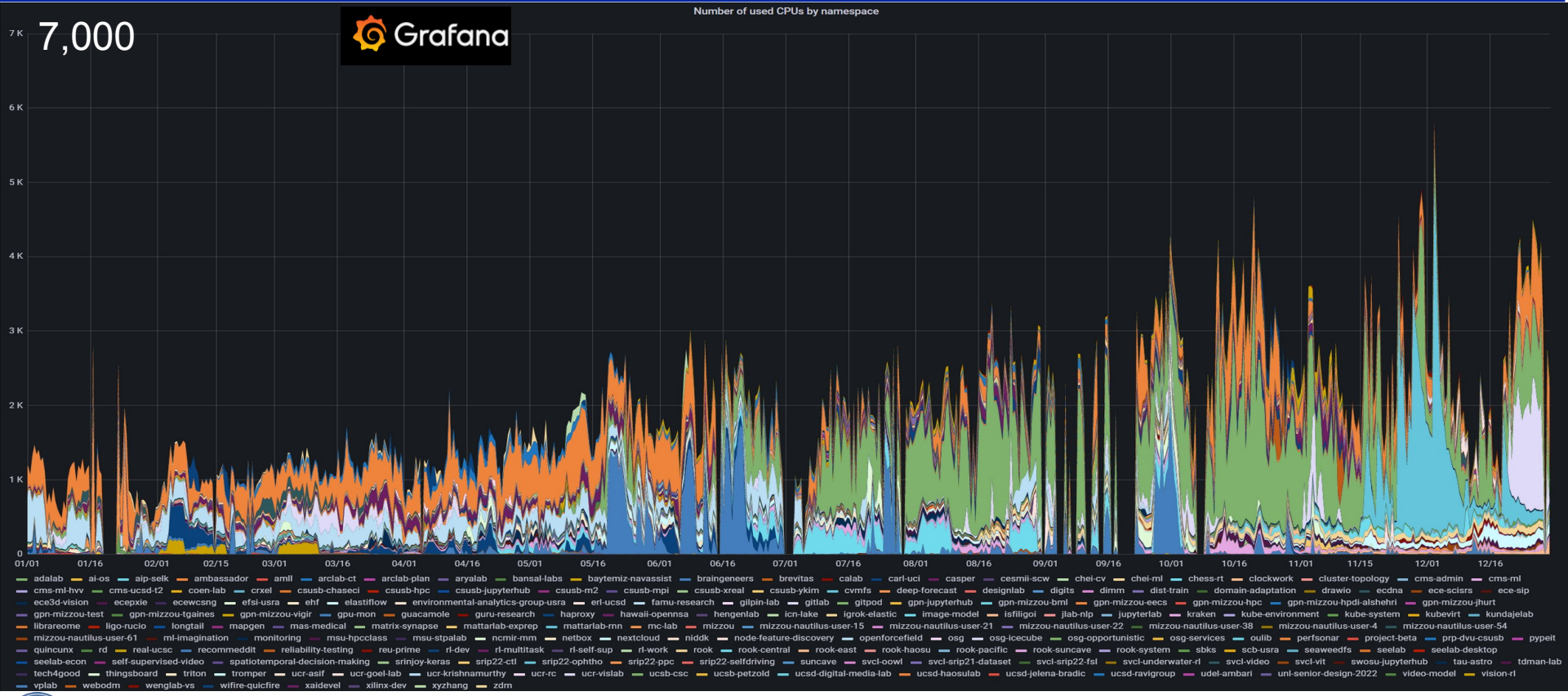
Nautilus

Grafana Graphs Nautilus Namespaces Usage Calendar 2022 GPUs



Nautilus

Grafana Graphs Nautilus Namespaces Usage
Calendar 2022 CPU Cores

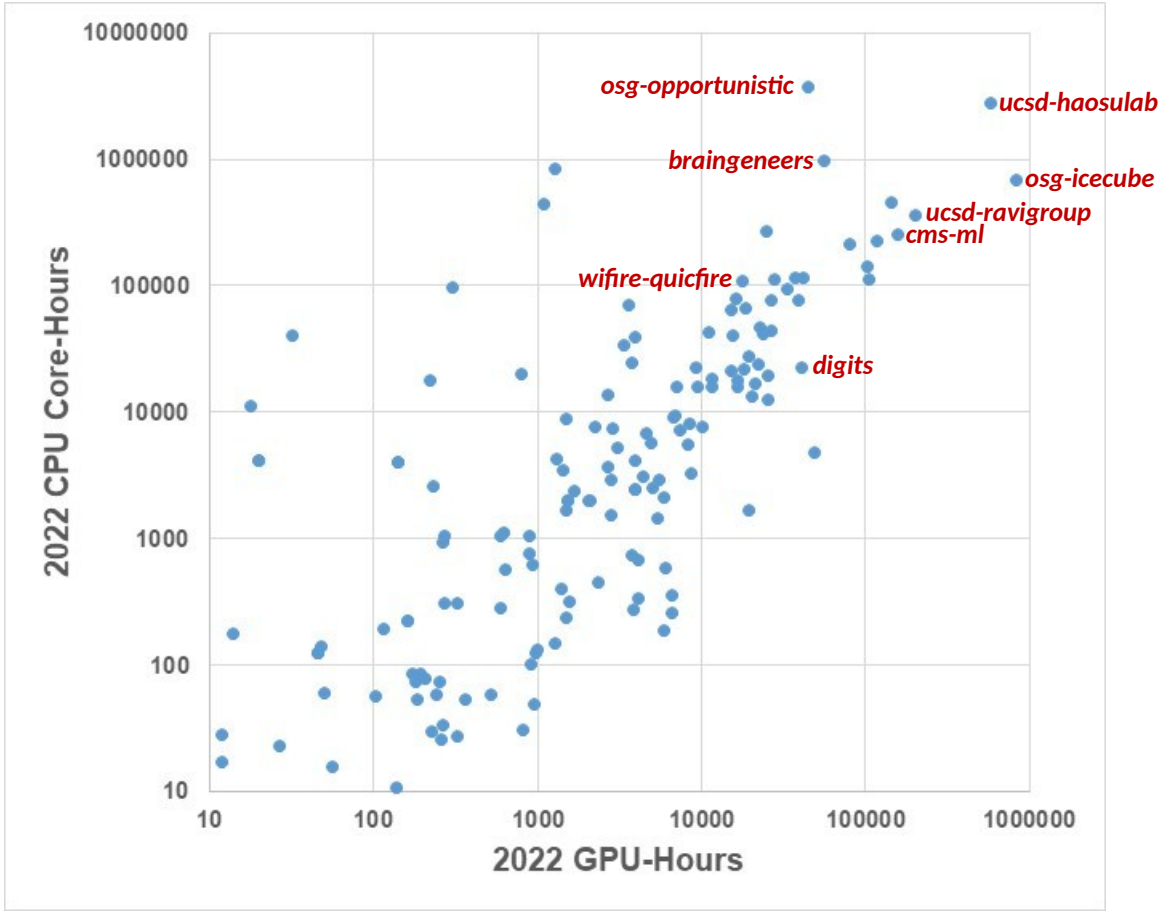


Nautilus

2022 Nautilus Namespace Users:
Largest User is One Million Times Smallest!

Nautilus Namespaces
Using >10 GPU-hrs/year
Or >10 CPU-hrs/year

I Will Look in Detail at the
Namespaces in Red



Nautilus

The New Pacific Research Platform Video Highlights 3 Different Applications Out of 800 Nautilus Namespace Projects



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

Nautilus

CITRIS BANATAO INSTITUTE

2015 PRP Grant Was Science-Driven: Connecting Multi-Campus Application Teams and Devices



Particle Physics

Biomedical 'omics

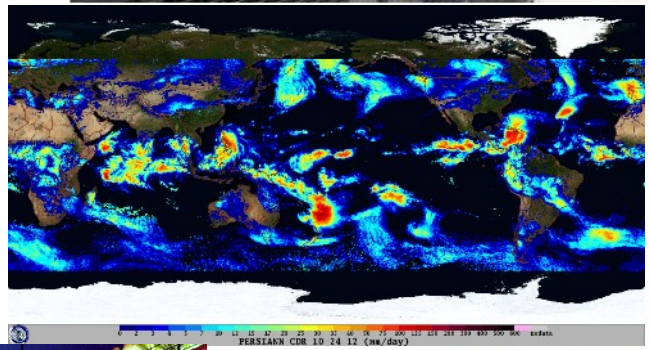


NSF



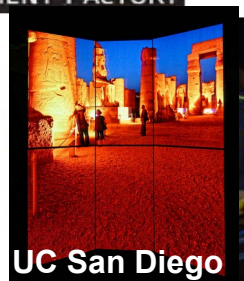
Telescope Surveys

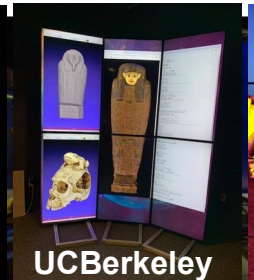
Earth Sciences

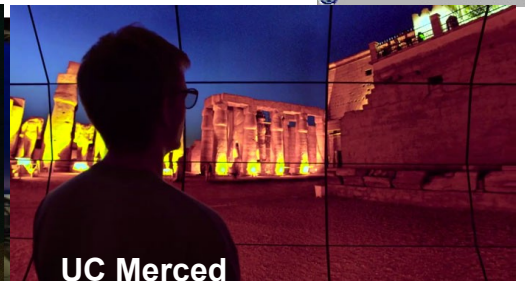


Visualization, Virtual Reality, Collaboration

PRP
PACIFIC RESEARCH PLATFORM







What Are The Largest 2022 PRP Users in Each Area?

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

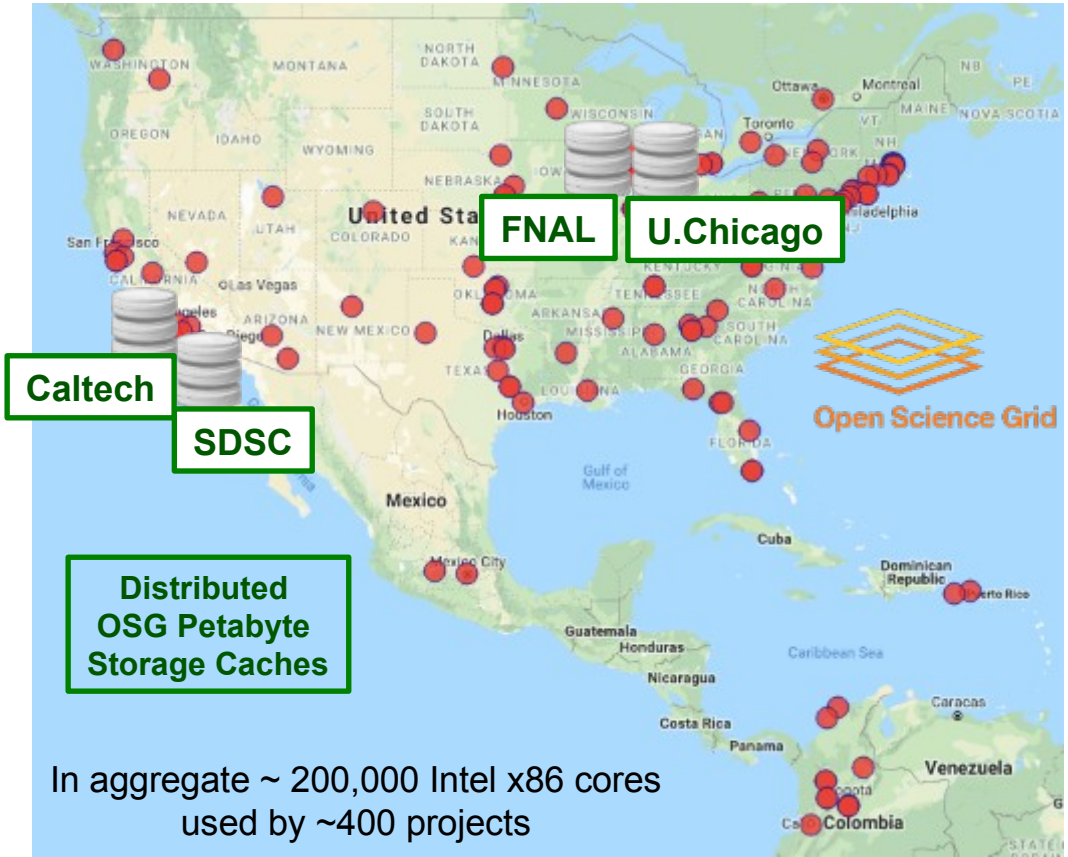
Source: Frank Würthwein,
OSG Exec Director; PRP co-PI; UCSD/SDSC

