Distributed Backends for Machine Learning-based Simulation Solvers

Allen Mao
Kliment Minchev

CTO Office

Ansys

Background

Instant Prediction of High-Fidelity Simulation

Cloud-first Machine Learning Platform

End-to-End Deployment

Industry landscape:

- Apple, Nvidia, Google, Intel
- DesignAI by Altair, Nvidia Modulus / SimNet + Omniverse

Cloud HPC integration

1000x or faster simulation

Distributed Computing + Microservices Architecture

- Input simulation data
- Build a deep learning model
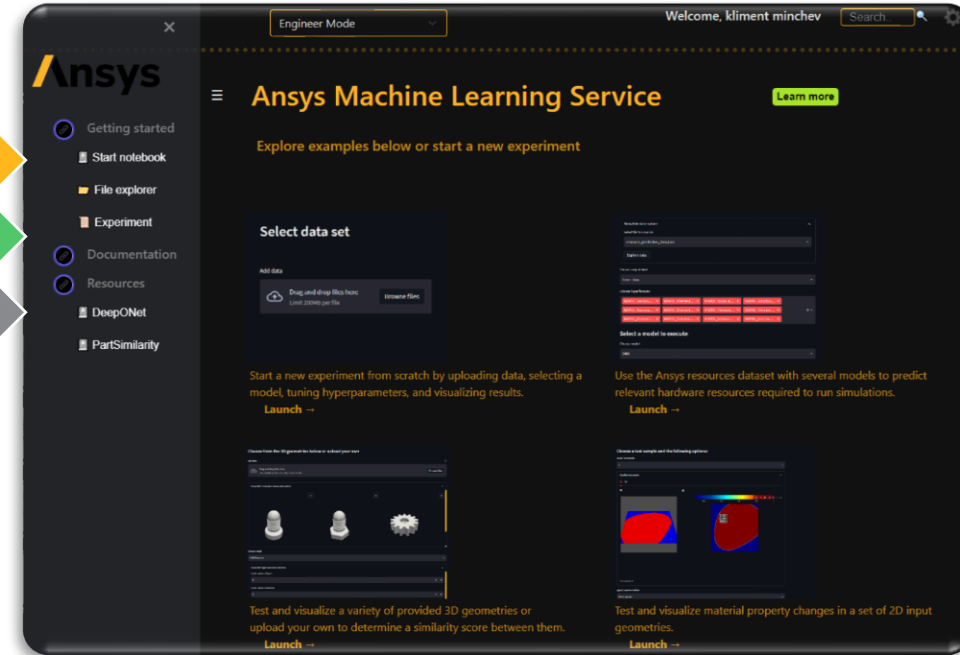- Use existing datasets, models from library

Focus on:
 simulation-based datasets
 visualization heavy

Peers:
- AWS SageMaker
- Azure ML

Improve Ansys ML developer productivity

Ansys Machine Learning Service

Why Ansys ▾   Products & Services ▾   Learn ▾

/Ansys

Home > Blog > Prepare for the Machine Learning Revolution with Emerging MLaaS Capabilities from Ansys
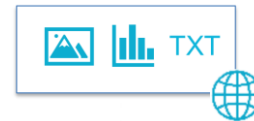
ANSYS BLOG   FEBRUARY 2, 2023

Prepare for the Machine Learning Revolution with Emerging MLaaS Capabilities from Ansys

Machine learning (ML) is, justifiably, receiving a lot of attention today. ML is helping companies in every industry identify performance

Public datasets

Private datasets

Synthetic datasets

Models + Code

/Ansys

Motivation for a Backend

Composable Machine Learning Simulator (CoMLSim)	Intricacies	Containerization & Deployment	Backend Consumption & UX

Design choices

- Pipeline of Neural Networks
- Built-in optimization
- Generated output and file formats

Solver: BCs, volumetric source terms, surface solution fields, geometry

Trains on and evaluates full-fidelity steady-state PDE solutions

R&D in progress

Distributed System

- Server + requests
- Functional isolation
- Data processing
- Model training
- Inference

