#### Dynamic Capability Composition at the Digital Continuum from Edge to HPC

Keynote presentation for the Chesapeake Large-Scale Analytics Conference 2022 October 26, 2022 – Annapolis, MD

#### İlkay ALTINTAŞ, Ph.D.

Chief Data Science Officer & Division Director of Cyberinfrastructure and Convergence Research and Development, San Diego Supercomputer Center Founding Fellow, Halicioğlu Data Science Institute Founding Director, Workflows for Data Science Center of Excellence Founding Director, WIFIRE Lab

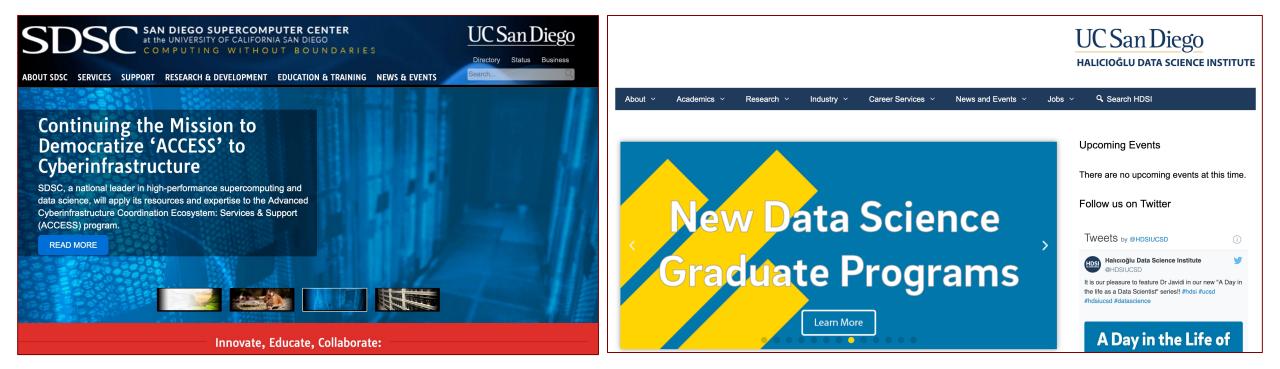
University of California, San Diego

Joint Faculty Appointee, Los Alamos National Laboratory





# UC San Diego





Ilkay Altıntaş, PhD (ialtintas@ucsd.edu)

DSC SAN DIEGO

# Cyberinfrastructure and Convergence Research @SDSC

Translating cyberinfrastructure research for impact at scale

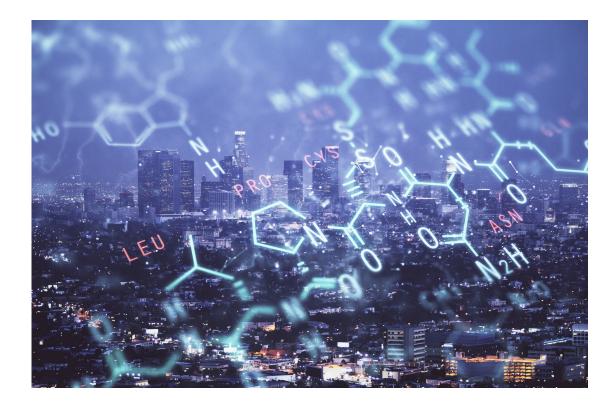
Convergence research is driven by a specific and compelling societal problem and works towards integrating innovative and sustainable solutions into society.

#### Why is data cyberinfrastructure and ML/AI critical?

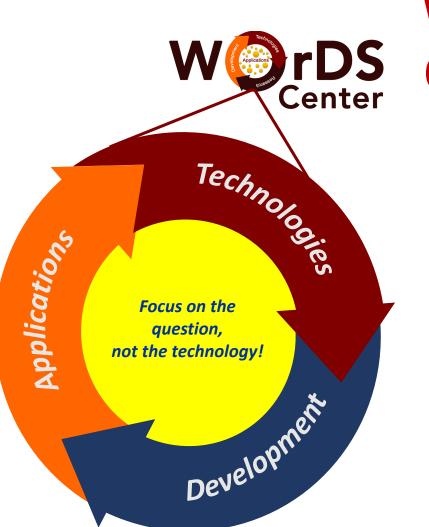
- Number of information sources
- Complexity of the data

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• Number and needs of different users







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# Workflows for Data Science Center of Excellence at SDSC

http://WorDS.sdsc.edu

#### **Research and Development Mission:**

- Methodology and tool innovation to enable collaborative workflow-driven science
- Create solutions on top of big data and advanced computing platforms.



Evolving advanced computing and workflow ecosystem...

# "Big" Data, Computational Science, Data Science, Cyberinfrastructure, and Their Applications



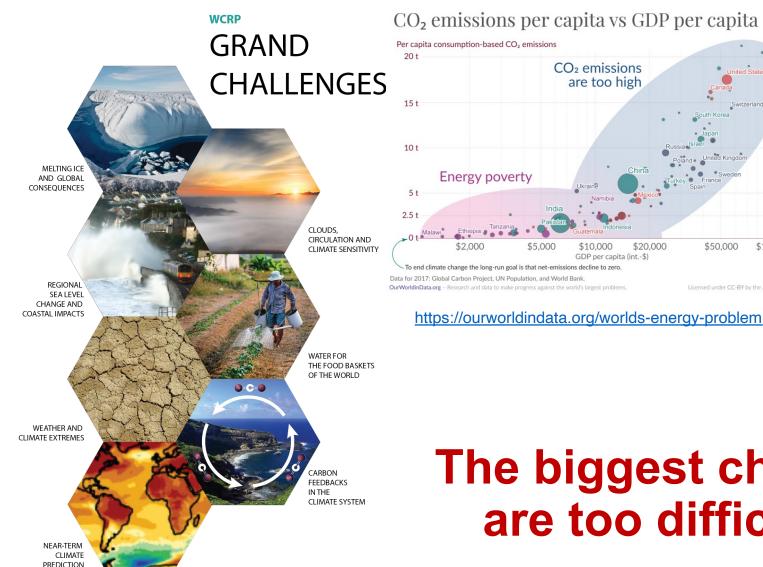


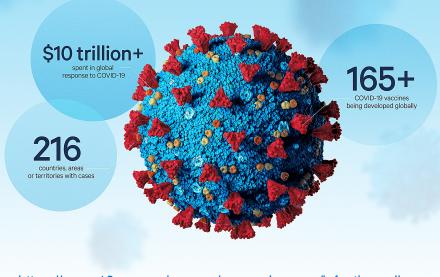
# **Application Context #1**

# We are in the age of complexity!









https://www.10xgenomics.com/research-areas/infectious-disease

#### The biggest challenges of our time are too difficult to solve alone!

Our World in Data

\$50,000

icensed under CC-BY by the author Max Rose

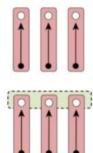
\$100,000

https://www.wcrp-climate.org/learn-grand-challenges





#### **Advanced computing and** data technologies can help, and ... ... we need to collaborate effectively.



#### Disciplinary

- Within one academic discipline
- Disciplinary gal setting
- Development of new disciplinary knowledge

#### Multidisciplinary

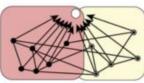
- Multiple disciplines
- Multiple disciplinary goal setting under one thematic umbrella



#### Interdisciplinary

Convergence

- Crosses disciplinary boundaries
- Development of integrated knowledge



 Crosses disciplinary and sectorial boundaries Common goal setting

0

- Develops integrated knowledge for science and society
- Creates new paradigms .

 Stakeholder Participants Discipline

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- Goal, Shared Knowledge Academic Knowledge
  - Thematic Umbrella Conventional Knowledge

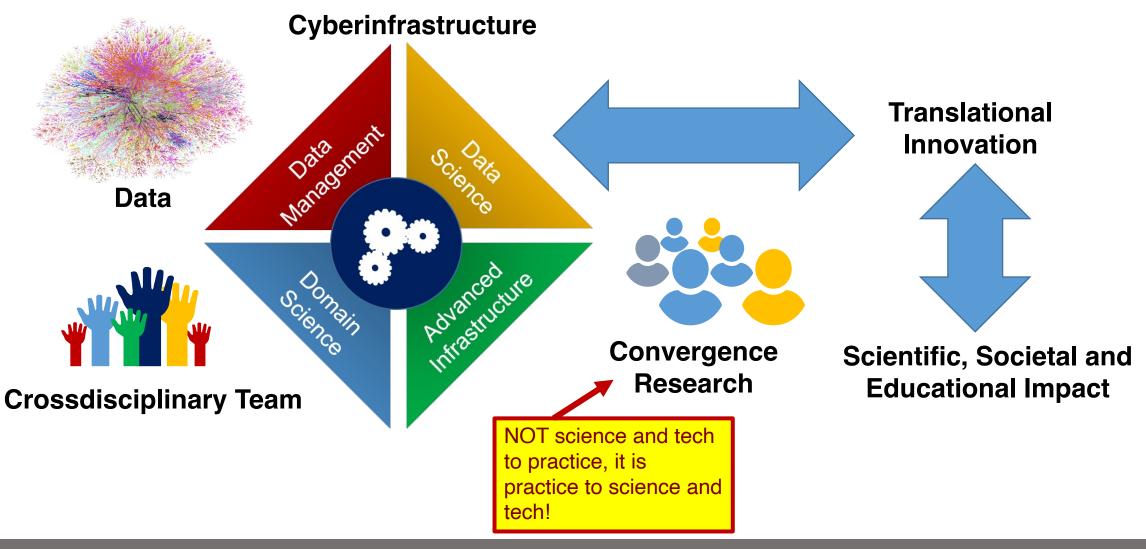
Ilkay Altıntaş, PhD (ialtintas@ucsd.edu)

Adapted from Wright Morton, L., S. D. Eigenbrode, and T. A. Martin. 2015. Architectures of adaptive integration in large collaborative projects. Ecology and Society 20(4):5.