All OSG User Communities Use HTCondor for Resource Orchestration

HTCondor
High Throughput Computing

NSF

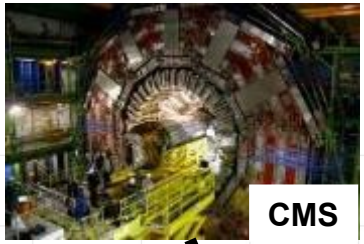
OSG Federates ~100 Clusters Worldwide



Nautilus

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

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





HTCondor Software Suite

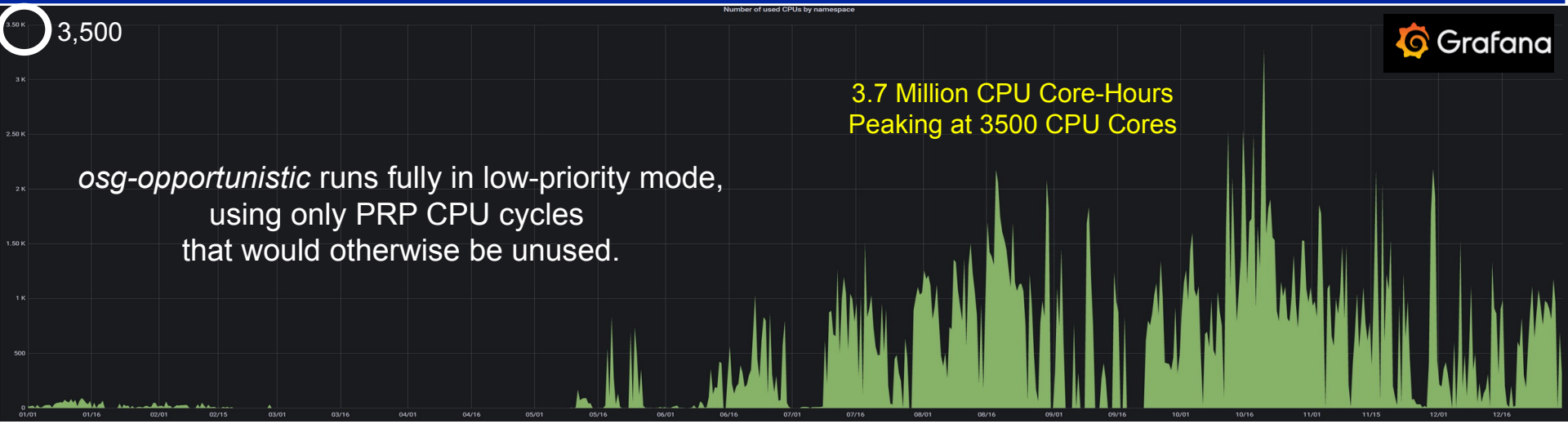
OSG

PRP's Nautilus Appears as Just Another OSG Resource

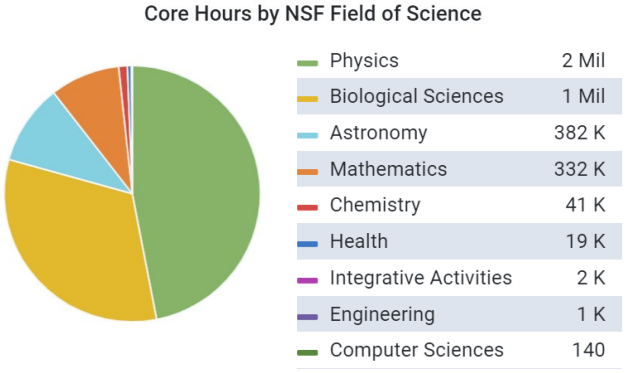
Nautilus

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

Nautilus Namespace *osg-opportunistic* Supported a Wide Set of Applications As the Largest Consumer of CPU Core-Hours in 2022



Source: Igor Sfiligoi, SDSC



OSG

Nautilus

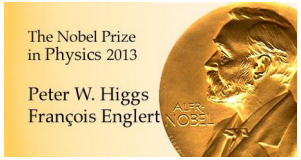
Particle Physics

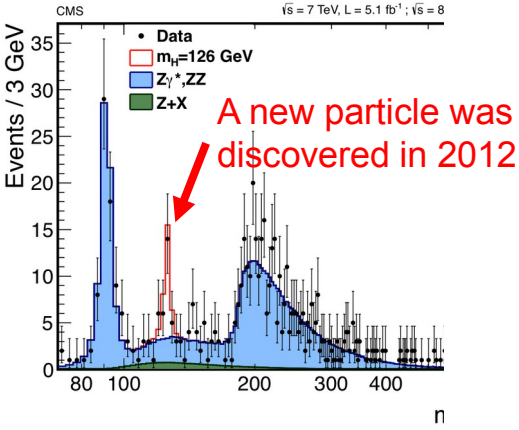


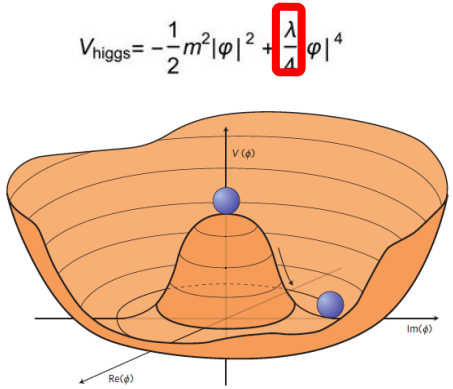


Nautilus

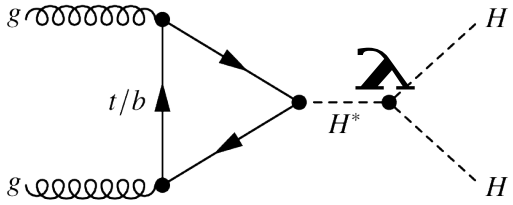
Bringing Machine Learning to Particle Physics







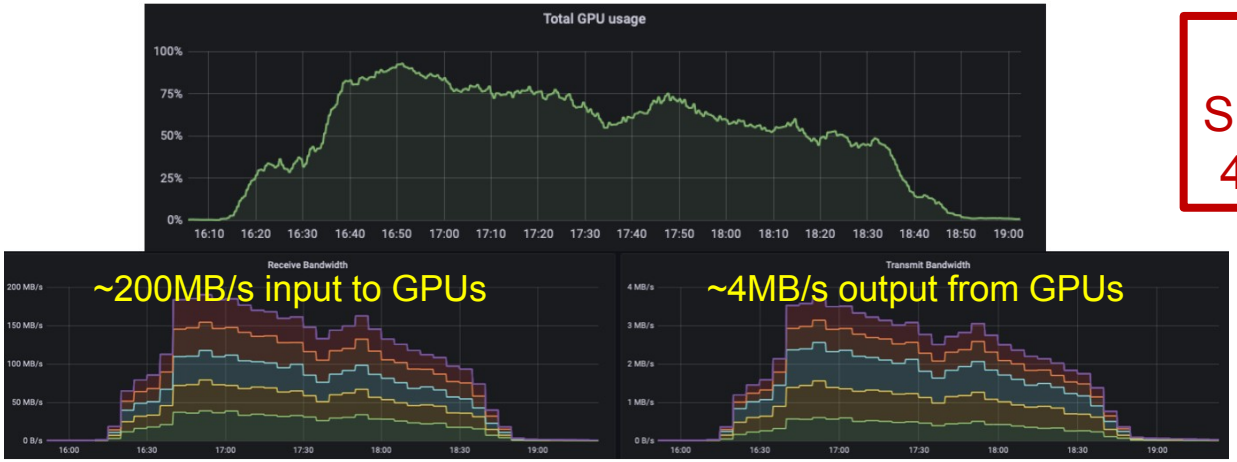
The “holy grail” of the LHC program today is measurement of di-higgs production **to infer the hhh coupling that determines the higgs potential**



Source: Frank Wuerthwein, SDSC

Nautilus

ML Inference as a Service on NRP



See Talk by Shih-Chieh Hsu 4NRP Friday

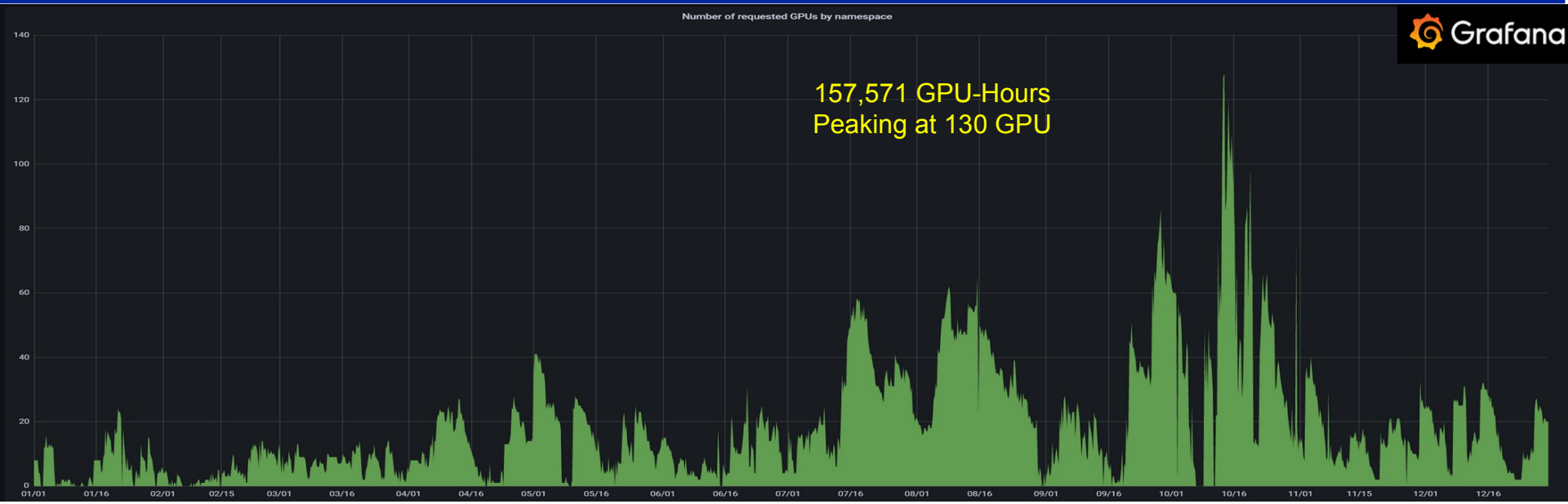
Raghav Kansal (grad. Stud. UCSD) runs ~1,000 CPU jobs calling out to ~10 GPUs on NRP for inference for his ML model for hh search.

80M events inferenced, sending 1.3TB of data from CPUs to GPUs in 3h

The ML model is too large to fit into the DRAM of the CPUs.
Fastest way to get the job done is "ML Inference as a service" on NRP

Source: Frank Wuerthwein, SDSC

Namespace *cms-ml* Was the 4th Largest Consumer of Nautilus GPU-Hours in 2022



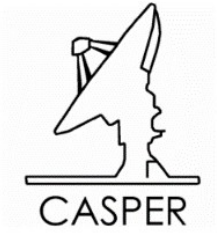
Nautilus

PI Frank Wuerthwein, UCSD

Telescopes



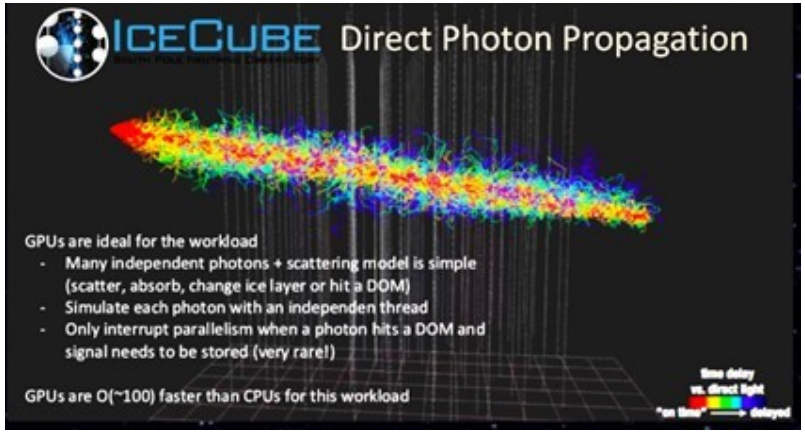




Nautilus

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

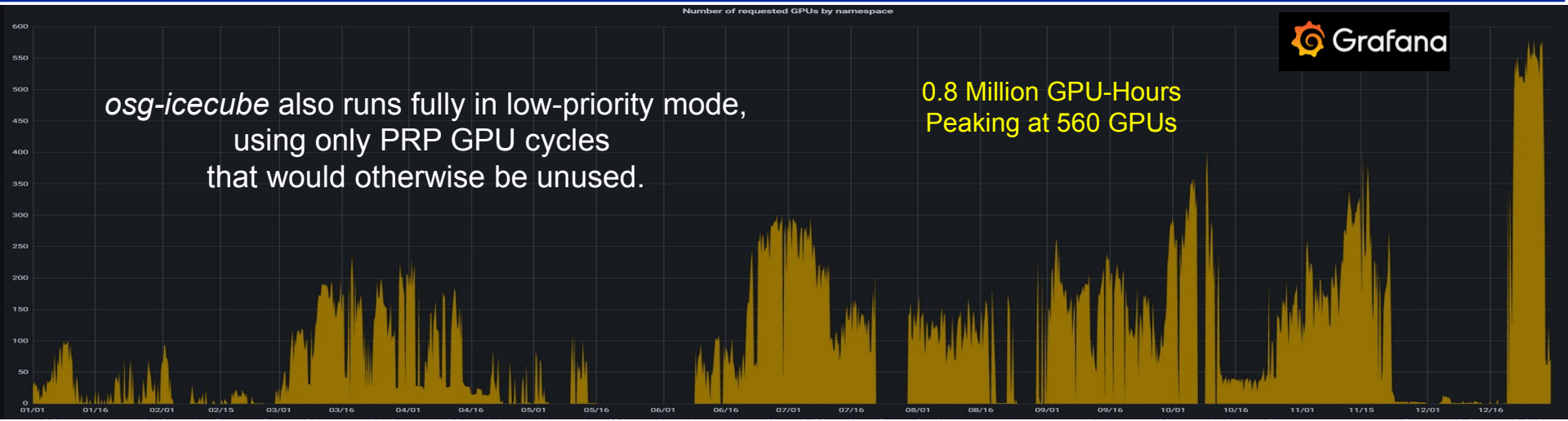
WISCONSIN
WIPAC
Wisconsin IceCube Particle Astrophysics Center
NSF

IceCube Peaked at 560 GPUs in 2022!

