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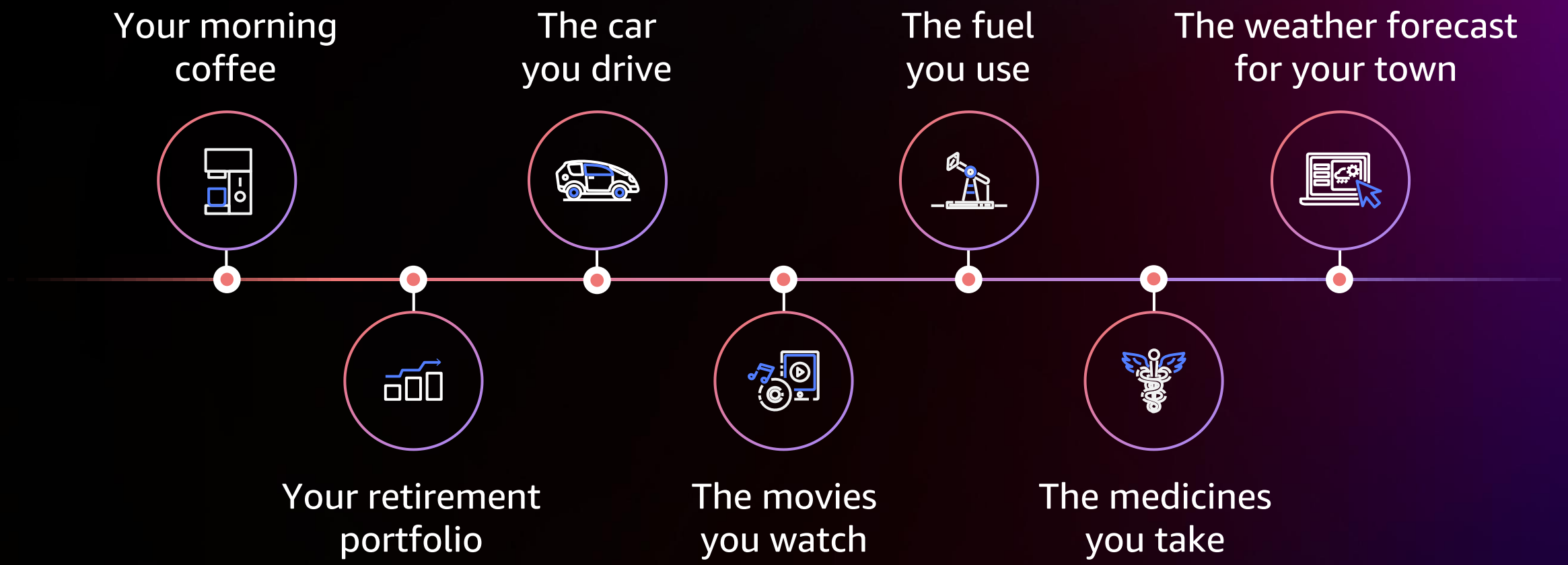
How AWS and aerospace and geospatial companies are rethinking HPC

Barry Bolding (he/him)
Director, HPC+ Worldwide GTM
AWS

Colin Haubrich
Head of IT
Wisk Aero

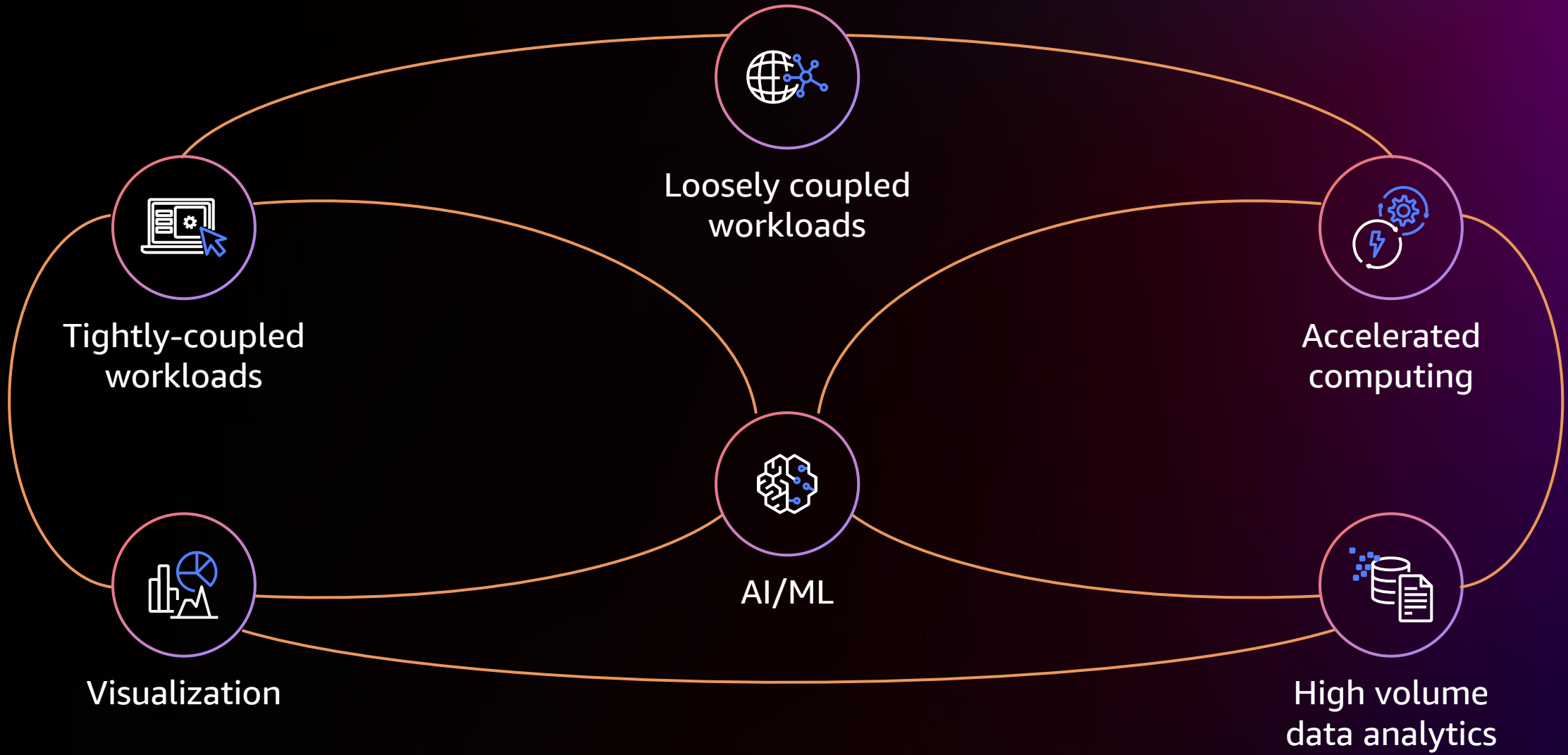
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HPC impacts your life every day