# **Building Cyberinfrastructure Systems for Impact**

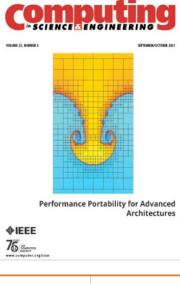






# **Translational Computer Science**

https://www.computer.org/csdl/magazine/cs/2021/05/09547673/1x9TDQr5c2c



Home / Magazines / Computing in Science & Engineering / 2021.05

Computing in Science & Engineering

# Translational Computer Science for Science and Engineering

Sept.-Oct. 2021, pp. 5-6, vol. 23 DOI Bookmark: 10.1109/MCSE.2021.3109962

#### Authors

Manish Parashar, University of Utah, Salt Lake City, UT, USA
 David Abramson, University of Queensland, Brisbane, QLD, Australia









# Systems should enable collaborative teams and thinking!

# Think "teamflows" along with individual workflows.





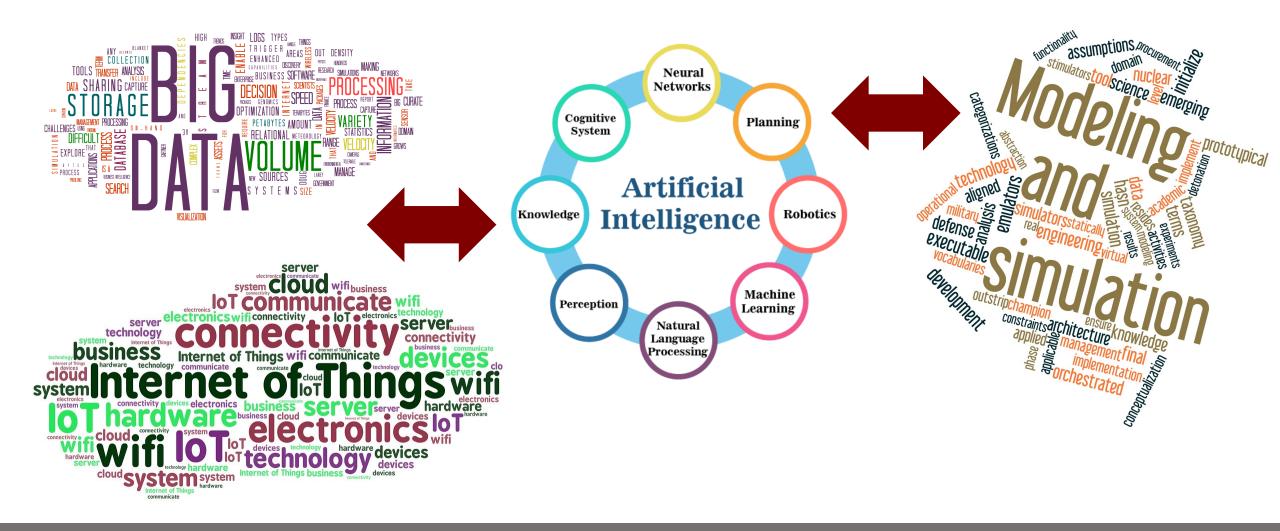
# **Application Context # 2**

### We are in the age of big data and Al!





### **Al-Integrated Applications at the Digital Continuum**

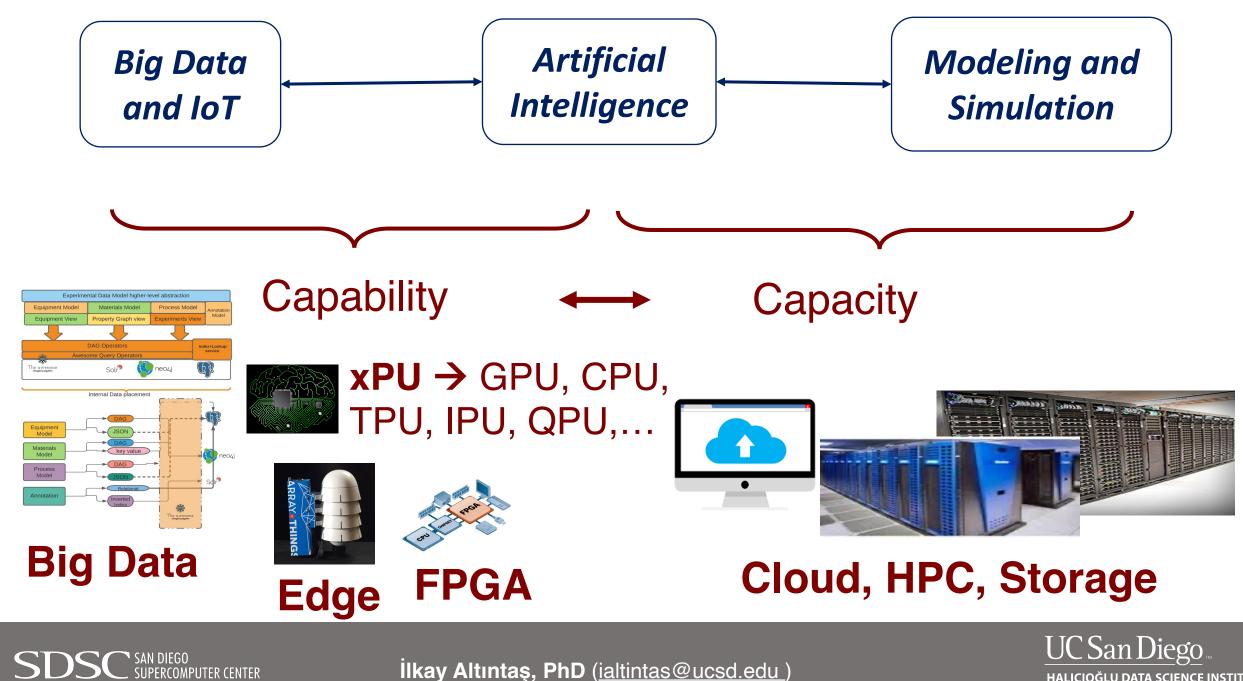




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HALICIOĞLU DATA SCIENCE INSTITUTE

# **Evolution of Applications with Al**

- Thinking in workflows moves AI closer to solutions in integrated applications.
- Teamwork is key to these workflows -- think workflows and teamflows!
- Enabling science and solutions requires open and transparent sharing and use of big data.
- Continuous integration of computing, data and AI into workflows needs dynamic systems capacity.

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#### Release Date: May 10, 2022



**Consensus Study Report** 

<u>https://www.nationalacademies.org/our-</u> <u>work/realizing-opportunities-for-advanced-and-</u> <u>automated-workflows-in-scientific-research</u>





# Systems should enable seamless integration of Al-integrated application workflows!





# **Application Context # 3**

## We are in the age of many systems!





# wire

#### NSF Funds Five New XSEDE-Allocated Systems August 7, 2020

Aug. 7, 2020 — This summer, five new National Science Foundation (NSF)-Jetstream 2 (Indiana University / Texas Advan University of Arizona / Arizona State University ded advanced computing systems have been awarded to partner University Corporation for Atmospheric Researcitutions across the country, all with their own unique specialties and

lications. Once deployed, all of these systems will be primarily allocated The NSF has awarded a \$10 million gran distributed cloud computing system to sur ugh XSEDE to help connect researchers, regardless of physical location artificial intelligence, and enhanced large he United States, to the system that best suits their research needs. nation. The project is led by the Pervasive

SDSC

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Indiana University. Jetstream 2 is a follow e recent was funded in 2014 as the NSF's first pro engineering research cloud system for the Ouncements

Delta (National Center for Supercomputing Apawards by

NCSA will integrate Delta into the nationa NSF is a through XSEDE. Integration into XSEDE ar indicator substantial portfolio of services and suppl deliver unprecedented advances in reseahe NSF's re-

collaboration will promote synergy among include campus, national, and commercia

#### Anvil (Purdue University)

University of Hawaii)

Anvil, which is funded by a \$10 million aw the People Who Bun The significantly increase the capacity availab has been a partner for the past nine year 2021 and will serve researchers for five y oloaies the NSF will support Anvil's operations ar

Neocortex (Pittsburgh Supercomputing Center

A \$5 million NSF award will allow PSC to performance artificial intelligence (AI) sys fundamentally new hardware to greatly st D-19 research organization of Carnegie Mellon of Pittsburgh, will build the new supercon with Cerebras Systems and Hewlett Packurce Library

Voyager (San Diego Supercomputing Center) dast

The NSFhas awarded DSC at UC San Div develop a high-performance resource for Channel research across a wide swath of science Called Voyager, the system will be the fire ank NSF resource portfolio. In addition to the our Authors equivalent amount of funding is expected anaggment and appration of the recou

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amazing feat of science and technology. But it was not designed for the massive data sets, machine-learning tools, advanced sensors and Internet of Things devices that have become central to many research and business endeavors and our homes.

ILLINOIS NCSA | National Center for

Supercomputing Applications

#### Funded with a \$20 million grant from the National Science

Foundation, FABRIC (Adaptive Programmable Research Infrastructure for Computer Science and Science Applications) is exploring ways to replace an internet infrastructure that's been showing its age for the last 20 years

NCSA is one of 13 collaborating institutions helping create a platform for testing novel internet architectures that could enable a faster, more secure Library internet better suited for today's users and future needs. One that's also able to do things not possible now. The FABRIC project is led by the Network Research and Infrastructure Group at RENCI at the University of North Carolina at Chapel Hill.

#### NCSA: First with the Gigs

Last fall, NCSA installed a 100-gigabit network connection that's dedicated solely to the FABRIC project, the first FABRIC collaborator to do so.

NCSA already had six 100-gigabit internet connections, says David Wheeler, leader of NCSA's ICI Data Management and Delivery Division and the

## Some recent news...

vire

#### **Business Wire**

#### **GigalO Awarded Lonestar6 Contract in TACC's First Bid for Composable Disaggregated Infrastructure**

2021

di Business Wire



#### September 24, 2021

nle Who Run Then

hannels

Authors

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"Exascale only becomes valuable when it's creating and using data that we care about," said Pete Beckman, co-director of the Northwestern-Argonne Institute of Science and Engineering (NAISE), at the most recent HPC User Forum. Beckman, head of an Argonne National Laboratory edge computing project called Waggle, was insistent on one thing: edge computing is a crucial part of delivering that value for exascale.

Beckman had opened with a guote from computer architect Ken Batcher: "A supercomputer is a device for turning compute-bound problems into I/Obound problems." "In many ways, that is still true today," Beckman said. "What we expect from supercomputers is that they're so blindingly fast that really it's bottlenecked on either reading or writing from input or output.'