Nautilus

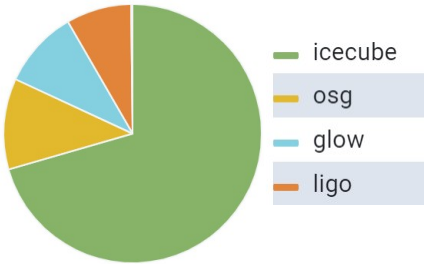
Open Science Grid

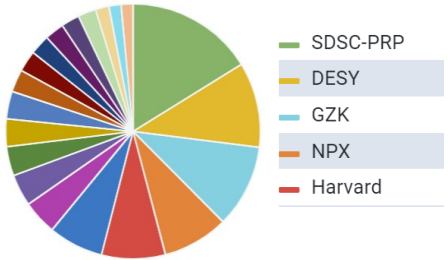
Namespace *osg-icecube*
Was the Largest Consumer of Nautilus GPU-Hours in 2022



In 2022 Icecube was the Largest consumer of OSG GPU-Hours
and PRP was the Largest Supplier of GPU-Hours to OSG

OSG GPU Consumers





OSG GPU Providers

Nautilus

https://gracc.opensciencegrid.org/d/ujFlp3vVz/gpu-payload-jobs

Laser Interferometer Gravitational-Wave Observatory (LIGO) Uses Nautilus/OSG Data Cyberinfrastructure

- **LIGO Runs Their Production Rucio Data Management System on Nautilus**
  - **Rucio is the De-Facto Data Management System for Many Large Instruments, LIGO, LHC, …**
  - **LIGO Continues to be One of the Major Users of the OSG Caching Infrastructure (A.K.A. Stashcache), Which is Deployed Mostly as PRP-Managed Kubernetes Pods.**
- **LIGO Does Not Use Much PRP Compute Given Their Dedicated Infrastructure**



Nautilus

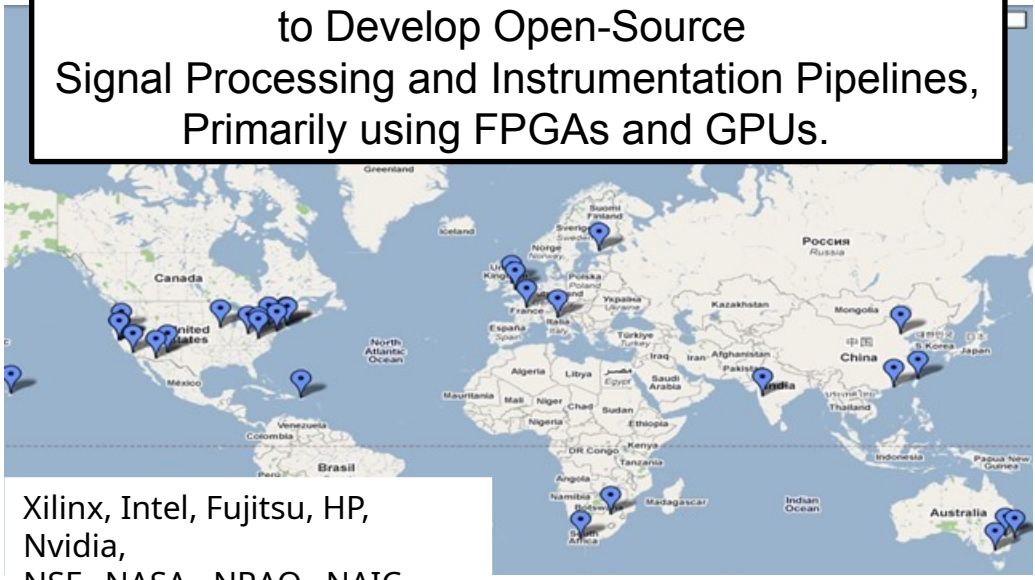
PRP Supports Radio Telescope Through Partnering with CASPER: the Collaboration for Astronomy Signal Processing and Electronics Research

https://casper.berkeley.edu/

The CASPER Collaboration of ~1000 Members and 50 Radio-Astronomy Instruments Worldwide to Develop Open-Source Signal Processing and Instrumentation Pipelines, Primarily using FPGAs and GPUs.

PRP Access Has Allowed CASPER to Expand in Several Aspects:

- PRP Portal to CASPER Tools/Libraries Was Developed by PRP's John Graham
- The PRP Team Added FPGAs to Nautilus FIONAs with the CASPER Software Stack
- Nautilus JupyterHub Used for FPGA Training
- Optical Fiber Connected Data Storage



Xilinx, Intel, Fujitsu, HP, Nvidia,
NSF, NASA, NRAO, NAIC

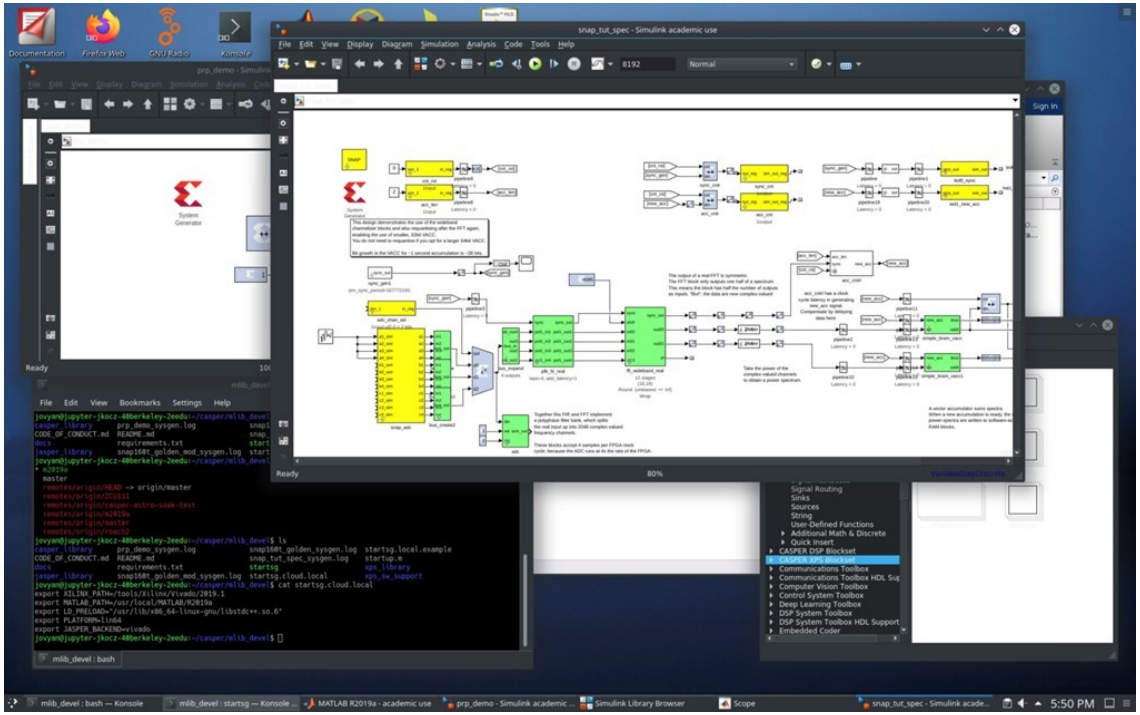
Radio Telescopes include:
- Event Horizon Telescope
- Square Kilometer Array
- Very Large Array

Source: Dan Werthimer
SETI Chief Scientist, UC Berkeley
SETI.berkeley.edu, CASPER.berkeley.edu

Nautilus

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

CASPER designs, compiles, tests and evaluates instrumentation on the PRP, then deploys dedicated FPGA and GPU clusters at the observatories



CASPER

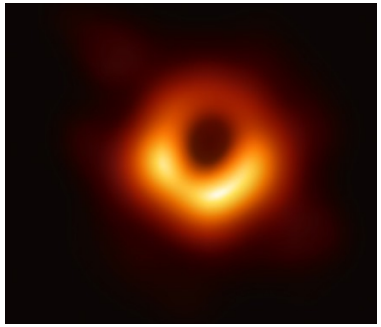
The Collaboration for Astronomy Signal Processing and Electronics Research

See John Graham's CASPER 2021 Workshop Talk and Tutorial:
https://casper.berkeley.edu/index.php/casper-workshop-2021/agenda/

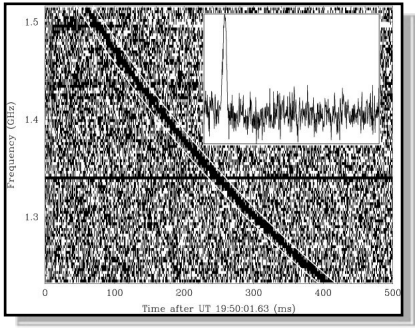
Nautilus

Discoveries Made with CASPER-Enabled Instrumentation

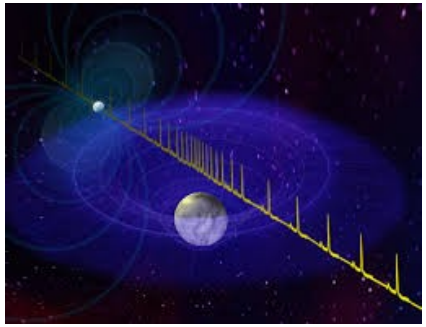
Radio Image of a Black Hole



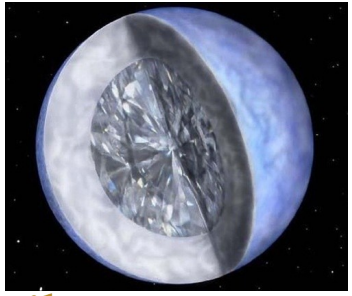
Fast Radio Bursts Weighing the Universe



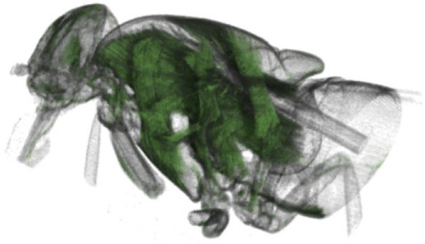
Pulsar Timing Gravitational Waves



Diamond Planet



Neutron Imaging



Protheses Control



Source: Dan Werthimer, UC Berkeley

Nautilus

Biomedical



open forcefield



TemPredict

UCSF Health | ŌURA

UC San Diego

NCMIR

National Center for Microscopy and Imaging Research

OpenForceField Uses OPEN Software, OPEN Data, OPEN Science and PRP 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

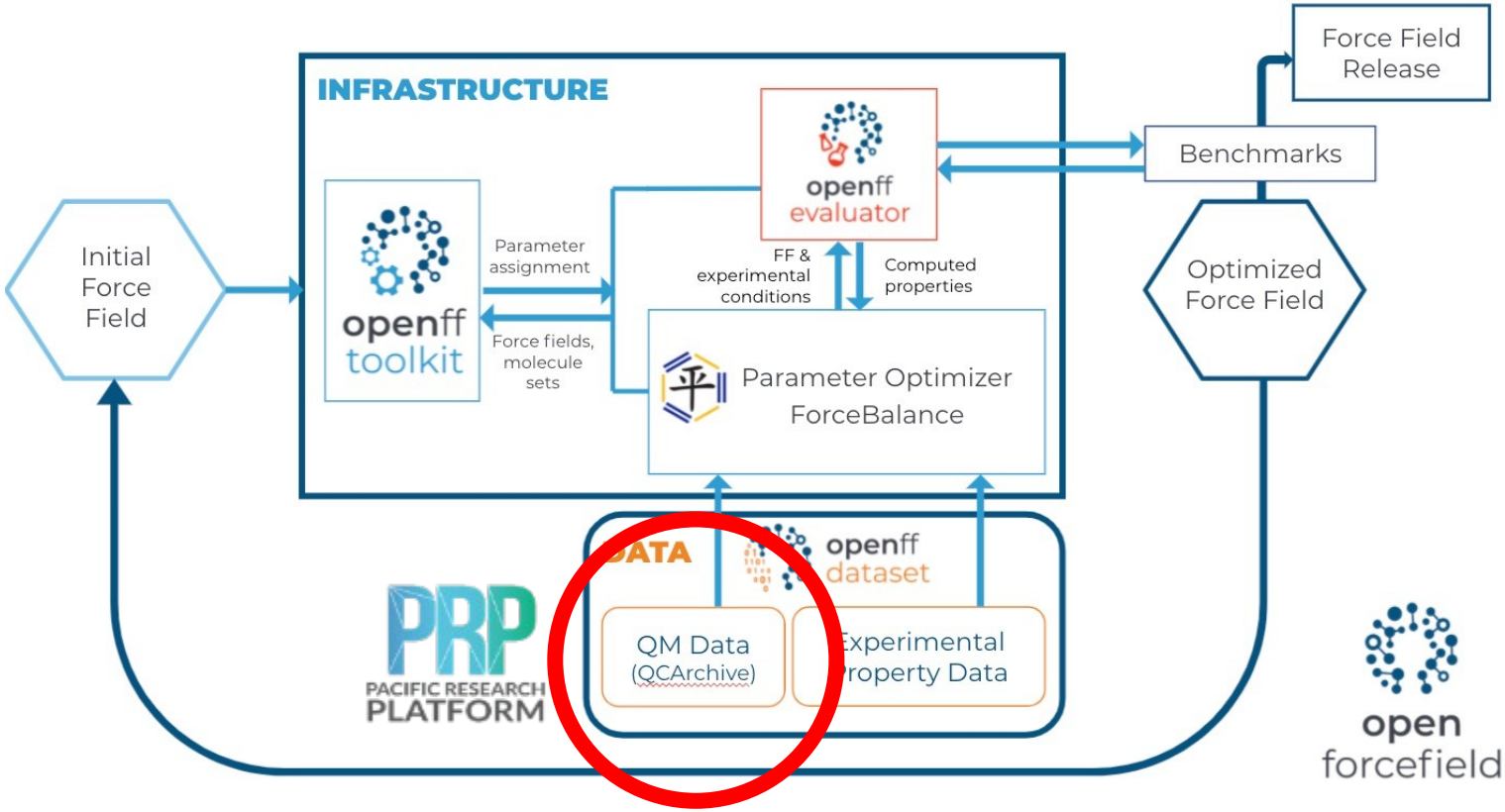
OFF Open-Source Models are Used in Drug Discovery, Including in the COVID-19 Computing on Folding@Home.

www.openforcefield.