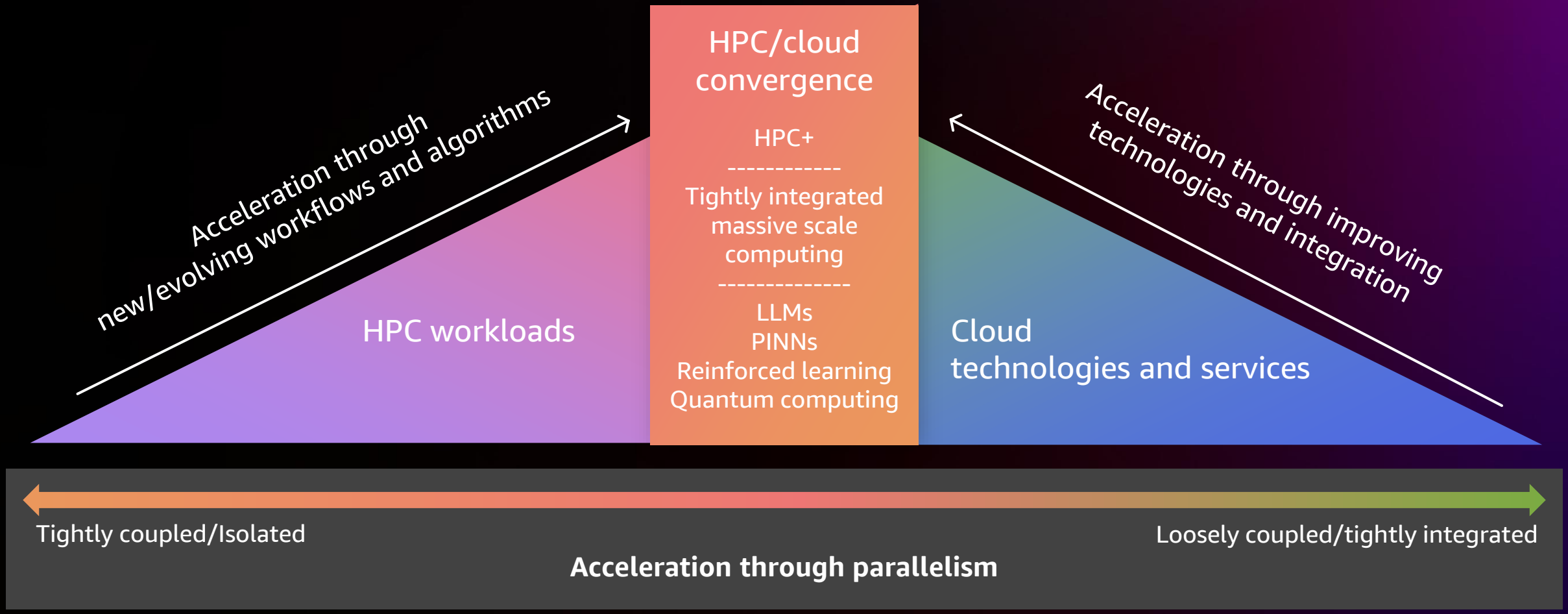
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Mapping HPC



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The convergence of cloud, HPC, and ML



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Acceleration through experience

Acceleration through new/evolving workflows and algorithms

Acceleration through improving technologies and integration

HPC workloads

HPC/Cloud convergence

HPC+

Tightly integrated massive scale computing

LLMs
PINNs
Reinforced learning
Quantum computing

Cloud technologies & services



CAE
CFD



Seismic reservoir



Financial services risk actuarial



EDA



Drug discovery
Genomics
Cryo-EM



Weather
Climate



Autonomous compute
Digital twins



Quantum computing



Autonomous vehicles



ML frameworks

aws

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Acceleration through scale

VirtualFlow

2.2M+ vCPUs
to analyze billions of cancer proteins

Woodside

1.1M vCPUs
to accelerate seismic processing workload by 150X



Descartes Labs

9.95 petaflop
high-performance LINPACK (HPL) benchmark to rank #50 on the TOP500

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Evolution of HPC at AWS

HPC workloads

Run and Scale all core-HPC workloads

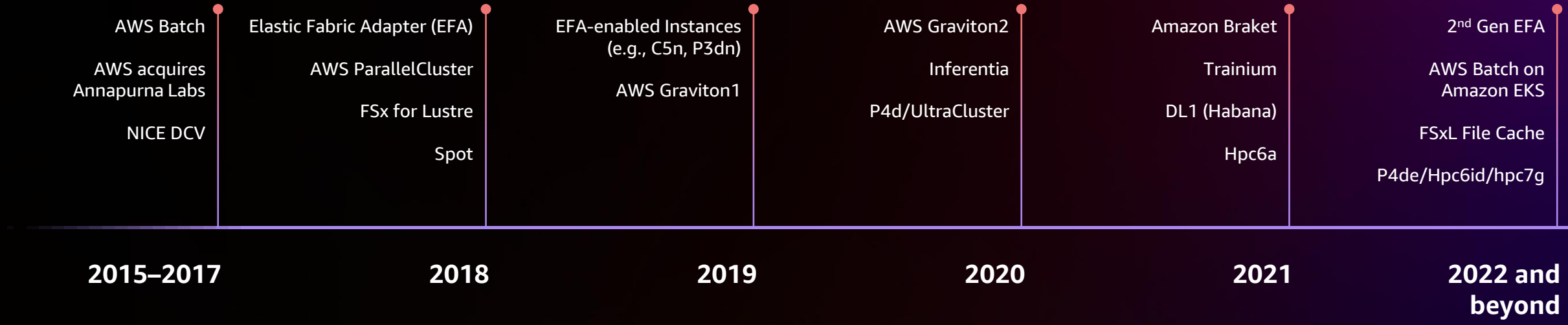
HPC+

Extend capabilities through ML and acceleration

- Quantum computing
- Digital twin
- Autonomous systems
- Reinforced learning

Empowering with ML and DL

Combination of SPDs and core technologies to scale inference and training workloads

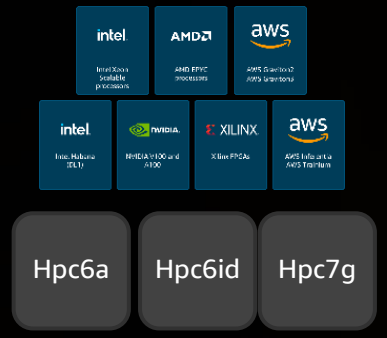


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Key services that enable HPC+ on AWS

Compute

Amazon EC2



Networking

Elastic Fabric Adapter (EFA)

Up to 400 Gbps networking

Storage

Amazon FSx for Lustre

Amazon FSx for NetApp ONTAP

Amazon FSx for OpenZFS

Orchestration

AWS Batch

AWS ParallelCluster

NICE EnginFrame

Visualization

NICE DCV

AWS takes a system view of workload and technology

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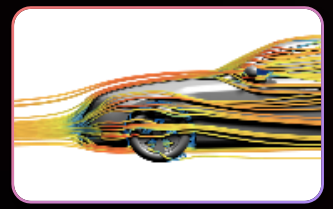
Putting HPC+ to work

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AWS HPC+ for engineering simulation



Crash[1]



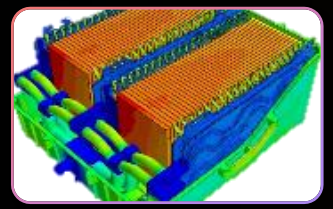
Aerodynamics[2]



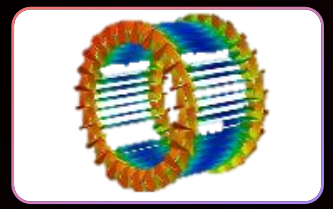
Thermal/cooling[2]



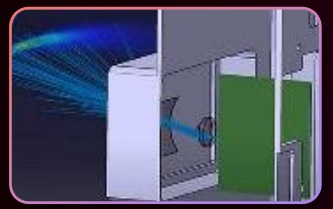
Engine[4]



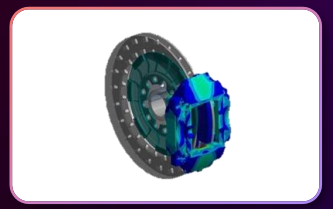
Battery[2]



Electric motor[3]



Sensors & electronics[3]



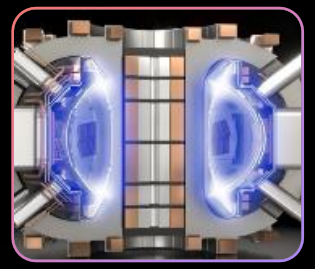
Body & chassis[3]

Images from AWS Partners:
www.altair.com; www.plm.automation.siemens.com; www.ansys.com; www.convergecfd.com

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AWS HPC+ enables science and engineering



Commonwealth Fusion Systems

CFS is leveraging decades of fusion research combined with the innovation and speed of the private sector

- Particle transport (LANL MCNP)
- Multi-physics sim. (FISPACT-II)

"As CFS works to bring clean, limitless commercial fusion energy to the grid, we're excited to work with AWS and their HPC team."
Nate O'Farrell, Head of IT Infrastructure, CFS



Boom Supersonic

Boom Supersonic leveraged AWS to accelerate the design and construction of its supersonic aircraft

