



Open Infrastructure for an Open Society

Frank Würthwein Director, San Diego Supercomputer Center

May 3rd 2023







Vision



Long Term Vision



- Create an Open National Cyberinfrastructure that allows the federation of CI at all ~4,000 accredited, degree granting higher education institutions, nonprofit research institutions, and national laboratories.
 - Open Science
 - Open Data
 - Open Source
 Open Compute

Open devices/instruments/IoT, …?

Openness for an Open Society





National Research Platform (NRP)

Community vs Funded Projects



NRP is "owned" and "built" by the community for the community



Cyberinfrastructure Stack



NRP operates at all layers of the stack, from IPMI up

- IPMI reduces TCO and lower threshold to entry
- Kubernetes allows service deployments
 - Also the natural layer for application container deployment
- Admiralty allows K8S federation with folks who want control
 - Including cloud integration to access TPUs & other cloud only architectures
- HTCondor allows NRP to show up as a "site" in OSG

The layer you integrate at depends on

Control you want



Effort you can afford





Pacific Research Platform

A distributed Kubernetes cluster (2015 – 2023)

• When the PRP Grant Was Funded in 2015, It Started With:

- 6 States Now 43 States
- 19 Campuses > Now 110 Campuses
- 9 Minority Serving Institutions >>>> Now 23 MSIs
- 2 NSF EPCoR States Now 19 EPSCoR States, 2 Territories, and Wash DC



Open Science Grid

A Federation of Compute and Storage Clusters (founded in 2005)







Complementarity in Implementation of "Bring Your Own Resource" model

OSG focuses on campus cluster integration. NRP focuses on individual node integration instead of clusters.



Cyberinfrastructure Stack



NRP operates at all layers of the stack, from IPMI up

- IPMI reduces TCO and lowers threshold to entry
- Kubernetes allows service deployments
 - Also the natural layer for application container deployment
- Admiralty allows K8S federation with folks who want control
 - Including cloud integration to access TPUs & other cloud only architectures
- HTCondor allows NRP to show up as site in OSG



- Under-resourced institutions
- Network providers and their POPs
- CS & ECE faculty specialized in:
 - AI/ML => gaming GPUs
 - systems R&D

All of these find it difficult to justify staff to support all layers

NKP Hardware on NRP is Global



NRP integrates hardware in USA, EU, and Asia





Cyberinfrastructure Stack



NRP operates at all layers of the stack, from IPMI up

- IPMI reduces TCO and lowers threshold to entry
- Kubernetes allows service deployments
 - Also the natural layer for application container deployment
- Admiralty allows K8S federation with folks who want control
 - Including cloud integration to access TPUs & other cloud only architectures
- HTCondor allows NRP to show up as site in OSG

NRP is unique in its support of global service deployments

- Open Science Data Federation
 - Origins & Caches in US, EU, Asia
- Protein Data Bank
 - (Future) Replicas in EU & Asia







Supporting Nautilus for the next decade

Nautilus = K8S infrastructure of PRP for the last 5+ years

Nautilus = K8S of NRP for the next 10 years



The NSF Cat-II Program



- NSF supports via the Cat-II program novel systems ideas.
 - 3 year "testbed" phase
 - The PI owns the resource, and has (some) freedom regarding who uses it.
 - No requirements for making it available via any specific allocation mechanism.
 - It is expected that not all features work on day 1.
 - 3 years of experimentation & development of features
 - 2 year "allocation" phase
 - The resource is made available via an NSF supported allocation mechanism.
 - The solicitation mentions the possibility of an additional 5 year renewal without re-competition if system is successful.
- We decided that this is an ideal program to try and secure NRP core operations funding for the next 10 years
 - And thus provide the stability necessary for growth of NRP.

Cat-II: Prototype National Research Platform (PNRP)





5 year project with \$5M hardware & \$6.45M people Supports Nautilus, and thus the core NRP infrastructure NSF Acceptance Review of System passed on March 9th 2023 PI = Wuerthwein; Co-PIs: DeFanti, Rosing, Tatineni, Weitzel Funded as NSF 2112167 15



Innovations



- I1: Innovative network fabric that allows "rack" of hardware to behave like a single "node" connected via PCIe.
- I2: Innovative application libraries to expose FPGAs hardware to science apps at language constructs scientists understand (C, C++ rather than firmware)
- I3: A "Bring Your Own Resource" model that allows campuses nationwide to join their resources to the system.
- I4: Innovative scheduling to support urgent computing, including interactive via Jupyter.
- I5: Innovative Data Infrastructure, including national scale Content Delivery System like YouTube for science.

I3 & I4 & I5 turn "PRP" into "NRP" and sustains it into the future. I1 & I2 are totally new.

Repara Infrastructure Model of NRP

- Support regional Ceph storage systems across the USA.
 - Campuses can join individual storage hosts to the Ceph system in their region.
 - All regional storage systems are Data Origins in OSG Data Federation (OSDF)
 - Deploy replication system such that researchers can decide what part of their namespace should be in which regional storage.
- Deploy caches in Internet2 backbone such that no campus nationwide is more than 500 miles from a cache.