Nautilus

open forcefield

OFF Runs Quantum Mechanical Computations on Many Molecules to Determine Their Optimized Force Fields

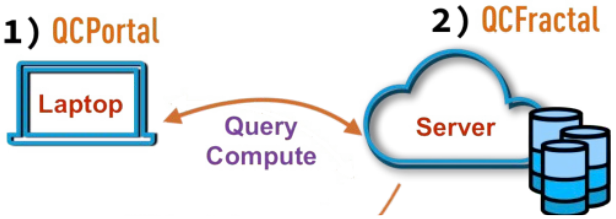


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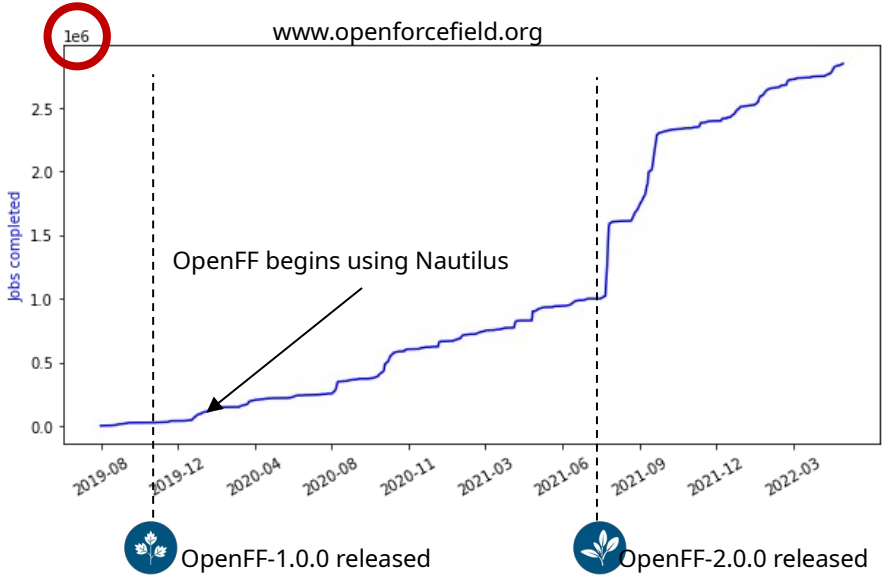
PRP is Capable of Running Millions of Quantum Chemistry Workloads

QC Archive
A MolSSI Project
VIRGINIA TECH





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 and scheduled on PRP's Kubernetes system. Due to the short job duration, these deployments can still be effective if interrupted every few hours.



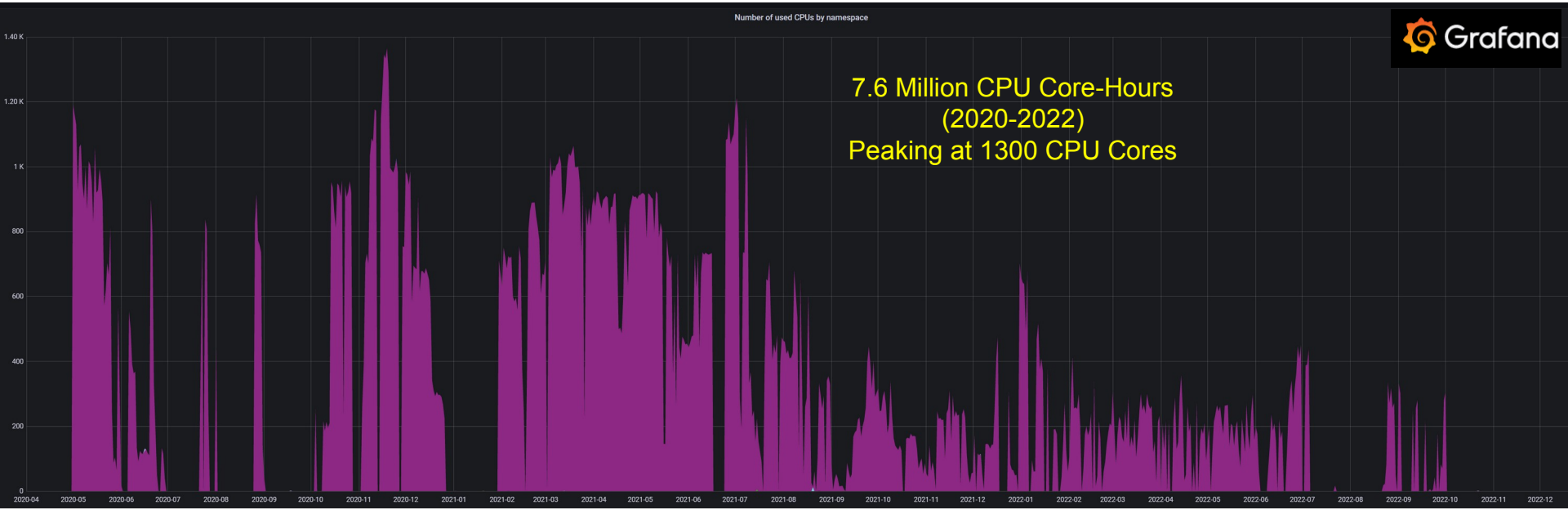
50% of OFF compute is run on Nautilus.

PRP PACIFIC RESEARCH PLATFORM

Nautilus

open forcefield

OFF Was the Top Nautilus CPU Core Consumer in 2020 & 2021, 4th Highest in 2022



OFF Datasets Consist of Hundreds to Millions of Jobs,
Each Requiring Tens to Thousands of CPU-Hours and 8-32 GB of RAM

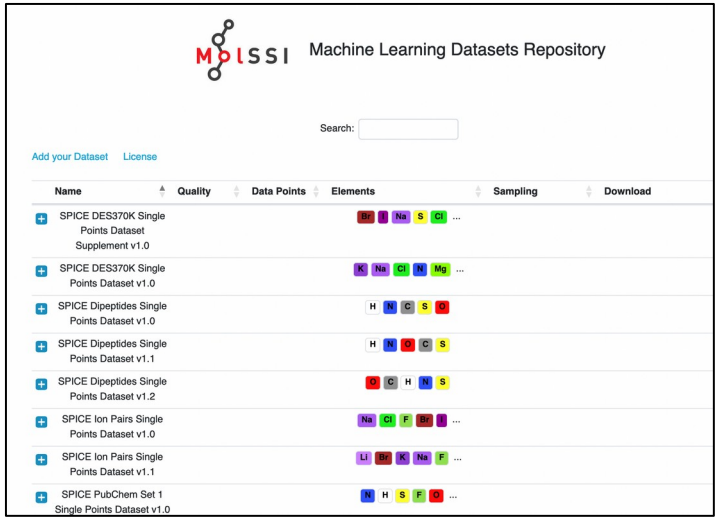
Nautilus

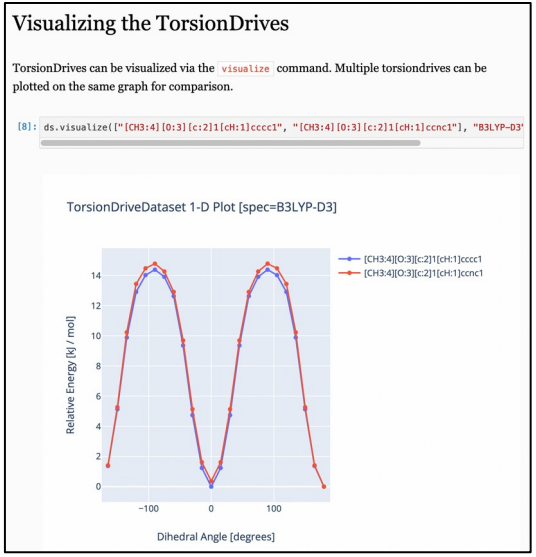
The OFF Datasets on QCArchive are Fully Open!

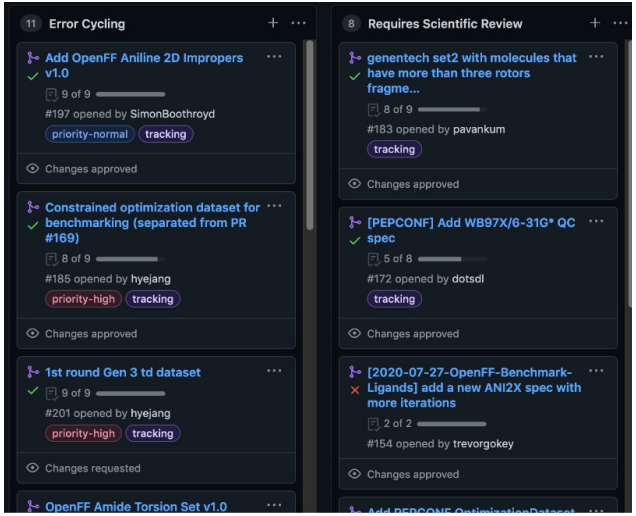
Dataset listing: https://qcarchive.molssi.org/apps/ml_datasets/

Python example notebooks for data access: https://qcarchive.molssi.org/examples/

OpenFF's dataset lifecycle: https://github.com/openforcefield/qca-dataset-submission/projects/1

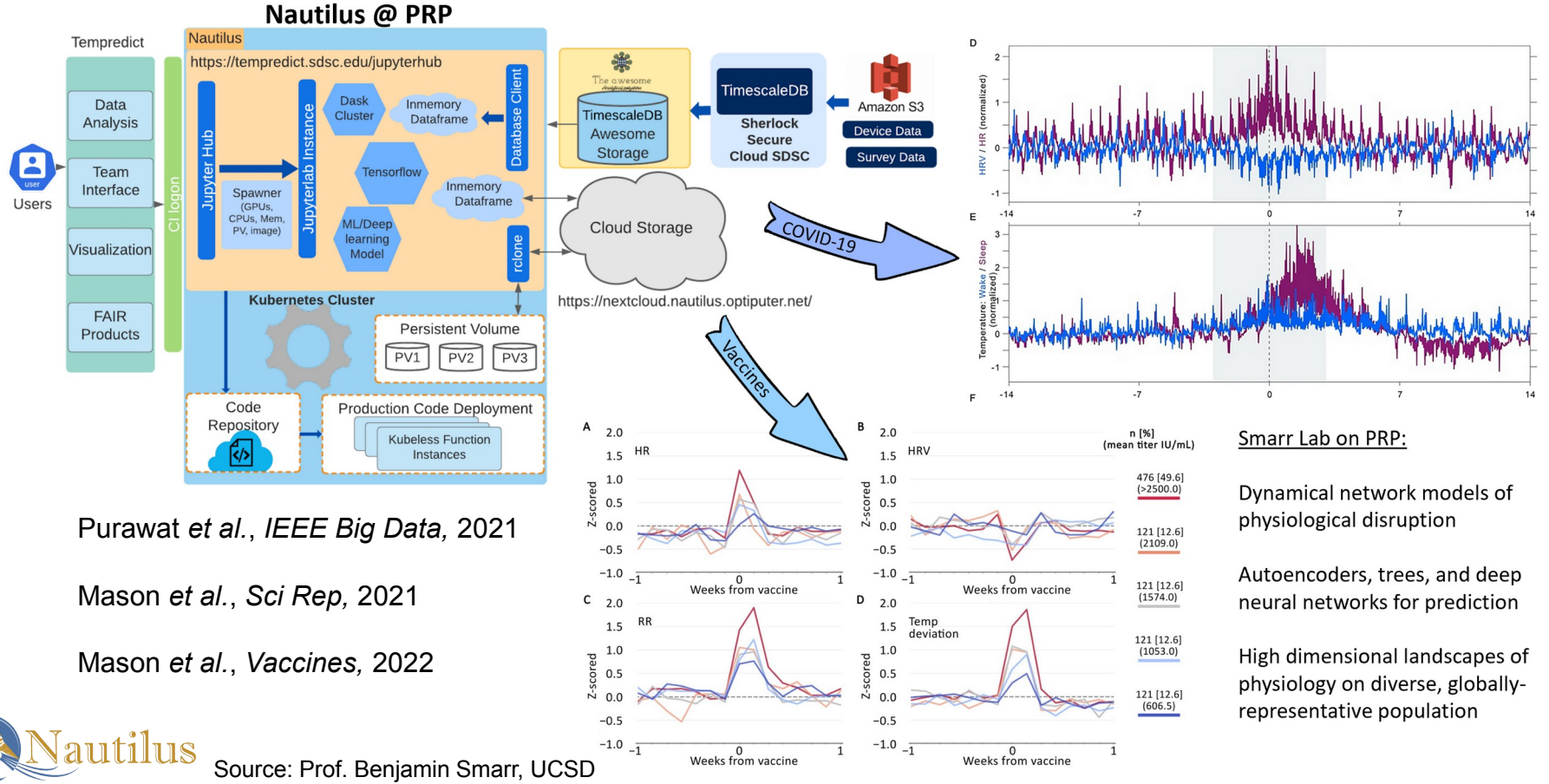






Nautilus

Nautilus Namespace *tempredict* Utilized PRP to Compute COVID-19 and Vaccine Responses ~65K Participants