Microservice Architecture

- Containerization
- Interoperability
- Scalability and compute resource requirements (RAM, GPU)

Cloud Resources

- AWS compute instances
- Storage, Container registry, Databases, Queue
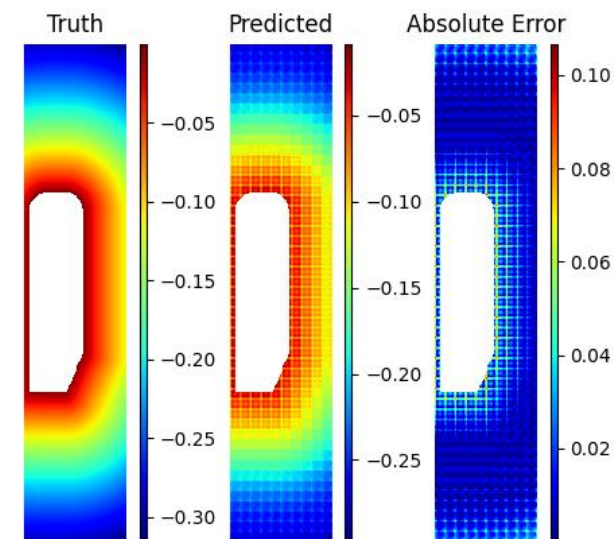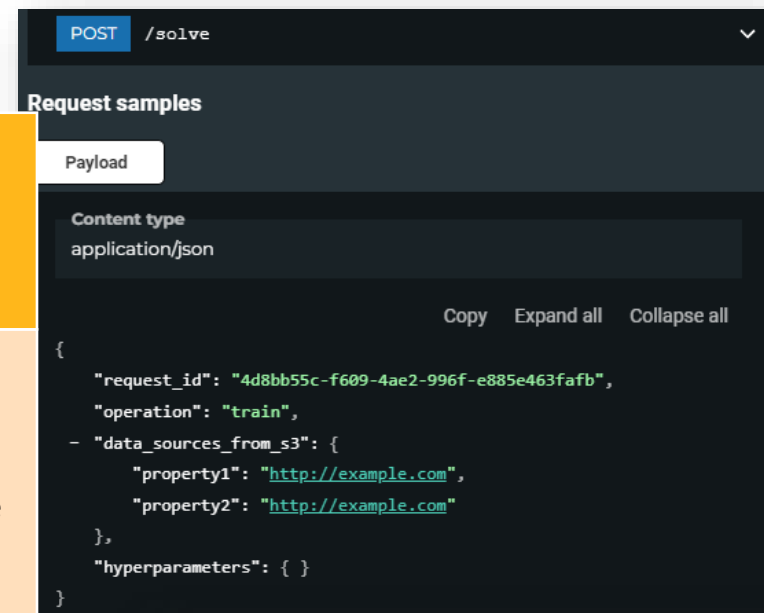- SageMaker, Kubernetes

Frontend

- No-Code Web Platform
- Notebook-style code execution

RESTful API

- Endpoints
- Payload schema
- Authentication

ML-based Simulation Paradigm

- Producer & Consumer Roles
- Custom workflow creation: training, model tuning, analysis, investigation
- Inference as a Service

POST /solve

Request samples

Payload

Content type
application/json

Copy   Expand all   Collapse all

{
    "request_id": "4d8bb55c-f609-4ae2-996f-e885e463fafb",
    "operation": "train",
  - "data_sources_from_s3": {
        "property1": "http://example.com",
        "property2": "http://example.com"
    },
    "hyperparameters": { }
}