"If we take that concept, though, and flip it over," he added, "then we end up with this idea that edge computing, therefore, is a device for turning an I/Ohound problem into a compute bound problem

GigalO Selected to Bring Composability to Bold New National Research Platform

\$BAD, Calif., July 16, 2021 — Building on the successes of past orations with the San Diego Supercomputer Center (SDSC) located at an Diego, GigalO, the creators of next-generation data center rack-scale ecture for artificial intelligence (AI) and high-performance computing solutions, is proud to be announcing its low latency universal dynamic FabreX, was selected as the technology of choice for the new type National Research Platform (NRP). This National Science dation-funded cyberinfrastructure ecosystem is an innovative, all-in-one -computing resources, research and education networks, edge uting devices and other instruments—designed as a testbed to expedite ce and enable transformative discoveries

plex computational and workflows underpin many of entific research ges we hope to address RP," says Dr. Frank vein. PI of NRP. and director of the San Diego computer Center. "In areas



rse as public health, high energy physics and wildfire response, this rch requires that we aggregate disparate computational elements, such GAs, GPUs, x86 processors and storage systems into highly usable and



# The problems we are solving are ... • heterogeneous

#### **EXISTING SYSTEMS:**

- data (storage + data/knowledge management)
- continuum of distributed computing (edge, cloud, HPC)
- high speed connectivity (programmable networks)

#### data and Al-integrated

- collaborative

#### **GROWING NEEDS:**

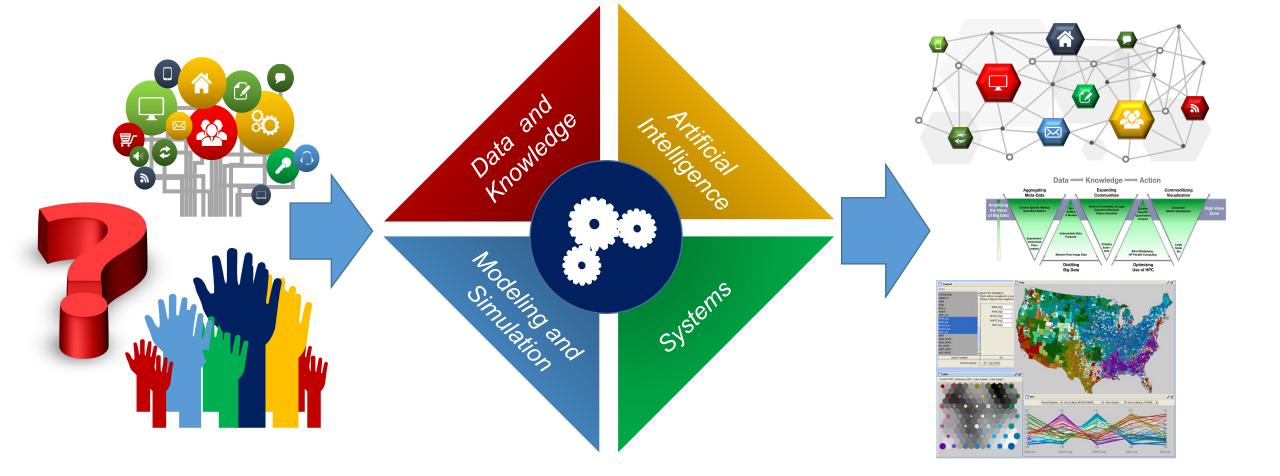
- Interoperability
- Dynamic scalability
- On-demand interactive access
- Performance measurement
- Composability





We need to think and build strategic ecosystems made up of reusable services and solutions toward capability integration!





# **A Typical Application Integration Ecosystem**



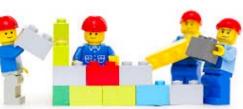


# Integration requirements...



Dynamic composability matters.

# Systems and services are only useful if



groups can integrate them into applications.

# **Teacher Coupled with responsible AI systems.**







#### **Dynamic composability matters.**

#### **COMPOSABLE SERVICES**

e.g., model and data archives, learning and analytics, simulation, training

#### **RESOURCE MANAGEMENT**

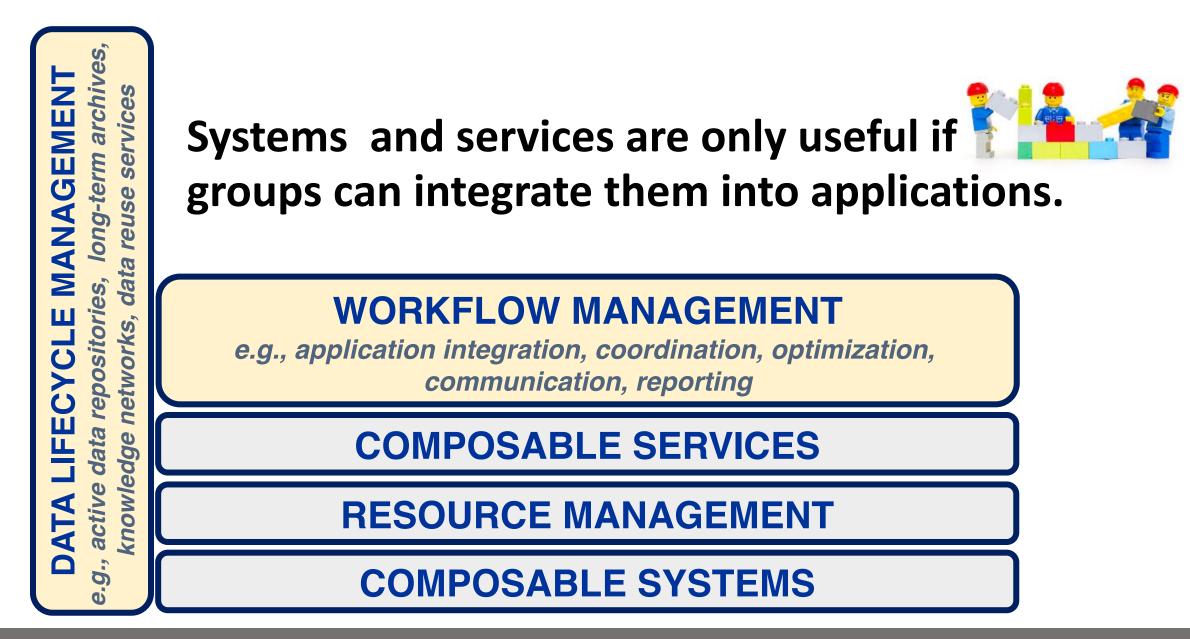
e.g., container orchestration, optimization

#### **COMPOSABLE SYSTEMS**

e.g., GPU, CPU, Big Data, quantum, neuromorphic, SDN, storage









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# REPRODUCIBILITY

**TEAM SCIENCE** 

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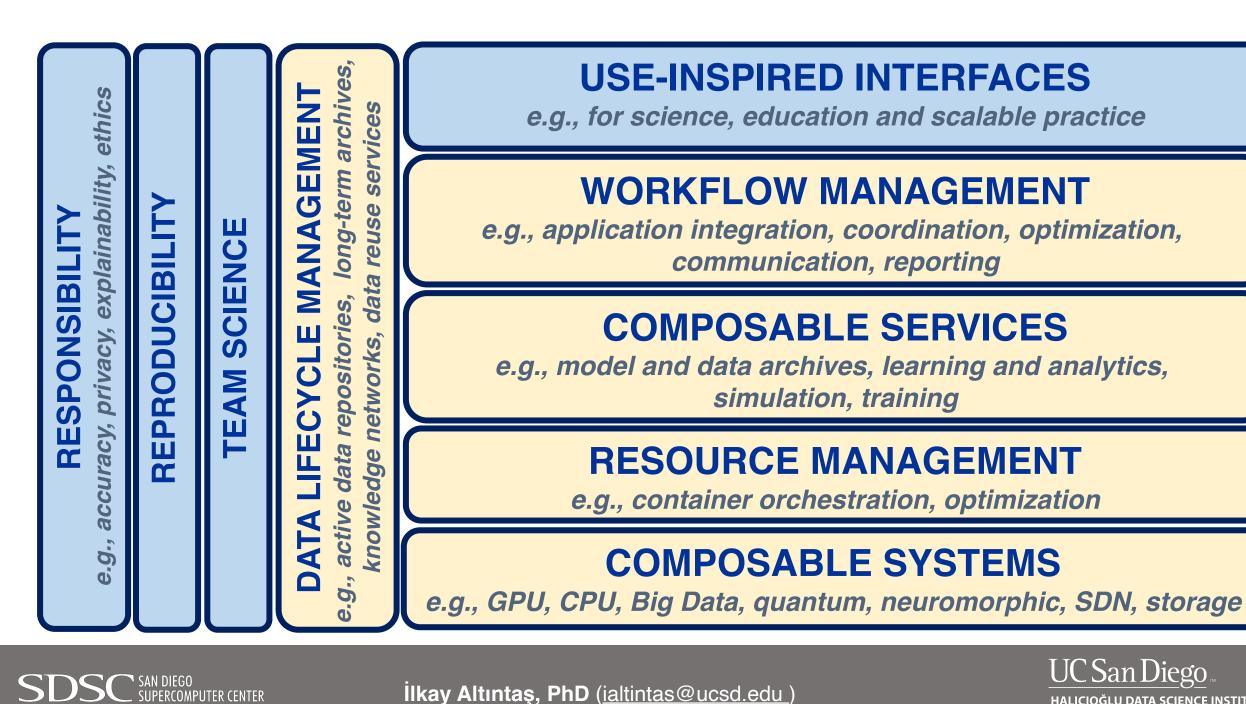
#### **USE-INSPIRED INTERFACES**

e.g., for science, education and scalable practice

# Tools that enhance teamwork and use need to be coupled with responsible AI systems.

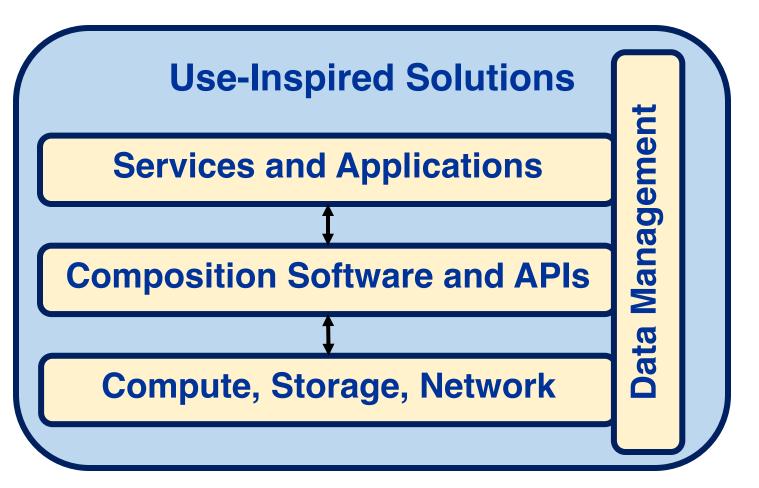








# **Smart Composability from Systems to Services**



- Dynamically measure, manage and provision resources
- Create plug and play microservices
- Run across many systems
- Capability-based integration
- Improved FAIR data capacity





