Composable Systems for AI-Integrated Scientific Computing

Presentation for Virtual Salishan Conference 2022
April 28, 2022 (Recorded talk.)

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Founding Fellow, **Halıcıoğlu Data Science Institute**

Founding Director, **Workflows for Data Science Center of Excellence**

Founding Director, **WIFIRE Lab**

Evolving advanced computing and workflow ecosystem…

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

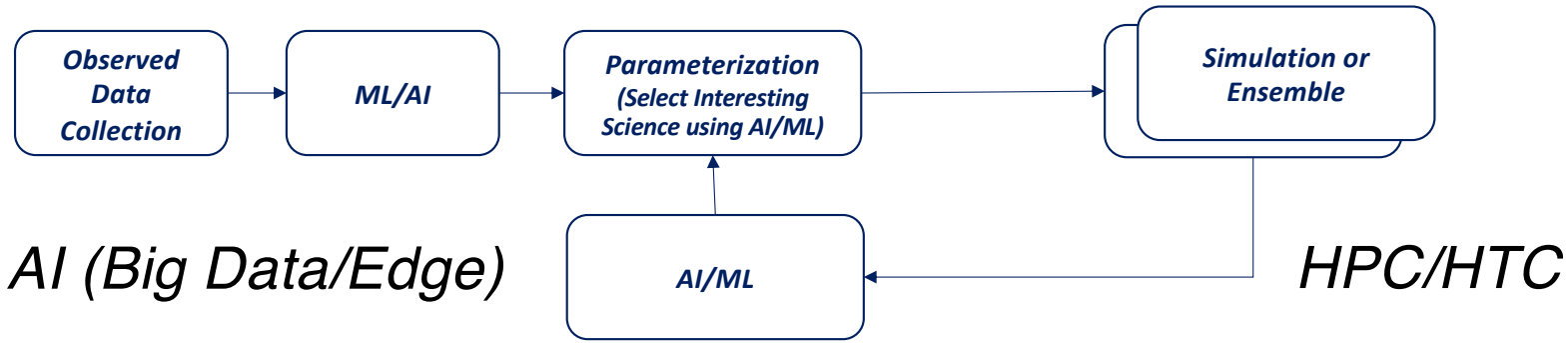
İlkay Altıntaş, PhD (ialtintas@ucsd.edu)

Continuous AI Integration at the Digital Continuum

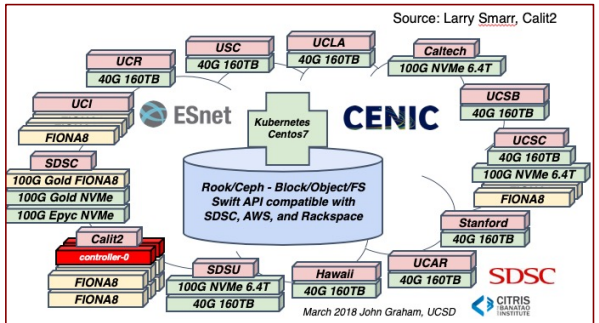
İlkay Altıntaş, PhD (ialtintas@ucsd.edu)

A Typical Heterogeneous AI-Integrated* Workflow

*AI-Integrated refers to **Dynamic Data-Driven** applications that require on-demand network capability to an instrument.



CI for AI : Capability ⟷ **CI for HPC/HTC** : Capacity



PRP + CHASE-CI

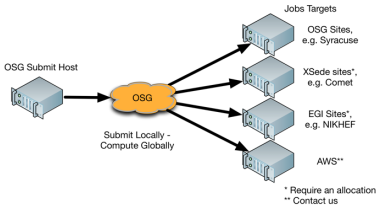
xPU → GPU, CPU, TPU, IPU, QPU,…

Edge

FPGA

hadoop

Big Data



Open Science Grid

amazon web services

Traditional HPC/Storage

1st National Exascale Day! – 10/18/2019

İlkay Altıntaş, PhD (ialtintas@ucsd.edu)
UC San Diego HALICIOĞLU DATA SCIENCE INSTITUTE

AI integration requirements…

Dynamic composability matters.

Systems are only useful if groups can integrate them into applications.

Tools that enhance teamwork need to be coupled with AI systems.

New requirements from systems…

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

RESPONSIBILITY
e.g., accuracy, privacy, explainability, ethics

REPRODUCIBILITY

TEAM SCIENCE

DATA LIFECYCLE MANAGEMENT
e.g., active data repositories, long-term archives, knowledge networks, data reuse services

USE-INSPIRED INTERFACES
e.g., for science, education and scalable practice

WORKFLOW MANAGEMENT
e.g., application integration, coordination, optimization, communication, reporting

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

İlkay Altıntaş, PhD (ialtintas@ucsd.edu)

Smart Composability from Systems to Services

- **Composable Systems**
  - dynamically measured and resourced
  - used as a resource based on need and availability
- **Resource Management**
  - container management
  - mapping tools for resource identification per task
- **Composable Services**
  - runs on composable systems (e.g., containers)
  - exposes a parametric interface for integration
  - continuously measured and profiled
- **Workflow Management**
  - focused on coordination and resource optimization
  - requires a number of AI-based tools and data processing to function

WORKFLOW MANAGEMENT
e.g., application integration, coordination, optimization, communication, reporting

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

Some Composable Systems

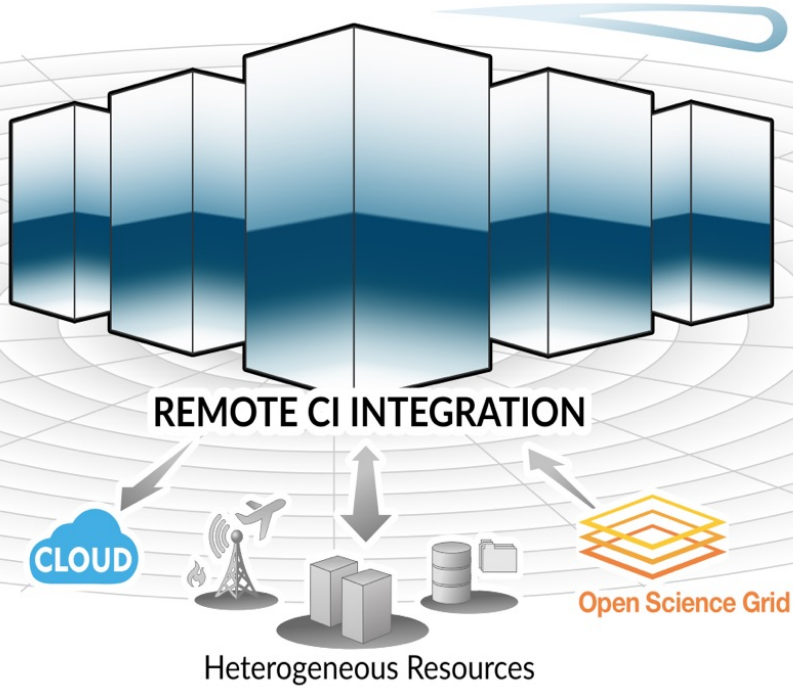
SDSC
SAN DIEGO SUPERCOMPUTER CENTER

EXPANSE

COMPUTING WITHOUT BOUNDARIES
5 PETAFLOP/S HPC and DATA RESOURCE

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

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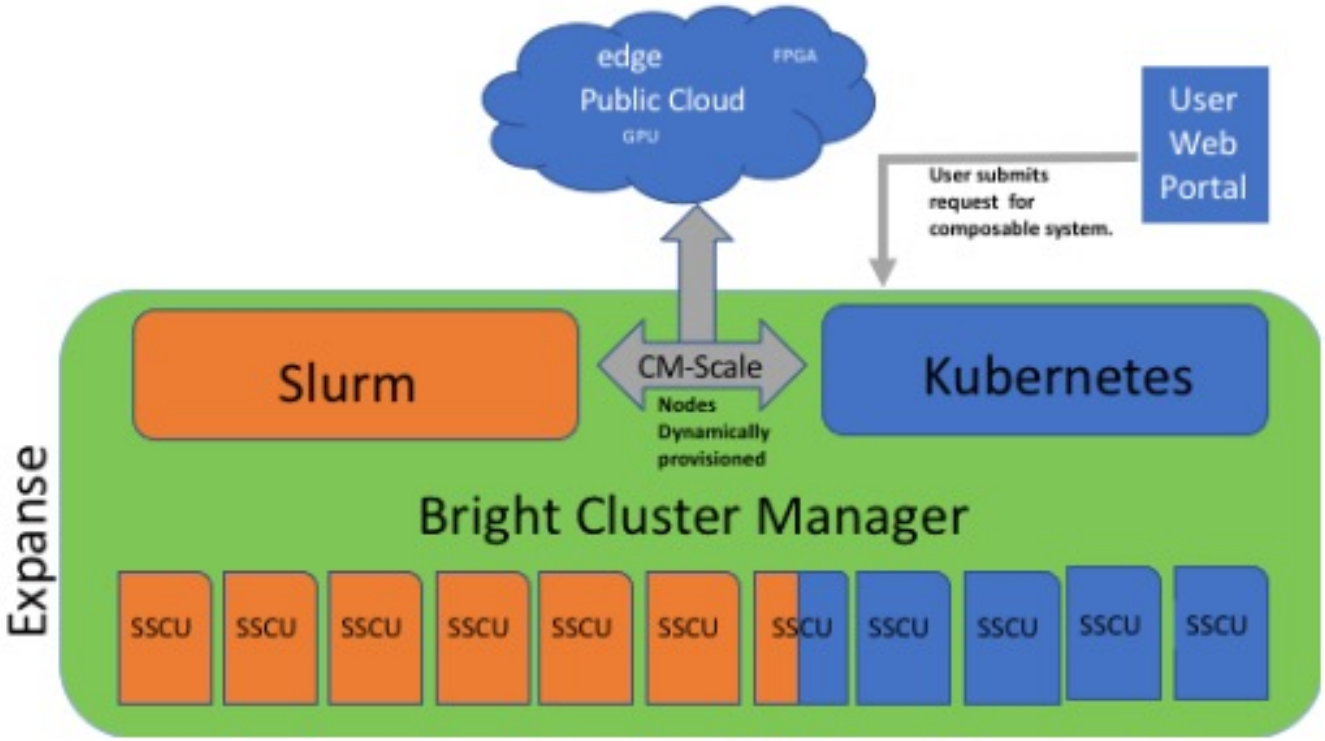
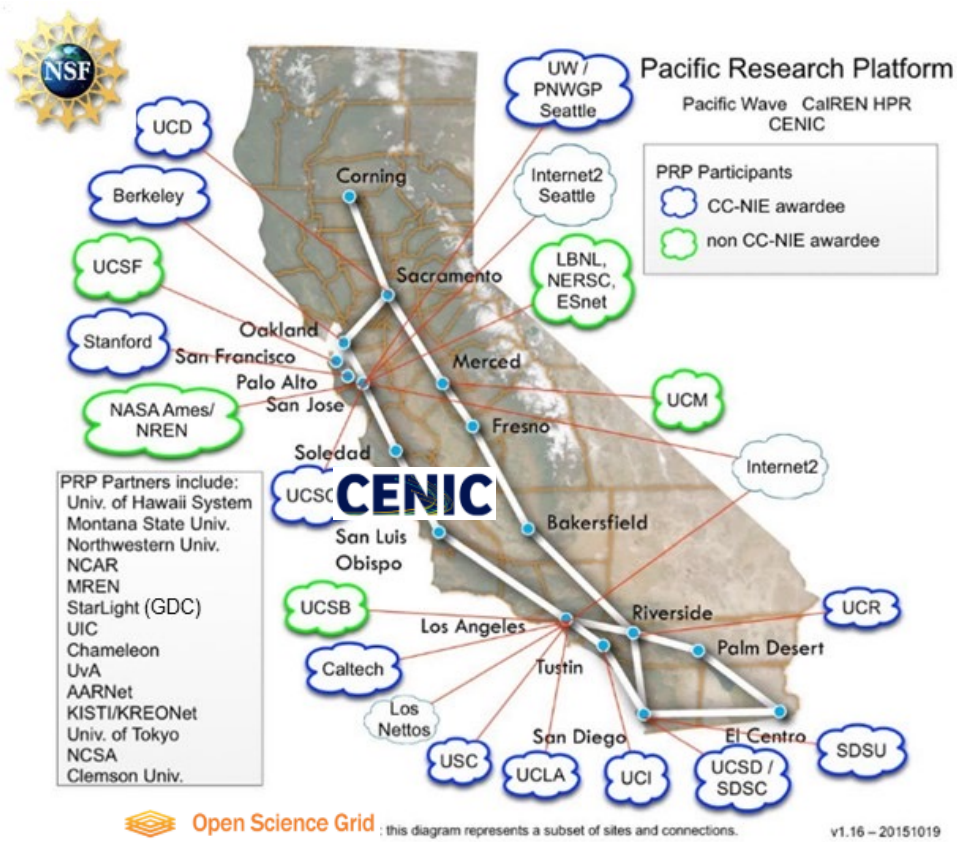


