This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2023-02999C

Exceptional service in the national interest

Computing-as-a-Service Infrastructure for Accelerating Digital Engineering

Salishan Conference on High Speed Computing
Gleneden Beach, Oregon
April 24 - 27, 2023

Kevin Pedretti
Principal Member of Technical Staff
Scalable System Software, Org. 1423
ktpedre@sandia.gov

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Collaborators

Computing-as-Service Team:

- Sylvain Bernard
- Ron Brightwell
- Wesley Coomber
- Mike Glass
- Eric Ho
- Todd Kordenbrock
- Cory Lueninghoener
- Aaron Moreno
- Kevin Pedretti
- Elliott Ridgway
- Gary Templet
- Andrew Younge

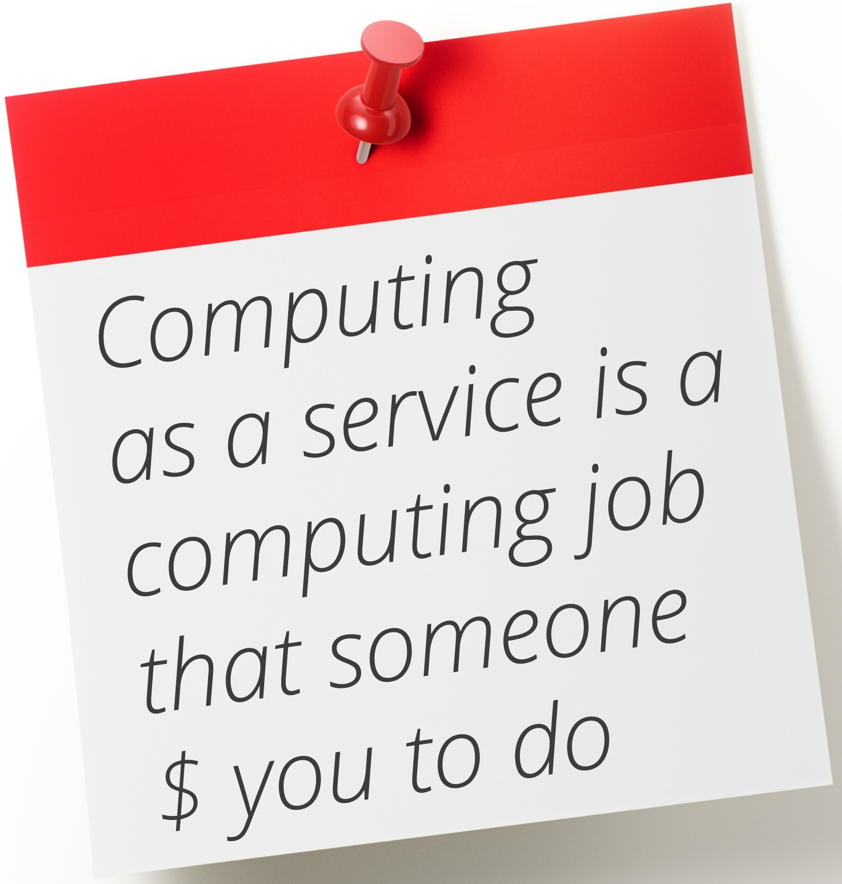
Guidance and Slide Material:

- Matthew Curry
- Ernest Friedman-Hill
- Chris Garasi
- Brenna Hautzenroeder
- Martin Heinstein
- Rob Hoekstra
- Jim Laros
- Scott Roberts
- Scot Swan

Outline

- Introduction
- Computing-as-a-Service Architecture
- R&D Directions / What’s Missing
- Conclusion

Computing-as-a-Service



Computing as a service is a computing job that someone $ you to do

11 year old's definition

- Cloud industry built around delivering things as a service
- Huge Business & Talent
- Software ecosystem for deploying turnkey services

Cloud vs. HPC – Different Usage Models, Customs, and Practices

1. They use the same underlying technology – servers, storage, and networks
2. Cloud has 100’s of services, HPC has ~ 1 **(HPC is the service)**
3. Cloud has APIs for managing all infrastructure and services, **(HPC APIs are ad hoc)**
4. Cloud uses token-based authentication, **(HPC uses passwords)**
5. Cloud runs the customer’s software stack, **(HPC runs the facility’s SW stack)**
6. Cloud charges by the hour (encouraging paranoia), **(HPC cycles are free)**

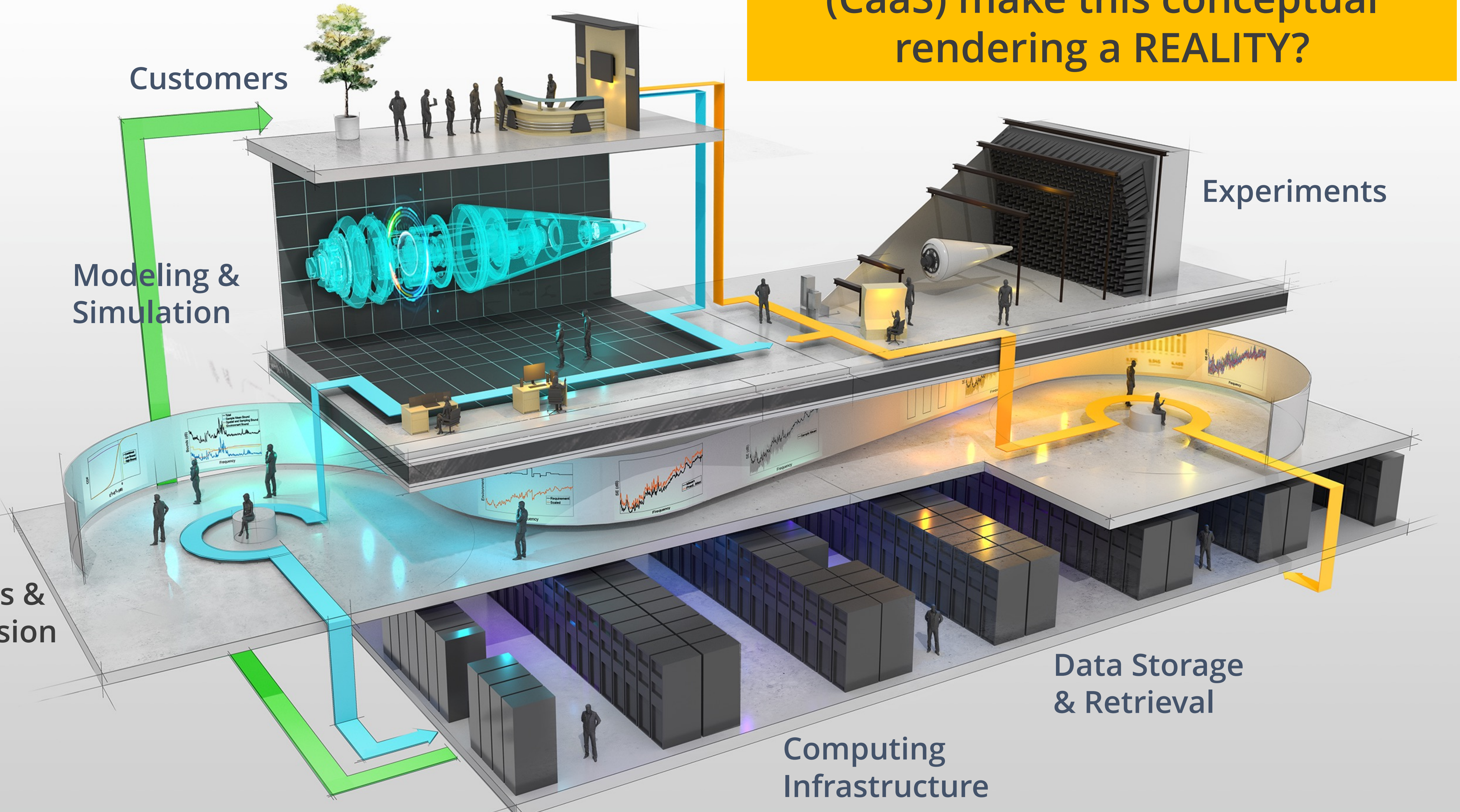
Cross-Pollination of Cloud & HPC Mutually Beneficial