Truth   Predicted   Absolute Error

/Ansys

# Backend Architecture Roadmap

Job Submission and Code Execution

- Server responds to requests
- AWS SageMaker Jobs (compute instance, S3 download/upload): training & inference
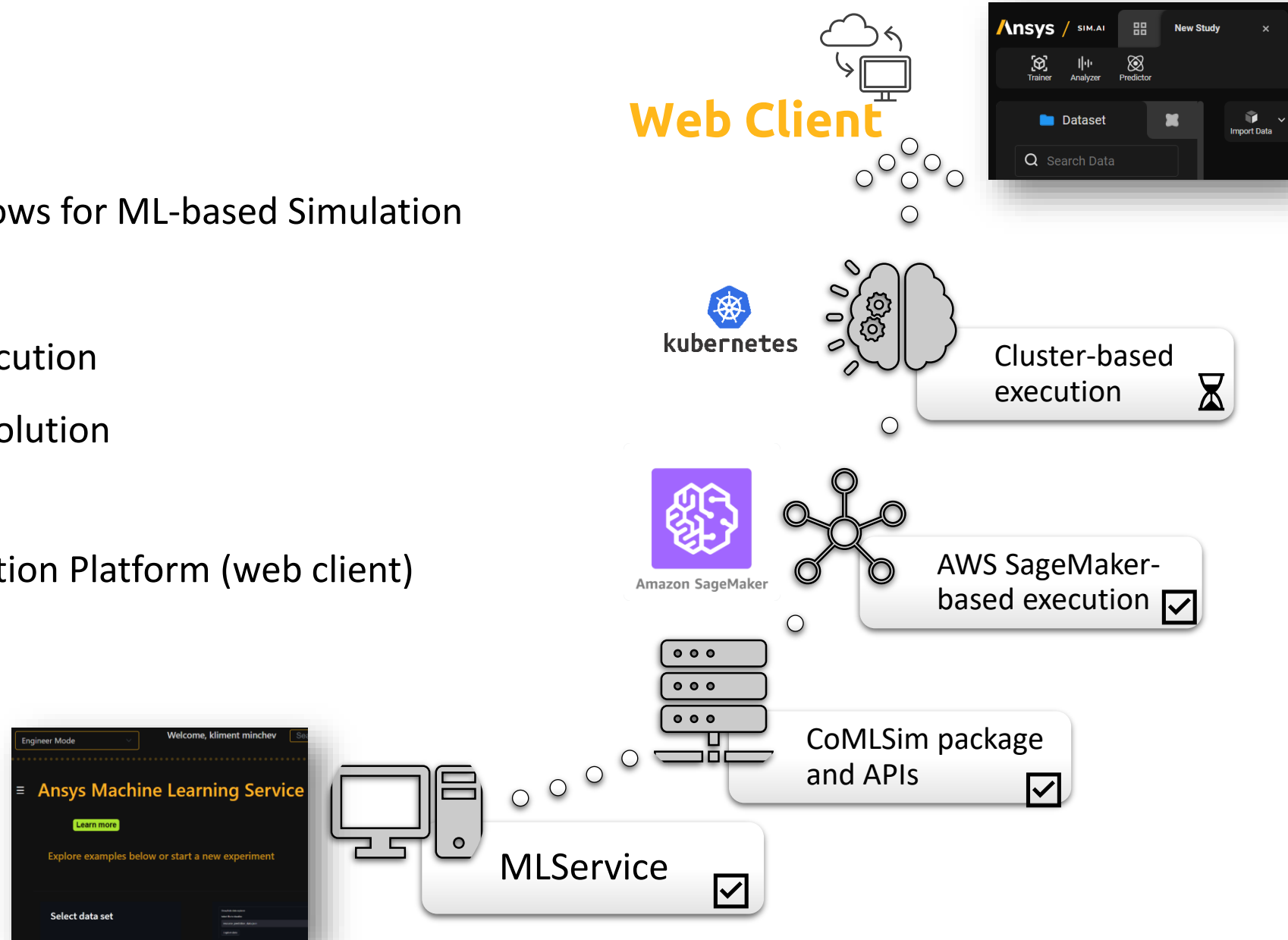- S3 input: case files, S3 output: results, DB: metadata
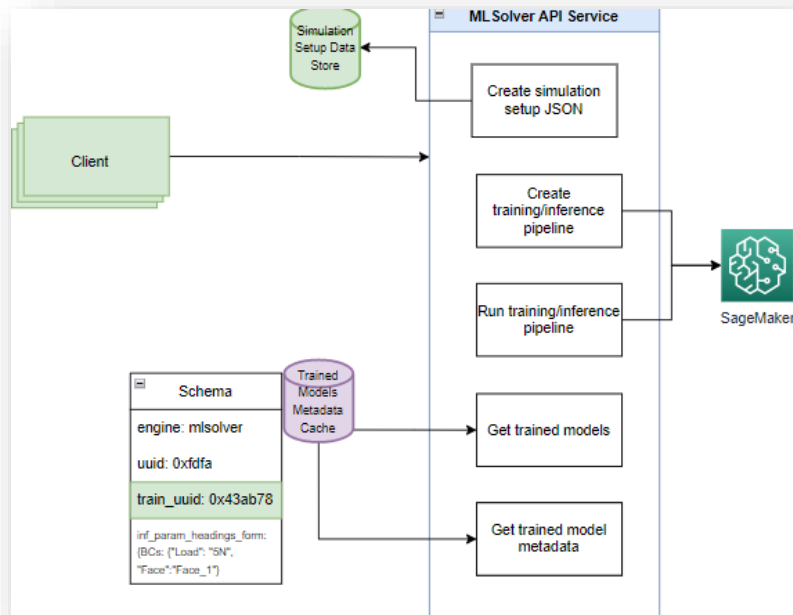
Service-based