Expanse Composable Systems Framework

The Pacific Research Platform Creates a Regional End-to-End Science-Driven "Big Data Superhighway" System



NSF CC*DNI Grant
$5M 10/2015-10/2020

PI: Larry Smarr, UC San Diego Calit2
Co-PIs:

- ***Camille Crittenden, UC Berkeley CITRIS,***
- ***Tom DeFanti, UC San Diego Calit2,***
- ***Philip Papadopoulos, UCSD SDSC,***
- ***Frank Wuerthwein, UCSD Physics and SDSC***

PRP PACIFIC RESEARCH PLATFORM

Slide Source: Larry Smarr, UCSD

Disk-to-Disk
10-100 Gbps

SDSC

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NSF CHASE-CI Grant Creates a Community Cyberinfrastructure Adding a Machine Learning Layer Built on Top of the Pacific Research Platform

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

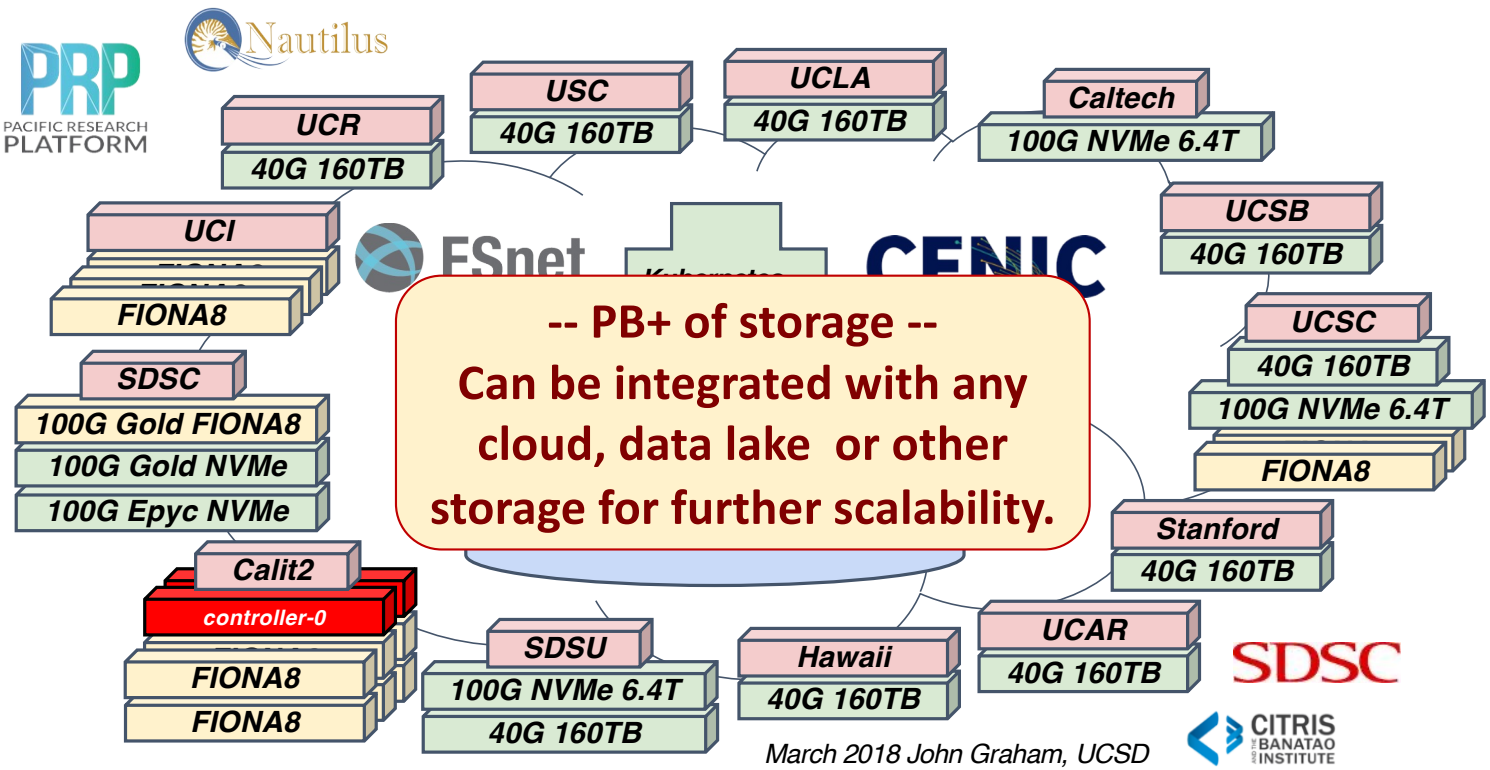
PI: Larry Smarr, Professor of Computer Science and Engineering, Director Calit2, UCSD
Co-PI: Tajana Rosing, Professor of Computer Science and Engineering, UCSD
Co-PI: Ken Kreutz-Delgado, Professor of Electrical and Computer Engineering, UCSD
Co-PI: Ilkay Altintas, Chief Data Science Officer, San Diego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

Slide Source: Larry Smarr, UCSD

JACOBS SCHOOL OF ENGINEERING

SDSC UC San Diego

NSF CHASE-CI : Nautilus – A Community Cyberinfrastructure Adding a Machine Learning Layer Built on Top of the Pacific Research Platform



*Five Racked **FIONAs** at Calit2*

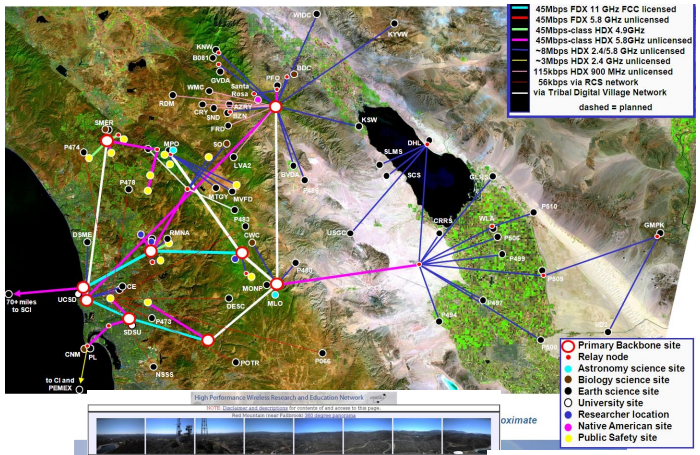
- *Each Contains:*
  - *Dual 12-Core CPUs*
  - *96GB RAM*
  - *1TB SSD*
  - *2 10GbE interfaces*
    - *Total ~$10,500*
  - *With 8 GPUs*
    - *total ~$18,500*

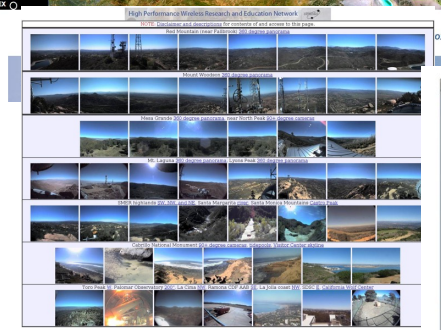
Phil Papadopoulos, SDSC & Tom DeFanti, Joe Keefe & John Graham, Calit2

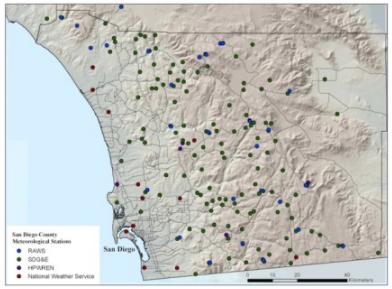
Source: Larry Smarr, Calit2

High Performance Wireless Research and Education Network

HPWREN







Major success to bring internet to incident command in the field. Used in over 20 fires over time.

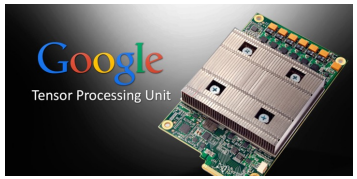
http://hpwren.ucsd.edu/cameras

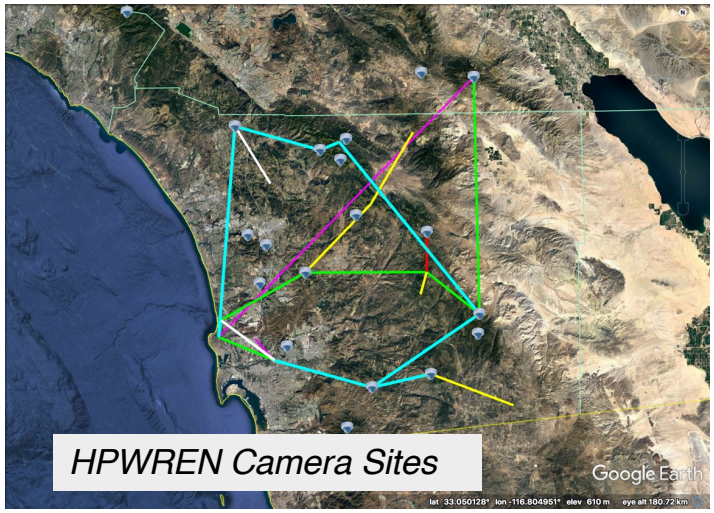
>160 Meteorological Sensors and Growing

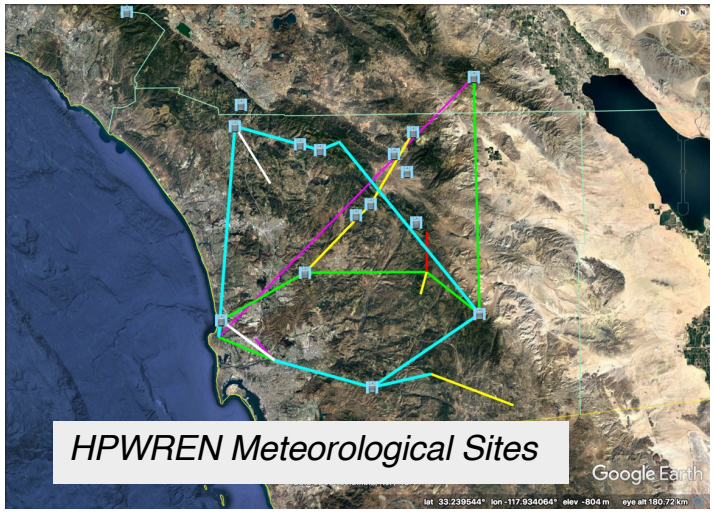
İlkay Altıntaş, PhD (ialtintas@ucsd.edu)

Ongoing Experiments to Extend CHASE-CI to the Edge of HPWREN

- Ground-based Smoke and Fire Detection from Web Camera Imagery at the edge to generate Alerts
- Continuous weather modeling at the edge (sensor -> higher resolution) to Weather Alerts
- Fuel and Soil Moisture Alerts