Cloud vs. HPC – Different Usage Models, Customs, and Practices

1. They use the same underlying technology – servers, storage, and networks
2. Cloud has 100’s of services, HPC has ~ 1 **(HPC is the service)**
3. Cloud has APIs for managing all infrastructure and services, **(HPC APIs are ad hoc)**
4. Cloud uses token-based authentication, **(HPC uses passwords)**
5. Cloud runs the customer’s software stack, **(HPC runs the facility’s SW stack)**
6. Cloud charges by the hour (encouraging paranoia), **(HPC cycles are free)**

Cross-Pollination of Cloud & HPC Mutually Beneficial

How can “Computing-as-a-Service” (CaaS) make this conceptual rendering a REALITY?



Customers

Experiments

Modeling & Simulation

Analytics & Data Fusion

Data Storage & Retrieval

Computing Infrastructure

Outline

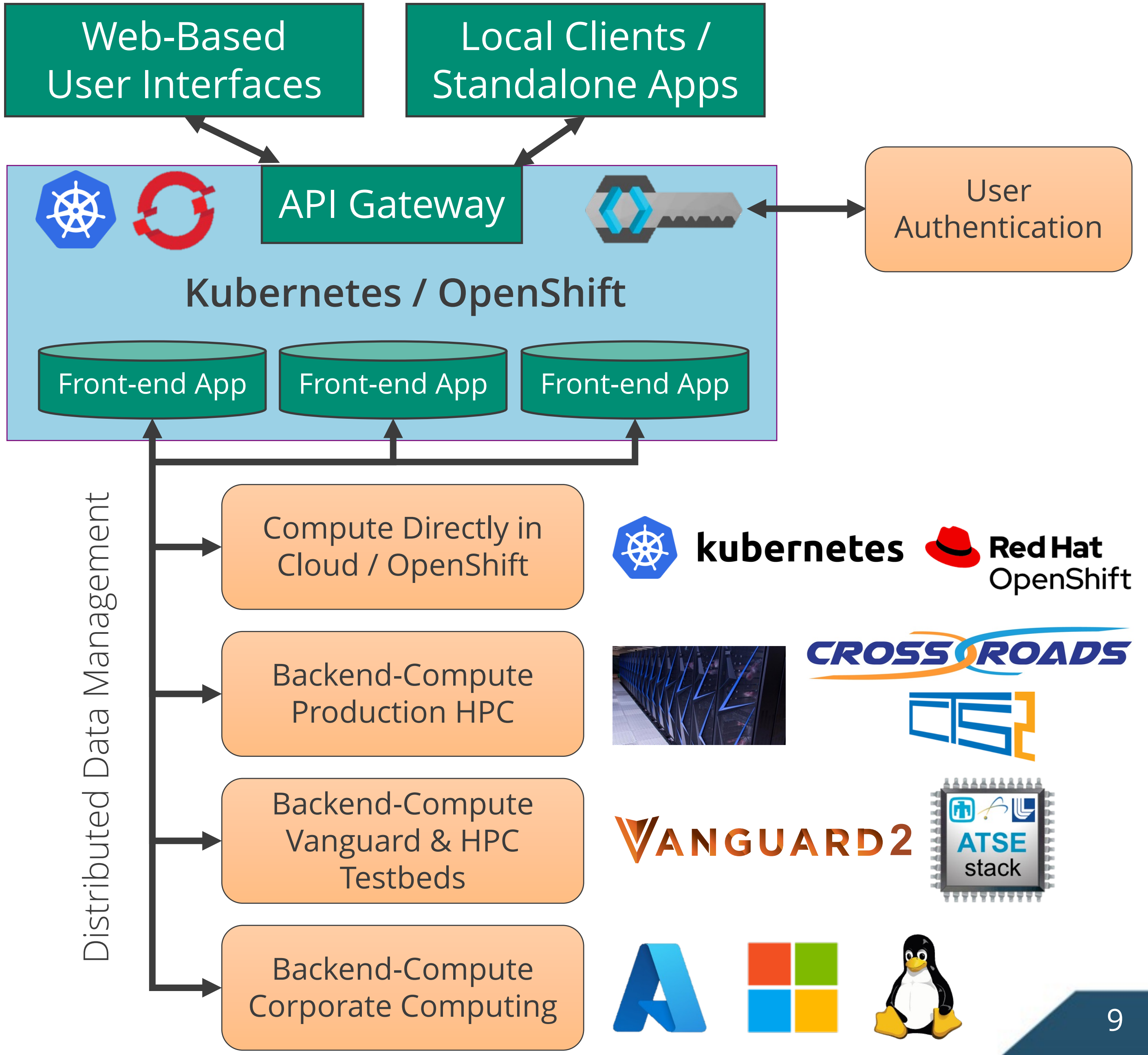
- Introduction
- Computing-as-a-Service Architecture
- R&D Directions / What’s Missing
- Conclusion

Connecting the Cloud Services to Backend Compute

- Kubernetes is a distributed operating system for managing ***containerized workloads & services***
  - Google open-sourced 2014
  - Now industry standard "Cloud OS"

- Sandia deploying production Kubernetes / OpenShift clusters

- Kubernetes not well suited for HPC
  - Bridging to HPC "on your own"
  - R&D efforts to improve Kubernetes support for HPC (RedHat Partnership)