# **Some Composable Systems**



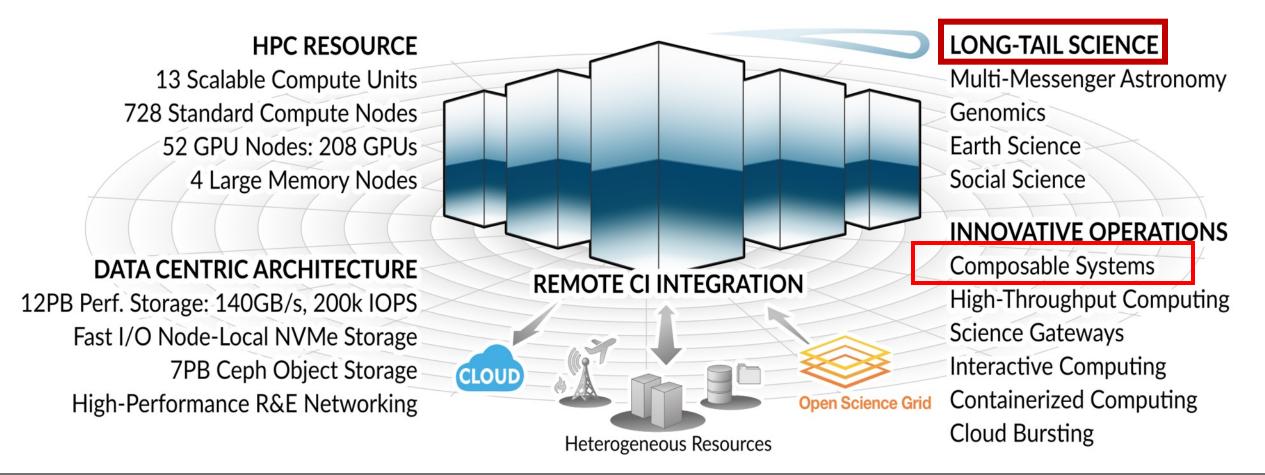




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#### EXPANSE COMPUTING WITHOUT BOUNDARIES 5 PETAFLOP/S HPC and DATA RESOURCE





- Two partitions exist in Expanse
  - Slurm
  - Kubernetes
- Dynamic provision
  via cm-scale (Bright
  Computing)
- User Web Portal (ACCESS)

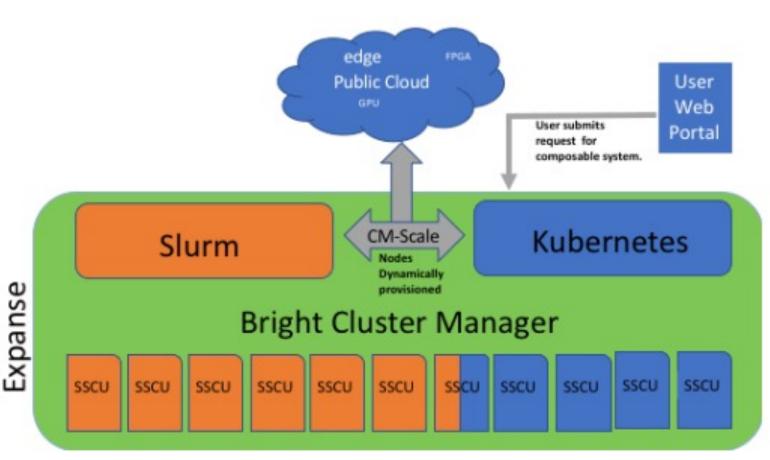


Figure 5.1 Expanse Composable Systems Framework





# Nautilus – PRP and NRP

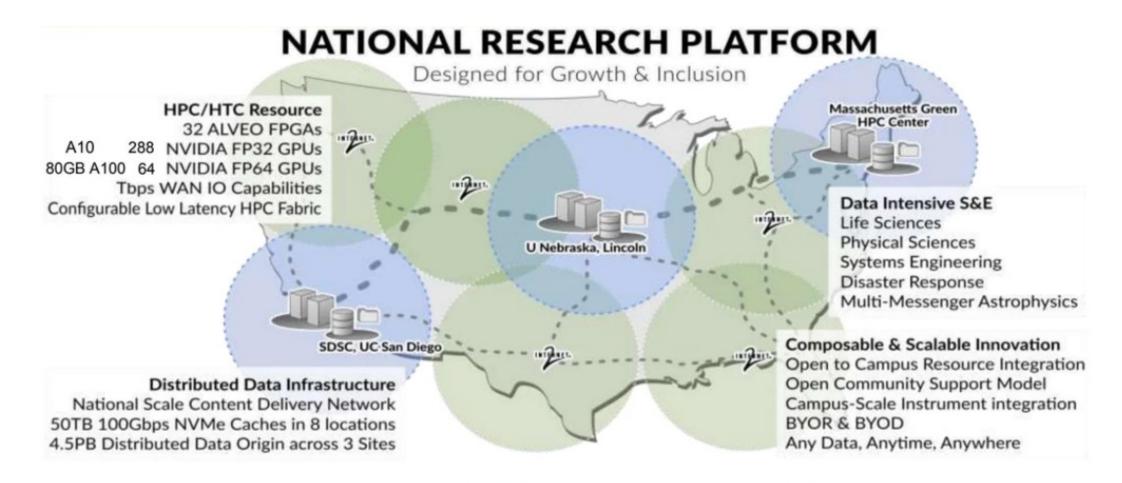


Image Source: https://pacificresearchplatform.org/nautilus

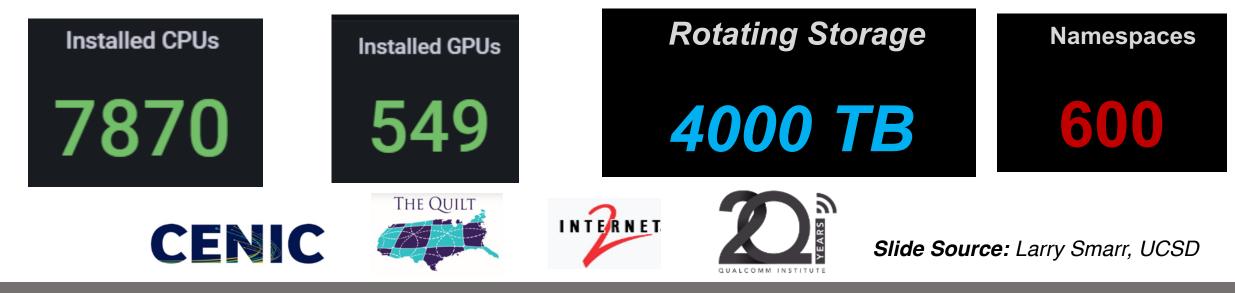




#### Nautilus is a Multi-Institution Hypercluster Connected by Optical Networks



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



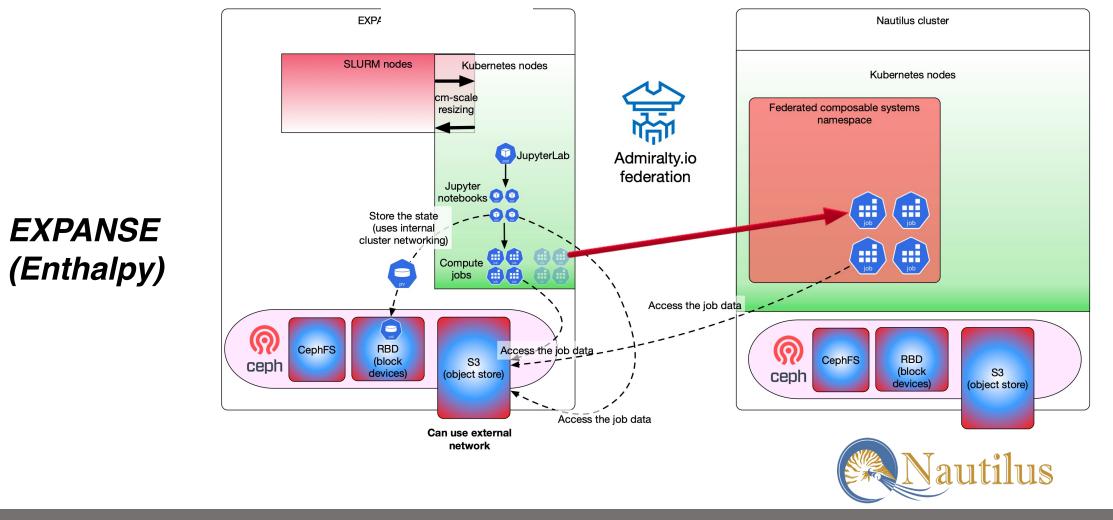


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#### **Composable System using Admiralty for Federation**

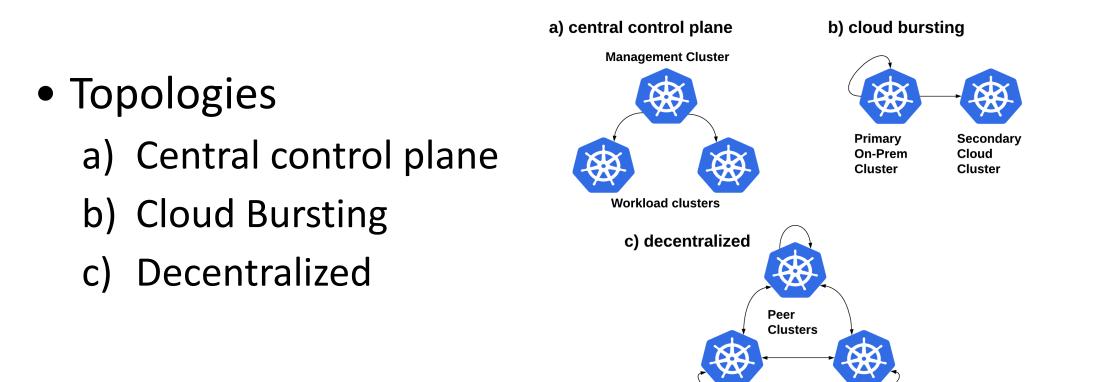
#### EXPANSE (Enthalpy) + CHASE-CI (Nautilus)





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# **Admiralty Federation Topologies**







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#### Sensor/Instrument

Put AI@Edge HERES

#### Al@Edge and the Digital Continuum



Slide Source: Pete Beckman, ANL















#### **Education & Training**







**Ao**T

**VUWI** 







Ilkay Altıntaş, PhD (ialtintas@ucsd.edu)

Triggered Computation Deep Learning Training



#### **Sensors**



Software Defined Radios



Hyperspectral Imaging

#### **Facilities**

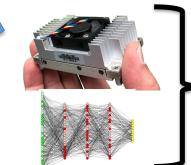


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Dynamic adaptation





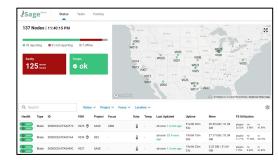
Scientific Data Analysis & Control

Artificial Intelligence Deep Learning Inference Lightweight Training

Slide Source: Pete Beckman, ANL

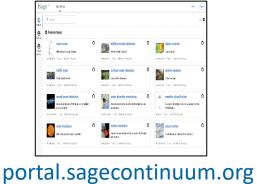
#### admin.sagecontinuum.org

**Scientific Digital Continuum in Sage** 



#### **Advanced Wireless & Networking**

#### New inference (model) Adaptive steering



#### Computation







Digital Twin Data Analysis Machine Learning

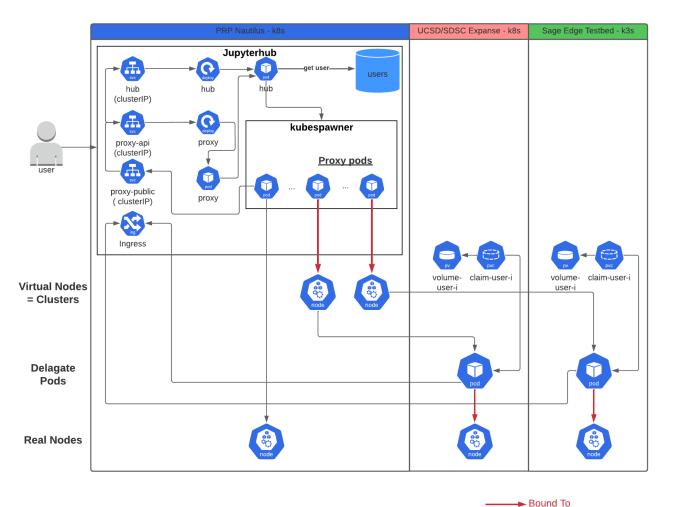


### Using Expanse, NRP and Sage for Edge Al Development





#### Integration of NSF EXPANSE, PRP and Sage A Composable System Deployment of JupyterHub



PRP Nautilus Expanse

- Edge-Cloud Unified Environment for prototyping AI models to deploy on the Edge
- A user can easily be provided the right environment for developing their AI Edge Application