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http://sagecontinuum.org/

SAGE

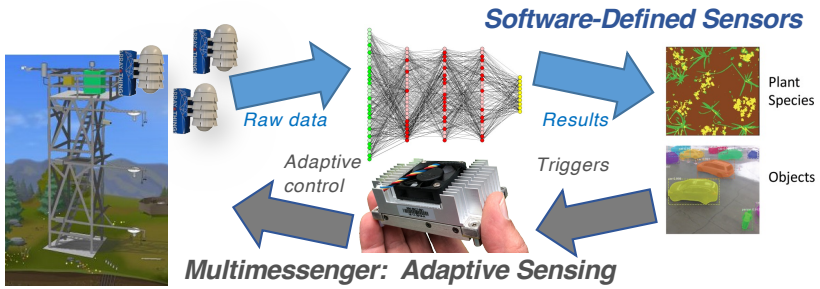
A Software-Defined Sensor Network

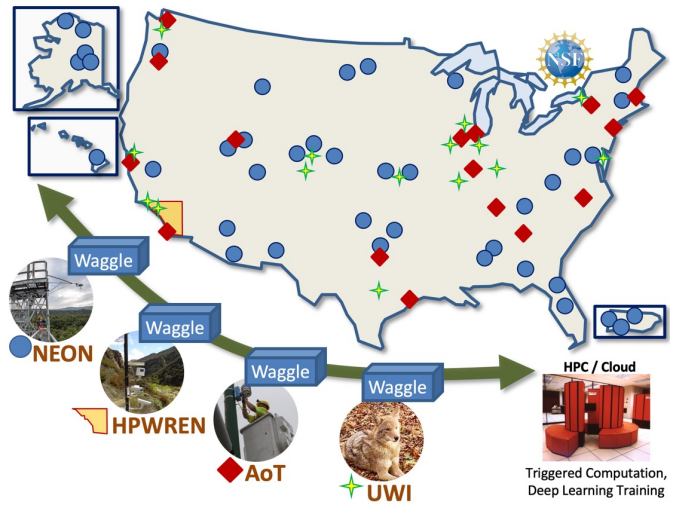
Cyberinfrastructure for **AI at the Edge**

sagecontinuum.org

Cyberinfrastructure Use Modalities

- Open Data, Open Calibration, Education
- Triggered Computation
- Scheduled Edge Computation
- Machine Learning for the Edge (AI@Edge)





Leadership Team

Pete Beckman (NU; Director)

Nicola Ferrier (NU; Deputy Dir.)

Ilkay Altuntas (SDSC; Data)

Charlie Catlett (UChicago; AoT)

Scott Collis (NU; ARM)

Valerie Taylor UChicago; Broader Impacts)

Jim Olds (GMU; Life Sci, Risk)

Dan Reed (Utah; Architecture)

Eugene Kelly (CSU; NEON)

Irene Qualters (LANL; Advisory Committee Chair)

Slide Source: Pete Beckman, NU

Application to Wildfire Modeling

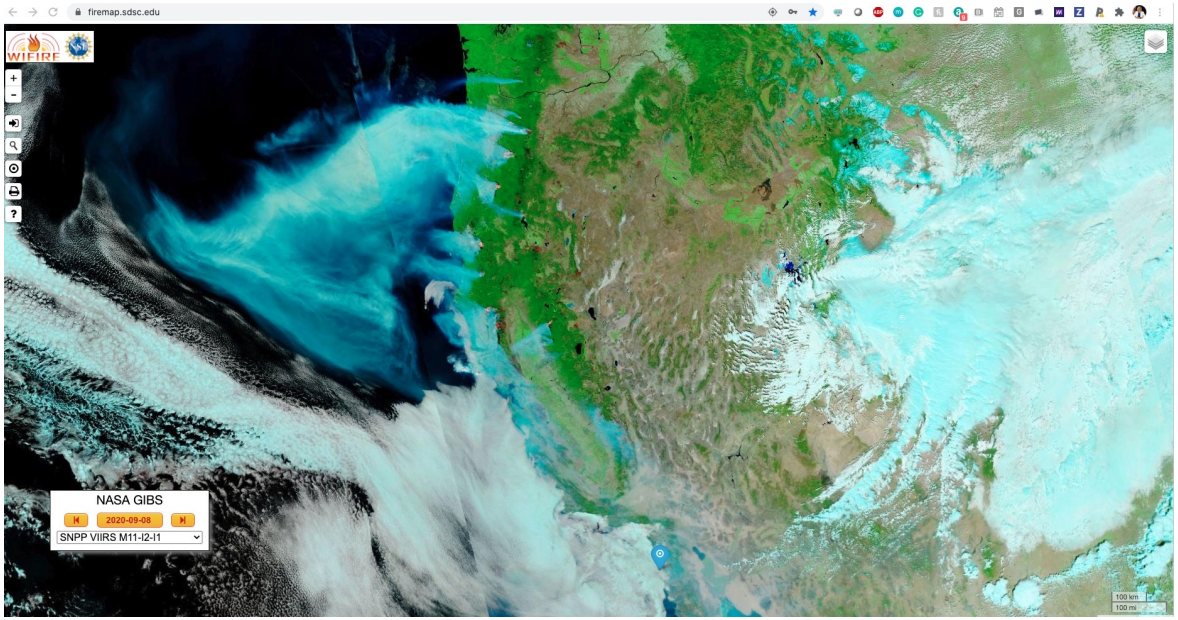


Image Source: https://commons.wikimedia.org/wiki/File:Cocos_fire_-_part_of_May_2014_San_Diego_County_wildfires.jpg

September 9, 2020
A view over the West Coast from NASA GIBS Satellite
Image Source: https://firemap.sdsc.edu/

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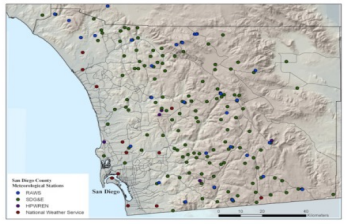
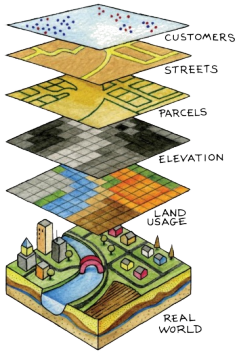
Next generation wildfire technology uses data from many sources.



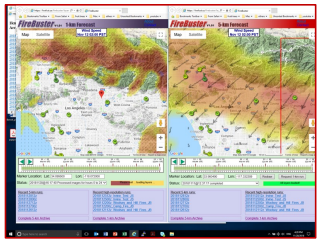
Ground-based real-time weather and camera imagery

Fire perimeter

Remote sensing

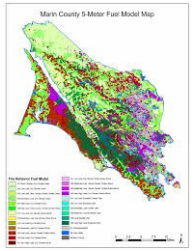


Landscape data



Weather forecast and modeling

Data-Driven Fire Preparedness, Mitigation and Response



Land cover and fuel

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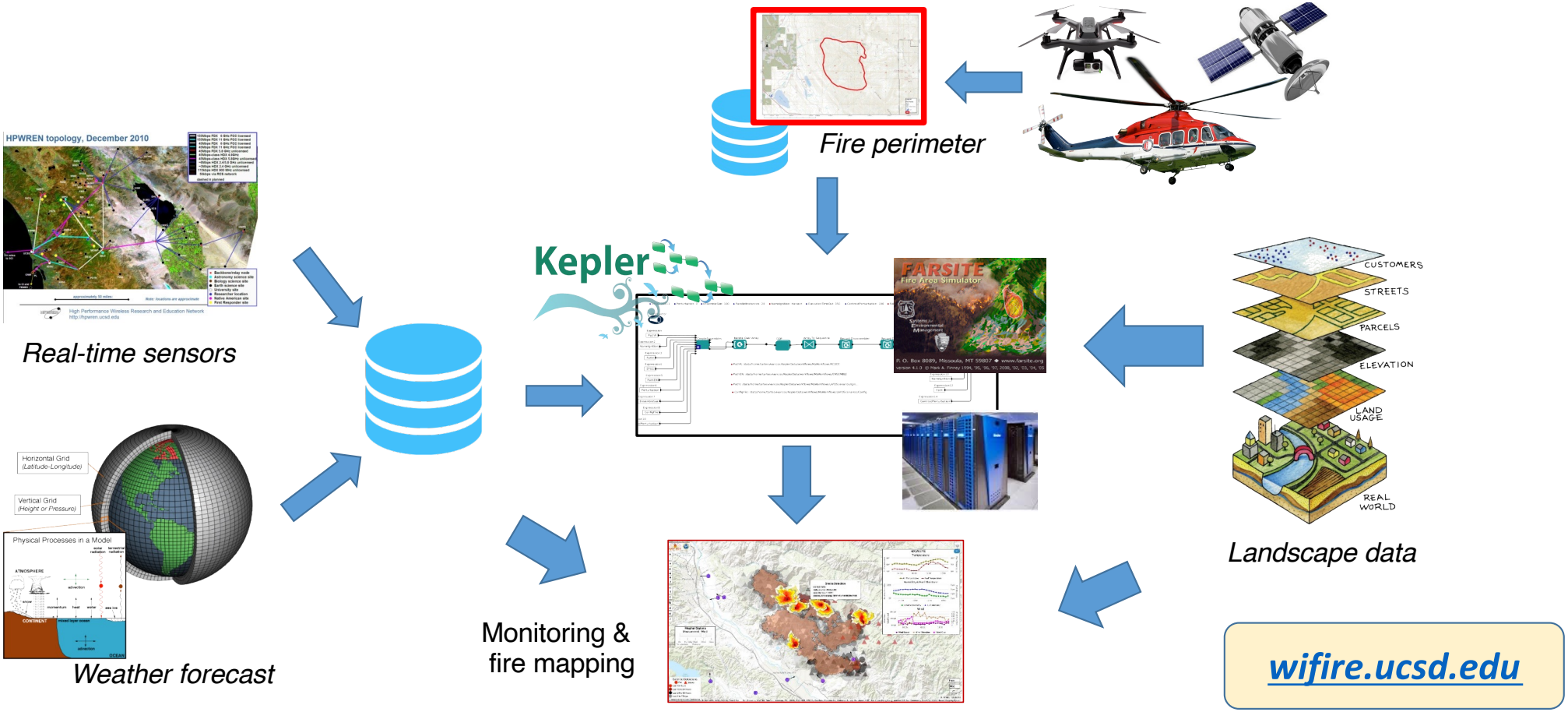
Dynamic Data-Driven Fire Modeling Workflows in WIFIRE



wifire.ucsd.edu

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During a fire: dynamic data-driven fire modeling

Where is the fire? Where will it go?

Direction and Rate of Spread

Continuous Iteration, Integration, Learning and Data Assimilation

at the Continuum of Computing using Automated Workflows

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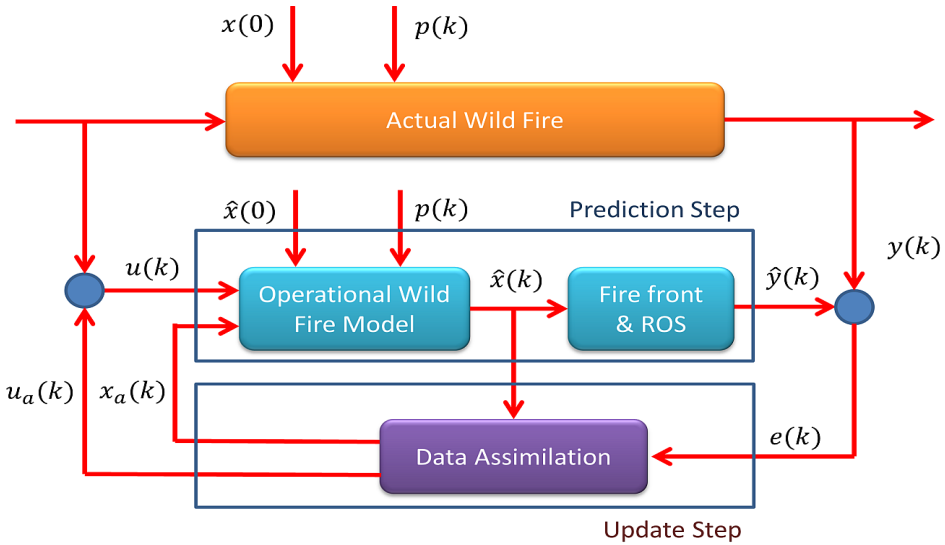
Closing the Loop using Big Data