- Server responds to requests
- AWS Fargate/ECS/Kubernetes cluster
- Pod in cluster executes compute job (highly available)
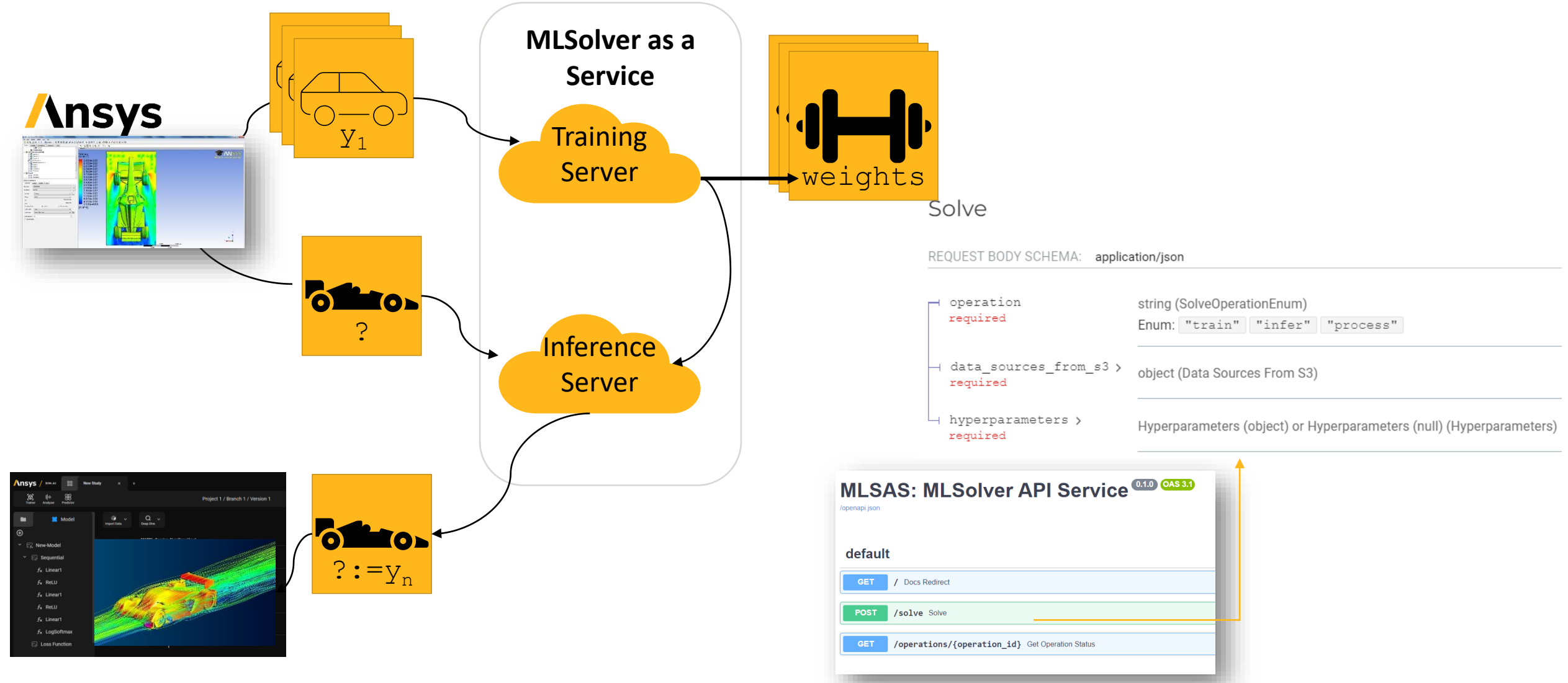- S3 input: case files, S3 output: results, DB: metadata
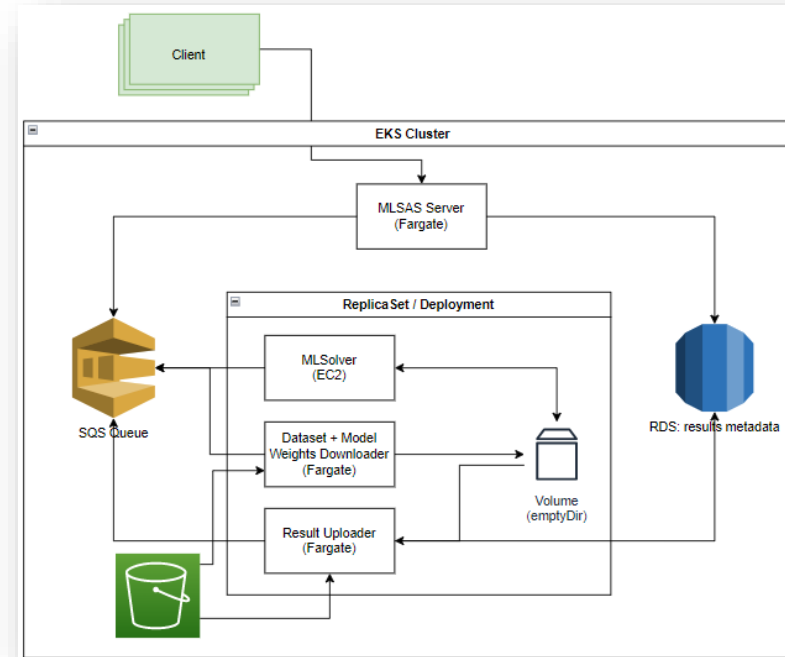
Project Evolution