Web-Based User Interfaces

Local Clients / Standalone Apps

API Gateway

User Authentication

Kubernetes / OpenShift

Front-end App

Front-end App

Front-end App

Distributed Data Management

Compute Directly in Cloud / OpenShift

Backend-Compute Production HPC

Backend-Compute Vanguard & HPC Testbeds

Backend-Compute Corporate Computing

DetNet Takes Leap of Faith and Teams with CaaS

DetNet PI: Chris Garasi

Goal:

- ***Provide simulation-as-a-service (SaaS) to the detonator community***
- *Speed development, reduce cost, reduce risk*

Challenges Experienced over 10+ years:

- Deploying software with antiquated input deck UI
- Software installation & upgrades
- User training – ***end-users were not HPC experts and didn't want to be***

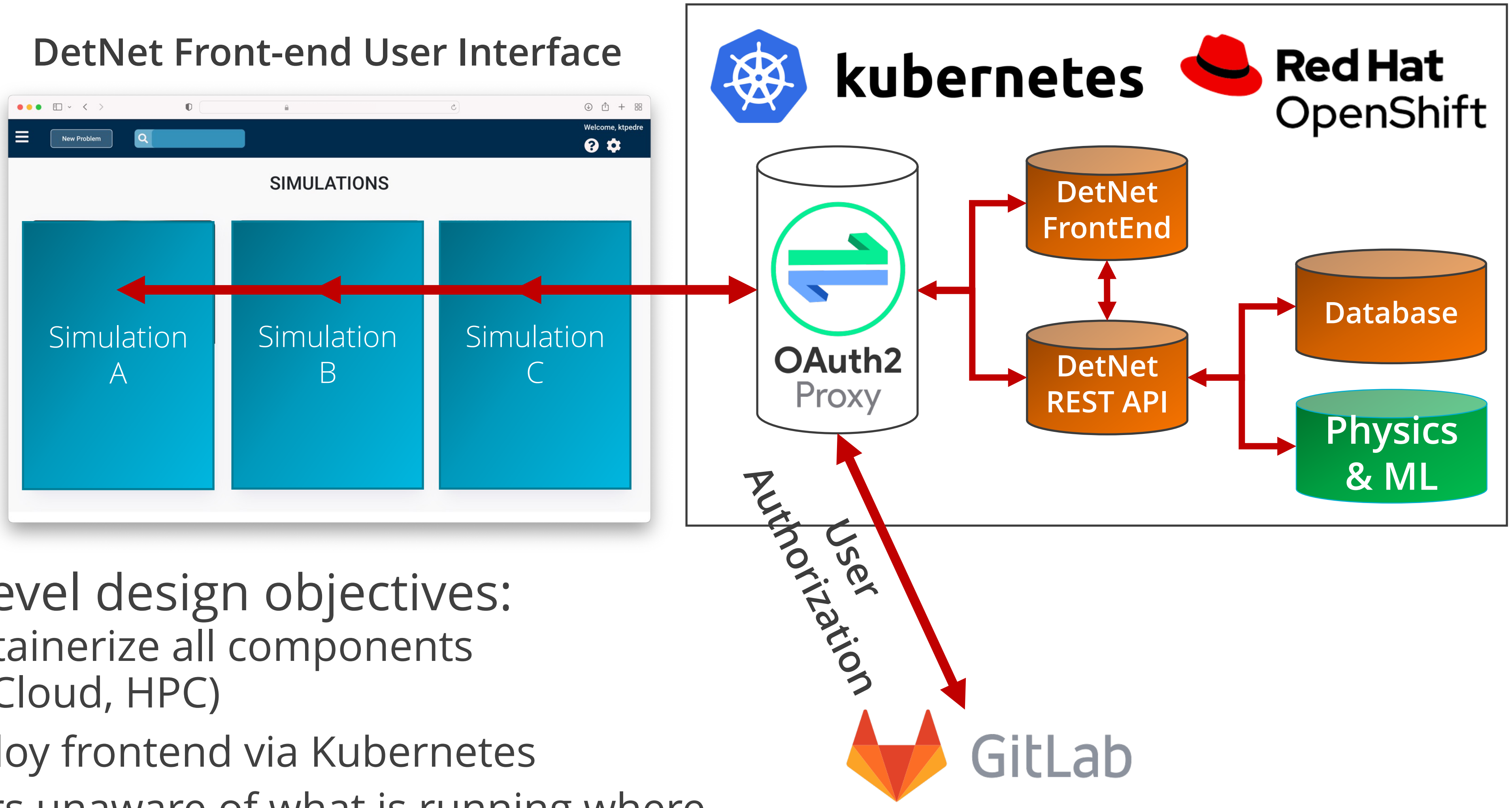
Why now?

- ***Massively faster compute***
- ***Cloud infrastructure & containerization***

Put the tools directly in the hands of the engineers
(not the analysts)