- Aerospace engineering
- Computational fluid dynamics (CFD)

"AWS, the world's leading cloud provider, will help us continuously refine our designs."
Blake Scholl, Founder and CEO, Boom Supersonic



Moderna Therapeutics

Moderna uses AWS services to reduce the time and cost of bringing new life-saving therapies to market

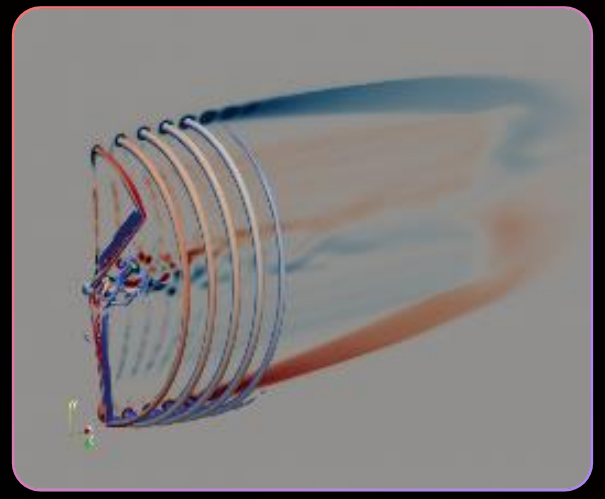
- Drug discovery
- AI/ML

"The science behind mRNA medicines is advancing at a rapid pace, and building Moderna's technology platform on AWS gives our scientists the insights, agility, and security they need to continue to lead in the industry."
Stéphane Bancel, CEO, Moderna

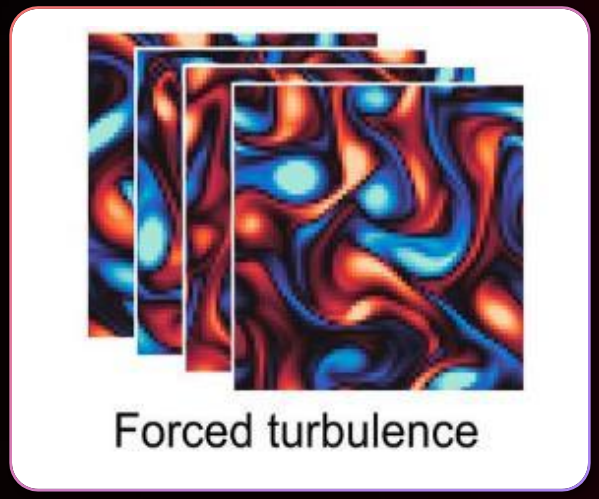
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From HPC simulations to predictive modeling

Computational fluid dynamics (CFD)

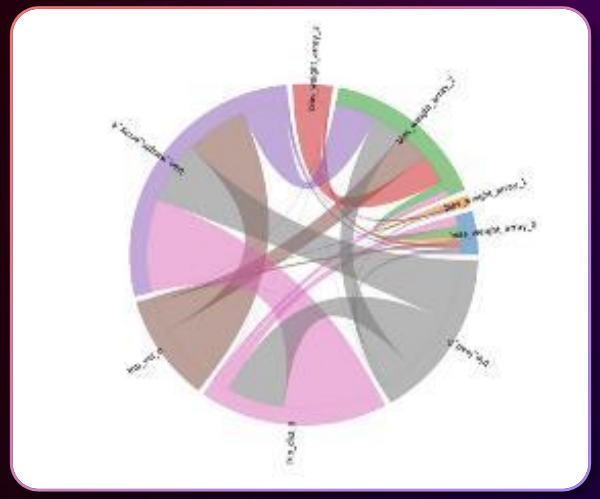


Accelerate CFD with AI/ML



Credit: “Machine learning–accelerated computational fluid dynamics” https://www.pnas.org/content/118/21/e2101784118

Predictive modeling for digital twins

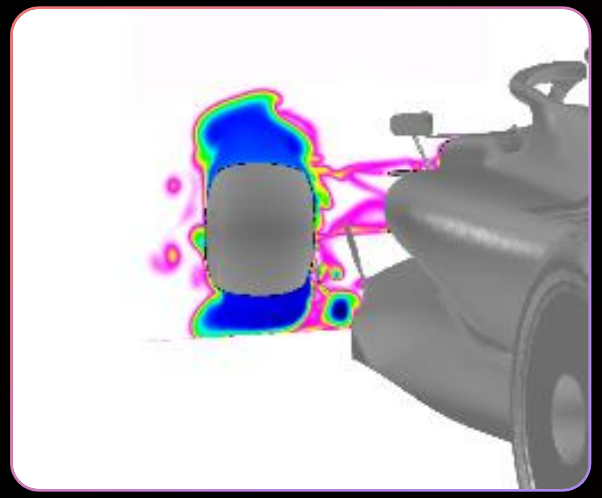


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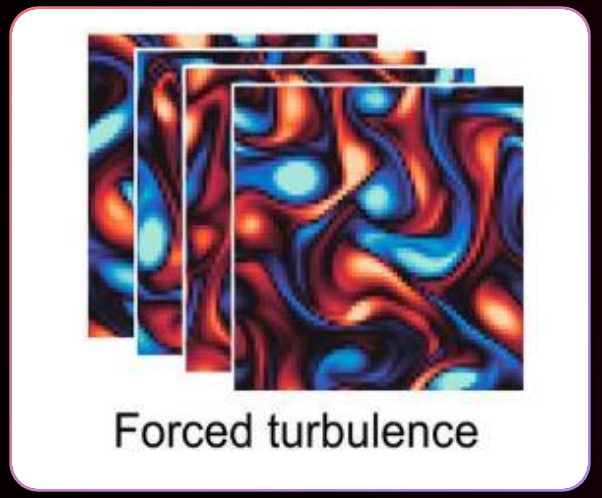
Accelerate CFD with AI/ML

Extract relationships from simulation data



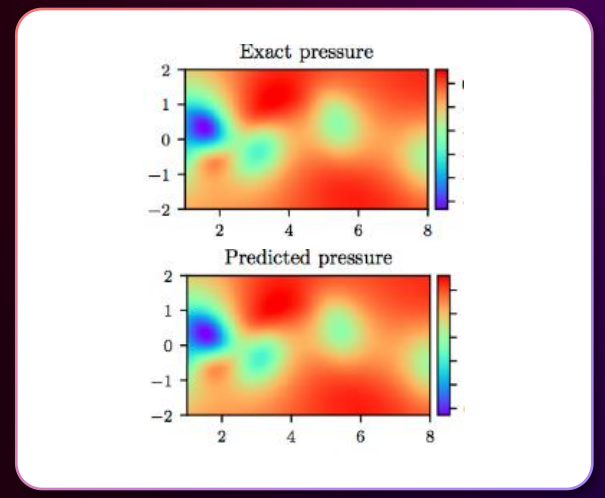
Credit: F1

Accelerate HPC simulations with embedded ML models



Credit: “Machine learning–accelerated computational fluid dynamics” https://www.pnas.org/content/118/21/e2101784118