Purawat *et al.*, *IEEE Big Data,* 2021

Mason *et al.*, *Sci Rep,* 2021

Mason *et al.*, *Vaccines,* 2022

Source: Prof. Benjamin Smarr, UCSD

Smarr Lab on PRP:

Dynamical network models of physiological disruption

Autoencoders, trees, and deep neural networks for prediction

High dimensional landscapes of physiology on diverse, globally-representative population

Nautilus Namespace *braingeneers:* One of the Most Advanced PRP projects - Uses Optical Fiber Connected Shared Storage, CPUs & GPUs

APR 27, 2020

CENIC



PRP Boosts Inter-Campus Collaboration on Brain Research

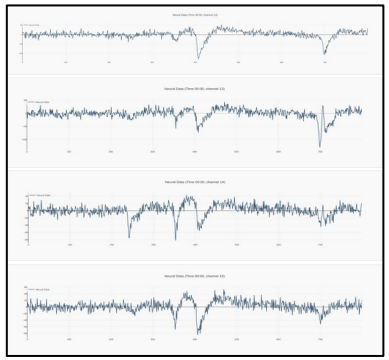
https://cenic.org/blog/prp-boosts-inter-campus-collaboration-on-brain-research



Nautilus

UCSC/Hengenlab Data Analysis Pipeline Using PRP





Hengenlab
UWSL

SCF05 (0.1 TB)
64 channel

EAB40 (1.1 TB)
256 channel

EAB50 (3.4 TB)
512 channel

EAB505 (3.3 TB)
512 channel

More coming...

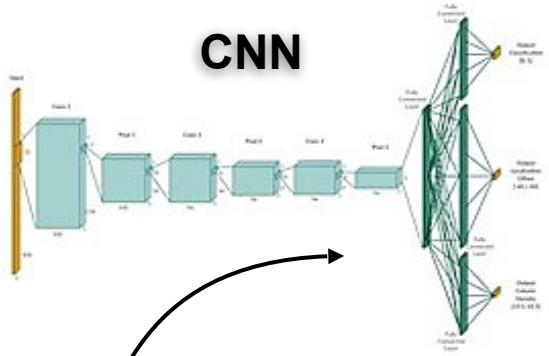
PRP/S3

PACIFIC RESEARCH PLATFORM

Results

PRP
Compute

CNN

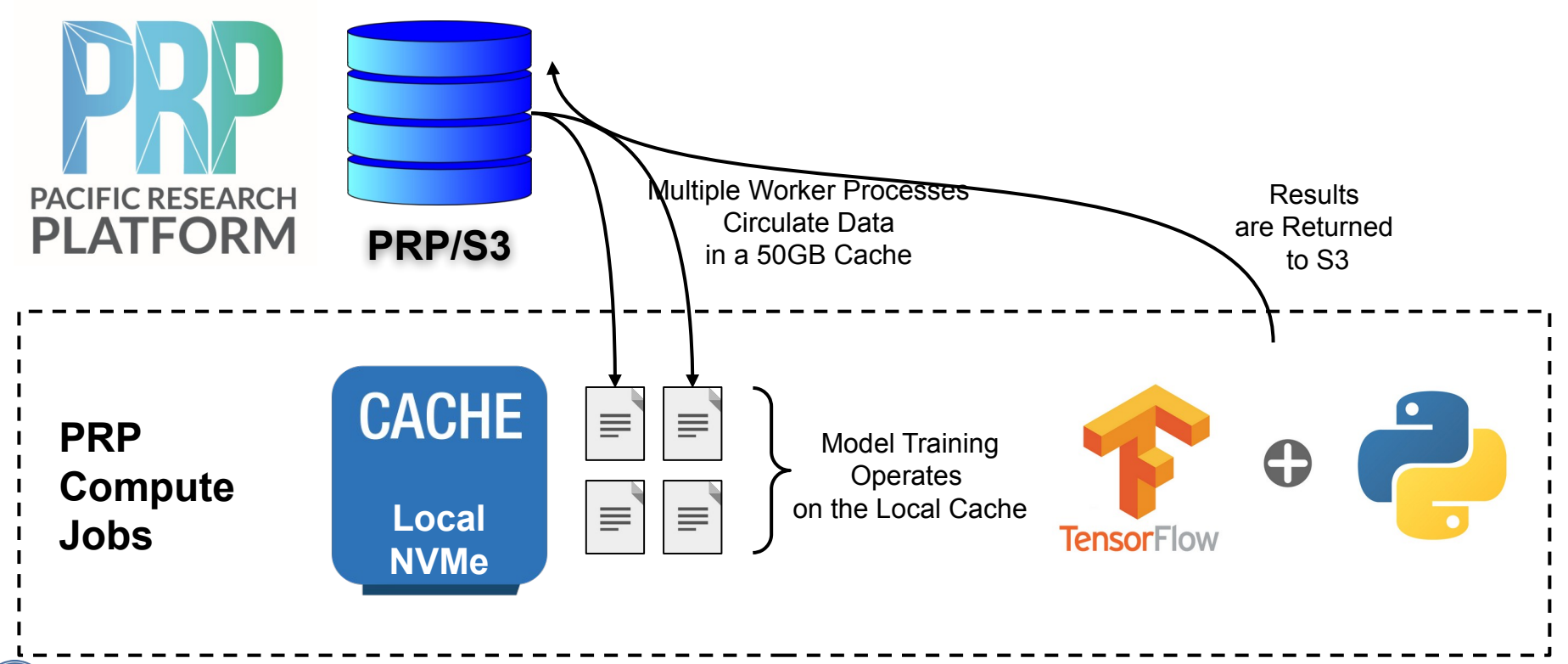


Braingeneers
UCSC and UCSF

Nautilus

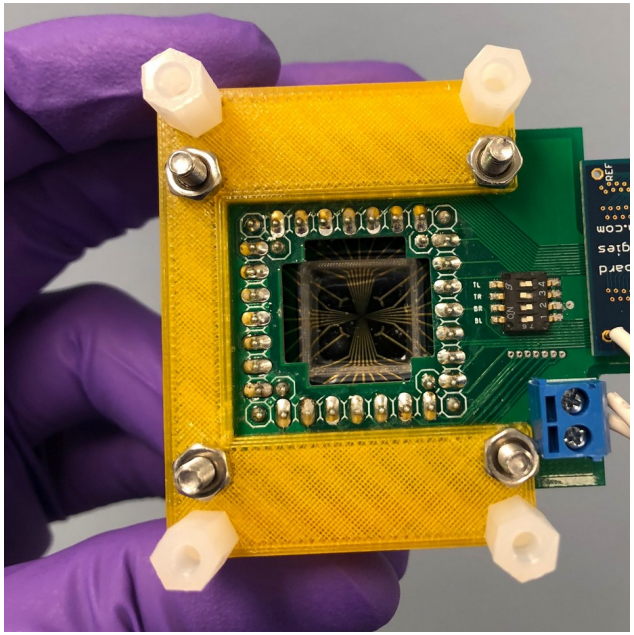
Source: David Parks, UCSC; *braingeneers* PI David Haussler

Sampling Strategy for *braingeneers* TB+ data

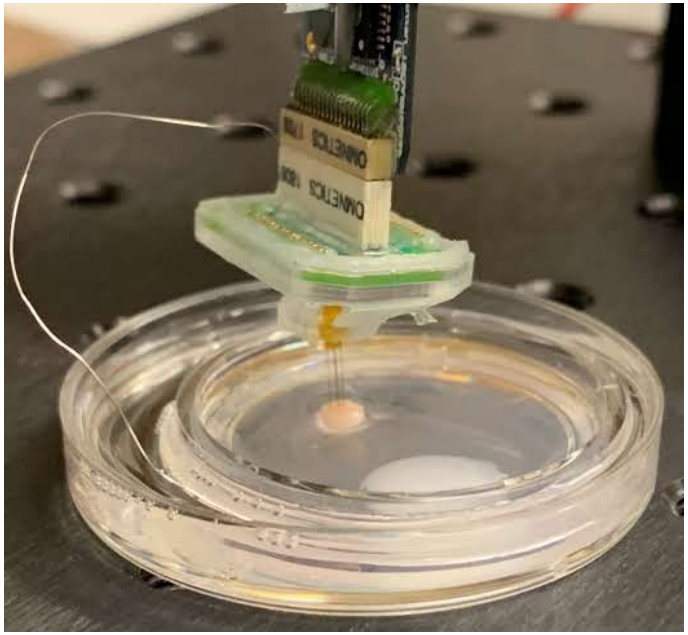


Source: David Parks, UCSC; *braingeneers* PI David Haussler

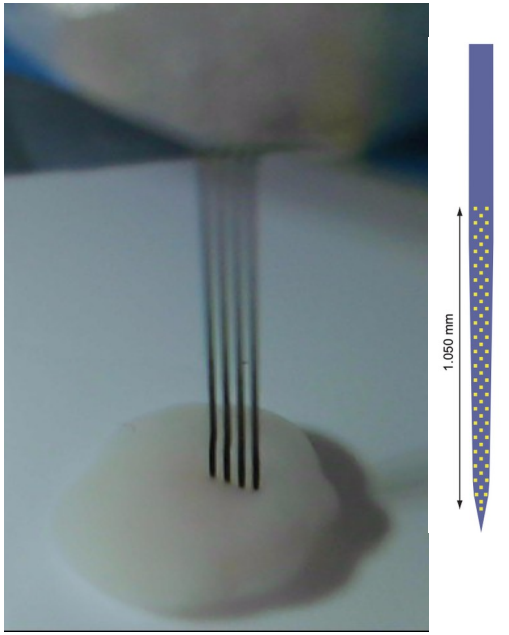
UCSC, UCSF & WUSL Are Collaborating To Grow Human Cerebral Organoids and Measure Their Neural Activity



Multi Electrode Array



Tetrodes

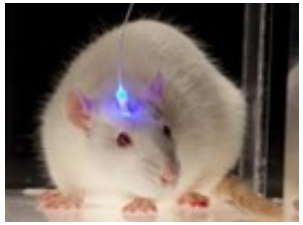


Silicon Probes

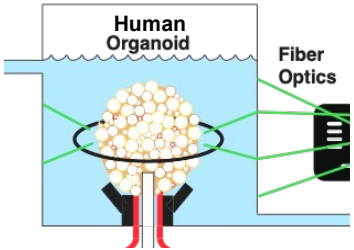
Source: David Parks, UCSC; *braingeneers* PI David Haussler

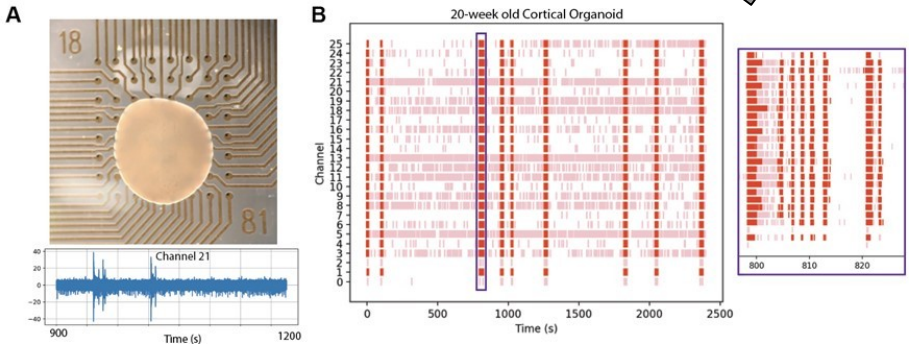
Goal: For Every Human Brain Slice, Grow 1000 Organoids, And For Every Organoid, Compute 1000 Simulated Organoids