Challenge 1: Containerize and Demonstrate End-to-End Prototype

DetNet Front-end User Interface

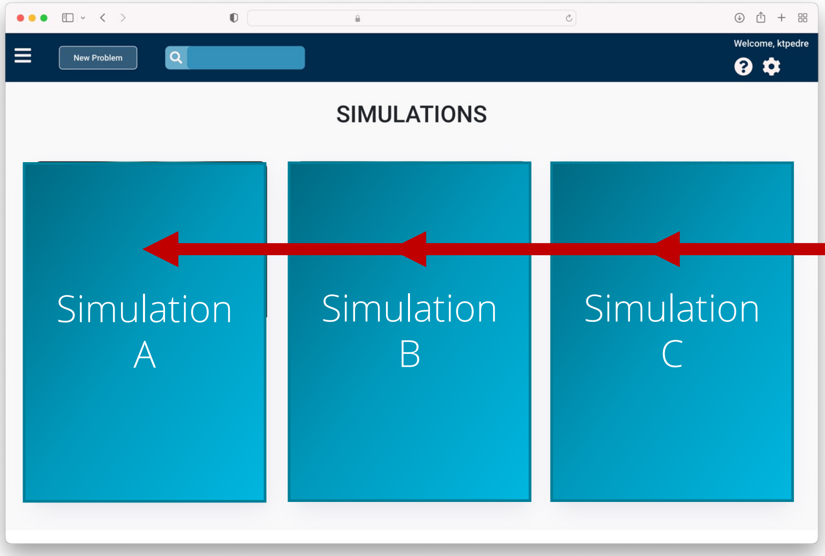


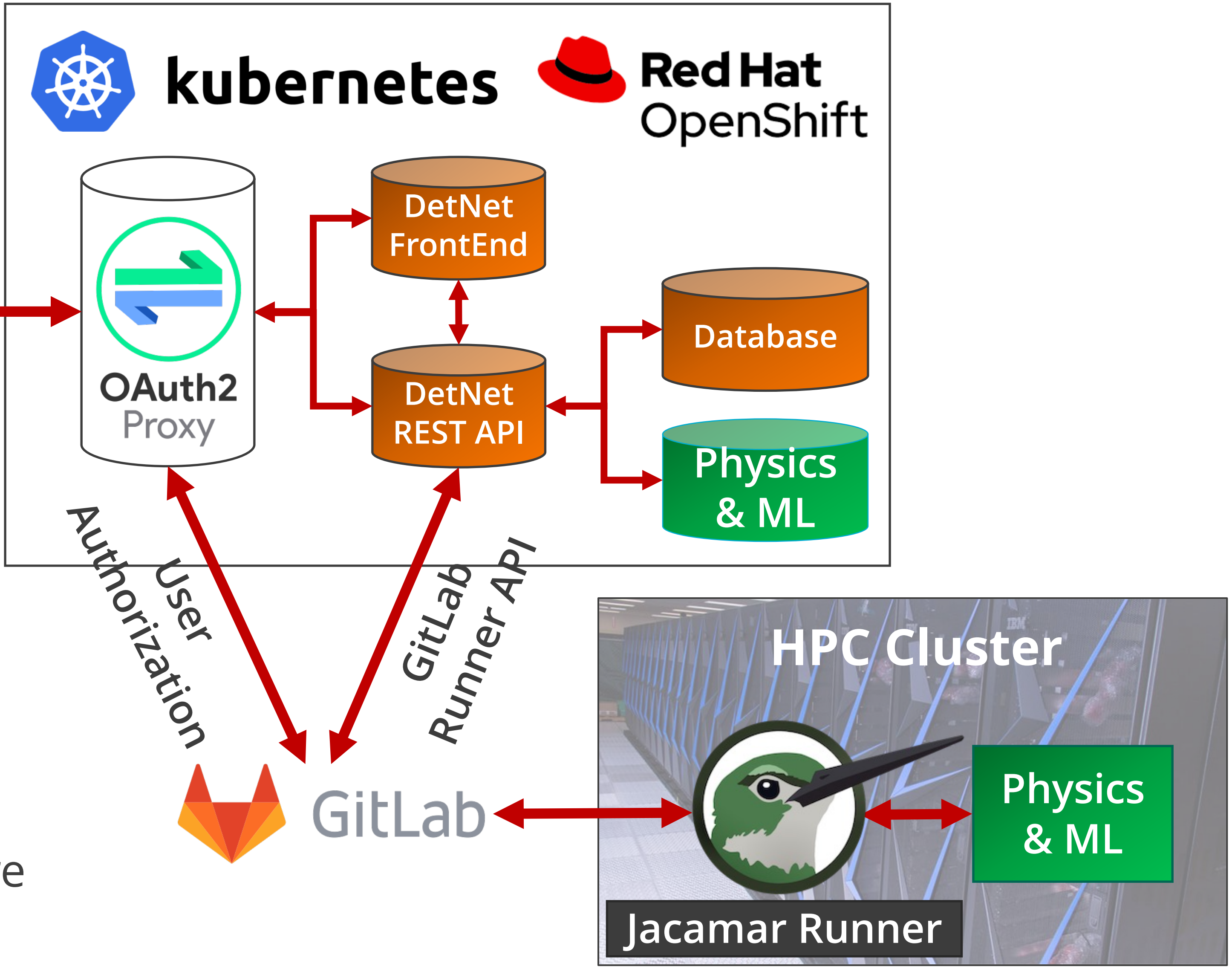
High-level design objectives:

- Containerize all components (UI, Cloud, HPC)
- Deploy frontend via Kubernetes
- Users unaware of what is running where

Challenge 2: Bridge to HPC with Jacamar Runners

DetNet Front-end User Interface





High-level design objectives:

- Containerize all components (UI, Cloud, HPC)
- Deploy frontend via Kubernetes
- Users unaware of what is running where

Jacamar @ Sandia push from Scot Swan & Allen Robinson

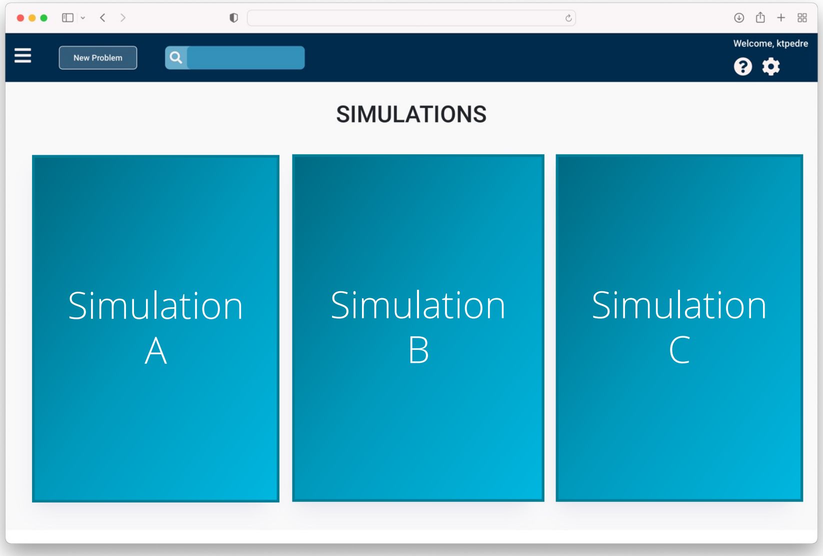
DetNet is Operational, Demonstrating Key Pieces