Learn solutions to governing equations directly



Credit: Physcs Informed Deep Learning, https://maziarraissi.github.io/PINNs/

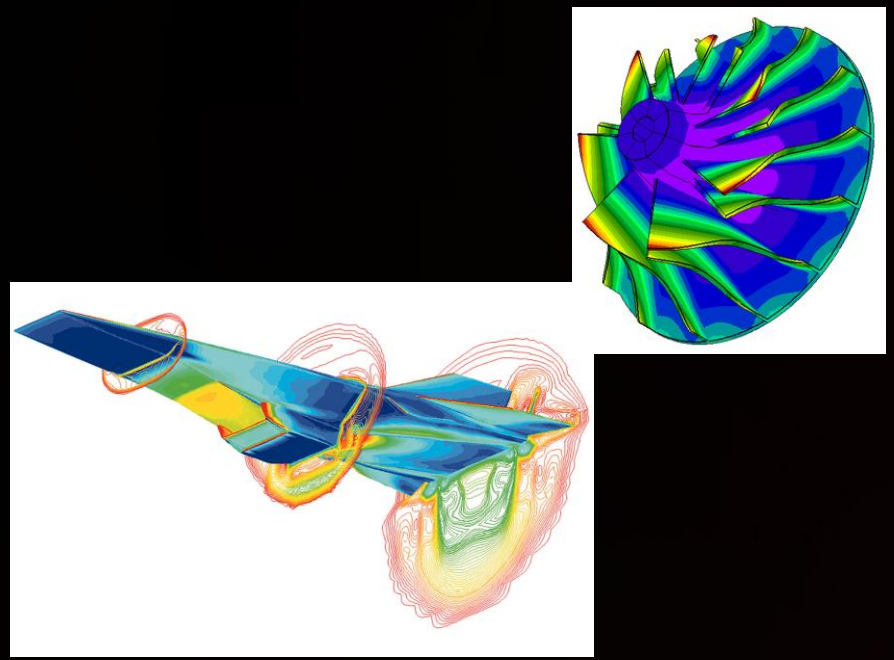
AI-driven infrastructure optimization

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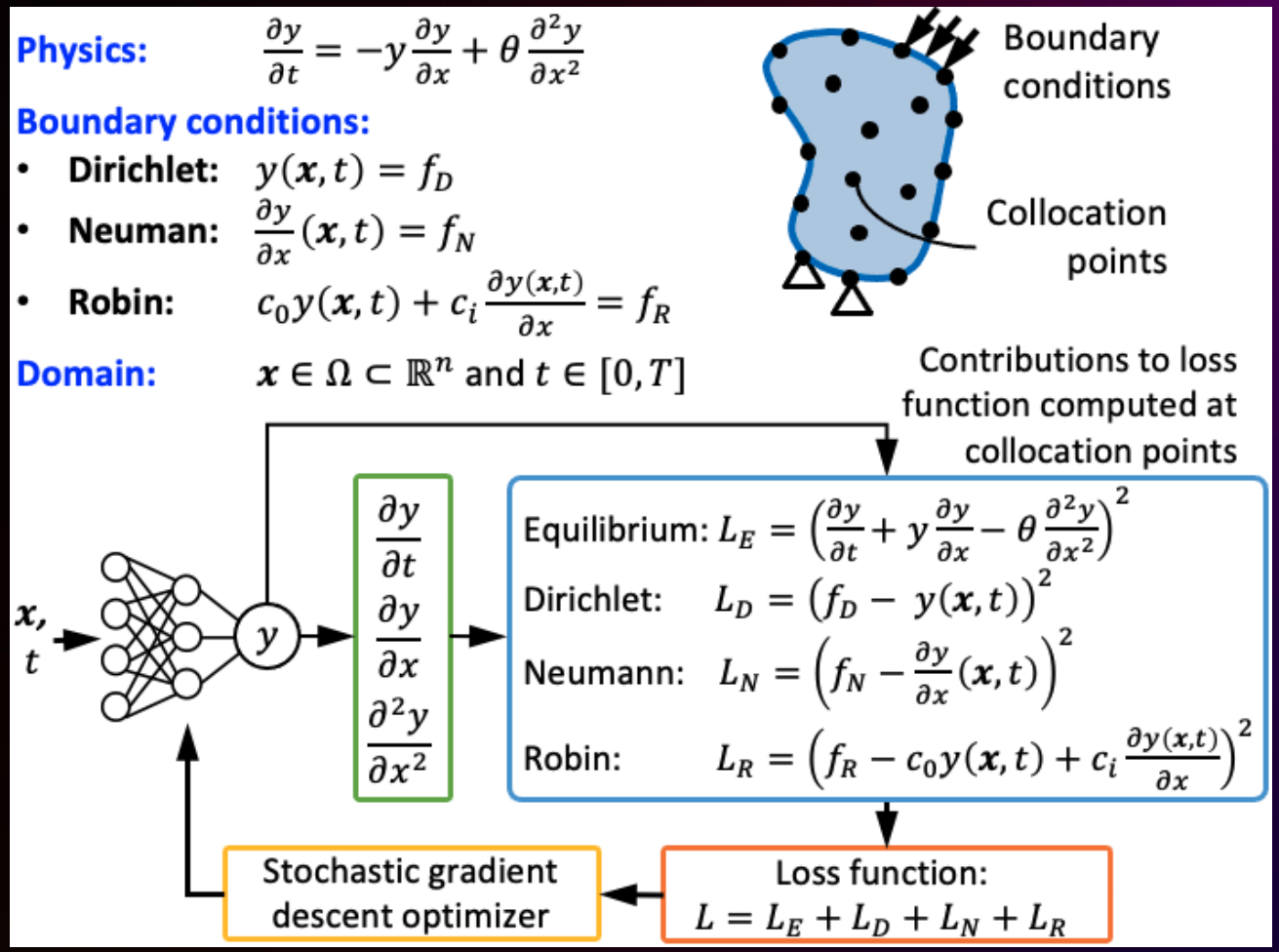
Physics-informed neural networks (PINNs) 101

Numerical methods used to solve partial differential equations (PDEs)

- Finite element modeling
- Computational fluid dynamics



Physics-informed neural networks



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State of the art

JOURNAL OF COMPUTATIONAL PHYSICS 91, 110–131 (1990)

Neural Algorithm for Solving Differential Equations

HYUK LEE

Department of Electrical Engineering, Polytechnic Institute of New York, Brooklyn, New York 11201

AND

IN SEOK KANG

Department of Chemical Engineering, California Institute of Technology, Pasadena, California 91125

Received August 17, 1988; revised October 6, 1989

Finite difference equations are considered to solve differential equations numerically by utilizing minimization algorithms. Neural minimization algorithms for solving the finite difference equations are presented. Results of numerical simulation are described to demonstrate the method. Methods of implementing the algorithms are discussed. General features of the neural algorithms are discussed. © 1990 Academic Press, Inc.

IEEE TRANSACTIONS ON NEURAL NETWORKS, VOL. 16, NO. 6, NOVEMBER 2005 1381

Finite-Element Neural Networks for Solving Differential Equations

Pradeep Ramuhalli, *Member, IEEE*, Lalita Udpa, *Senior Member, IEEE*, and Satish S. Udpa, *Fellow, IEEE*

***Abstract*—The solution of partial differential equations (PDE) arises in a wide variety of engineering problems. Solutions to most practical problems use numerical analysis techniques such as finite-element or finite-difference methods. The drawbacks of these approaches include computational costs associated with the modeling of complex geometries. This paper proposes a finite-element neural network (FENN) obtained by embedding a finite-element model in a neural network architecture that enables fast and accurate solution of the forward problem. Results of applying the FENN to several simple electromagnetic forward and inverse problems are presented. Initial results indicate that the FENN performance as a forward model is comparable to that of the conventional finite-element method (FEM). The FENN can also be used in an iterative approach to solve inverse problems associated with the PDE. Results showing the ability of the FENN to solve the inverse problem given the measured signal are also presented. The parallel nature of the FENN also makes it an attractive solution for parallel implementation in hardware and software.**

***Index Terms*—Finite-element method (FEM), finite-element neural network (FENN), inverse problems.**

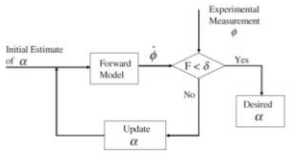


Fig. 1. Iterative inversion method for solving inverse problems.

resulting in the corresponding solution to the forward problem ($\hat{\phi}$). The model output is compared to the measurement (ϕ), using a cost function $F(\phi, \hat{\phi})$. If $F(\phi, \hat{\phi})$ is less than a tolerance δ, the estimate α is used as the desired solution. If not, α is updated to minimize the cost function.