**Spawner Options** /home/jovyan is persistent volume, 5GB by default. Make sure you don't fill it up - jupyter won't start next time. You can request increasing the size in Matrix GPUs 0 Cores 1 RAM, GB 8 GPU type Any  $\sim$ /dev/shm for pytorch Mount CephFS (if assigned) You can request assignment in Matrix Kubernetes Stack options are described in docker-stacks Image Spawned 0 Stack Minimal 0 Stack Minimal + Desktop GUI Exploration 0 Stack Scipy 0 Stack R 0 Stack Tensorflow ۲ Stack Tensorflow + PRP added libs 0 Stack Datascience 0 Stack Pyspark 0 Stack All Spark

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Tensorflow 1.14 (deprecated, choose one above)

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Pod

for

#### **Data federation is still a big deal!**

Needs to be coupled with data systems, knowledge networks, and commons frameworks.





### Application of Composable Systems in Fire Science and Management





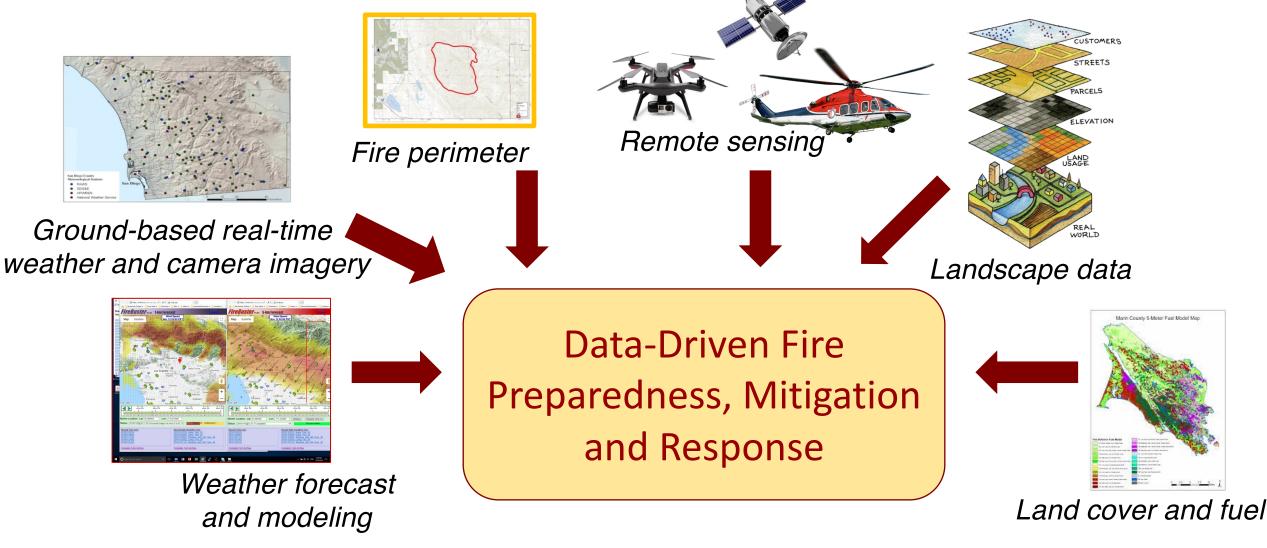
### Fire is an inevitable part of nature, but megafires are not.







#### Next generation fire prediction combines emerging fire science with data from many sources.





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### WIFIRE

wifire.ucsd.edu

### **F**<sup>†</sup>**REMAP**

Initial Attack Fire Response





Edge AI services and data plugins





BurnPro<sup>3D</sup>

**Prescribed Fire Optimization** 



Powered By

(**WIFIRE**)) Commons

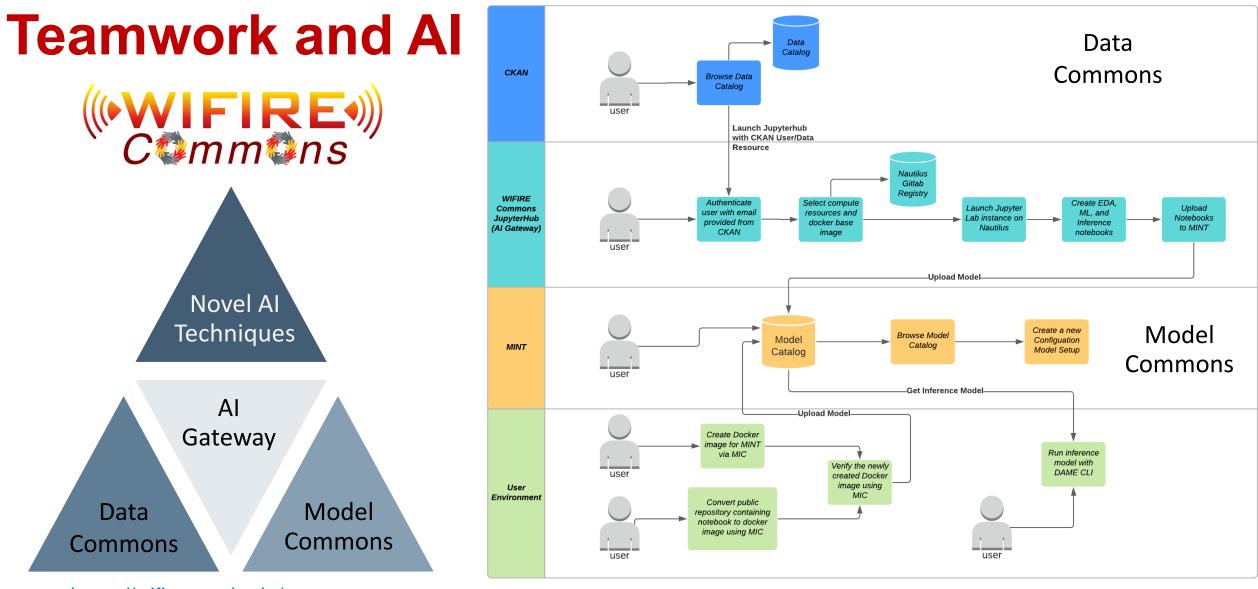
FAIR Data and Model Catalog and AI Gateway









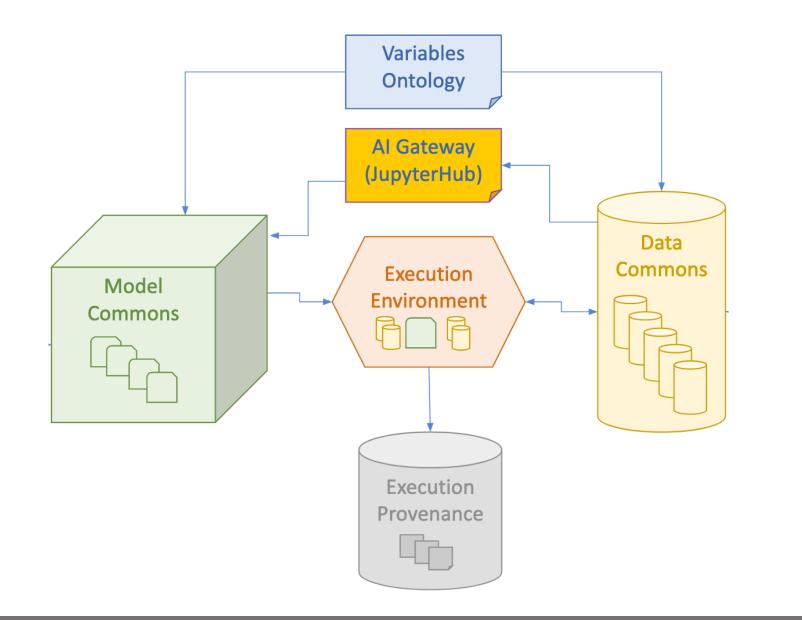


https://wifire.ucsd.edu/commons

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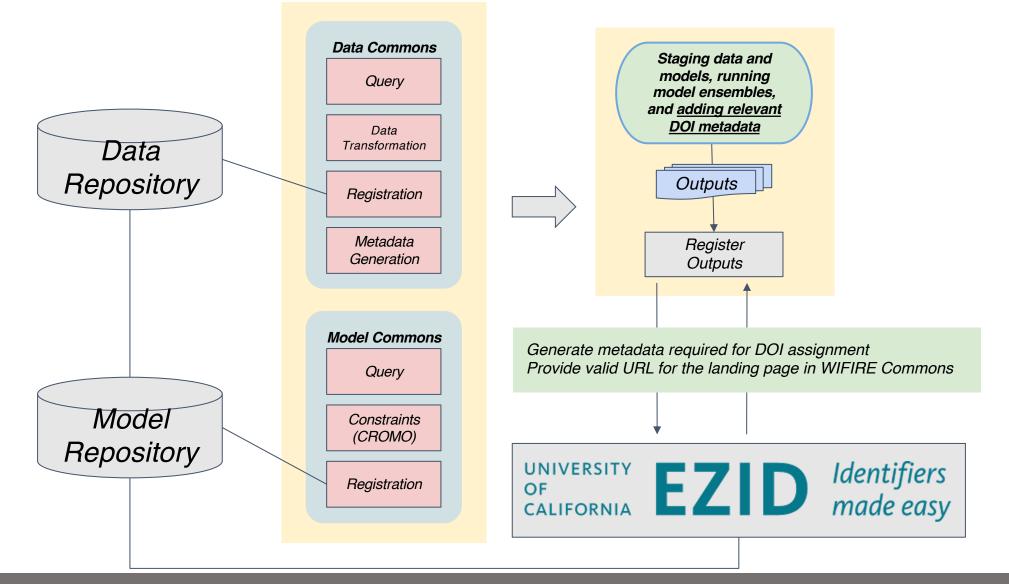


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#### Linking Data and Models to Open Knowledge Networks