From Neural Activity in Living Mouse Brain



PACIFIC RESEARCH PLATFORM



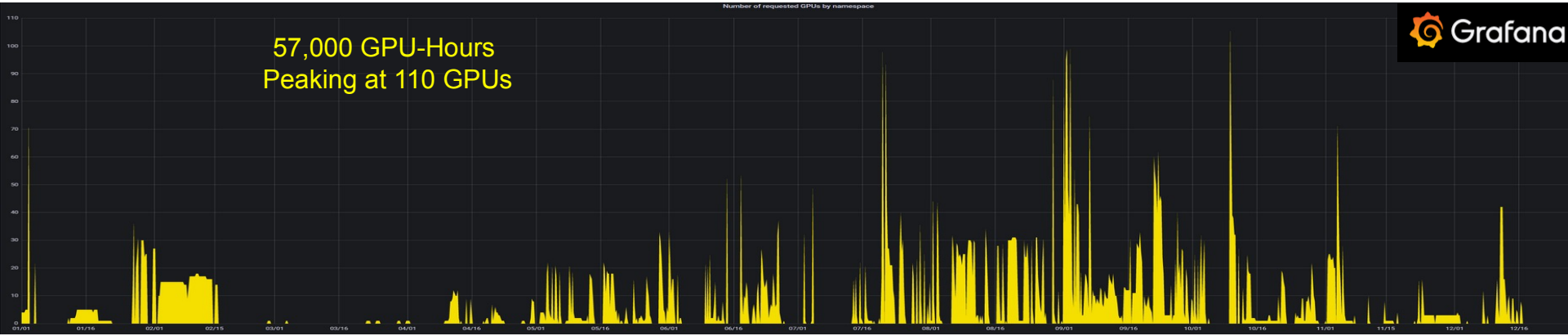


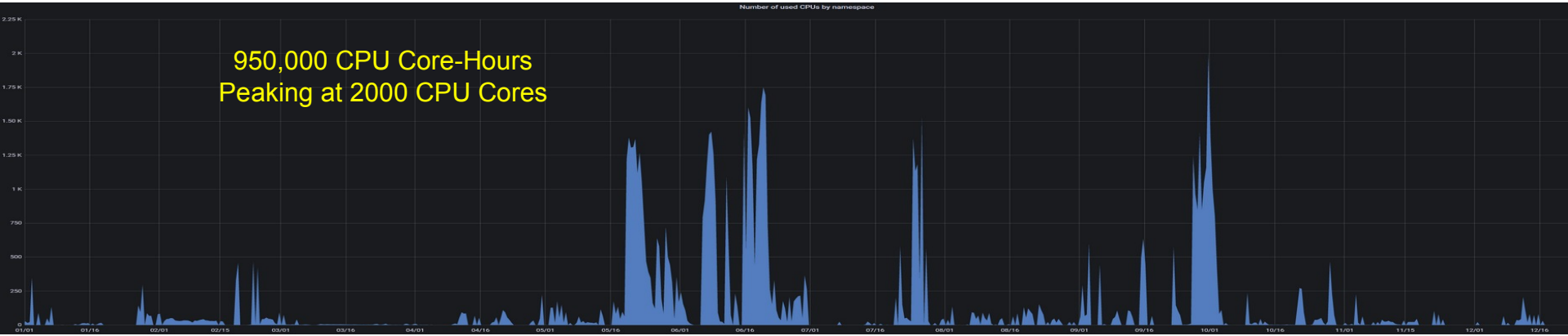
To Neural Activity in Human Brain Organoids

Nautilus

Source: David Parks, UCSC; *braingeneers* PI David Haussler

Nautilus Namespace *braingeneers*
Was The 3rd Largest Consumer of CPU Core-Hours in 2022





Nautilus

https://braingeneers.ucsc.edu/

NeuroKube: An Automated Neuroscience Reconstruction Framework Uses Nautilus for Large-Scale Processing & Labeling of Neuroimage Volumes

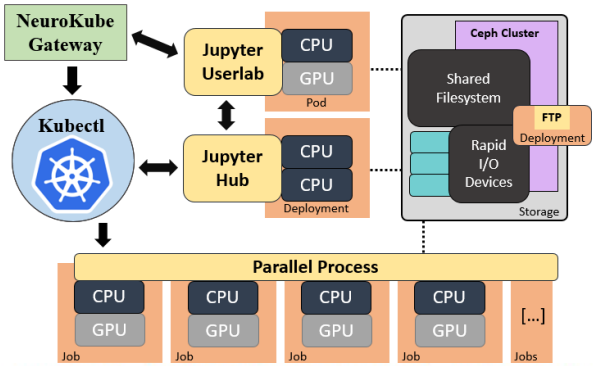


Figure 2. NeuroKube Framework Architecture

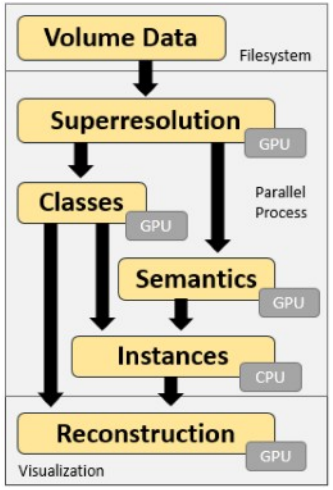


Figure 4. Workflow Steps

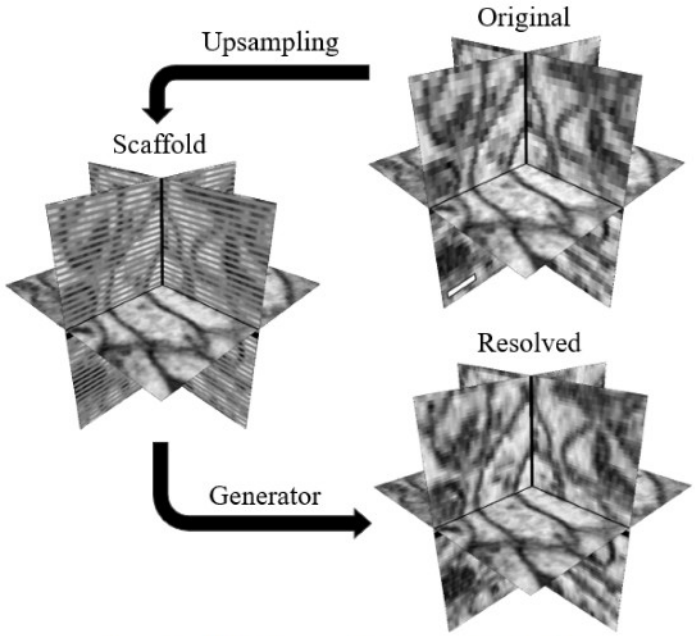
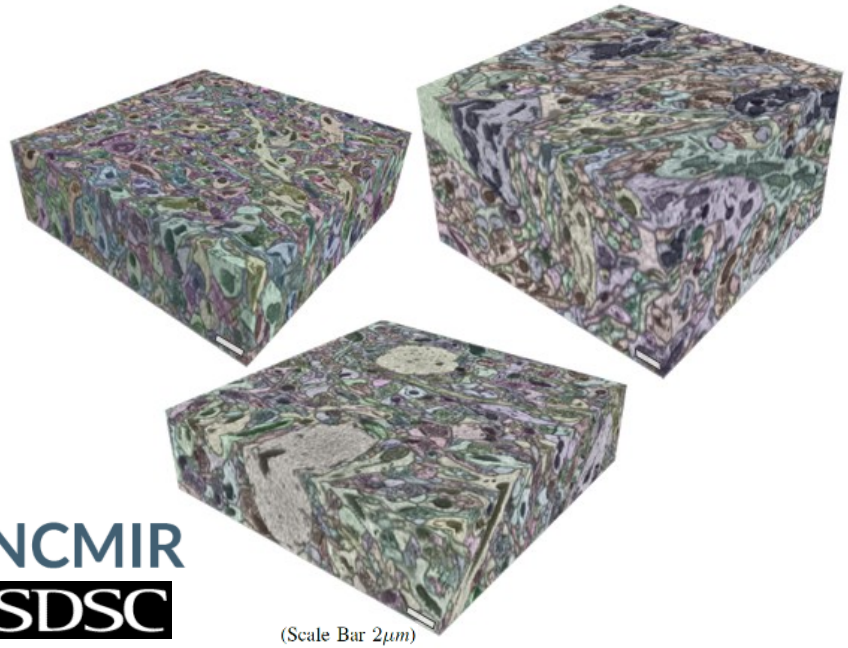


Figure 5. VEM Superresolution (Scale Bar 250nm)

Figures 2, 4, & 5 in “NeuroKube:
An Automated and Autoscaling Neuroimaging Reconstruction Framework
Using Cloud Native Computing and A.I.,”
Matthew Madany, et al. (IEEE Big Data ’20, pp. 320-330)

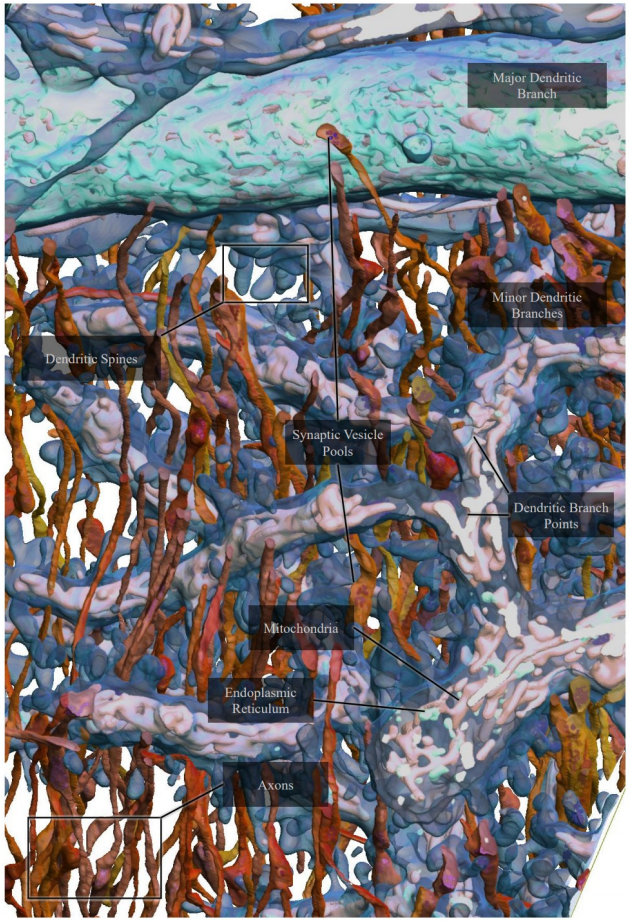
Computer Vision-Based Approach Provides the Potential to Automatically Generate Labels Using ML



NCMIR

SDSC

Volumetric Electron Microscopy (VEM) Data with Colorized Labels



Subset of Neurites from Cerebellum Neuropil Extracted & Rendered in 3D with Structures of Interest Labeled

Figures 1 & 14 in "NeuroKube: An Automated and Autoscaling Neuroimaging Reconstruction Framework using Cloud Native Computing and A.I.," Matthew Madany, et al. (accepted to IEEE Big Data '20)