SCIENCE ADVANCES | RESEARCH ARTICLE

APPLIED MATHEMATICS

Data-driven discovery of partial differential equations

Samuel H. Rudy,[1]* Steven L. Brunton,[2] Joshua L. Proctor,[3] J. Nathan Kutz[1]

We propose a sparse regression method capable of discovering the governing partial differential equation(s) of a given system by time series measurements in the spatial domain. The regression framework relies on sparsity-promoting techniques to select the nonlinear and partial derivative terms of the governing equations that most accurately represent the data, bypassing a combinatorially large search through all possible candidate models. The method balances model complexity and regression accuracy by selecting a parsimonious model via Pareto analysis. Time series measurements can be made in an Eulerian framework, where the sensors are fixed spatially, or in a Lagrangian framework, where the sensors move with the dynamics. The method is computationally efficient, robust, and demonstrated to work on a variety of canonical problems spanning a number of scientific domains including Navier-Stokes, the quantum harmonic oscillator, and the diffusion equation. Moreover, the method is capable of disambiguating between potentially nonunique dynamical terms by using multiple time series taken with different initial data. Thus, for a traveling wave, the method can distinguish between a linear wave equation and the Korteweg–de Vries equation, for instance. The method provides a promising new technique for discovering governing equations and physical laws in parameterized spatiotemporal systems, where first-principles derivations are intractable.

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

M. Raissi [a], P. Perdikaris [b,*], G.E. Karniadakis [a]

[a] Division of Applied Mathematics, Brown University, Providence, RI, 02912, USA
[b] Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA, 19104, USA

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Nonlinear dynamics

ABSTRACT

We introduce *physics-informed neural networks* – neural networks that are trained to solve supervised learning tasks while respecting any given laws of physics described by general nonlinear partial differential equations. In this work, we present our developments in the context of solving two main classes of problems: data-driven solution and data-driven discovery of partial differential equations. Depending on the nature and arrangement of the available data, we devise two distinct types of algorithms, namely continuous time and discrete time models. The first type of models forms a new family of *data-efficient* spatio-temporal function approximators, while the latter type allows the use of arbitrarily accurate implicit Runge–Kutta time stepping schemes with unlimited number of stages. The effectiveness of the proposed framework is demonstrated through a collection of classical problems in fluids, quantum mechanics, reaction-diffusion systems, and the propagation of nonlinear shallow-water waves.

REVIEWS

Check for updates

Physics-informed machine learning

George Em Karniadakis[1,2], Ioannis G. Kevrekidis[3,4], Lu Lu[5], Paris Perdikaris[6], Sifan Wang[7] and Liu Yang[1]

Abstract | Despite great progress in simulating multiphysics problems using the numerical discretization of partial differential equations (PDEs), one still cannot seamlessly incorporate noisy data into existing algorithms, mesh generation remains complex, and high-dimensional problems governed by parameterized PDEs cannot be tackled. Moreover, solving inverse problems with hidden physics is often prohibitively expensive and requires different formulations and elaborate computer codes. Machine learning has emerged as a promising alternative, but training deep neural networks requires big data, not always available for scientific problems. Instead, such networks can be trained from additional information obtained by enforcing the physical laws (for example, at random points in the continuous space-time domain). Such physics-informed learning integrates (noisy) data and mathematical models, and implements them through neural networks or other kernel-based regression networks. Moreover, it may be possible to design specialized network architectures that automatically satisfy some of the physical invariants for better accuracy, faster training and improved generalization. Here, we review some of the prevailing trends in embedding physics into machine learning, present some of the current capabilities and limitations and discuss diverse applications of physics-informed learning both for forward and inverse problems, including discovering hidden physics and tackling high-dimensional problems.

Archives of Computational Methods in Engineering
https://doi.org/10.1007/s11831-021-09539-0

SURVEY ARTICLE

A Survey of Bayesian Calibration and Physics-informed Neural Networks in Scientific Modeling

Felipe A. C. Viana[1] · Arun K. Subramaniyan[2]

Received: 28 September 2020 / Accepted: 7 January 2021
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Abstract

Computer simulations are used to model of complex physical systems. Often, these models represent the solutions (or at least approximations) to partial differential equations that are obtained through costly numerical integration. This paper presents a survey of two important statistical/machine learning approaches that have shaped the field of scientific modeling. Firstly we survey the developments on Bayesian calibration of computer models since the seminal work by Kennedy and O'Hagan. In their paper, the authors proposed an elegant way to use the Gaussian processes to extend calibration beyond parameter and observation uncertainty and include model-form and data size uncertainty. Secondly, we also survey physics-informed neural networks, a topic that has been receiving growing attention due to the potential reduction in computational cost and modeling flexibility. In addition, in order to help the interested reader to familiarize with these topics and venture into custom implementations, we present a summary of applications and software tools. Finally, we close the paper with suggestion for future research directions and a thought provoking call for action.

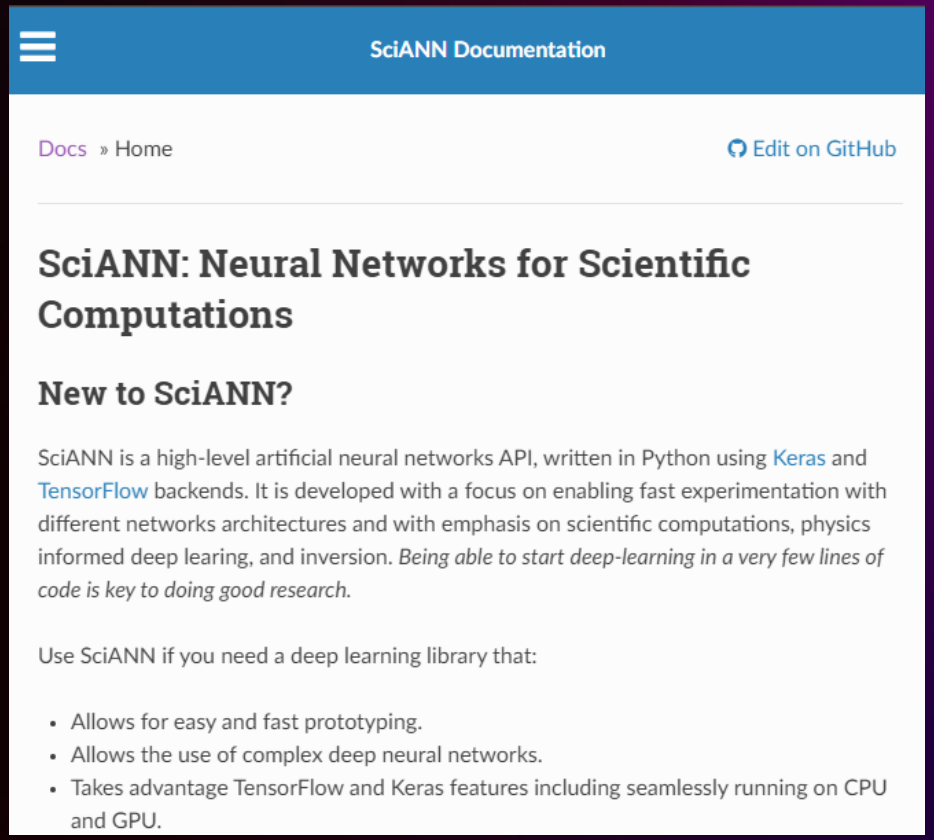
How about software?