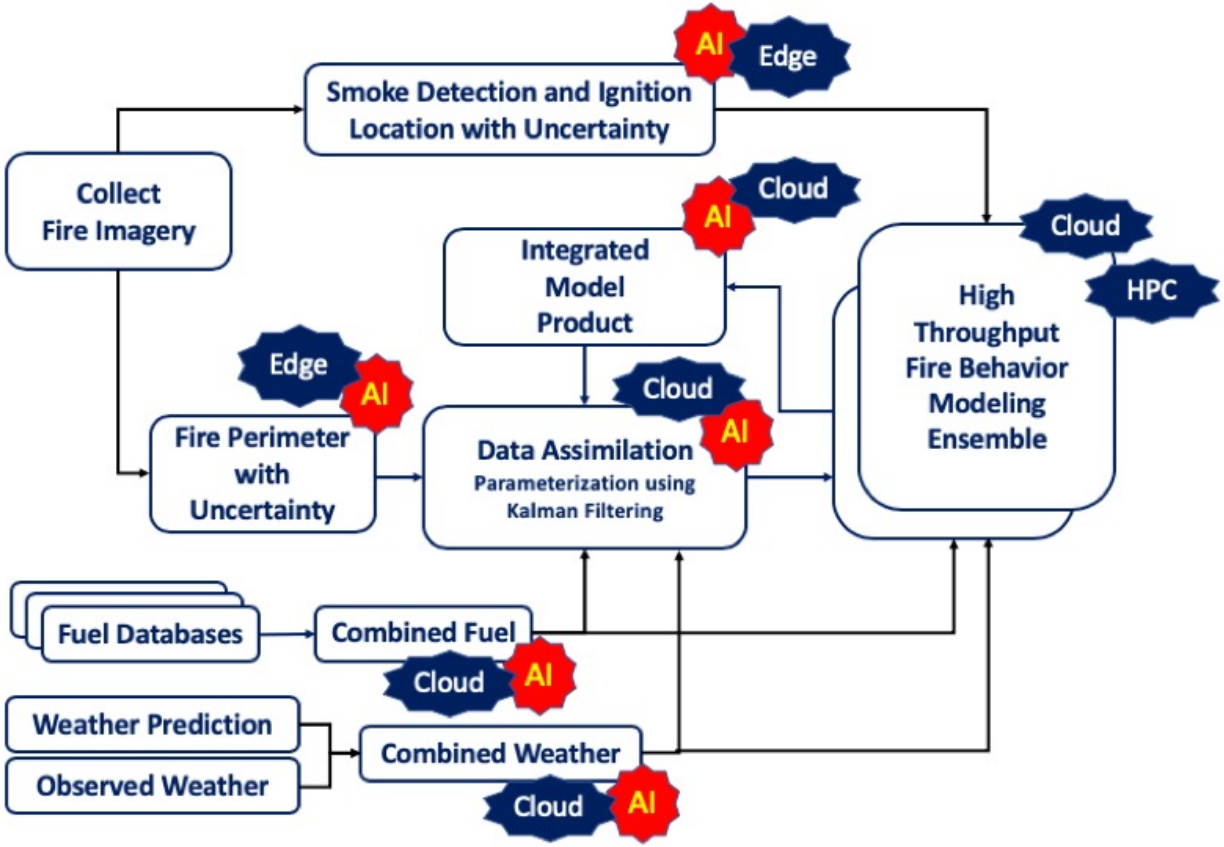
-- Autopilot for Wildfire Behavior Modeling using Data Assimilation --



Conceptual Data Assimilation Workflow with Prediction and Update Steps using Sensor Data

- Srivas, T., Artés, T., de Callafon, R., Altintas, I., **Wildfire Spread Prediction and Assimilation for FARSITE Using Ensemble Kalman Filtering**. doi:10.1016/j.procs.2016.05.328
- Srivas, T., de Callafon, R., Crawl, D., Altintas, I., **Data Assimilation of Wildfires with Fuel Adjustment Factors in FARSITE using Ensemble Kalman Filtering.** doi:10.1016/j.procs.2017.05.197

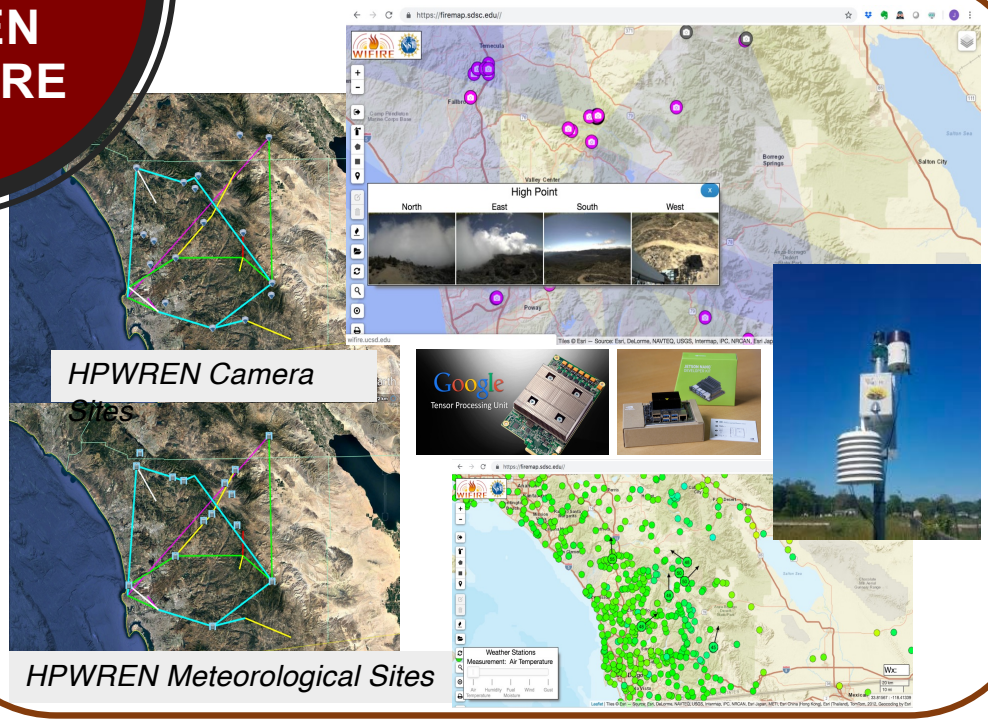
AI integration needs a computing ecosystem…



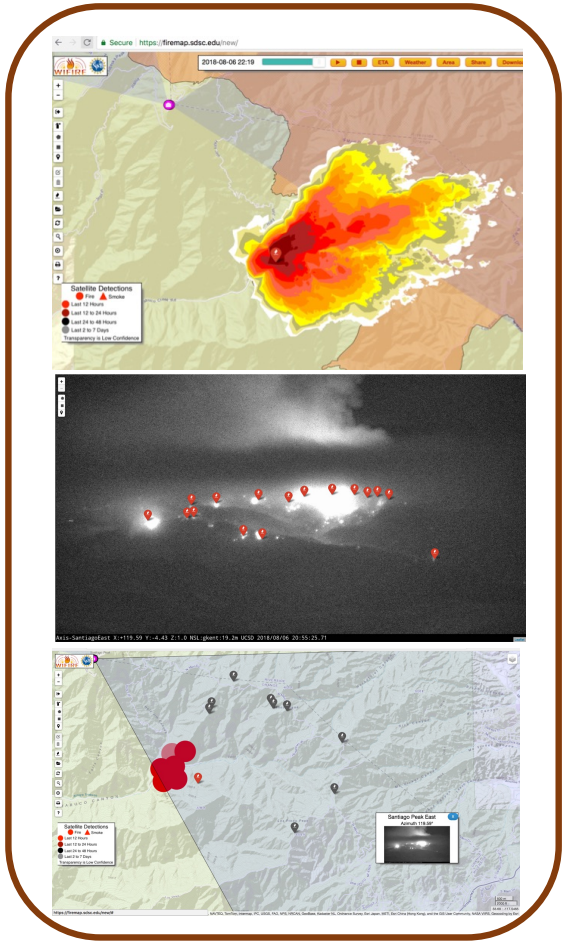
SAGE Integration with HPWREN and WIFIRE

- *Smoke detection*
- *Perimeter detection*
- *High-resolution weather modeling*
- *Fuel and soil moisture alerts*

Inference at the EDGE



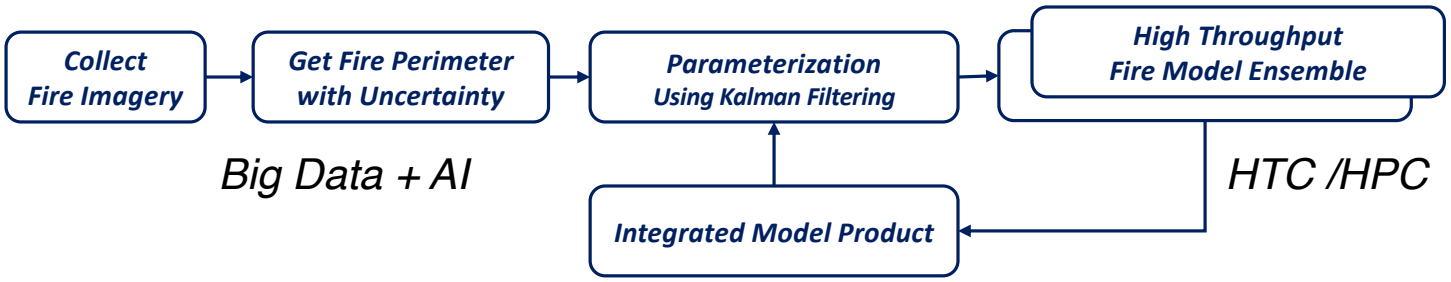
Fire Modeling on the CLOUD

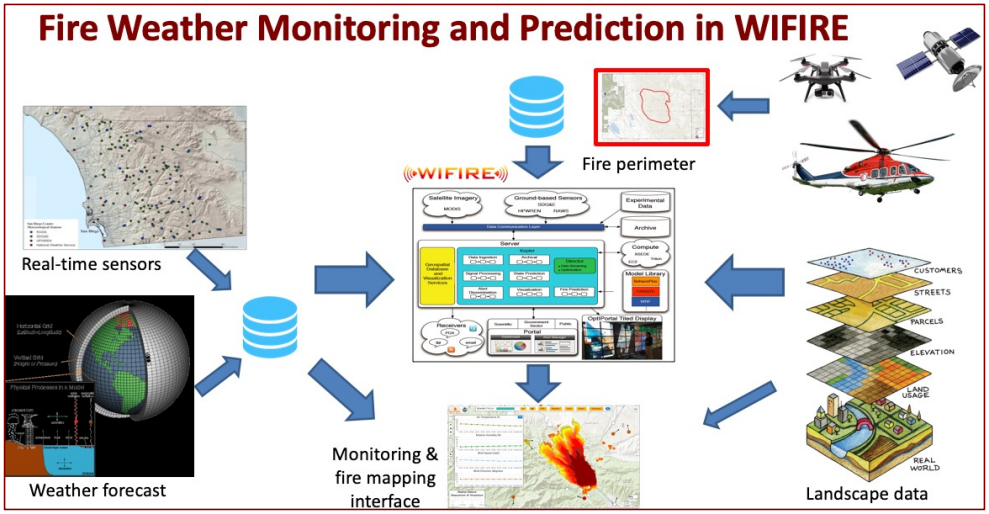


Automated Dynamic Data-Driven Fire Modeling in WIFIRE
using HPWREN, PRP+CHASE-CI, SAGE, Comet and Cloud

WIFIRE

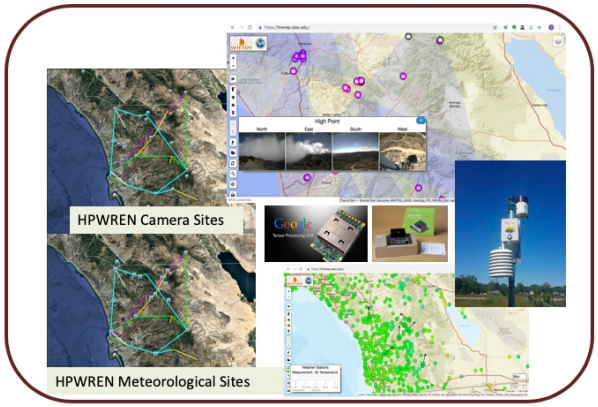
wifire.ucsd.edu



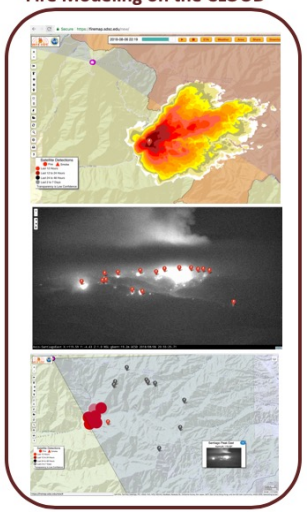


- Smoke detection
- Perimeter detection
- High-resolution weather modeling
- Fuel and soil moisture alerts

Inference at the EDGE



Fire Modeling on the CLOUD



First composable cluster is federated!