NRP data infrastructure model combines best of PRP & OSG

From PRP we take the regional Ceph storage concept From OSG/PATh we take the data origin & caching concepts

And then we add as a totally new feature: User controlled replication of partial namespaces across regions. (We will develop this during 3 year "testbed" phase)

Want Others to build higher level data services on top

Open Science Data Federation



Global data distribution driven by LIGO, Virgo, DUNE, ...

NKP Matrix of Science x Innovations

Table 3.1 Representative Science and Engineering Use Cases				Lot's of AI
Application domain	Lead researcher & Institution	Science Driver Themes	NRP Innovations	but so much mor
LIGO	Peter Couvares, LIGO Lab; Erik Katsavounidis, MIT	BGS, UC, AI	12, 13, 14, 15	- NSF MREFCs
IceCube	Benedikt Riedel, UW Madison	BGS, UC, AI	13, 14	
Astronomy (DKIST & Sky Surveys)	Curt Dodds, U. Hawai'i	BGS, AI	13, 15,	
Campus Scale Instru- ment Facilities	Mark Ellisman, NCMIR; Sa- mara Reck-Peterson, Nicon Imaging Center; Johannes Schoeneberg, Adaptive Op- tics Lightsheet Microscopy; Kristen Jepsen, Institute for Genomic Medicine; Tami Brown-Brandl, Precision Ani- mal Management	SD, UC, H	11, 12, 13, 14, 15	Incl. 4 campus sca instrument facilities
Molecular Dynamics	Rommie Amaro, UCSD; An- dreas Goetz, SDSC; Jona- than Allen, LLNL	MD, AI, H	11, 12, 13	Incl. a very divers set of sciences an engineering
Human microbiome	Rob Knight, UCSD	G, AI, H	1, 2, 3	
Genomics & Bioinfor- matics	Alex Feltus, Clemson	G, AI, H	13, 14, 15	
Fluid Dynamics	Rose Yu, UCSD	AI	11, 12, 13	
Experimental Particle Physics, IAIFI	Phil Harris, MIT	AI, BGS, SD	11, 12	
Computer Vision	Nuno Vasconcelos, UCSD	AI, CV	13	
Computer Graphics	Robert Twomey, UNL	CV, AI	13	
Programmable Storage	Carlos Malzahn, UCSC	SD	11, 12, 15	
AI systems software stack for FPGAs	Hadi Esmaeilzadeh , UCSD	SD	11, 12	
WildFire Analysis & Prediction	Ilkay Altintas, UCSD	UC, AI, CV	13, 14	

Key: The NRP innovations column lists those innovations among 11 through 15 listed in Section 2.1 that a given science driver most benefits from.

cl. 4 campus scale strument facilities

so much more ...

ncl. a very diverse et of sciences and engineering



FKW's Wishlist for NRP



- Growth of NRP infrastructure
 - 1,000++ GPUs end of 2022 => 1,300 GPUs as of April 2023
 - 50 PB storage end of 2024
 - Growth in diversity of community
 - # and types of campuses and their researchers
- Introduce new capabilities to NRP
 - Machine learning at 100TB scale
 - Support Domain Specific Architecture R&D on NRP
 - Expand NRP into Wireless, Edge, IoT
 - Towards "FAIR" on OSDF
- New Directions initiated by the Community

"Domain Specific Architectures"

- 11: Innovative network fabric allowing "composable hardware".
- I2: Innovative application libraries allowing "domain optimized architectures" on FPGAs



"end of Moore's law" motivates new architectures









- The NSF CC* 2022 program awarded 9 campuses with \$500k storage awards each.
 We guess this pays for 5PB of storage each.
- Some of these campuses may decide to integrate their CC* storage into the OSDF.
- Some of these campuses have storage from other projects that they may integrate with the OSDF in addition.
- NSF 23-523 includes \$500k storage solicitation again, Spring & Fall 2023.





New Infrastructure Coming up in USA

High Performance Data Facility

- DOE is competing (LAB 23-3020) HPDF
 - \$300-500M program that is a Hub & Spokes model.
 - Deadline for proposals was May 5th 2023
- HPDF will serve as foundational element of the "Integrated Research Infrastructure" (IRI)
- IRI = "federated" infrastructure across DOE labs
- IRI Science Patterns:
 - Time-sensitive, e.g. streaming data, instrument steering, ...
 - Data-integration, e.g. analysis of combined data from multiple independent sources, …
 - Long-term campaigns, e.g. large scale archiving and processing for collaborative use and reuse, ...



- Compute resources
- Computing continuum resources

NAIRR gets off the ground.



Summary & Conclusions



- 10 year program to support Federation at multiple locations within the vertical stack
 - From IPMI through K8s to clusters
 - Supporting IPMI & K8s implies a distributed open devOps infrastructure => much more than just federating compute & storage
- DOE sees a need for federated cyberinfrastructure
- USA sees a need to invest into AI Research Resources as an initiative that is coordinated across federal agencies.







 This work was partially supported by the NSF grants OAC-1541349, OAC-1826967, OAC-2030508, OAC-1841530, OAC-2005369, OAC-21121167, CISE-1713149, CISE-2100237, CISE-2120019, OAC-2112167