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Academic and industry-grade software

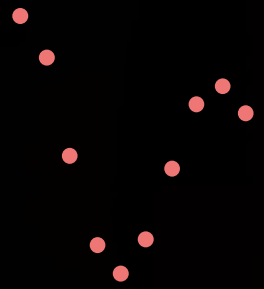
Non-comprehensive list of libraries/packages

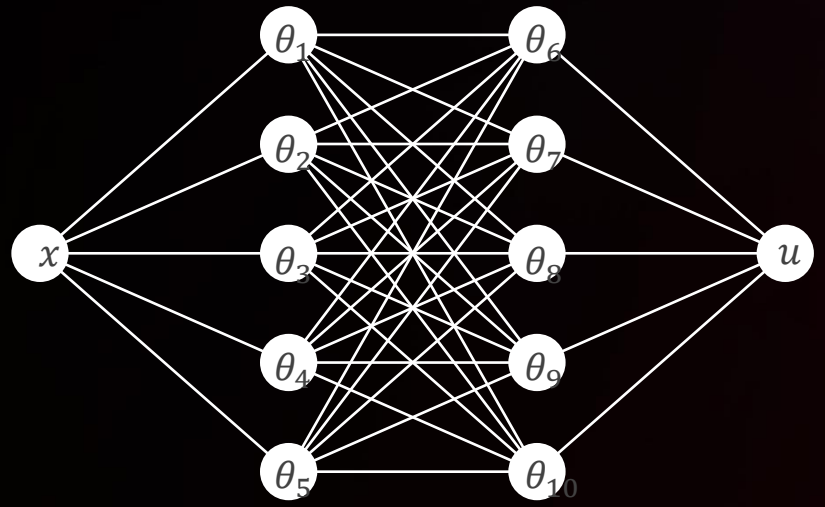
Package	Language	Link
SciANN	Python	https://www.sciann.com
Modulus	Python	https://developer.nvidia.com/modulus
DeepXDE	Python	https://deepxde.readthedocs.io
PyDEns	Python	https://github.com/analysiscenter/pydens
NeuroDiffEq	Python	https://neurodiffeq.readthedocs.io/
NeuralPDE	Julia	https://github.com/SciML/NeuralPDE.jl
ADCME	Julia	https://github.com/kailaix/ADCME.jl

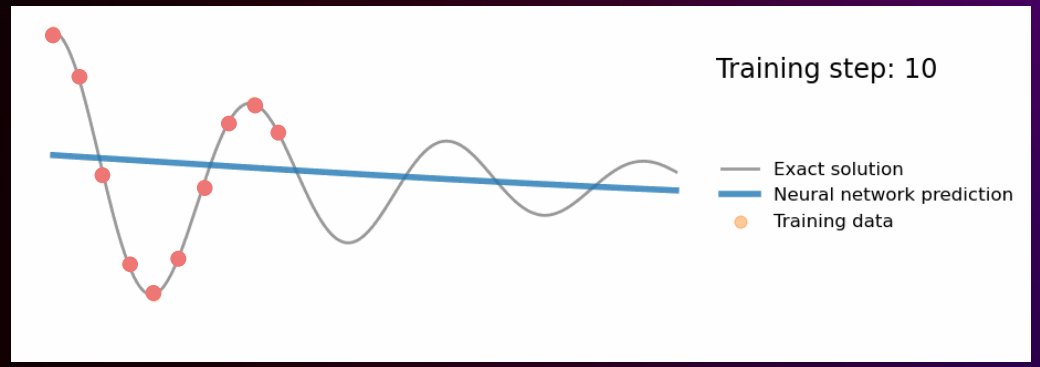


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Neural network







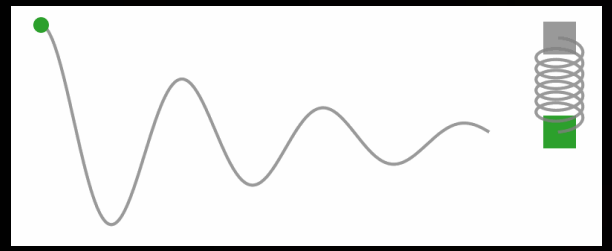
experimental data

$$\min \frac{1}{n} \sum_{i}^{n} \left(u_{nn}(x_i, \theta) - u_{true(x_i)} \right)^2$$

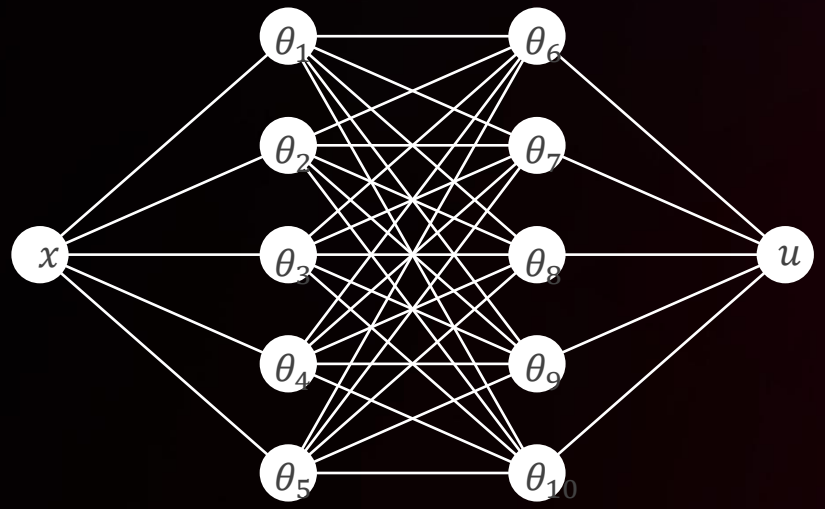
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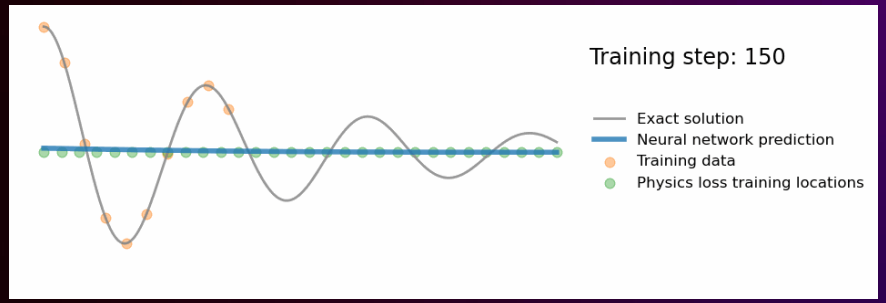
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Physics Informed Neural Network (PINN)



$$m\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \mu\frac{du}{dx} + ku$$



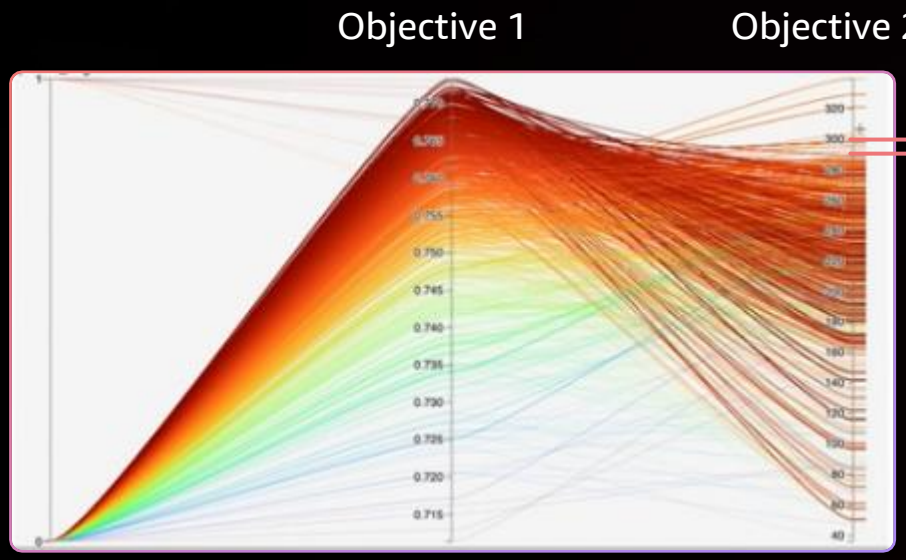


$$\min \frac{1}{n}\sum_{M}^{i}\left(u_{nn}(x_i,\theta) - u_{true(x_i)}\right)^2$$

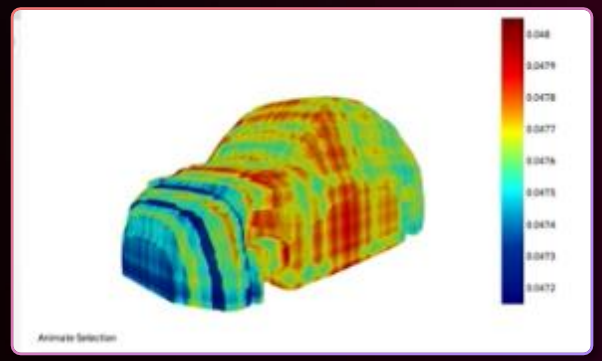
$$+\frac{1}{M}\sum_{j}([m\frac{d^2}{dx^2} + \mu\frac{d}{\mathrm{d}x} + k]u_{nn}(x_j,\theta))^2$$