EXPANSE (Enthalpy) + CHASE-CI (Nautilus)

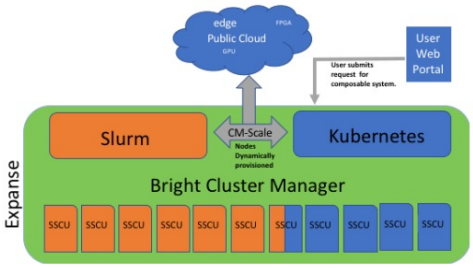
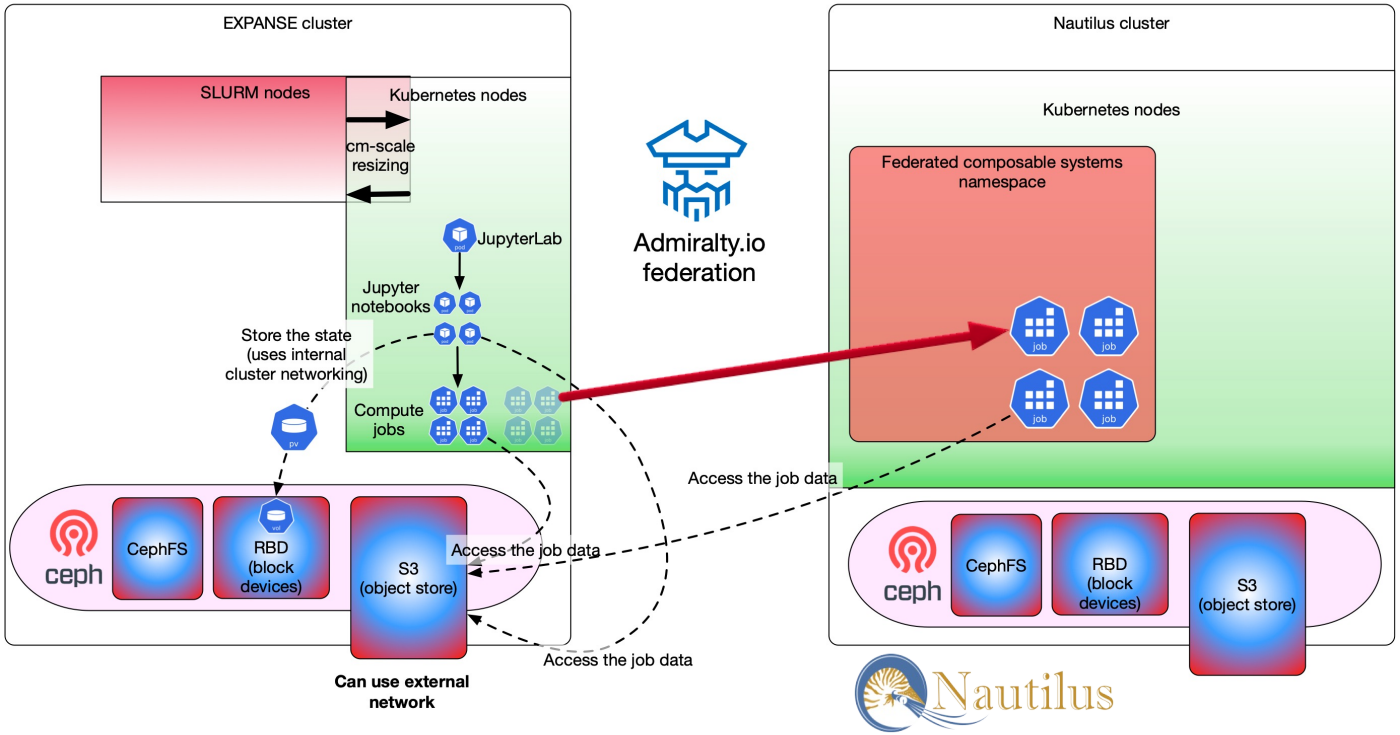


Figure 5.1 Expanse Composable Systems Framework

EXPANSE (Enthalpy)



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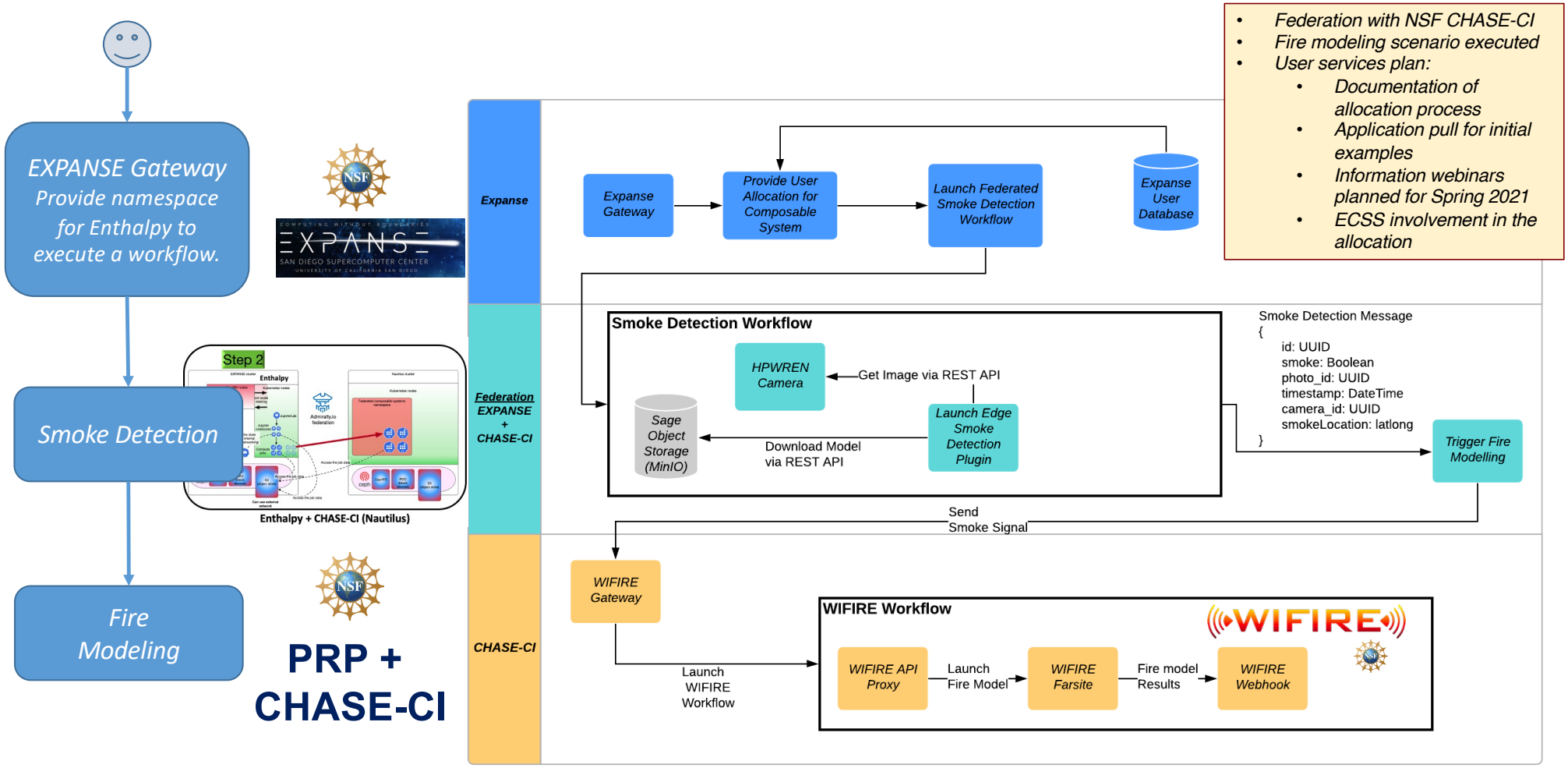

- *Federation with NSF CHASE-CI*
- *Fire modeling scenario executed*
- *User services plan:*
  - *Documentation of allocation process*
  - *Application pull for initial examples*
  - *Information webinars planned for Spring 2021*
  - *ECSS involvement in the allocation*

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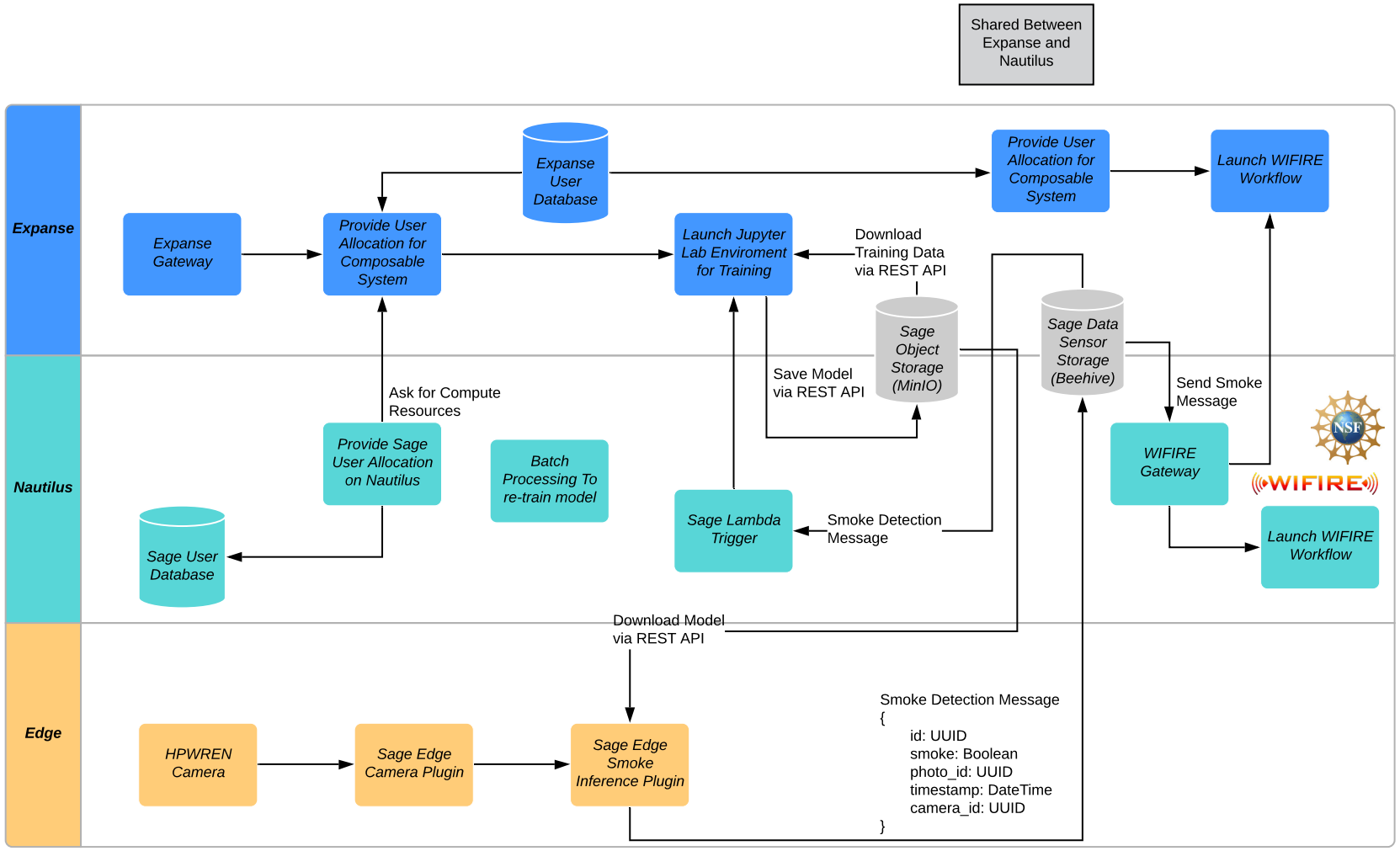
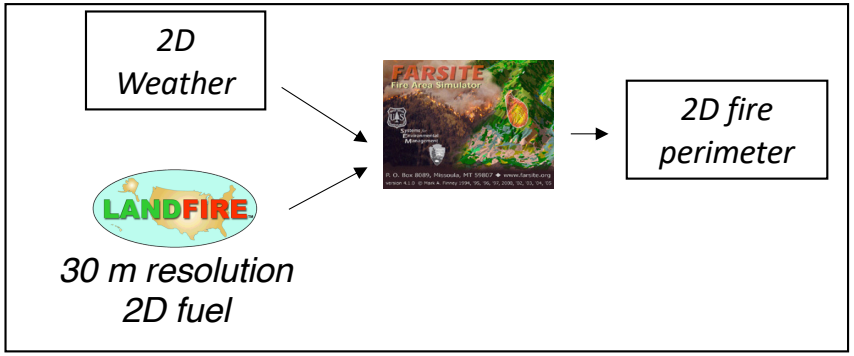

