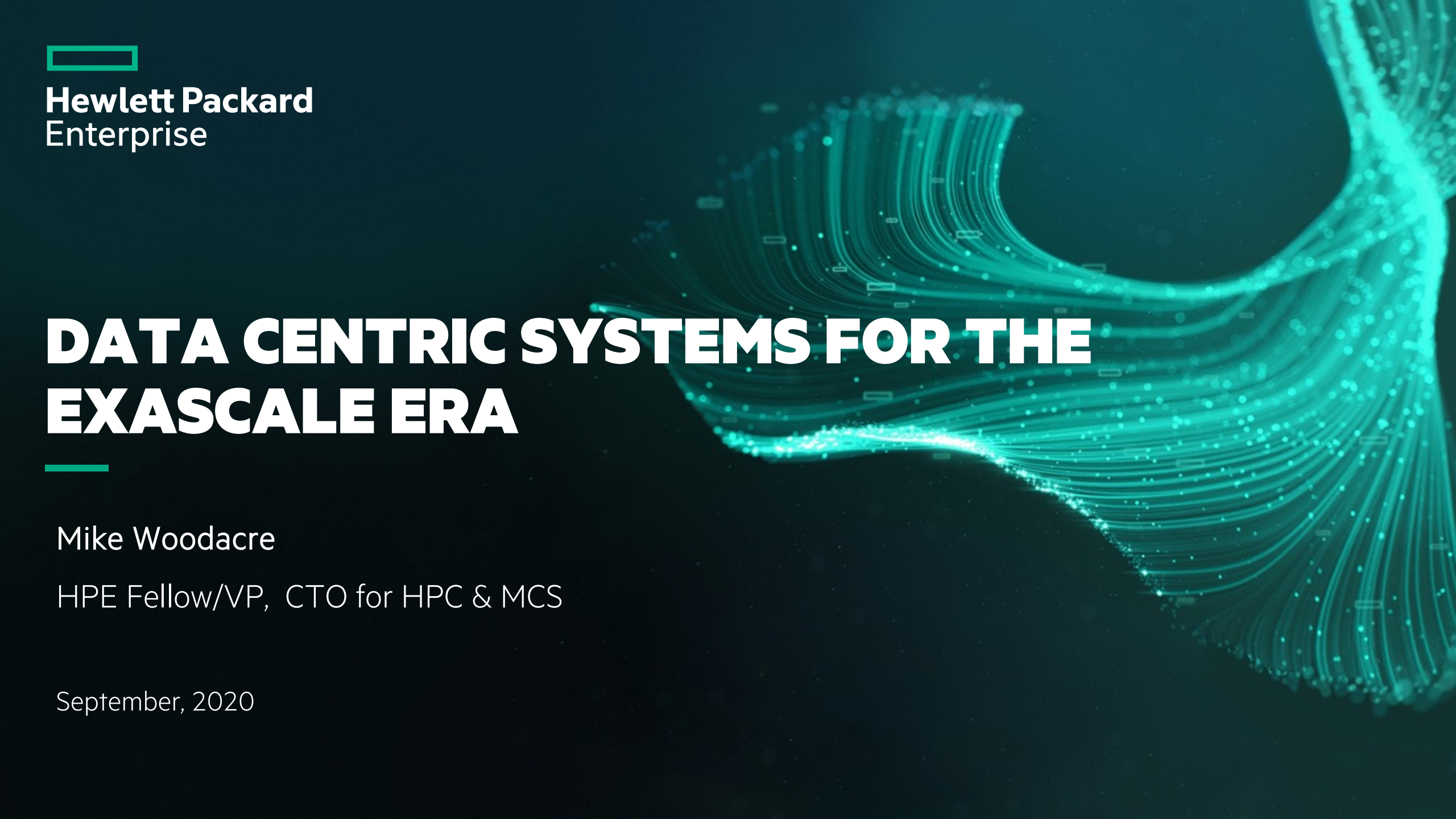


Hewlett Packard Enterprise

DATA CENTRIC SYSTEMS FOR THE EXASCALE ERA

Mike Woodacre

HPE Fellow/VP, CTO for HPC & MCS

September, 2020

LEADING THE NEXT GENERATION OF HIGH PERFORMANCE COMPUTING (HPC)

Hewlett Packard Enterprise

Global leader focused on developing intelligent solutions to capture, analyze and act upon data seamlessly from edge to cloud

CRAY

Premier provider of high-end supercomputing solutions, addressing customers' most challenging data-intensive workloads for critical decisions

DEALING WITH YOUR MASSIVE GROWTH OF DATA
→ 2X GROWTH EVERY YEAR!