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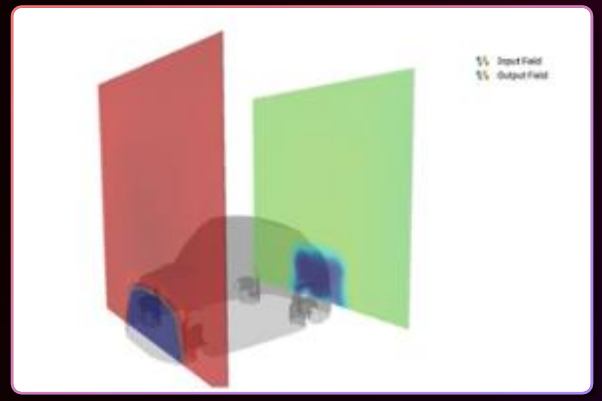
Mapping trajectories to design solutions



10,000 designs explored



Optimal geometry



Optimal flow field

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Safe, Everyday Flight for Everyone



wisk

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wisk

Previous Environment & Challenges

- Wisk had an aging, complex, and fixed CFD infrastructure capacity
- Limited power and cooling availability in our co-location facility
- Original skill set no longer at the company
- Diverse technology components driving operational complexity and risk



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Goals

- Ability to accommodate the legal constraints of export-controlled software provided by NASA
- Quickly scale to support Gen 6 aircraft development
- Fault-tolerant and redundant system
- Supportable by common skill sets and well documented
- Minimize cash outlay

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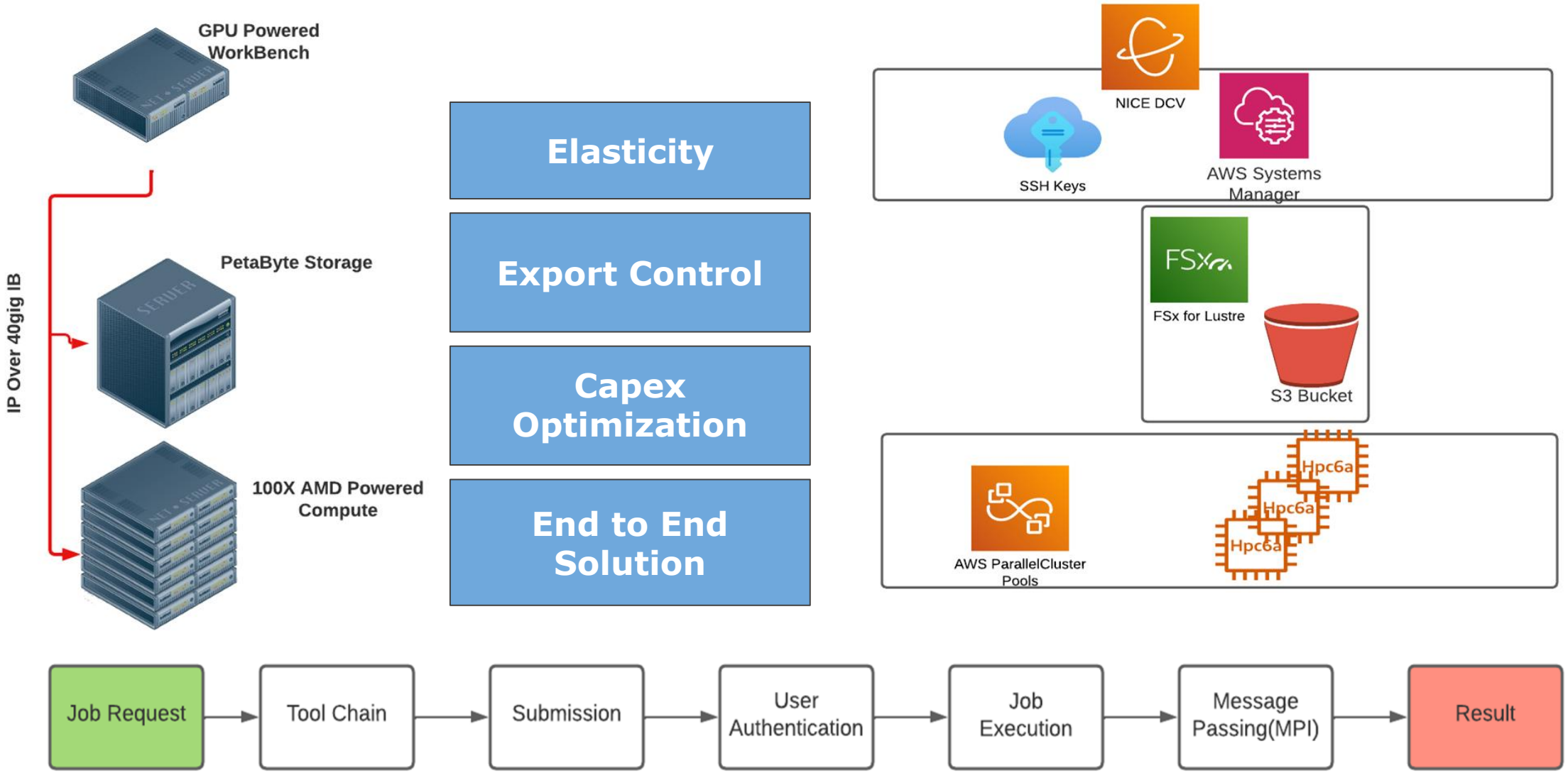
Solution

- Partnered with Converge to POC and Validate Parallel Cluster on AWS GovCloud (US)
- Solved for low latency and high IO requirements with Amazon FSx for Lustre and Hpc6a (EFA)
- Addressed custom CFD software requirement by recompiling Fun3D and overflow for AWS support on the AMD (**EPYC 7003)**
- Validated pre- and post-processing data uploads through FSx for Lustre and Amazon S3 integration
- Tested post-processing artifact validation with the Nice DCV GPU enabled solution all within the AWS ecosystem

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Data Center On Premise

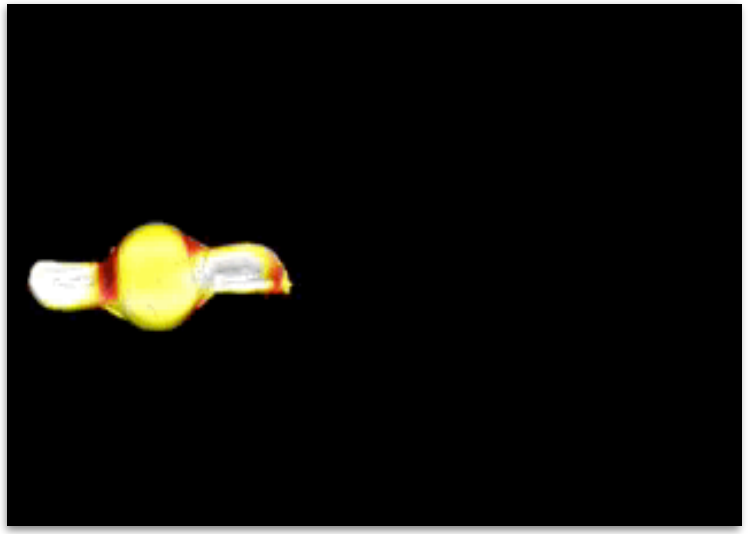
AWS Cloud Native



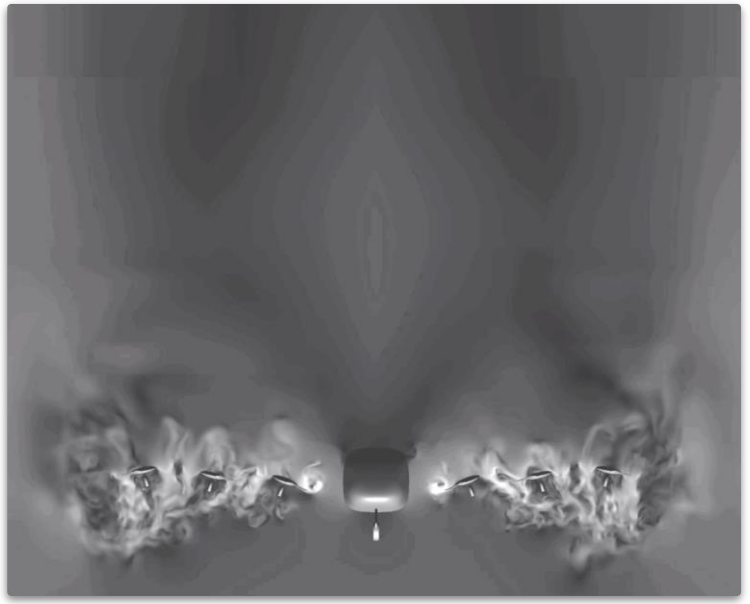
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CFD Simulation Artifacts