Shared Between Expanse and Nautilus
Expanse
Nautilus
Edge
Expanse Gateway
Provide User Allocation for Composable System
Expanse User Database
Launch Jupyter Lab Enviroment for Training
Download Training Data via REST API
Provide User Allocation for Composable System
Launch WIFIRE Workflow
Sage Object Storage (MinIO)
Sage Data Sensor Storage (Beehive)
Save Model via REST API
Ask for Compute Resources
Provide Sage User Allocation on Nautilus
Batch Processing To re-train model
Sage User Database
Sage Lambda Trigger
Smoke Detection Message
Send Smoke Message
WIFIRE Gateway
Launch WIFIRE Workflow
Download Model via REST API
HPWREN Camera
Sage Edge Camera Plugin
Sage Edge Smoke Inference Plugin
Smoke Detection Message
{
id: UUID
smoke: Boolean
photo_id: UUID
timestamp: DateTime
camera_id: UUID
}

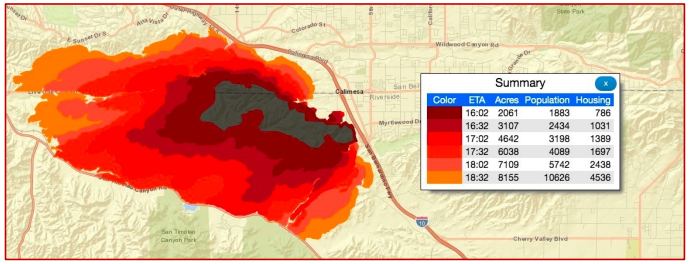
PRP + CHASE-CI

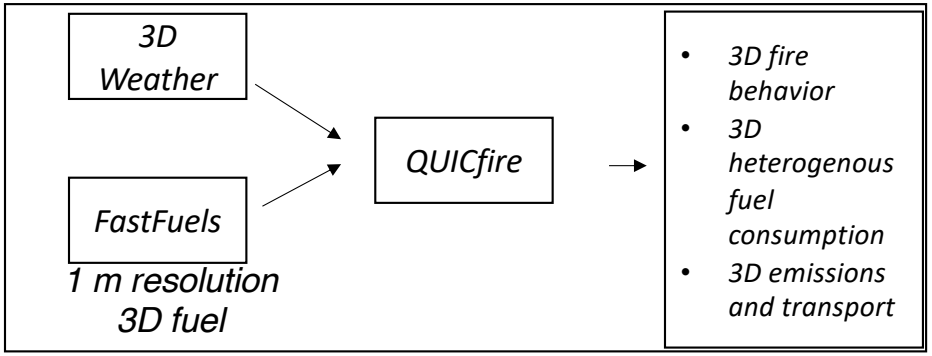
https://wifire.ucsd.edu/commons

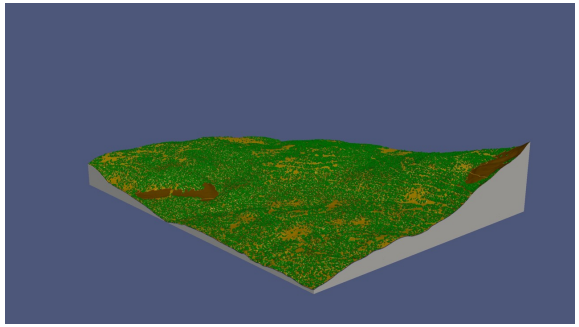
Transformative Science: more detailed and informative

From *30m resolution in 2D* ... ***to*** *1m resolution in 3D*









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

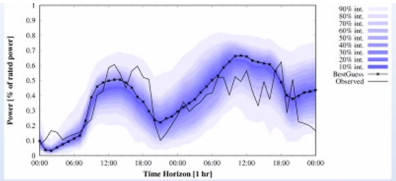
İlkay Altıntaş, PhD (ialtintas@ucsd.edu)

https://wifire.ucsd.edu/commons

Major AI Capability Integration Needs

Collaboration with Yolanda Gil, Mike Pazzani, Raymond de Callafon

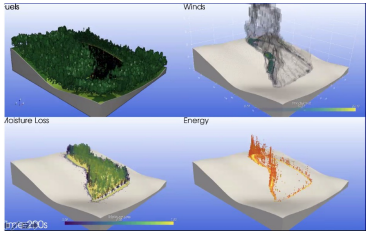
DYNAMIC DATA FUSION



Bessa et al, "Towards Improved Understanding of the Applicability of Uncertainty Forecasts in the Electric Power Industry", Energies 2017.

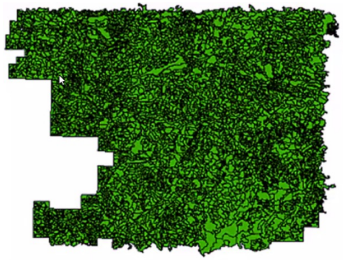
- *Multiple sensors, inconsistent data*
- *Hard to create a common operating picture*

ACCURATE MODELING



- *Fire models include many complex processes*
- *Hard to fine-tune models to make accurate predictions*

DECISION SUPPORT



- *Many possibilities for preventive fires/actions*
- *Hard to minimize cost and maximize impact of preventive fires*

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NeuroKube

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.

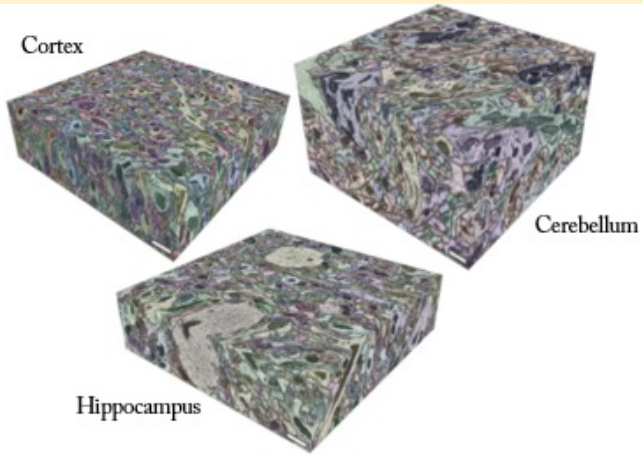
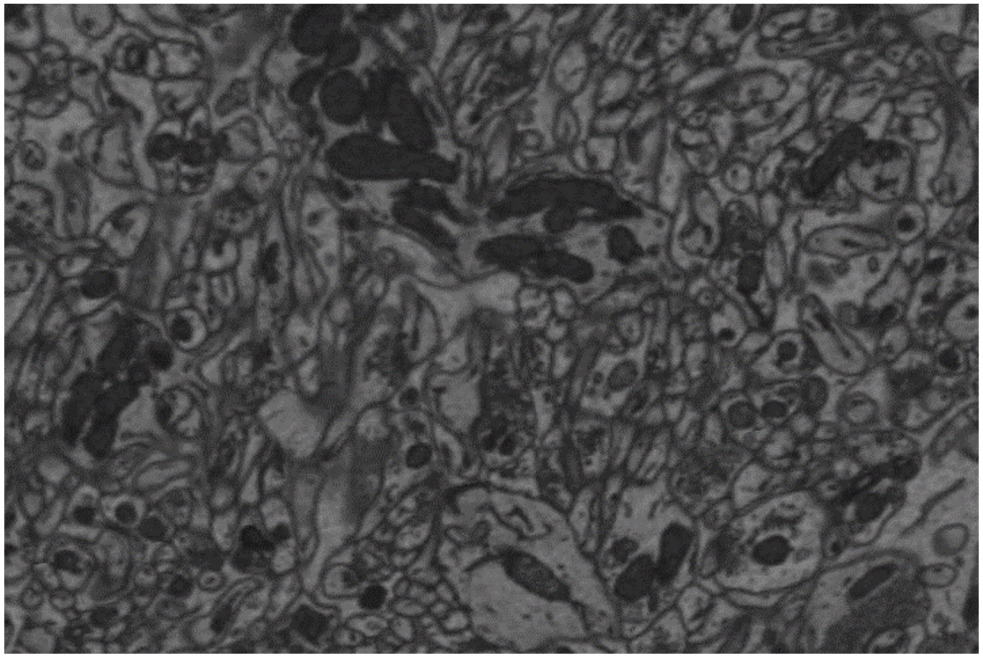


Figure 1. Volumetric electron microscopy (VEM) data with colorized labels. (Scale Bar $2\mu m$)

- Neuroscientists rely on volumetric electron microscopy imaging (VEM) because it is one of the only ways to acquire images that contain resolutions sufficient to see synapses and extents large enough to contain circuits of neurons
- However, these datasets are constantly inhibited from analysis due to the size of the data, as well as complex challenges stemming from the uncertainty of biological protocols and microscope engineering.