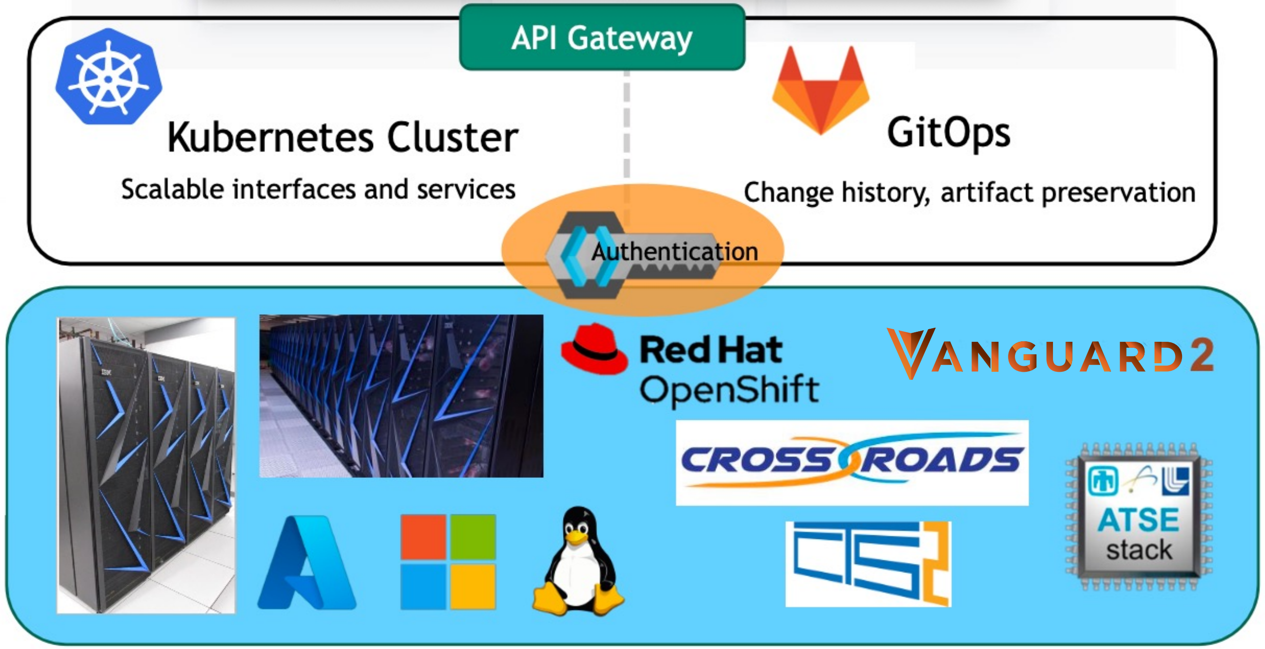
Designers / Engineers navigate web browser to DetNet front end

Presented with ***menu of simulations***, able to customize as needed

Computing-as-a-Service layer executes ***containerized simulation*** on appropriate computing resources

Results presented ***interactively*** and stored for later retrieval & analysis





What DetNet is Putting in the Hands of the Engineers

Simple Example: 2-D Detonator Simulation

1) User Enters Desired Parameters

Param A	100
Param B	200
Param C	300

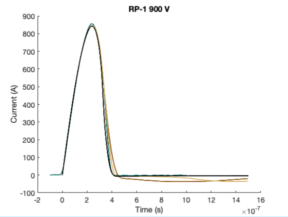
Simulate

2) 2D Simulation, ~1 min turnaround

Containerized Code

Cloud or HPC

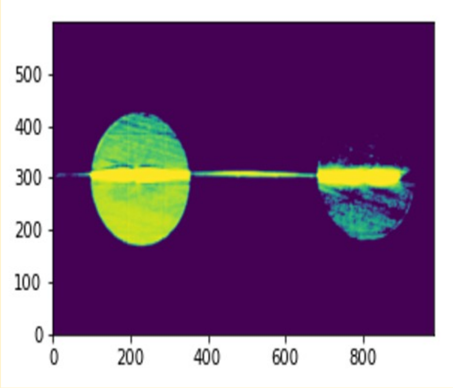
3) Interactive Exploration of Result



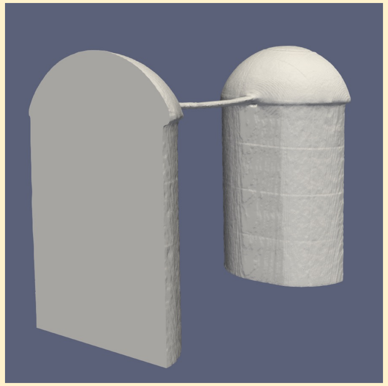
Ensemble Runs & Uncertainty Quantification

More Complex Example: Credible Automated Meshing of Images (CAMI), Surveillance Pathfinder

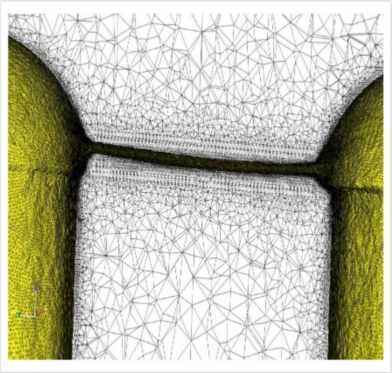
1) CT Scan Segmentation (ML, Python)



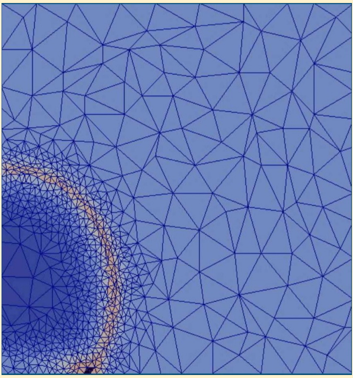
2) Surface Extraction & Smoothing (Python)



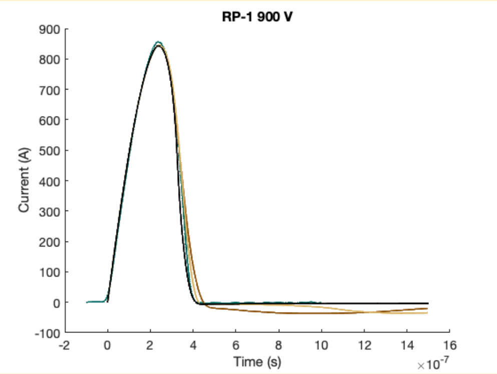
3) Surface & Volumetric Meshing (Krino & CUBIT)



4) Shock physics simulation (LGR)