- Vorticity magnitude simulation
- Restrained ground testing
- High speed descent







Images by Wisk Aero LLC generated via NASA Overflow software

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Key Results

- Scalability
  - September peak/October lull – pay for what you need
- Performance
  - ~30+% runtime improvement, ~50%+ job turnaround time improvement
- Supportability
  - Supported by our partner Converge
  - Built knowledge within with current IT team
  - Enterprise support with AWS and Converge
- Secure
  - Set up in AWS GovCloud (US)
  - Integrated with Okta with MFA
  - Defined roles and and ownership
- Visibility
  - Cost and dashboard metrics available in real time

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Future Outlook

CFD was a starting point for Wisk for AWS to validate a solution

Some of the possible areas of expanding our AWS partnership are

- Expand AWS for areas in flight automation, flight autonomy and simulation, and business support systems
- Exploring data storage and management solutions
- Standup dev environments on demand for our software development
- Support external collaboration opportunities for our partners

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HPC+ through partners and collaborators

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AWS Partner solutions to accelerate time to value

Ansys SIEMENS AUTODESK

HEXAGON cadence SYNOPSYS

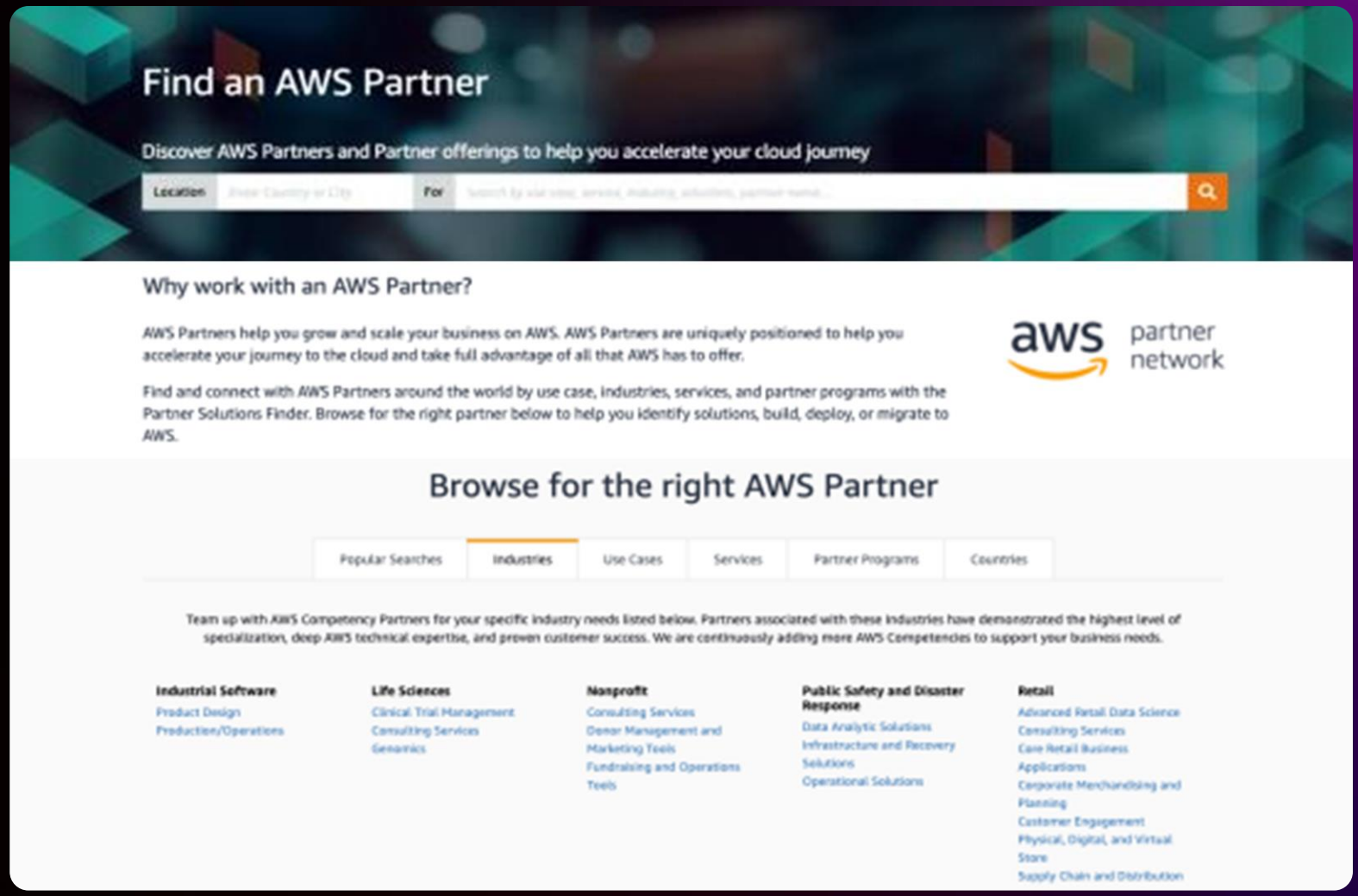
CFD Direct ALTAIR SIMSCALE

rescale TotalCAE RONIN

AtoS CADFEM ZENOTECH SIMULATION UNLIMITED

intel NVIDIA AMD arm

. . . and several more



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This list of partners is current as of November, 17, 2022.

Transforming design and engineering with a cloud-first approach

Companies partner to **simplify product and production complexity** through technology collaborations and new offerings

re:Invent, Las Vegas, 30 November 2021

Siemens Expands Partnership with AWS to Facilitate Cloud-Based Digital Transformation



Siemens Digital Industries Software and Amazon Web Services, their collaboration, which combines Siemens' deep industry exp help industrial companies accelerate digital transformation in t

PRESS RELEASE

DATE: 2/2/2022

Ansys Announces Strategic Collaboration with AWS to Transform Cloud-Based Engineering Simulations

Global leader in engineering simulation solutions partners with comprehensive cloud services provider to develop Ansys Gateway powered by AWS for cloud-based simulation

Key Highlights

- Ansys welcomes AWS as the preferred and recommended cloud service provider (CSP) for Ansys Gateway powered by AWS
- Ansys Gateway powered by AWS will facilitate seamless access and deployment of Ansys products on AWS — enabling customers to accelerate innovation while reducing costs
- Ansys and AWS are expanding high-performance computing (HPC) in the cloud to advance electronic design automation (EDA), computer-aided engineering (CAE), and simulation solutions

PITTSBURGH, PA, February 2, 2022 – Ansys (NASDAQ: ANSS) announced a strategic collaboration with Amazon Web Services, Inc. (AWS), identifying the CSP as the preferred and recommended partner for Ansys Gateway powered by AWS. The collaboration will enable deployment of Ansys products on AWS — making simulation workloads more user-friendly, while offering scalability and flexibility with easy access to software and storage solutions from anywhere with a web browser. By leveraging connected ecosystem applications in a cloud environment, Ansys customers will reduce time to market, reduce costs, and innovate faster.

Building on a longstanding relationship, the newly formed collaboration will provide a browser-based, location-independent solution for Ansys customers — particularly product developers, designers, and engineers that have traditionally utilized on-prem HPC resources. Customers will manage and advance their complete CAE, EDA, and Computer-aided design (CAD) product development in the cloud by leveraging scale, flexibility, elasticity, and global reach of AWS.

aws

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Thank you!



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