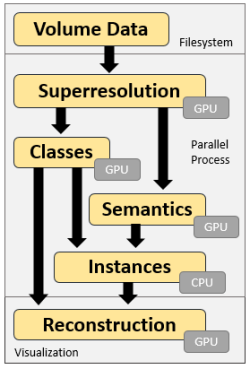
- *Example video of instance-level segmentation in 3D brain volumes to automatically label all the neurons in the field*
- *This requires a consort of A.I. methods, from deep-learning image processing, to DNN volumetric classifiers orchestrated in complex workflows.*

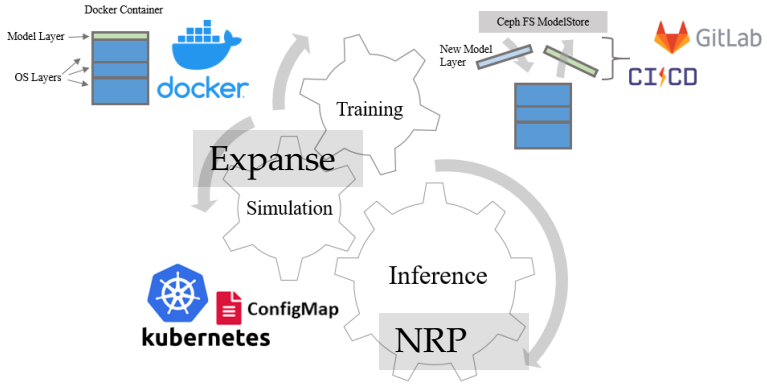
NeuroKube

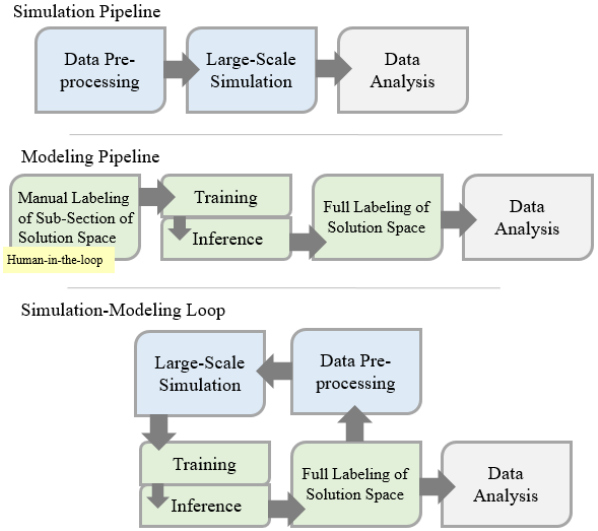
Frameworks, Gateways, & Architecture

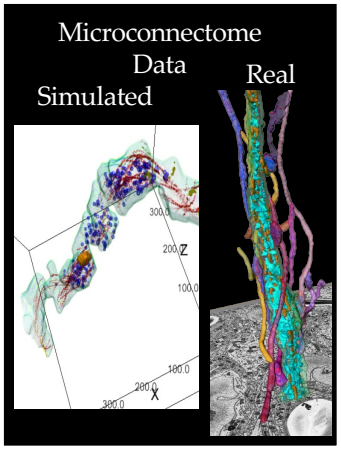
Workflow overview, many GPU-stages each with training/inference

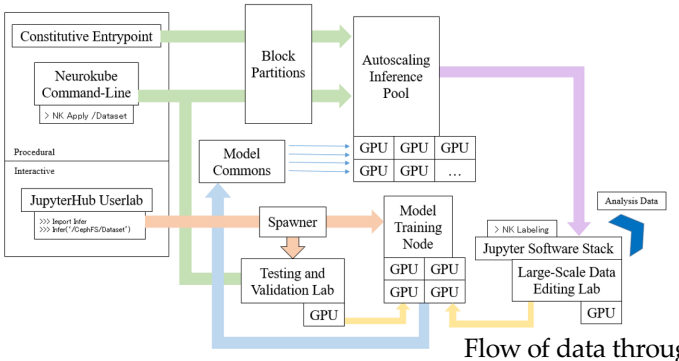
Training-Inference-Simulation cycles *will run permanently* on NRP-Expanse and individual *components* will scale *independently*











Flow of data through serviced A.I. modules

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.

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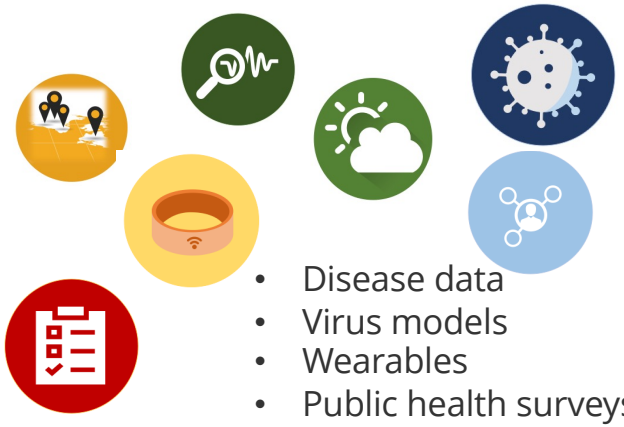
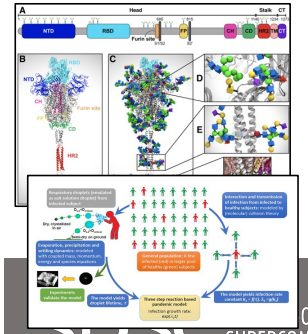
COVID-19 problems require a holistic approach to knowledge management and simulation.

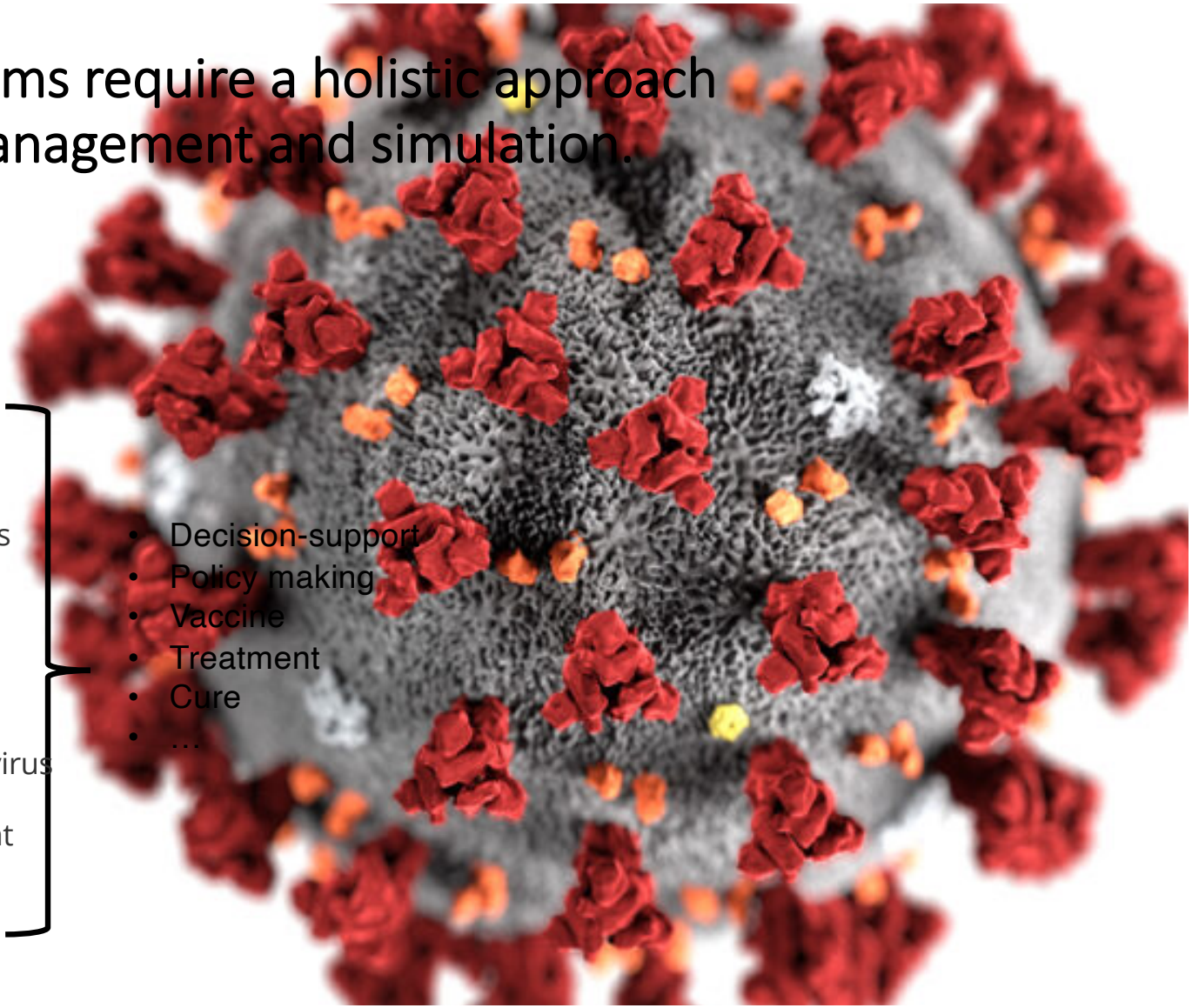


- Disease data
- Virus models
- Wearables
- Public health surveys
- Social media
- Contact data
- …



- Spread modeling
- Understanding the virus
- Drug design
- Vaccine development
- Economical impact
- Mental health
- …

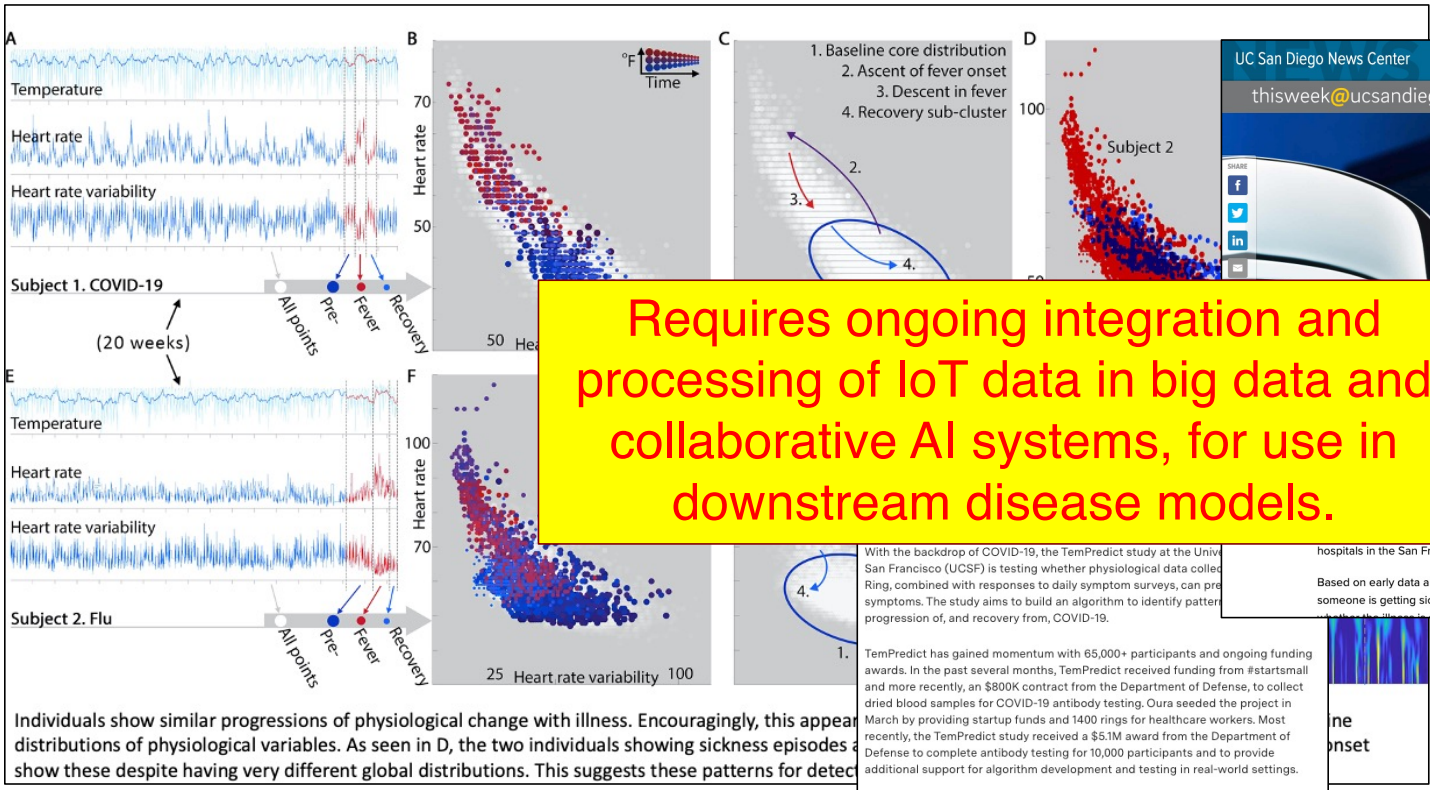
- Decision-support
- Policy making
- Vaccine
- Treatment
- Cure
- …



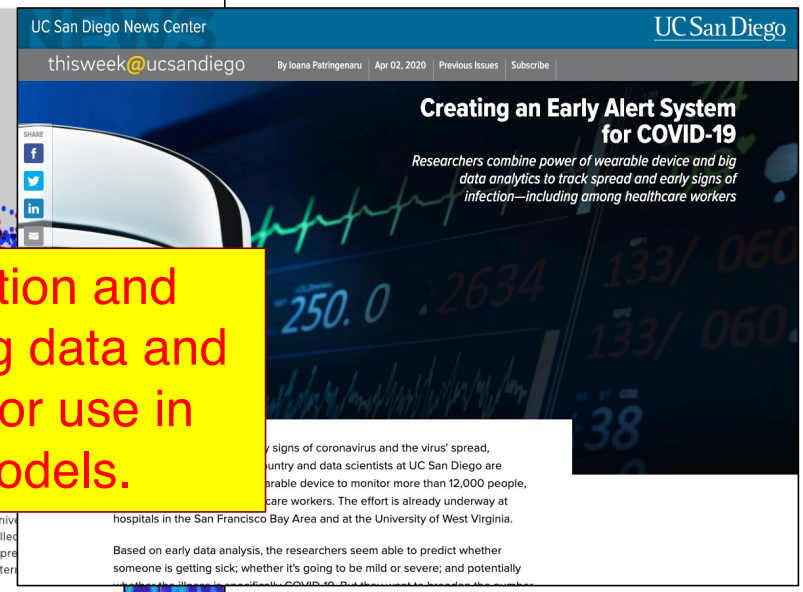
https://www.tacc.utexas.edu/-/locks-and-loads-coronavirus-for-infection

https://www.nist.gov/news/2020-06-resolution-droplet-motion-evaporation-covid-type.html

TemPredict: illness detection through wearables



Requires ongoing integration and processing of IoT data in big data and collaborative AI systems, for use in downstream disease models.



https://ucsdnews.ucsd.edu/feature/creating-an-early-alert-system-for-covid-19

With the backdrop of COVID-19, the TemPredict study at the Univ
San Francisco (UCSF) is testing whether physiological data collec
Ring, combined with responses to daily symptom surveys, can pre
symptoms. The study aims to build an algorithm to identify patter
progression of, and recovery from, COVID-19.