#### **DOIs for Models and Datasets**

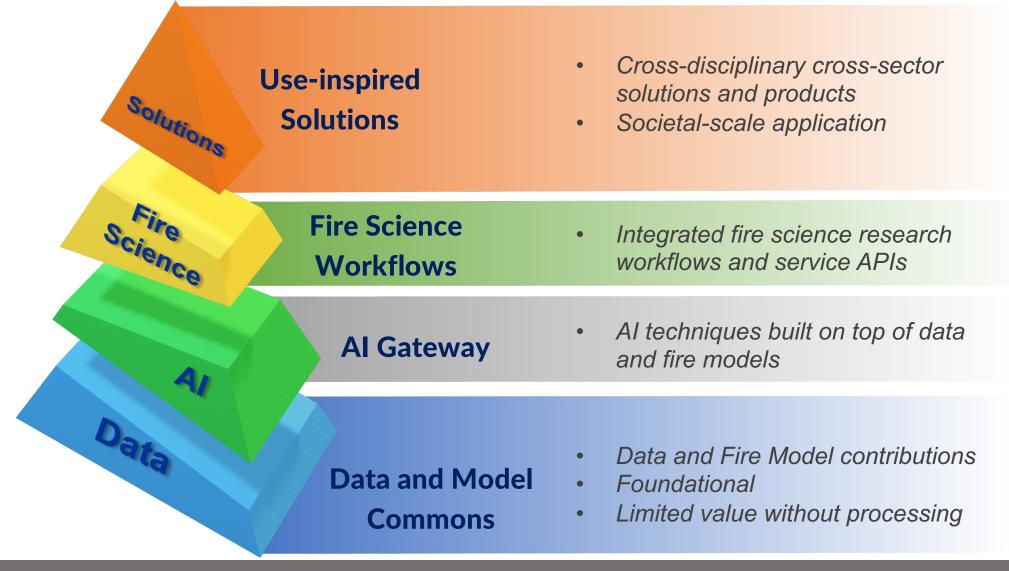




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### **Data to Value in WIFIRE Commons**







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### **AI Gateway** → Pangeo Customized for AI and Fire Science

https://wifire-commons-pangeo-jupyter.nrp-nautilus.io/

INTAKE

DASK .

Al-Ready Ensemble Datasets stored in cloud-optimized Zarr format

Ceph

distributea

FastFuel

Zarı

format for cloud-optimized

N-dimensional arrays

storage of chunked, compressed,

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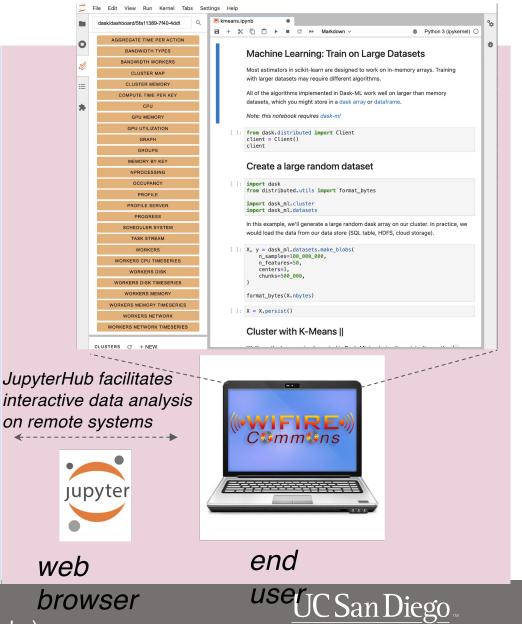
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Tech stack supporting scalable analysis of large wildfire datasets Nautilus PRP Label-based indexing and arithmetic Wide range of input/output xarray options: netCDF, HDF, geoTIFF, Zarr

Data cataloging utility

Parallel processing

browser



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### (•WIFIRE•) Focus on Two Ways to Manage Wildland Fires



#### **Fighting Severe Wildfires**

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#### Conducting Prescribed Burns



#### **AI-Integrated Real-time Fire Response In WIFIRE**

#### WIFIRE Firemap





**FIRIS** 



### **Dynamic Data-Driven Fire Modeling**

#### **Data and AI Needs**

- -- Characterizing the dynamic fire environment : Variation of wind, smoke, moisture, fuels, fire perimeter, ...
- -- Detection of fire ignitions
- -- Decision support for fire management
- -- Prediction of potential fire ignitions

#### **Heterogenous Computing Needs**

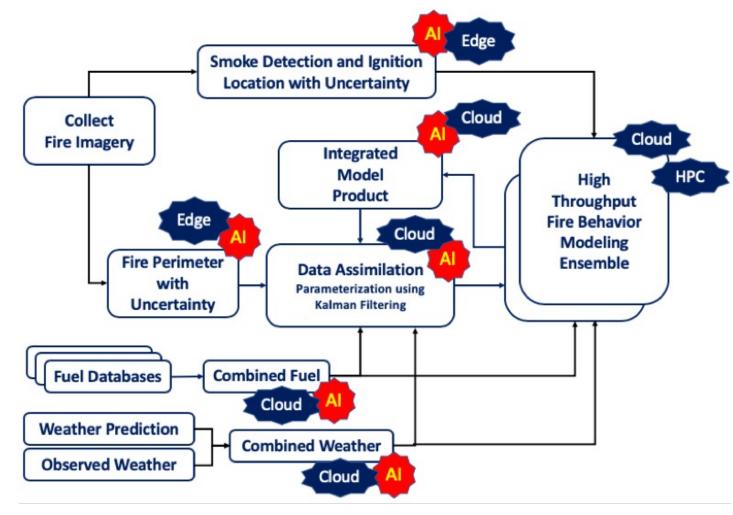
-- Edge

-- AI processors

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- -- Cloud
- -- HPC





### **Deep Learning-Based Smoke Detection**

#### **CITE:** <u>https://www.mdpi.com/2072-4292/14/4/1007</u>



**Data:** Camera images of wildland fires

 System Architecture: Several deep learning models to extract spatio-temporal information from camera imagery to detect smoke plumes.

**Training Data:** Labeled camera images

**Computing:** Edge and composable systems







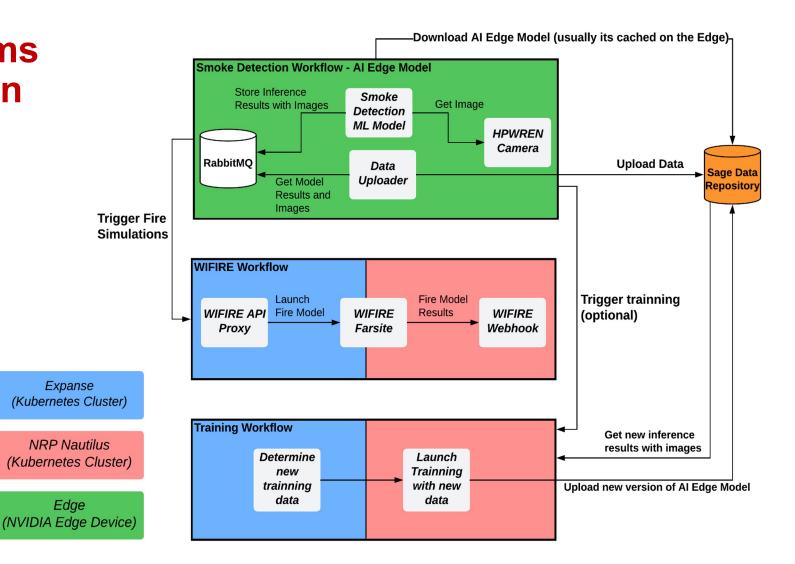
#### Fire Simulations using Composable Systems and Edge Smoke Detection

- Three workflows
  - Smoke Sage Edge App
  - Fire simulator
  - Al Training

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 Both the fire simulator and training workflows are can be run on Expanse or Nautilus through the federation layer





## **Prescribed Burns**

### **Transformational Science**

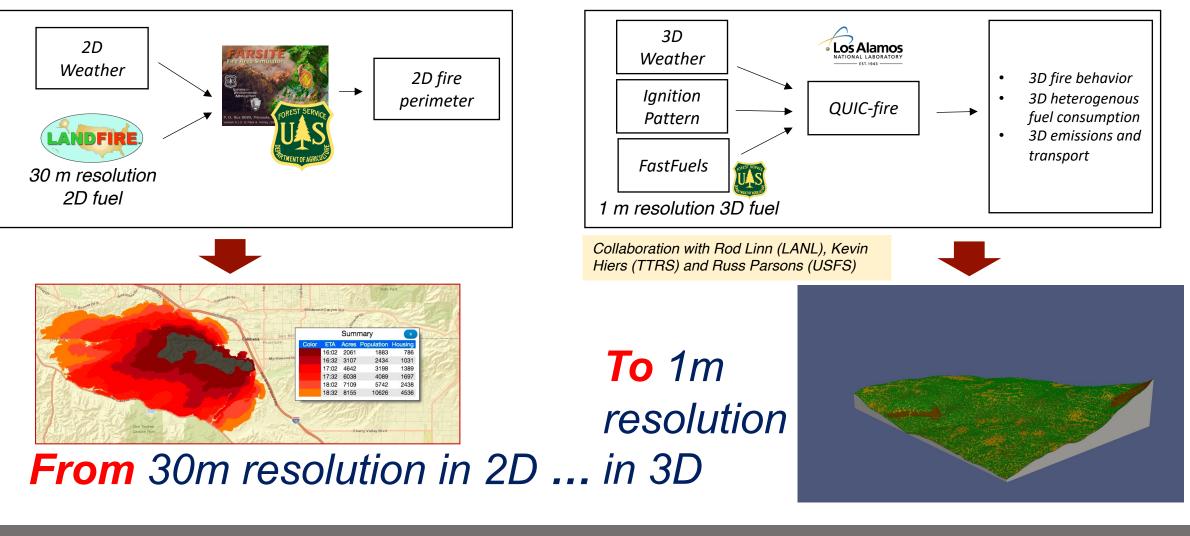
### Fast 3D is better than 2D!