Nautilus

Earth Sciences







Nautilus

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



Real-Time Meteorological Sensors

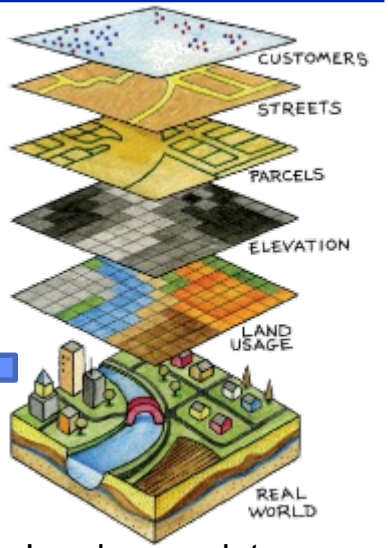
HPWREN

Fire Perimeter

Source: Ilkay Altintas, SDSC

WIFIRE



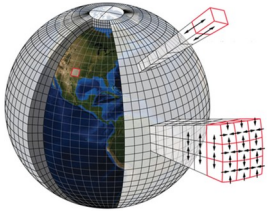


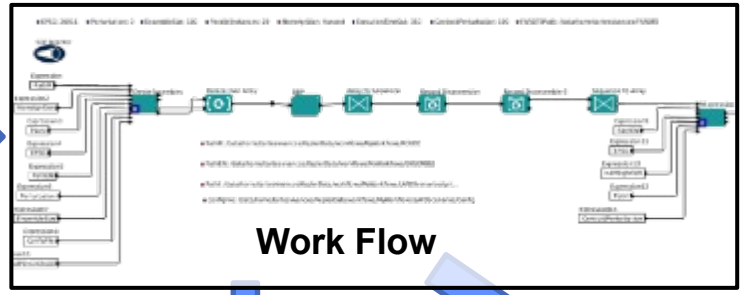
Landscape data

PRP

CENIC

Weather Forecasts



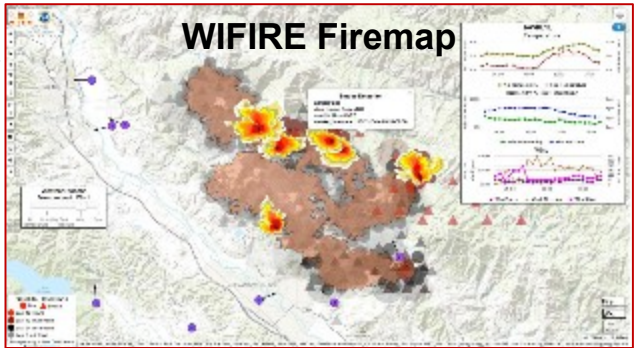


Work Flow



SDSC

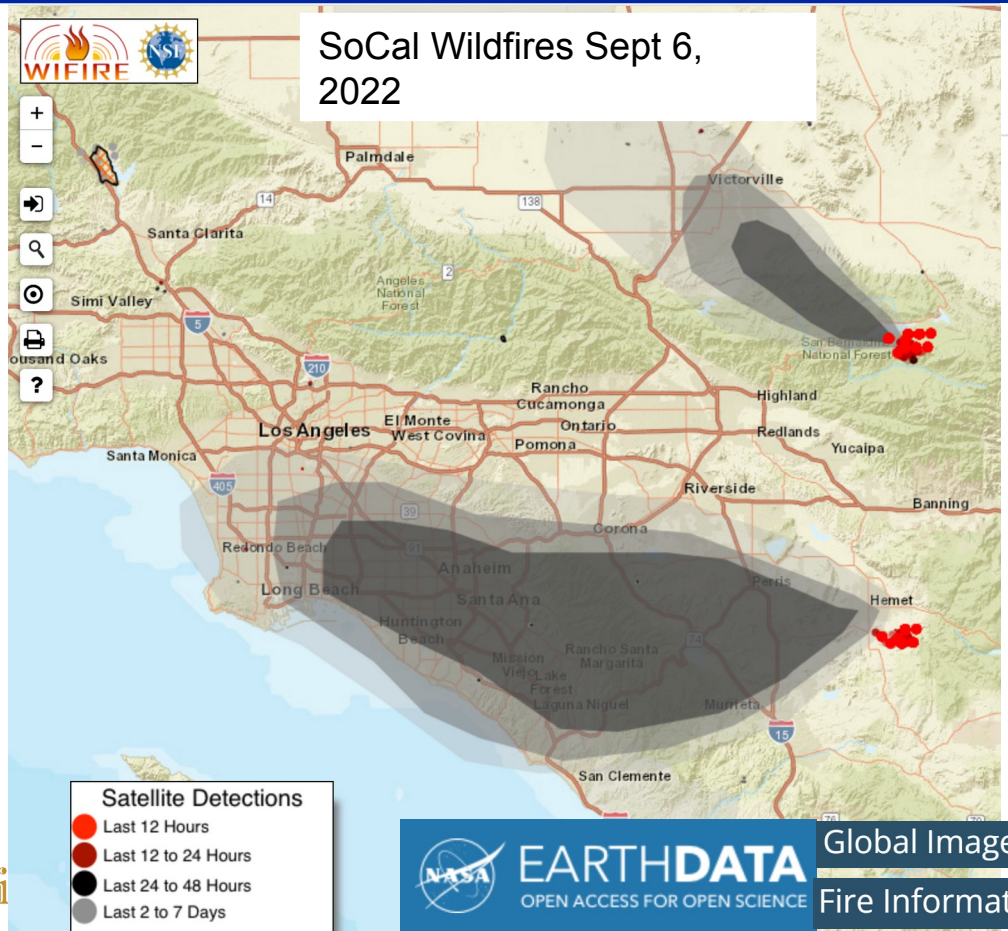


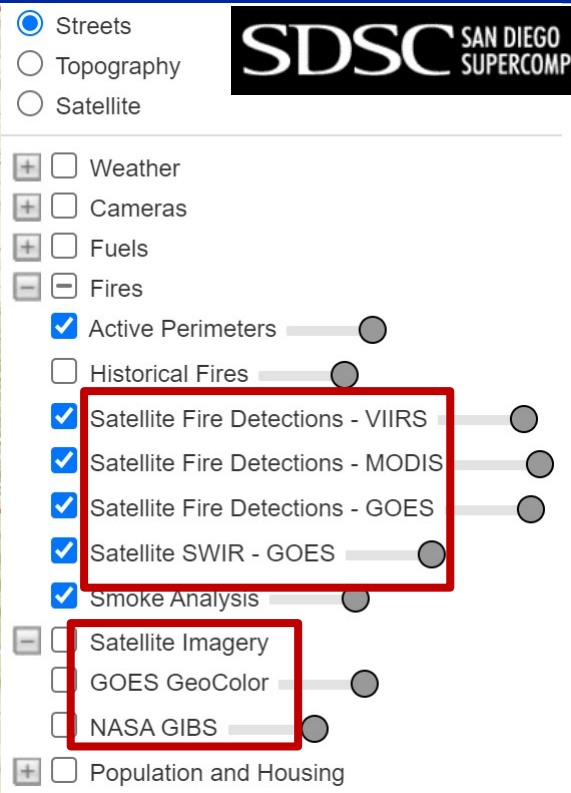


Nauti

NSF

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





SDSC SAN DIEGO SUPERCOMPUTER CENTER

EARTHDATA OPEN ACCESS FOR OPEN SCIENCE

Global Imagery Browse Services (GIBS)

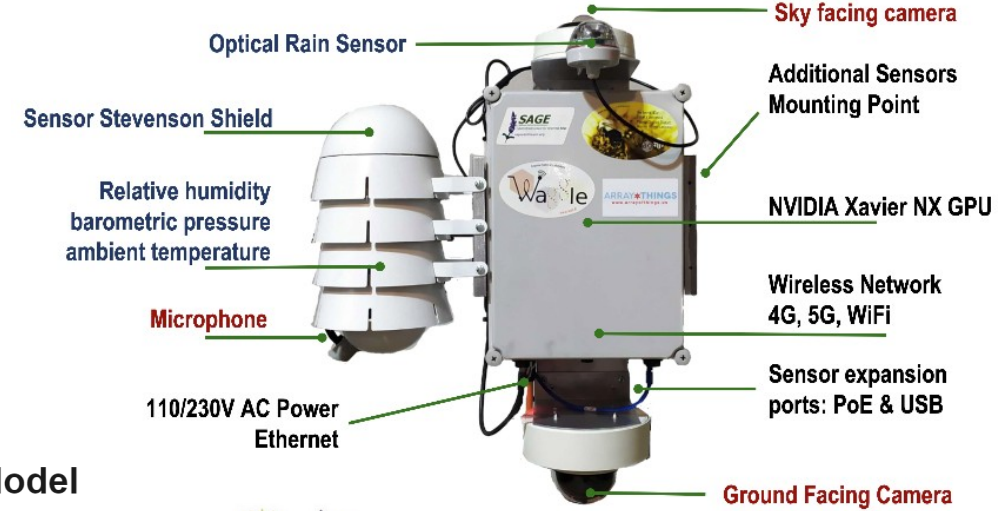
Fire Information for Resource Management System (FIRMS)

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



FIgLib & 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

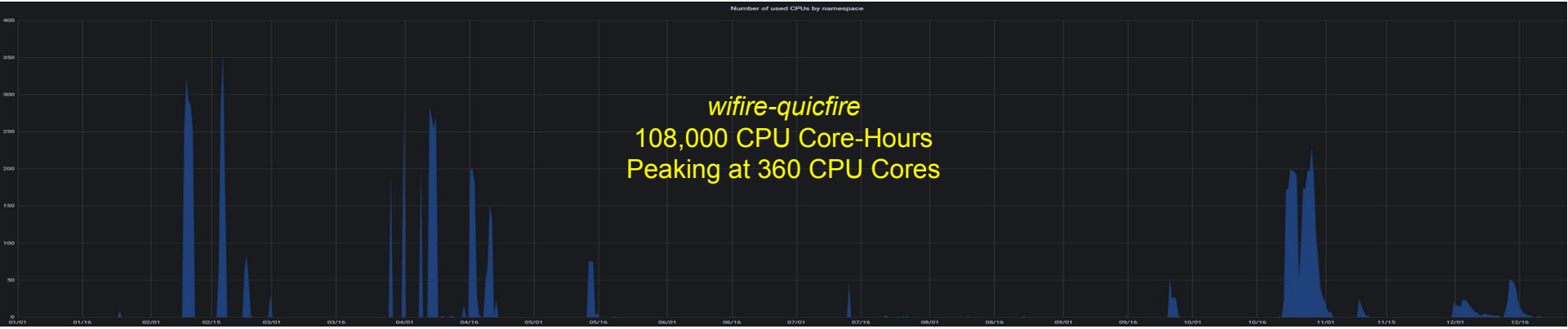
PRP namespace *digits*

Sage

Building atop standard community software:

Source: Charlie Catlett, Pete Beckman, Argonne National Lab

Nautilus Namespace *wifire-quicfire* was the 25th Largest 2022 Consumer of CPU Core-Hours; *digits* was the 14th Largest GPU Consumer





Nautilus

Visualization and Virtual Reality



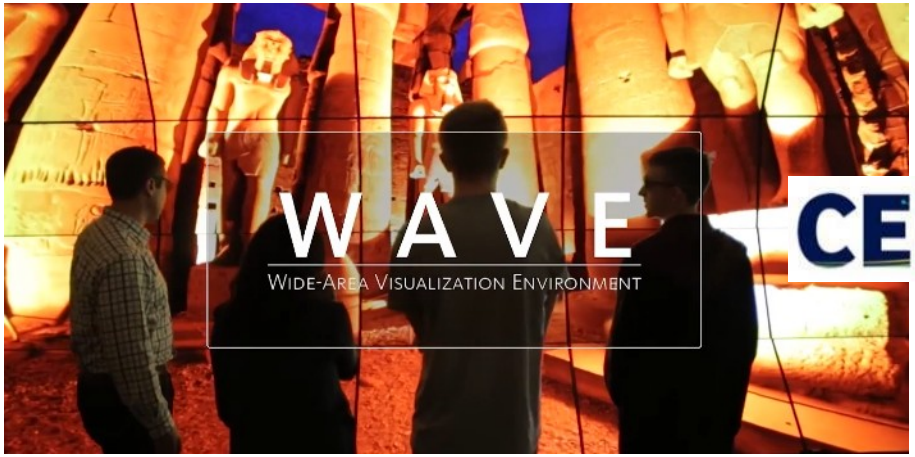
UC San Diego
SU Lab

NeRF

Representing Scenes as Neural Radiance Fields for View Synthesis

Nautilus

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

Nautilus

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

PRP Has Been Bringing Machine Learning to Building Virtual Worlds, Including Robotics and Autonomous Vehicles

- **Goal: Train Robots That Can Manipulate Arbitrary Objects**
  - **Open Drawer, Turn Faucet, Stack Cube, Pull Chair, Pour Water, Pick And Place, Hang Ropes, Make Dough, …**

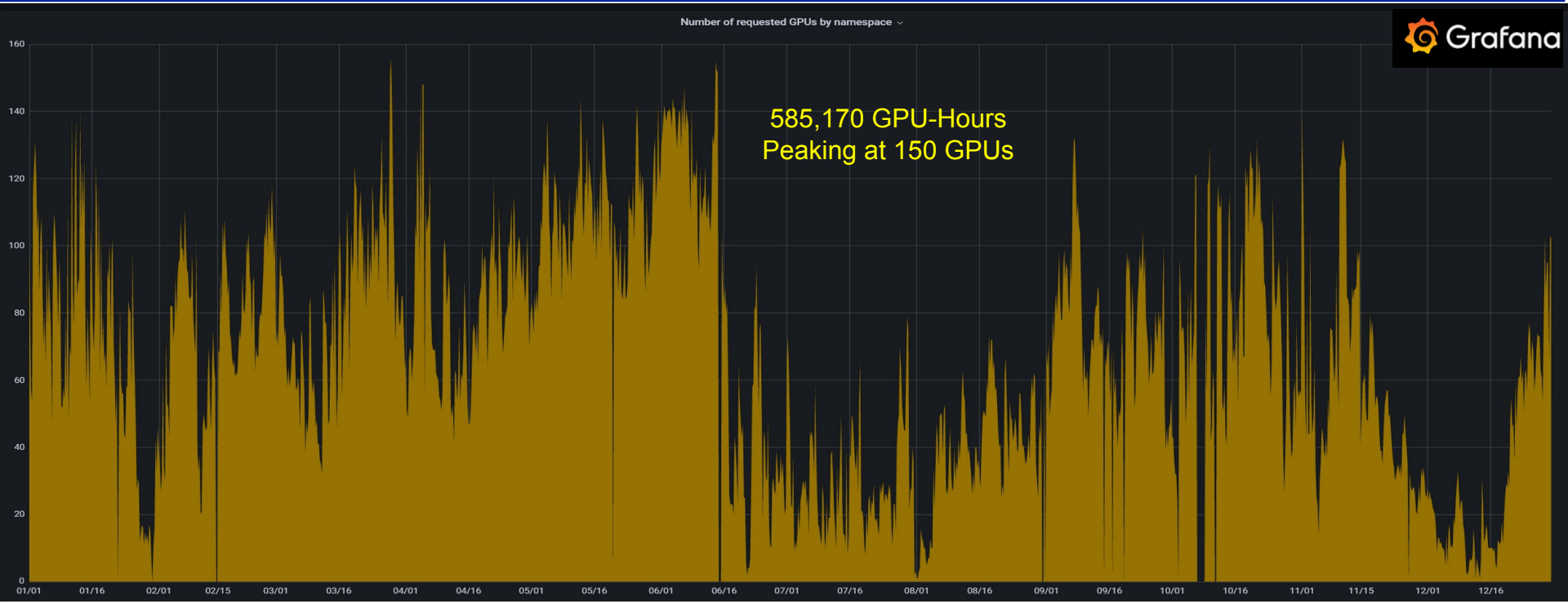


(video)

UCSD's Hao Su Lab Uses NRP GPUs for 3D Deep Learning and Embodied AI (Robotics and Self-Driving Cars)

Nautilus

Namespace *ucsd-haosulab*
Consumed the 2nd Most Nautilus GPU-Hours in 2022 (1st is Icecube)