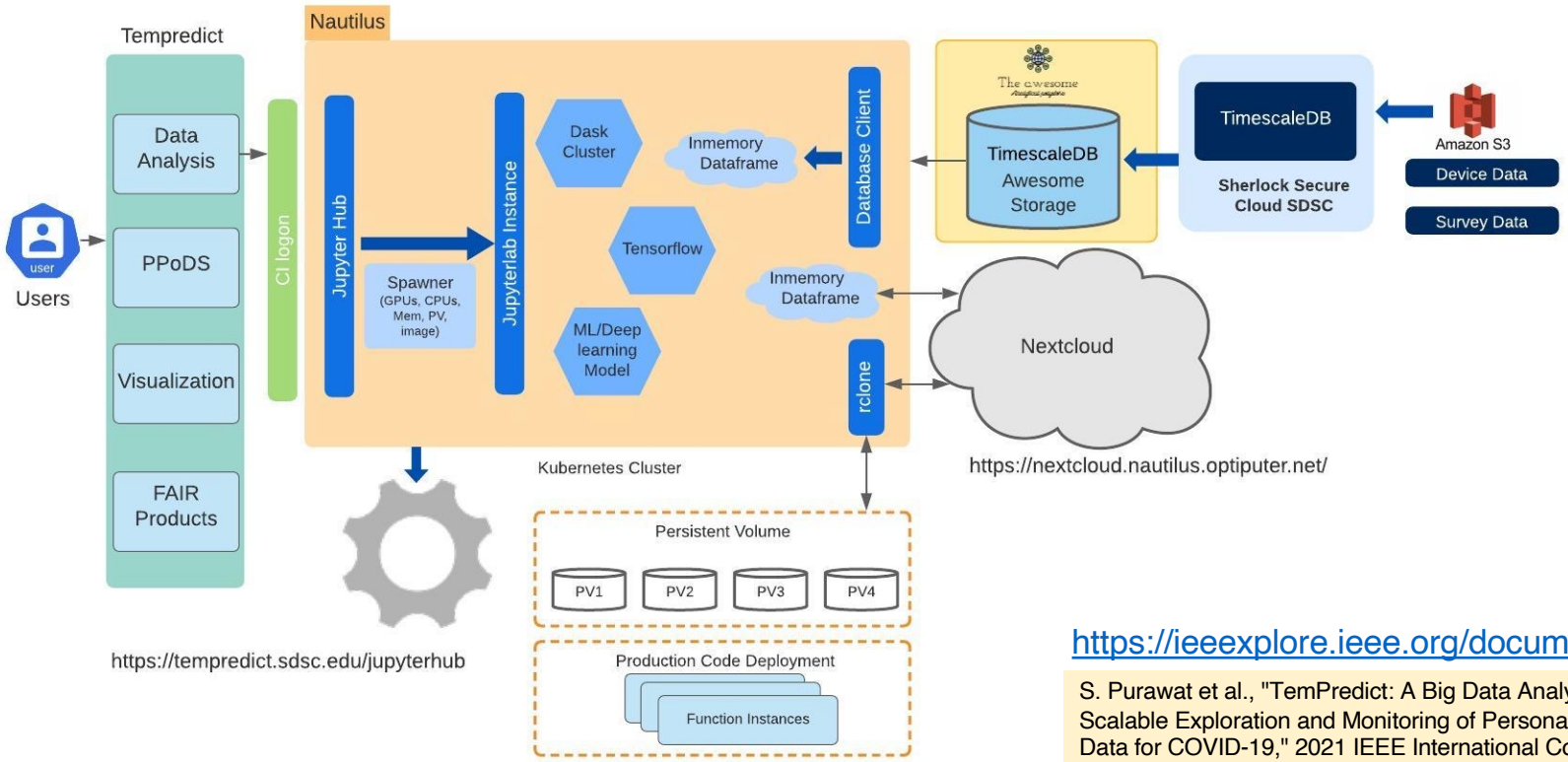
TemPredict has gained momentum with 65,000+ participants and ongoing funding awards. In the past several months, TemPredict received funding from #startsmall and more recently, an $800K contract from the Department of Defense, to collect dried blood samples for COVID-19 antibody testing. Oura seeded the project in March by providing startup funds and 1400 rings for healthcare workers. Most recently, the TemPredict study received a $5.1M award from the Department of Defense to complete antibody testing for 10,000 participants and to provide additional support for algorithm development and testing in real-world settings.

This effort includes researchers at UCSF and UC San Diego as well as researchers at the Massachusetts Institute of Technology (MIT) Lincoln Laboratory, the US Army, and the US Navy. To see more, visit: https://osher.ucsf.edu/news/51m-awarded-tempredict

https://blog.ouraring.com/ucsf-tempredict-study/

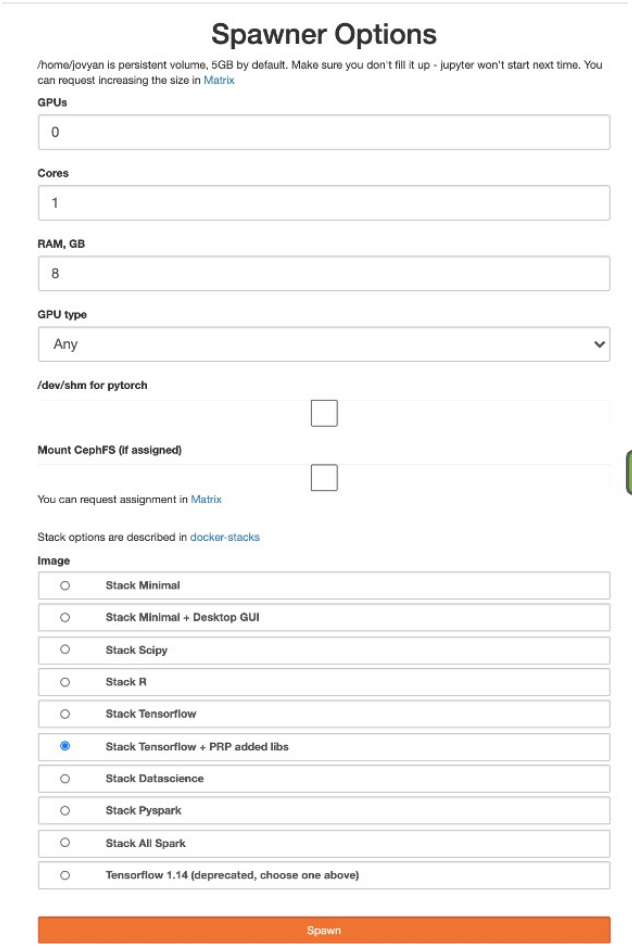
Above: COVID-19 vs. flu analysis
by Prof. Benjamin Smarr from UC San Diego.

TemPredict System Architecture

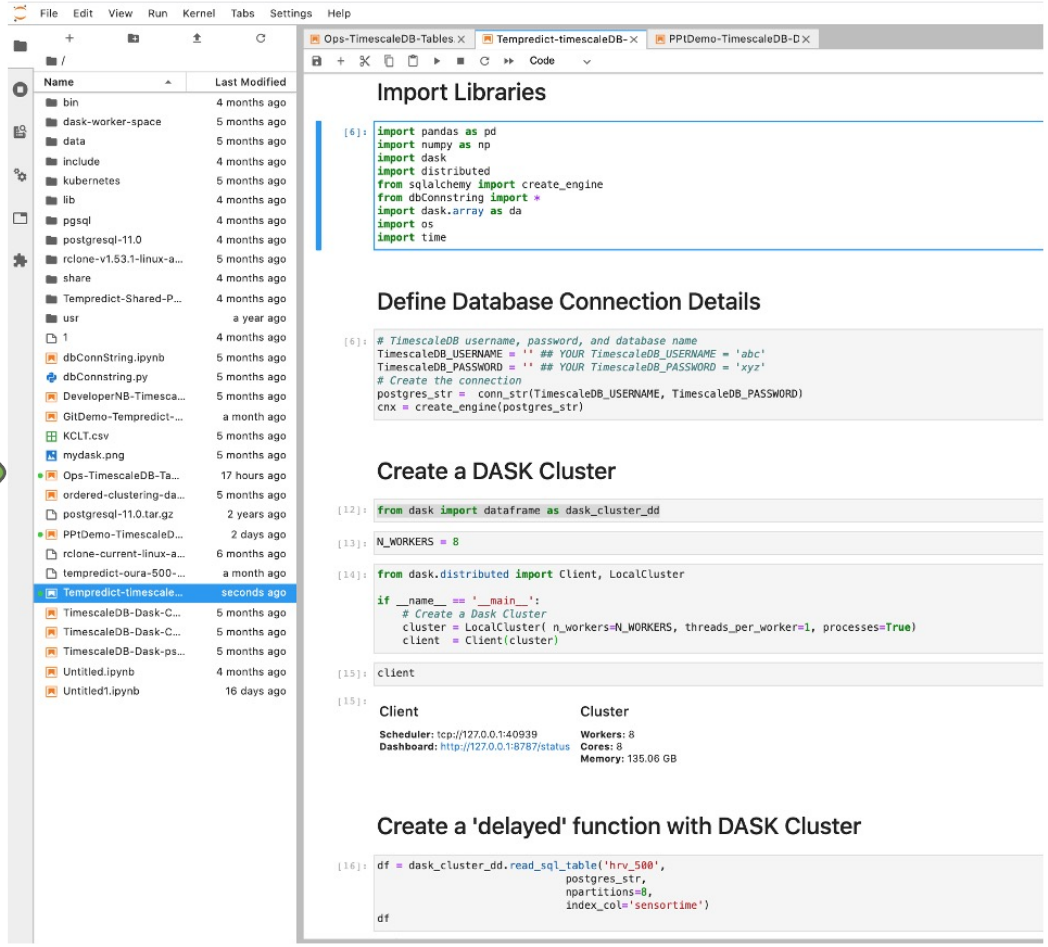


https://ieeexplore.ieee.org/document/9671441

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.



Kubernetes Pod Spawned for Exploration



To sum up…

- Emerging new applications require heterogeneous CI and integrated AI in dynamic workflows
- Composable systems is not a turnkey functionality
  - Requires collaboration with and between infrastructure providers
  - Unique for heterogenous application workflow across multiple systems in the Kubernetes ecosystem
  - Storage and computing requirements, and end-to-end data pipelines need to be defined for each application

UC San Diego

Contact: Ilkay Altintas, Ph.D.
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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 partners.