- MLService: configurable workflows for ML-based Simulation

- CoMLSim python package

- AWS SageMaker: job-based execution

- Cluster-based highly-available solution

  - ECS, EKS

- Ansys Machine Learning Simulation Platform (web client)

Web Client

Cluster-based execution

AWS SageMaker-based execution ☑

Amazon SageMaker

CoMLSim package and APIs ☑

MLService ☑

Training as a Service, Inference as a Service

©2023 ANSYS, Inc.

The Stack and its Properties

Raw Case Files
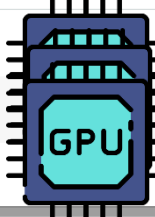
Data Processor

Machine Learnable Data

Trainer

Machine Learning Models + Weights

Inference Solver

Vector Field Predictions

Accelerated Computing	vCPU	Memory
ml.p3.2xlarge	8	61 GiB
ml.p3.8xlarge	32	244 GiB
ml.p3.16xlarge	64	488 GiB

MLSAS: MLSolver API Service 0.1.0 OAS 3.1
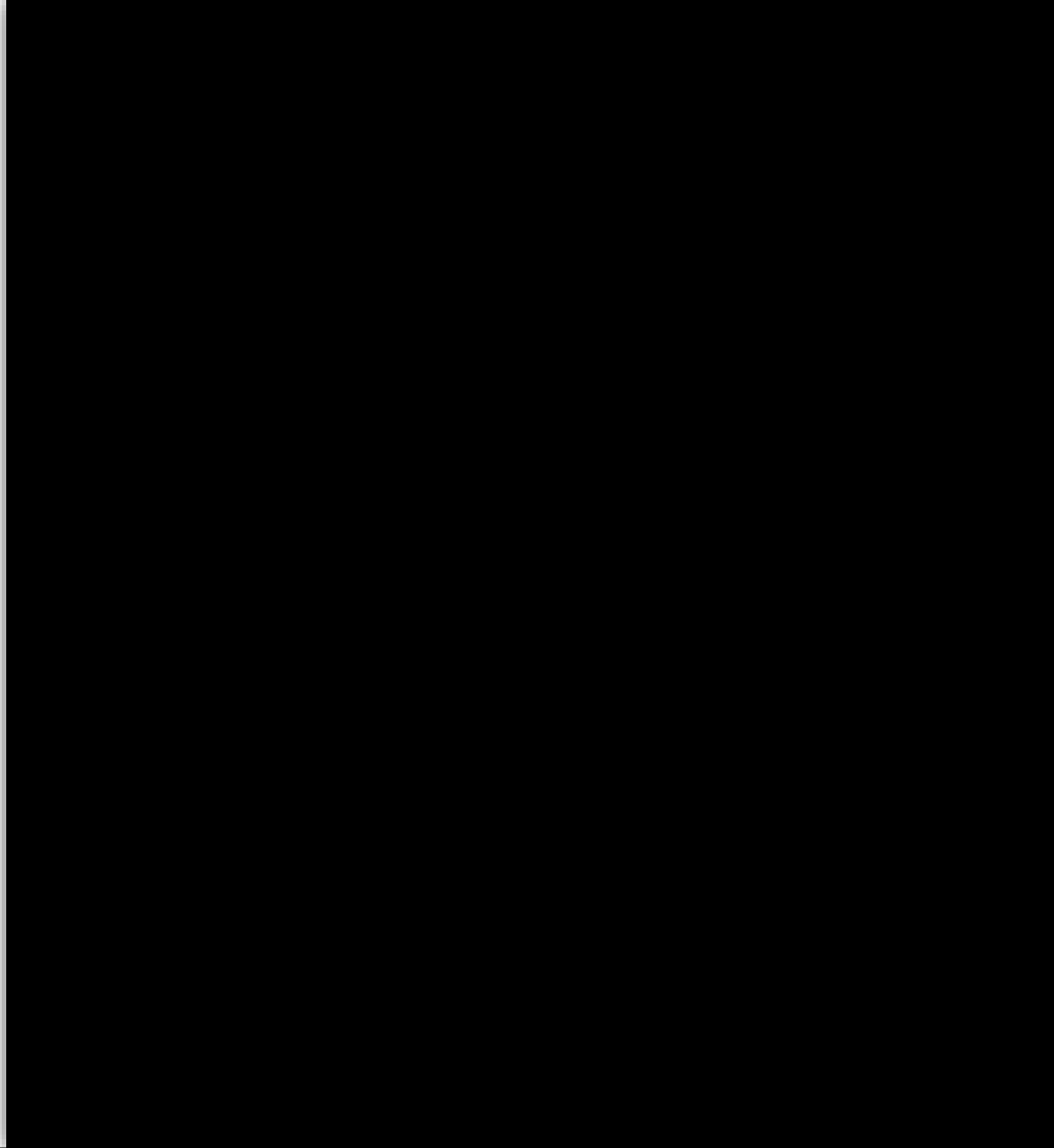/openapi.json

API Request

Amazon SageMaker

Amazon EC2

Ansys

Demo Video

Summary

- Cloud backend and web API for the Composable Machine Learning Simulator (CoMLSim)

  - Next generation ML-based simulation

  - Universally accessible

- Evolving CoMLSim package, maturing cloud backend in parallel

  - Sophisticated, distributed (compute cluster), Infrastructure req's

- Compute jobs-based execution for initial rollout

  - Training as a Service, Inference as a Service