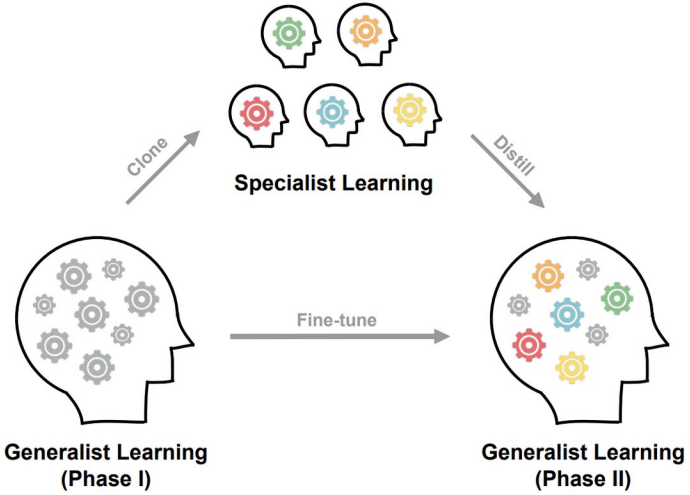


Nautilus

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**

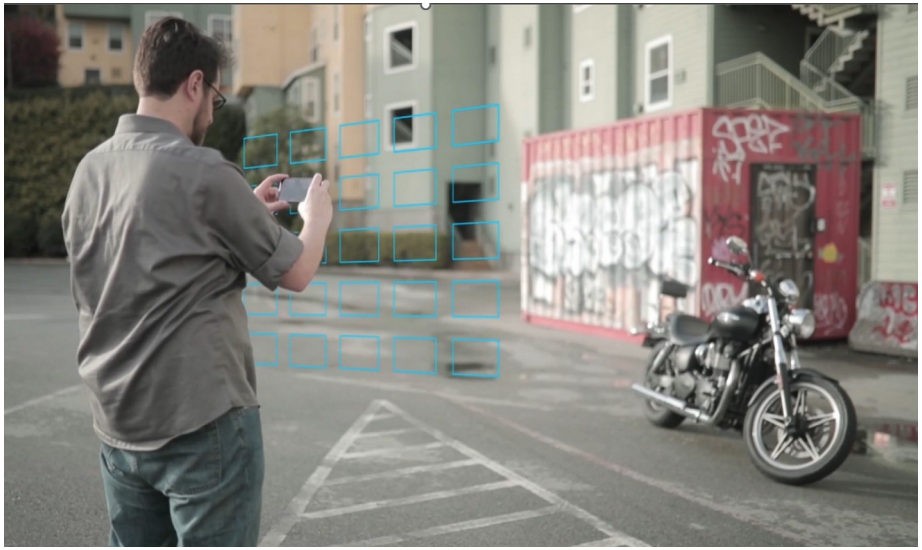
- On **Nautilus**:
  - *Hundreds* of specialists have been trained
  - Each specialist is trained in *millions* of environment variants
  - ~10,000 GPU hours per run



Source: Prof. Hao Su, UCSD

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

Machine Learning Using NRP GPUs
Transforms a Series of 2D Images
Into a 3D View Synthesis





Nautilus

Source: Prof. Ravi Ramamoorthi, UCSD

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 R&D

Spatial Journalism

Creating Workflows for NeRF Portraiture

September 27, 2022

← THE BEST INVENTIONS OF 2022

TIME

Automated 3D Rendering

NVIDIA Instant NeRF

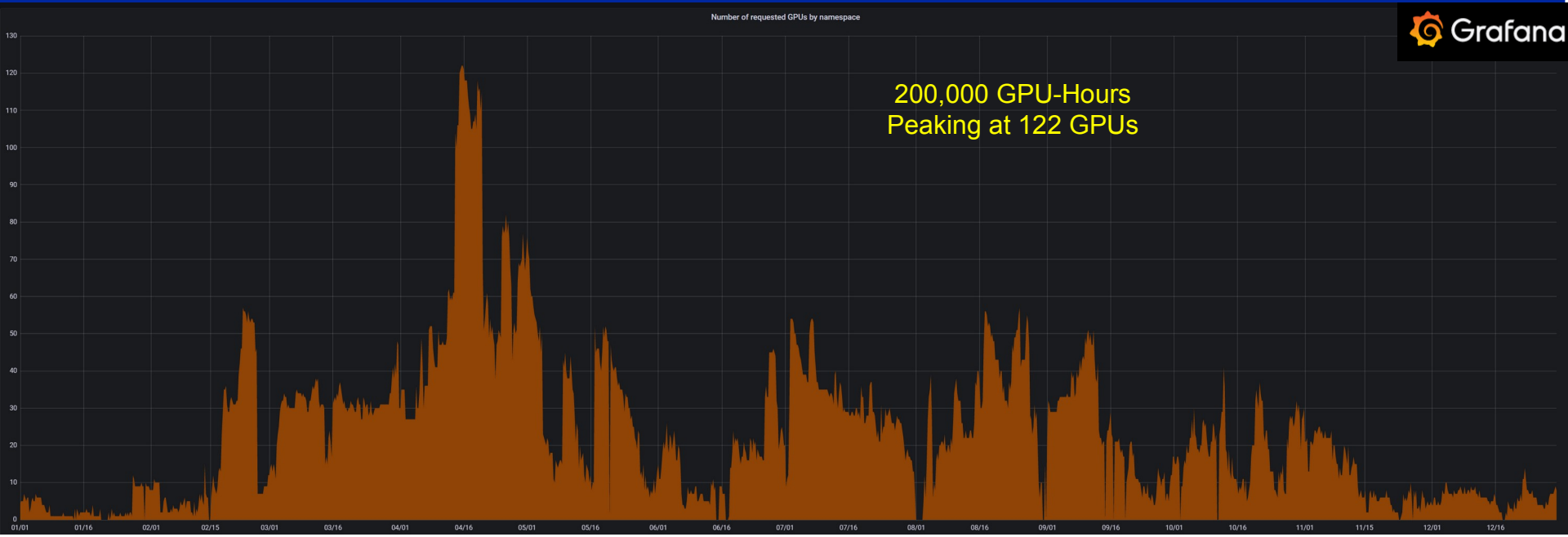
BY JARED LINDZON
NOVEMBER 10, 2022

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

Namespace *ucsd-ravigroup*
Consumed the 3nd Most Nautilus GPU-Hours in 2022

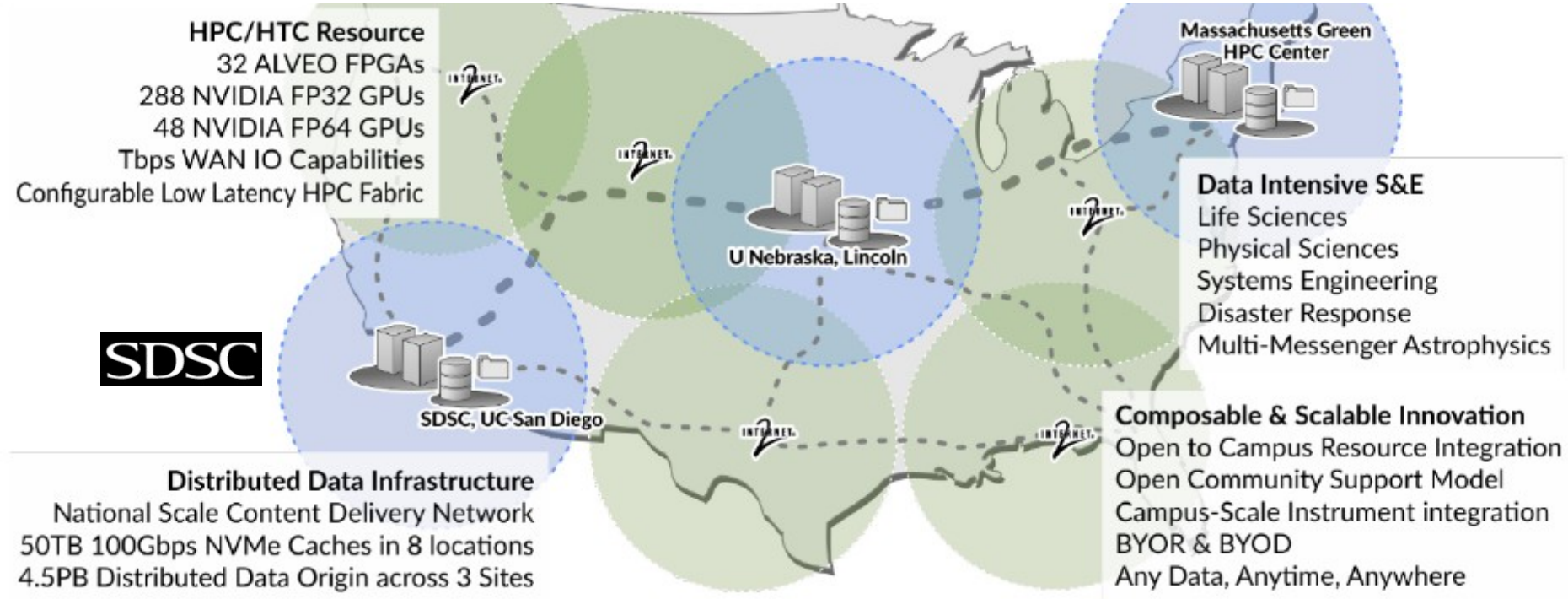


- Much of the compute involves training computationally expensive NeRFs.
- Training time to learn a representation of a single scene on a GPU can vary from seconds to a day.
- NeRFs that can see behind occlusions may require a week of training on 8 GPUs simultaneously.

Nautilus

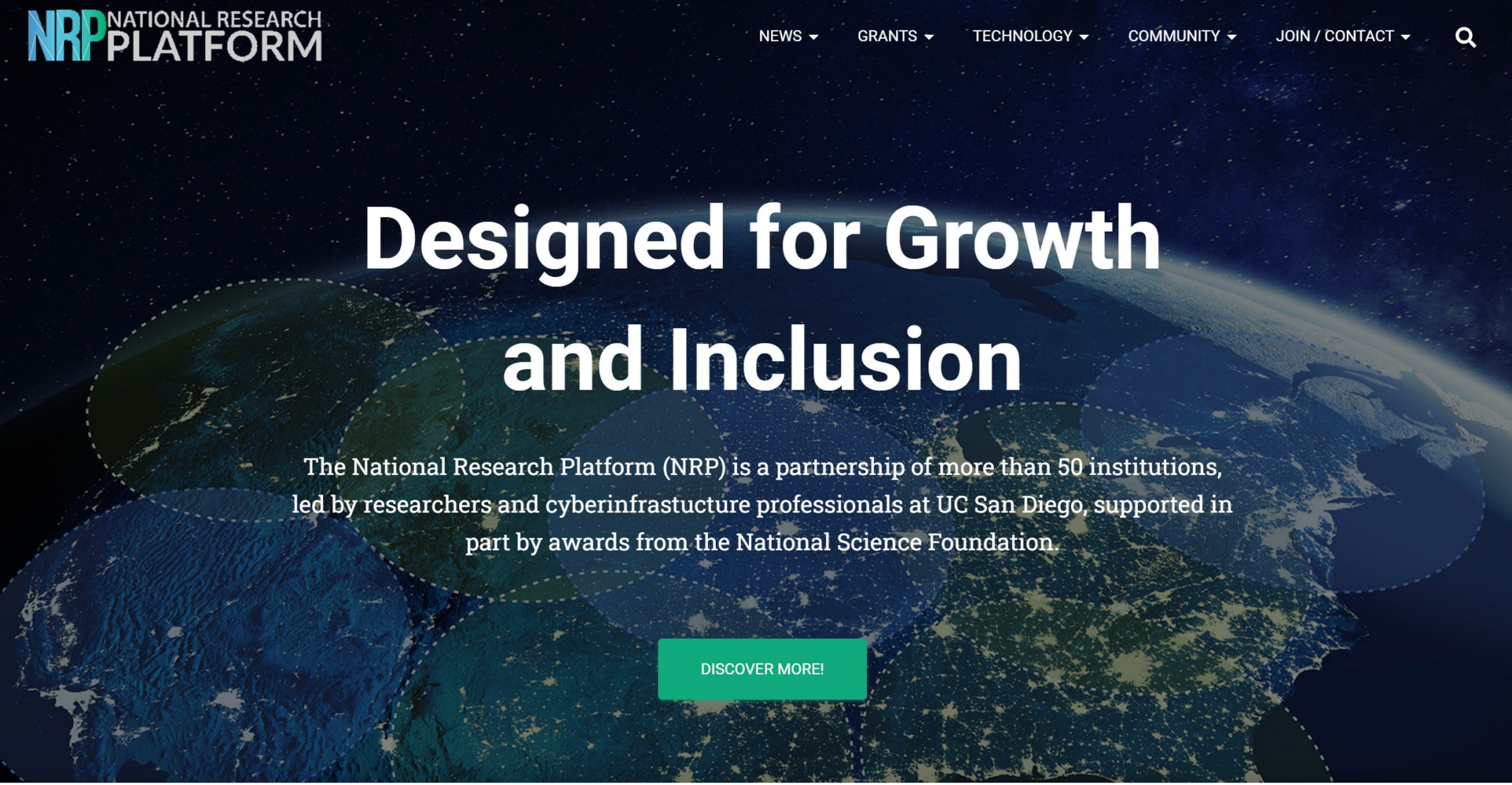
Source: Alexander Trevithick, UCSD Ravi Group

2022-2026 NRP Future: PRP Federates with NSF-Funded *Prototype National 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)

Nautilus



Nautilus

https://nationalresearchplatform.org/