# Next-generation fire models provide the right science basis for proactive mitigation and management decisions.

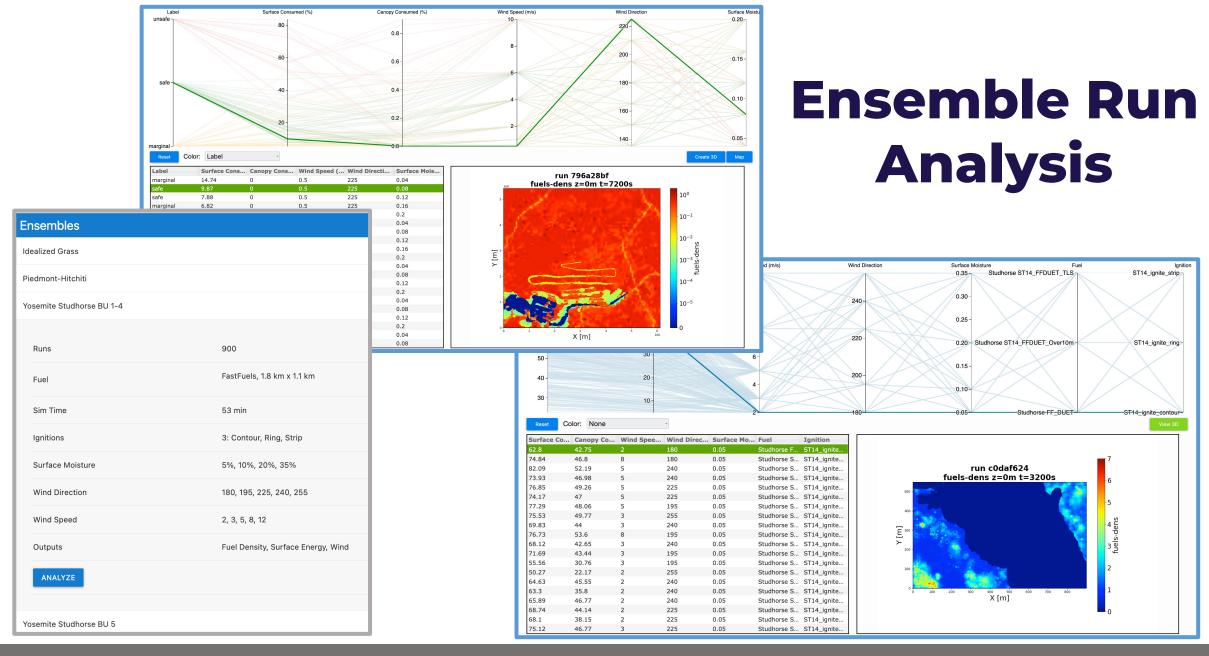




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### **Emerging AI Needs for Next Generation Fire Modeling**

• High-res, 3D and dynamic fire environment data

• Speed, flexibility, and interpretability of fire models























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The BurnPro<sup>3D</sup> platform gives our public sector partners next-generation fire science using data and AI to optimize prescribed burns at an unprecedented scale.





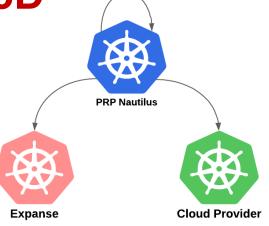








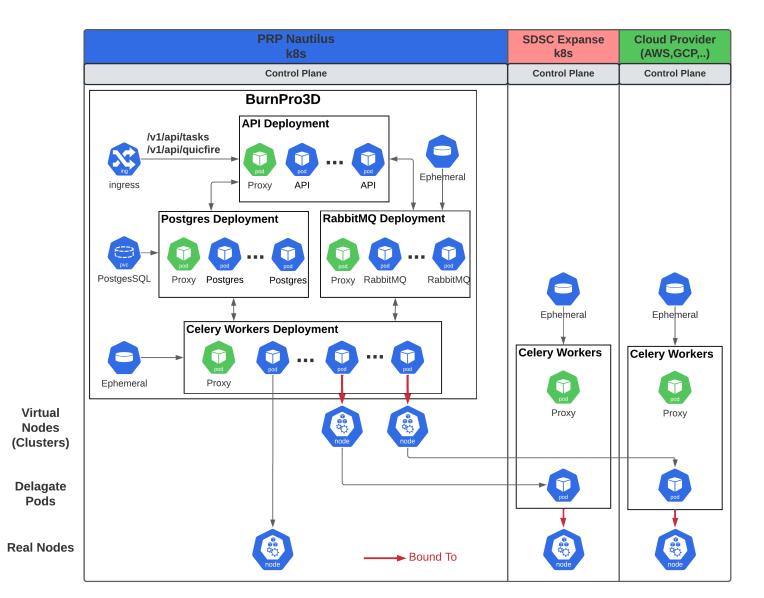
#### 3D Fire Simulation Ensembles using Composable Systems in BurnPro3D



 Instead of deploying all the services on each cluster we only federate over the pods that are performing the fire simulation

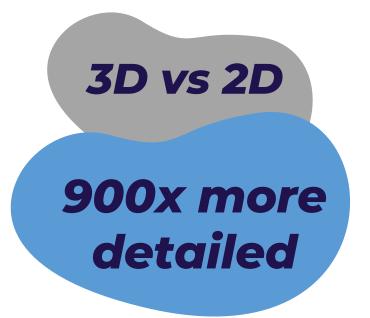
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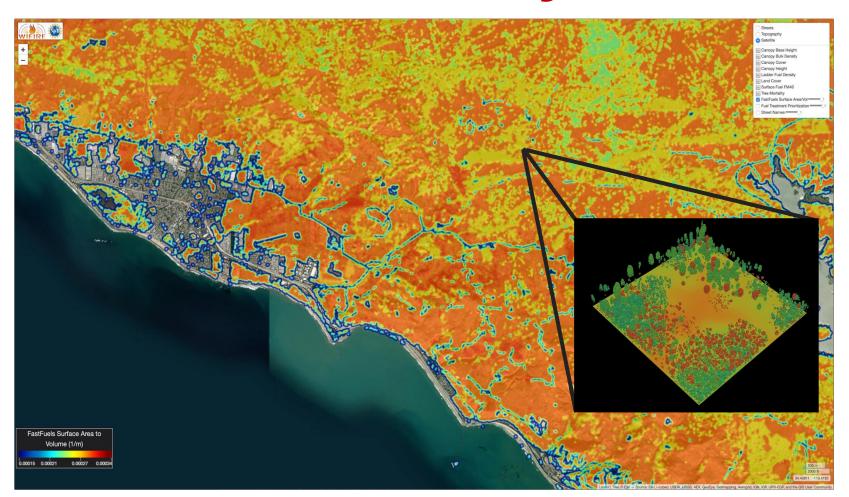


### Al Techniques to Condition Data and Improve Model Accuracy

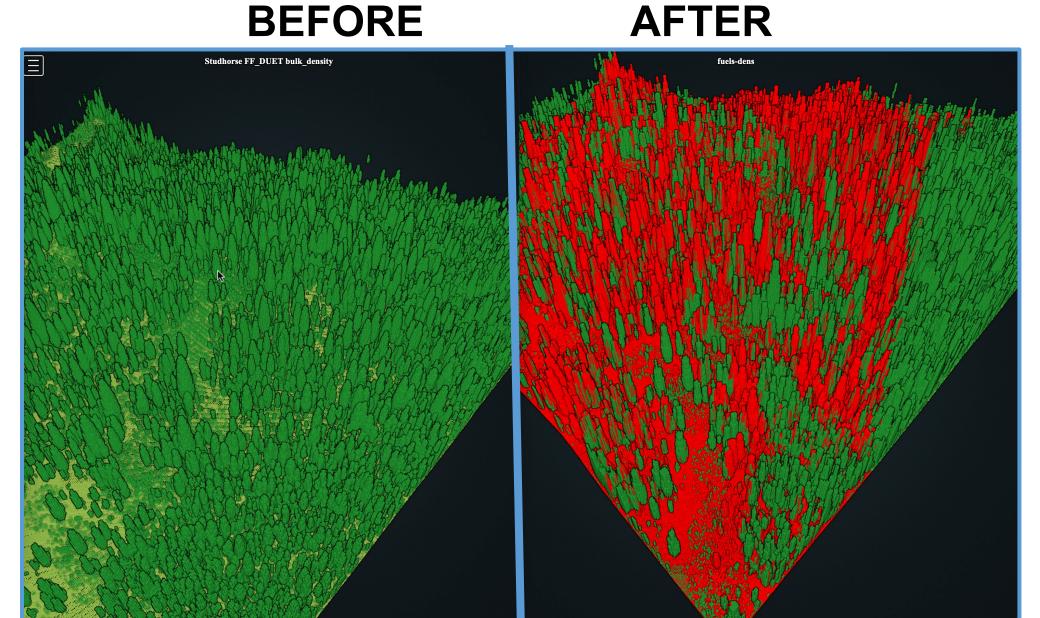


Collaboration with Rod Linn (LANL), Kevin Hiers (TTRS) and Russ Parsons (USFS)

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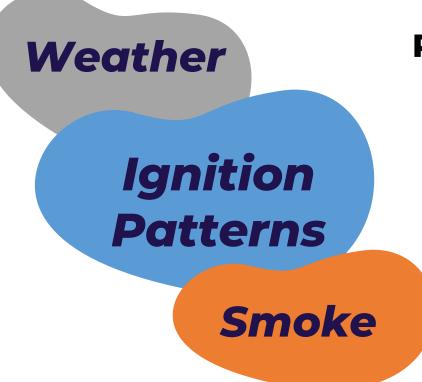




#### Yosemite National Park

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### **AI Techniques to Improve Decision Making**



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#### **PHYSICS-GUIDED MACHINE LEARNING**

To improve predictive fire behavior models

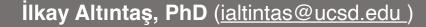
#### **OPTIMIZATION**

To address complex tradeoffs and prioritization

#### **EXPLAINABLE AI**

To increase scientific understanding and interpretability all along the decision-making chain



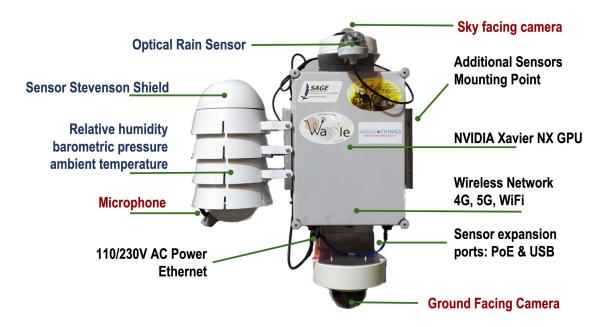


### High resolution data from Sage is needed for understanding of the prescribed fire environment at the resolutions required.

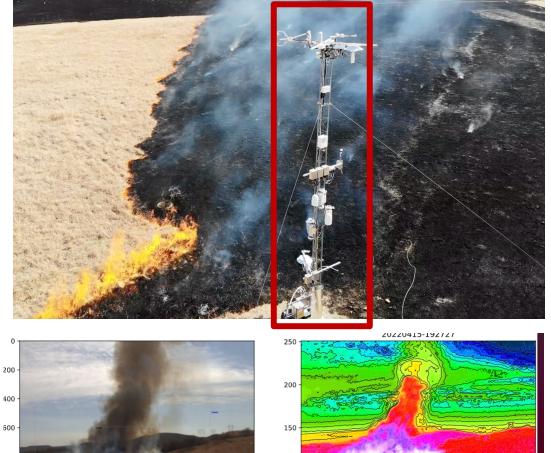




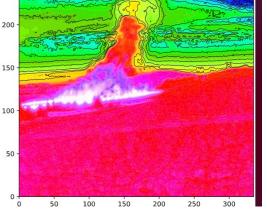
#### NEON Mobile Deployment Platform (MPD) with SAGE Konza Prairie for controlled burn: April 2022.