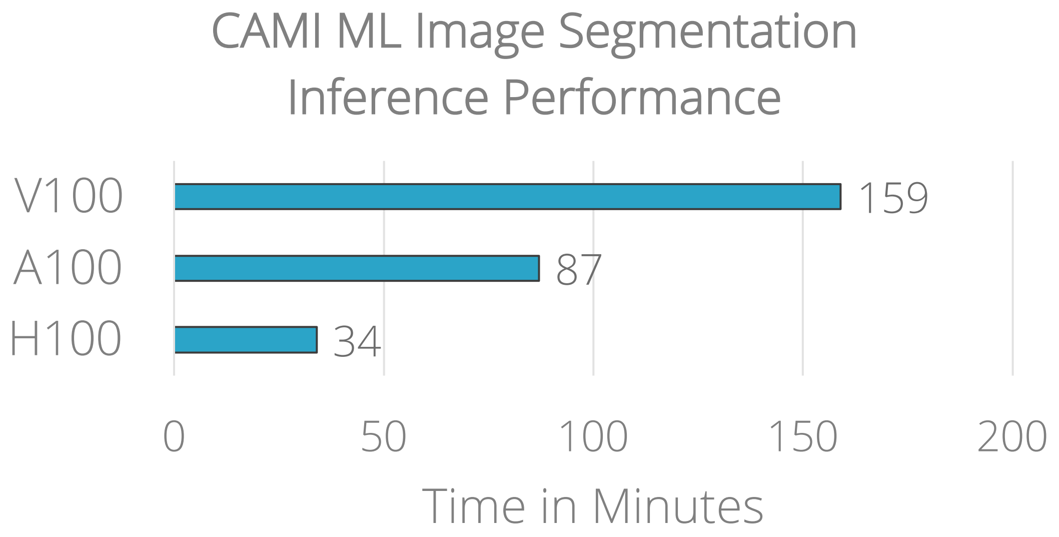
5) Simulated Response With UQ



DetNet Success Driving CaaS Expansion

- Hands-on engagement with DetNet team built relationships & translated "Leap of Faith" healthy skepticism to **"This is Working!"** ☺
  - Key aspect was cross-disciplinary teaming (HPC ModSim, Web Apps, Infrastructure)
- Rapid progress & demos have attracted attention from other teams
- Adding GPU hardware to Sandia OpenShift clusters

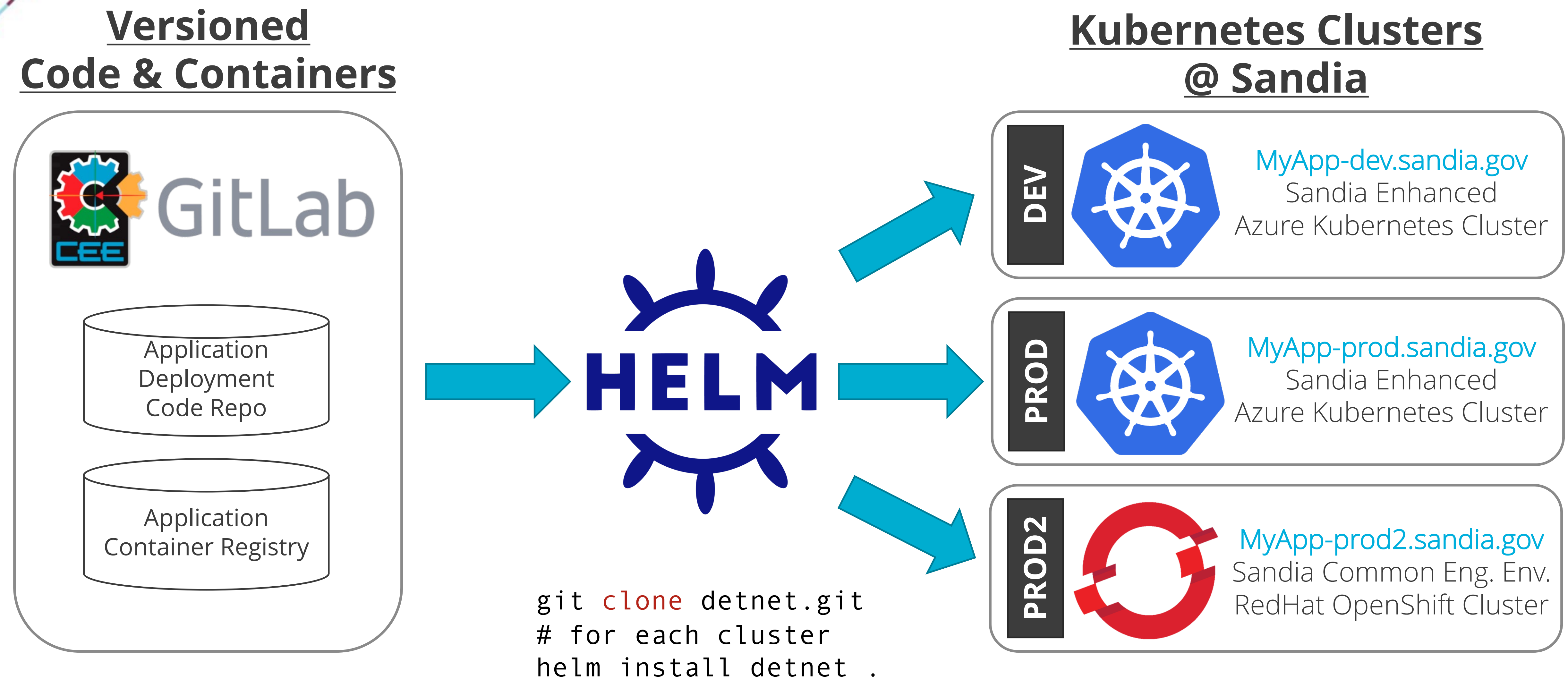
Example:
CAMI ML-based
Image Segmentation
Requires GPUs For
"Coffee Break"
turnaround speed



Outline

- Introduction
- Computing-as-a-Service Architecture
- R&D Directions / What’s Missing
- Conclusion

The Need for Automated Deployment



Versioned Code & Containers

GitLab CEE

Application Deployment Code Repo

Application Container Registry

HELM

```
git clone detnet.git
# for each cluster
helm install detnet .
```

Kubernetes Clusters @ Sandia

DEV

MyApp-dev.sandia.gov
Sandia Enhanced
Azure Kubernetes Cluster

PROD

MyApp-prod.sandia.gov
Sandia Enhanced
Azure Kubernetes Cluster

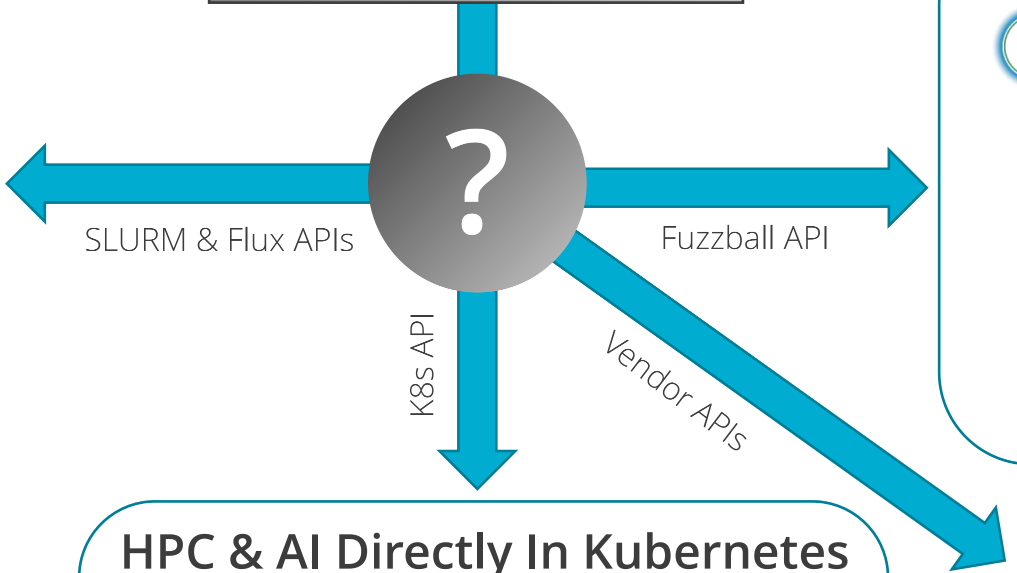
PROD2

MyApp-prod2.sandia.gov
Sandia Common Eng. Env.
RedHat OpenShift Cluster

The Need for an Intelligent Job Routing Layer

Where's the best place to run this job?