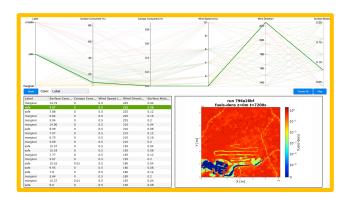


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#### Konza Site Prescribed Fire Scenario



#### BEFORE

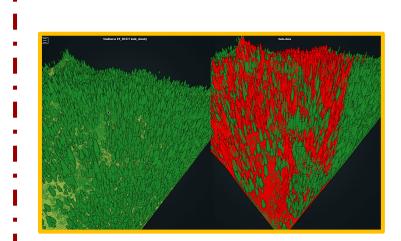


- Run ensemble
  models of the burn
- Decide on burn prescription

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Make Sage NEON
 mobile unit request

**DAY OF** 



 Make Go/No Go decision

- Deploy edge AI for smoke detection and environment monitoring
- Set up Sage dashboard

| (WIFIRE)<br>Commons  | DATASETS ORGANIZATIONS ABOUT Search   |
|--|---|
| # / Organizations / SAGE - NEO   | DN / NEON MDP / Sage / WIFIRE   |
| NEON MDP / Sage / WIFIRE<br>BP3d: Konza Prairie Burn<br>Experiment   | NEON MDP / Sage / WIFIRE BP3d: Konza Prairie Burn   |
|  | Experiment  |
| Dataset extent   | The Korean Parisine Biological Solitonis, Nozardi in the File Hills of entreheusteen to searce, in our of the bist statistic tubyra<br>paralises, Weinking with the Korean Parising Statistics (ROM and the Sang Parises than caliboand to diagity a IKOU<br>mobile diagityment platform (MOP) suppresented with Sang and Tables and |
|  | Data collected on April 15, 2022 include images from a thermographic camera, RGB cameras, particle sensors, and<br>more. Al algorithms analyzed some of the data streams in real time, while other data streams logged the events and<br>will be used later with advanced self-supervised Al algorithms to improve algorithms, build training data sets, and he<br>scientists better understand the earth's atmospheric and environmental processes.  |
| Titles by Stamen Design (CC BY 3.0)  | See the following jupyter notebook as a reference for accessing the data:<br>https://github.com/iperezr/sage-smoke-detection/blob/master/post-processing/sage-data-client.lpynb   |
| *  | Data and Resources  |
| <b>SAGE</b>  | reading.sensor.csat3.pkl  |
|  | reading.sensor.g2131L.raw.pkl   |
| SAGE - NEON  | reading.sensot.hfp01sc.pkl  |
| The Sage project is designing and<br>building a new kind of national-scale<br>reusable cyberinfrastructure to enable | reading.sensor.hmp1SS.pkl   |
| Al at the edge.<br>https://sagecontinuum.org/ The  | reading.sensor.(2130L.raw.pkl 🛹 Explore   |
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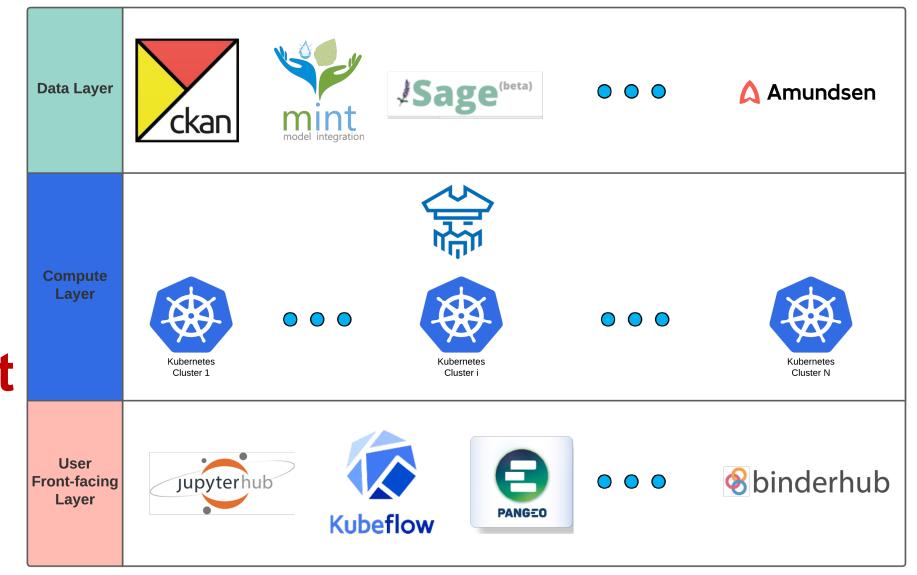
- Publish data in WIFIRE
  Commons
- Conduct post-fire model evaluation
- Create adaptive prescribed burn strategies



Use Case: Generalized Application Development

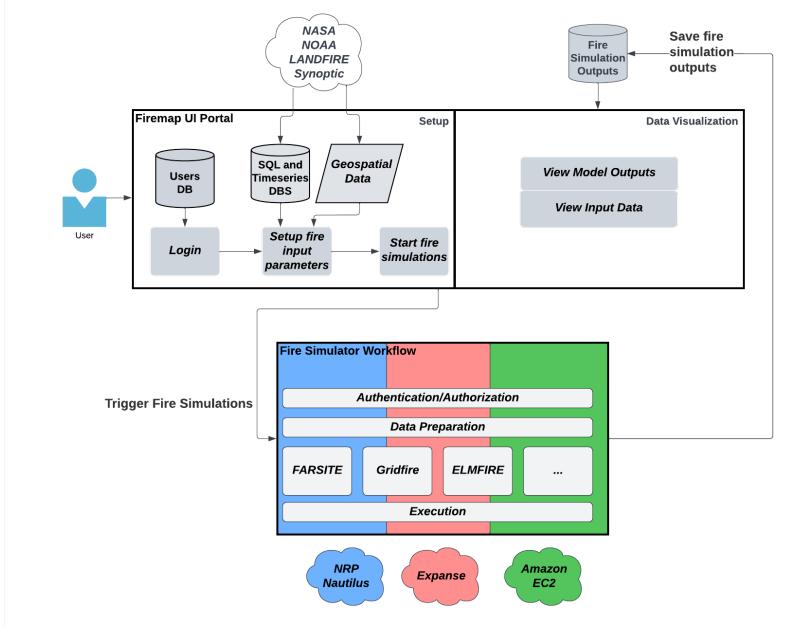
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Use-Case: Many Fire Simulators Workflow

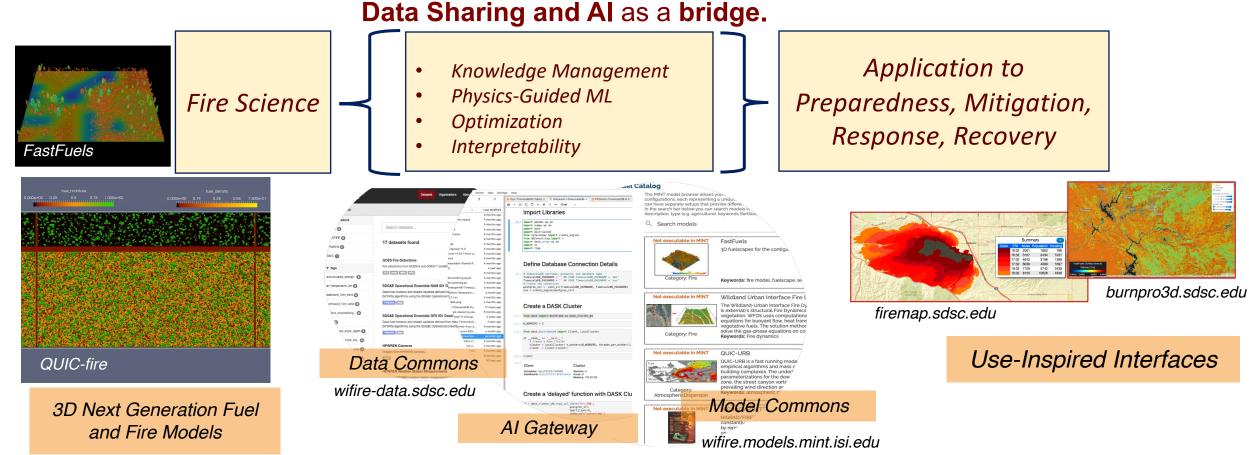






### powered by WIFIRE Commons

A Data and AI Framework for Convergence in Wildland Fires





Ilkay Altıntaş, PhD (ialtintas@ucsd.edu)

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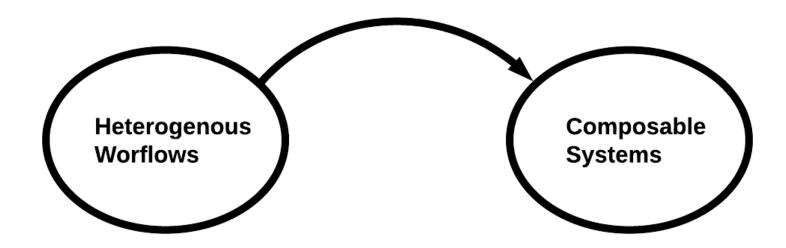
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### Mapping between Heterogenous Workflows to Composable Systems

Ikay Altıntaş, PhD (ialtintas@ucsd.edu)

- Burnpro3D: Prescibed Fire Planning Platform
- JupyterHub: Sage Edge App Development and WIFIRE AI Gateway
- Other projects
  - Neurokube: Al Neuroscience imaging
  - TemPredict for IoT use in COVID detection

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M. Madany, K. Marcus, S. Peltier, M. H. Ellisman and I. Altintas, "NeuroKube: An Automated and Autoscaling Neuroimaging Reconstruction Framework using Cloud Native Computing and A.I.," 2020 IEEE International Conference on Big Data (Big Data), Atlanta, GA, USA, 2020, pp. 320-330, doi: 10.1109/BigData50022.2020.9378053.

S. Purawat et al., "TemPredict: A Big Data Analytical Platform for Scalable Exploration and Monitoring of Personalized Multimodal Data for COVID-19," 2021 IEEE International Conference on Big Data (Big Data), 2021, pp. 4411-4420, doi: 10.1109/BigData52589.2021.9671441.



Artwork: Jen Stark, Cosmographic, 2014, acid-free paper, holographic paper, glue, wood, acrylic paint, 34 x 37 x 4 in.

### To sum up...

Emerging new applications require integrated AI in dynamically composed workflows.



#### **Embrace Complexity!**

#### **Complexity comes at a cost!**

- Composable systems is not a turnkey functionality
- Requires collaboration with and between infrastructure providers
- End-to-end data pipelines need to be defined for each application along with microservice execution





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The presented work is collaborative work with many wonderful individuals, and parts of it are funded by NSF, DOE, NIH, UC San Diego and various industry, government and foundation partners.

of Health



Ilkay Altıntaş, PhD (ialtintas@ucsd.edu)



Science