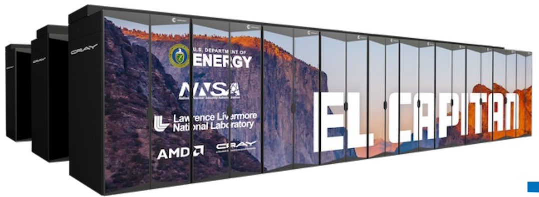
ADE Frontend Clients



Traditional HPC Platforms

slurm flux

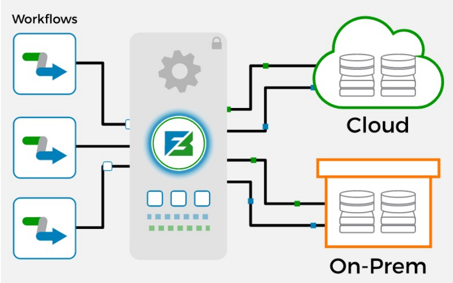
CROSSROADS


U.S. DEPARTMENT OF ENERGY
NNSA
Lawrence Livermore National Laboratory
AMD
CRAY
EL CAPITAN

CTS2

Emerging "HPC 2.0"

FUZZBALL https://ciq.co/



Exploring in VANGUARD

HPC & AI Directly In Kubernetes

KUBERNETES BATCH + HPC DAY NORTH AMERICA

kubeflow/mpi-operator

multi-nic-cni-operator

Fluence (KubeFlux)

Cloud Services & HW

AWS Lambda & Batch

Azure Functions & Batch

Google Cloud Dataflow

The Need for Integrated Data Management Solutions

Spawned "informal" data management working group to find solutions

Sandia has deployed S3 (Simple Storage Service)

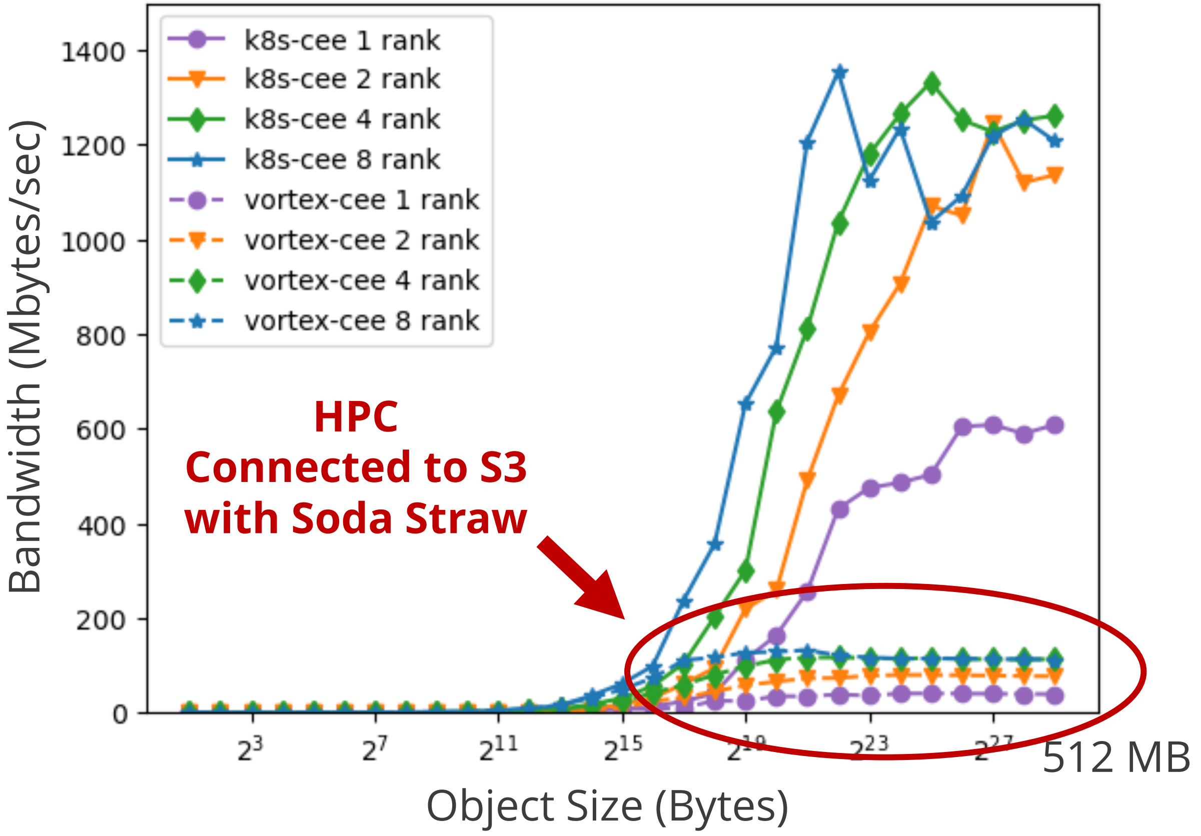
Sandia data management services:

DataSEA
Data for Systems Engineering Applications

SAW SDM
Simulation Data Management

Sandia MPI S3 Client Benchmark

Aggregate Get Bandwidth

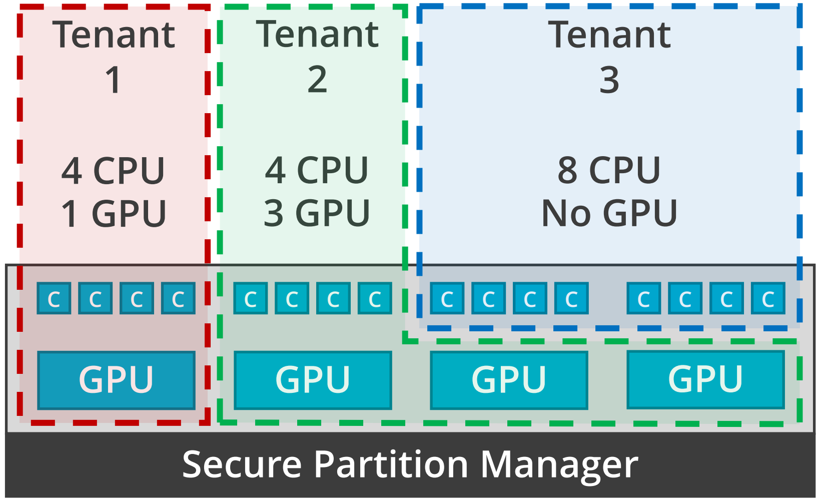


HPC Connected to S3 with Soda Straw

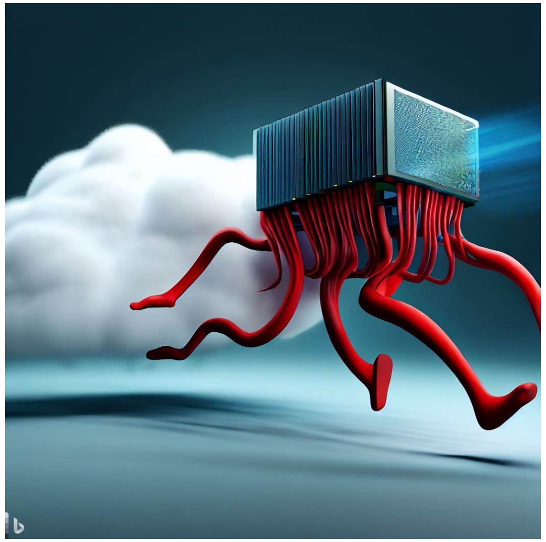
512 MB

Future Directions

- Cloud-style multi-tenancy
- Digital twins linking sensors & simulation
- ChatGPT style interfaces to ModSim tools



Split-up complex nodes to reduce waste & improve security



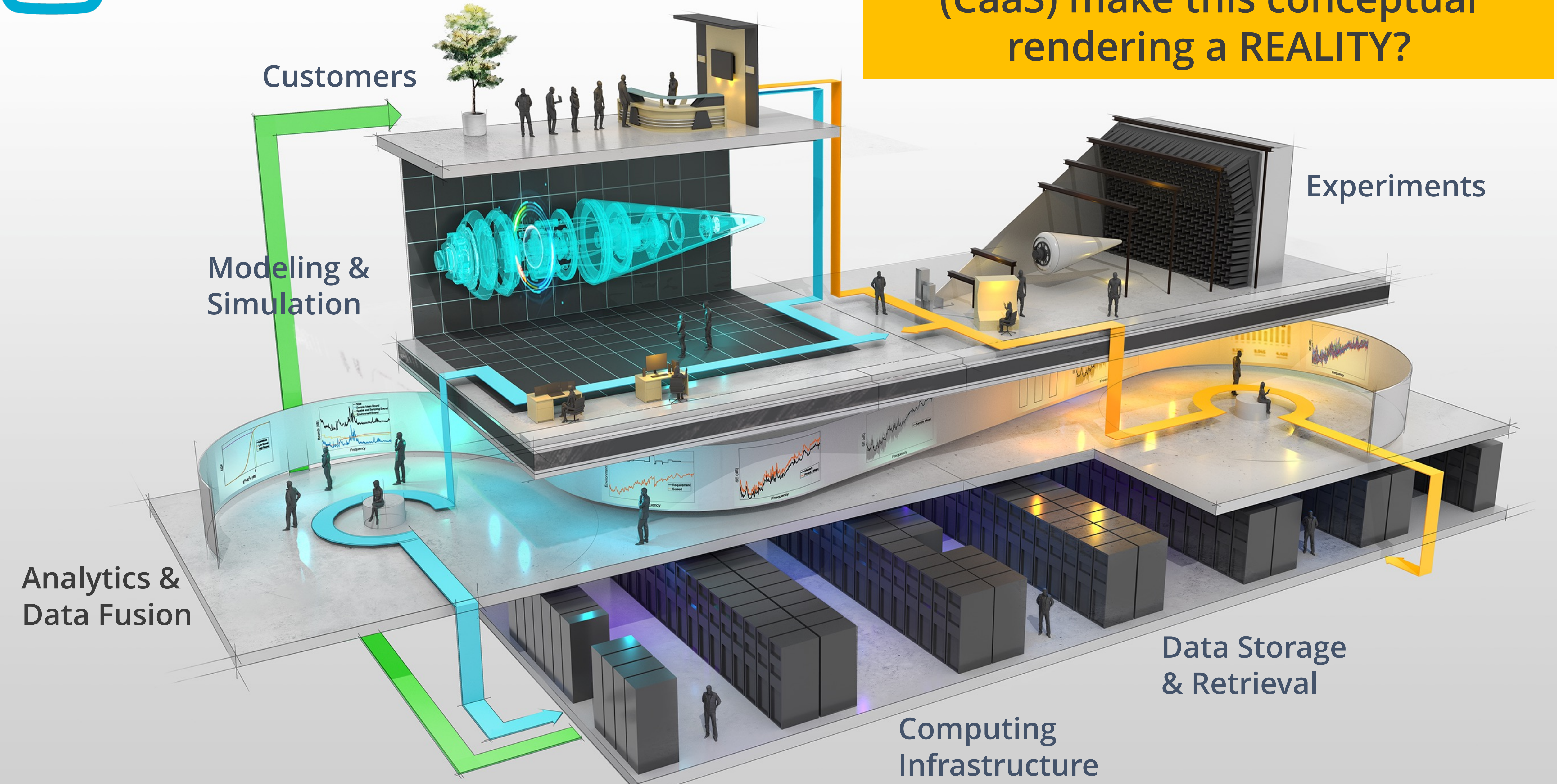
Supercomputer sprouting legs and running from a cloud

Supercomputer sprouting wings and flying in the clouds

Outline

- Introduction
- Computing-as-a-Service Architecture
- R&D Directions / What's Missing
- Conclusion

How can “Computing-as-a-Service” (CaaS) make this conceptual rendering a REALITY?



CaaS is Enabling Digital Engineering

- Delivering simulation capabilities as turnkey services
- Forming cross-disciplinary teams key to success
- Pioneered Approach with DetNet

BEFORE: HPC Specialist Required,
Turnaround time **Days**

AFTER: Engineers directly access web-based detonator performance assessment tools,
Containerized backend HPC & ML pipelines,
Results within **1 hour**

Thank you to the Sandia CEE, Testbeds, CapViz, ASC DevOps, Azure Stack, CSSE, and ADE teams for supporting this work.

Reshaping How We Deploy Codes to Users and Designing our Computing Infrastructure to Match