175 **zettabytes of data by 2025**

– IDC

75% **of data will be created outside the traditional data center or cloud**

– Gartner

New business models

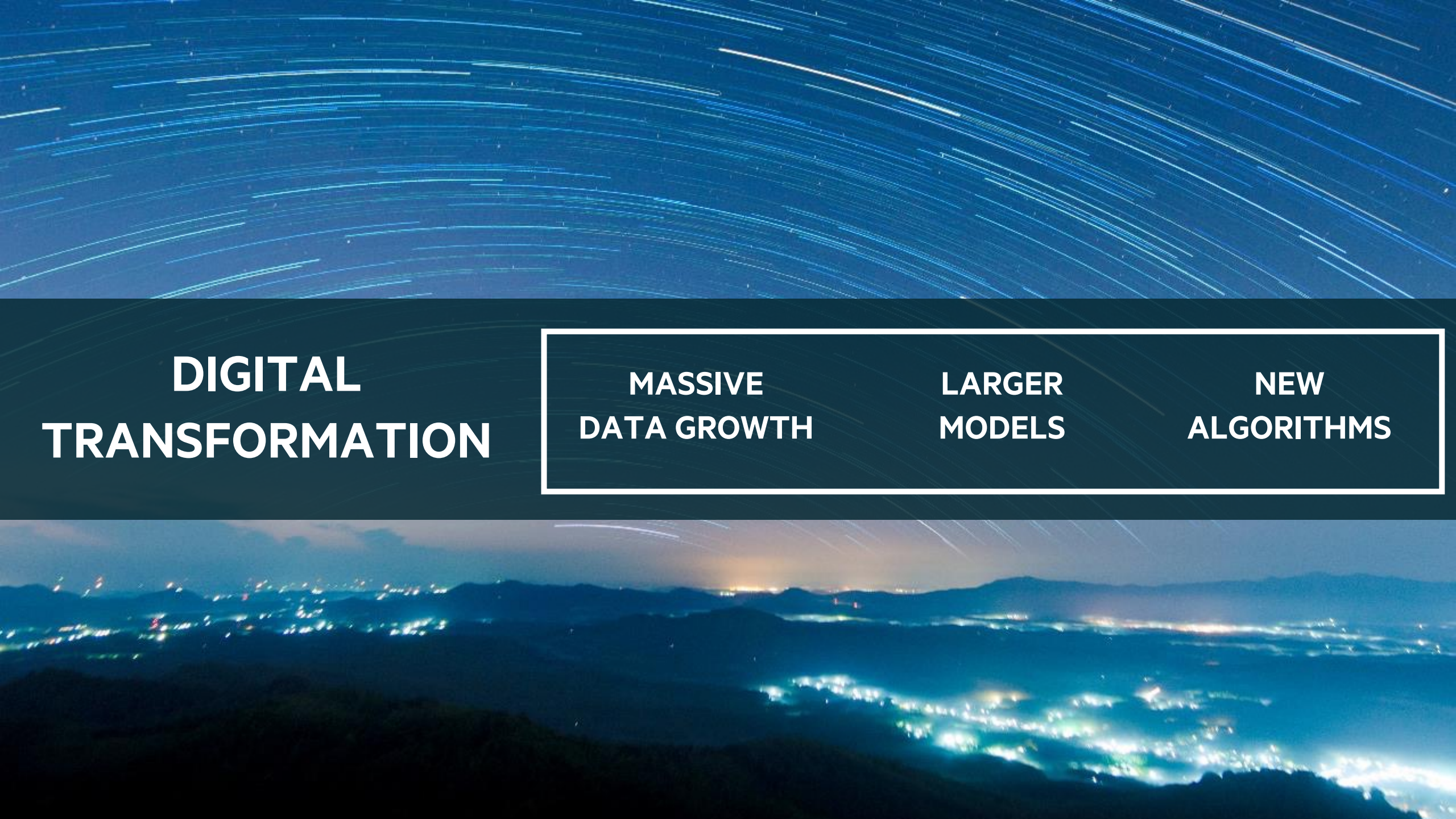
New insights

Always on

Always fast

New revenue streams

Automated and on-demand



DIGITAL TRANSFORMATION

MASSIVE DATA GROWTH

LARGER MODELS

NEW ALGORITHMS

DX requires a different type of infrastructure...

THE EXASCALE ERA IS UPON US

All three worldwide announced Exascale systems are based on HPE Cray EX systems

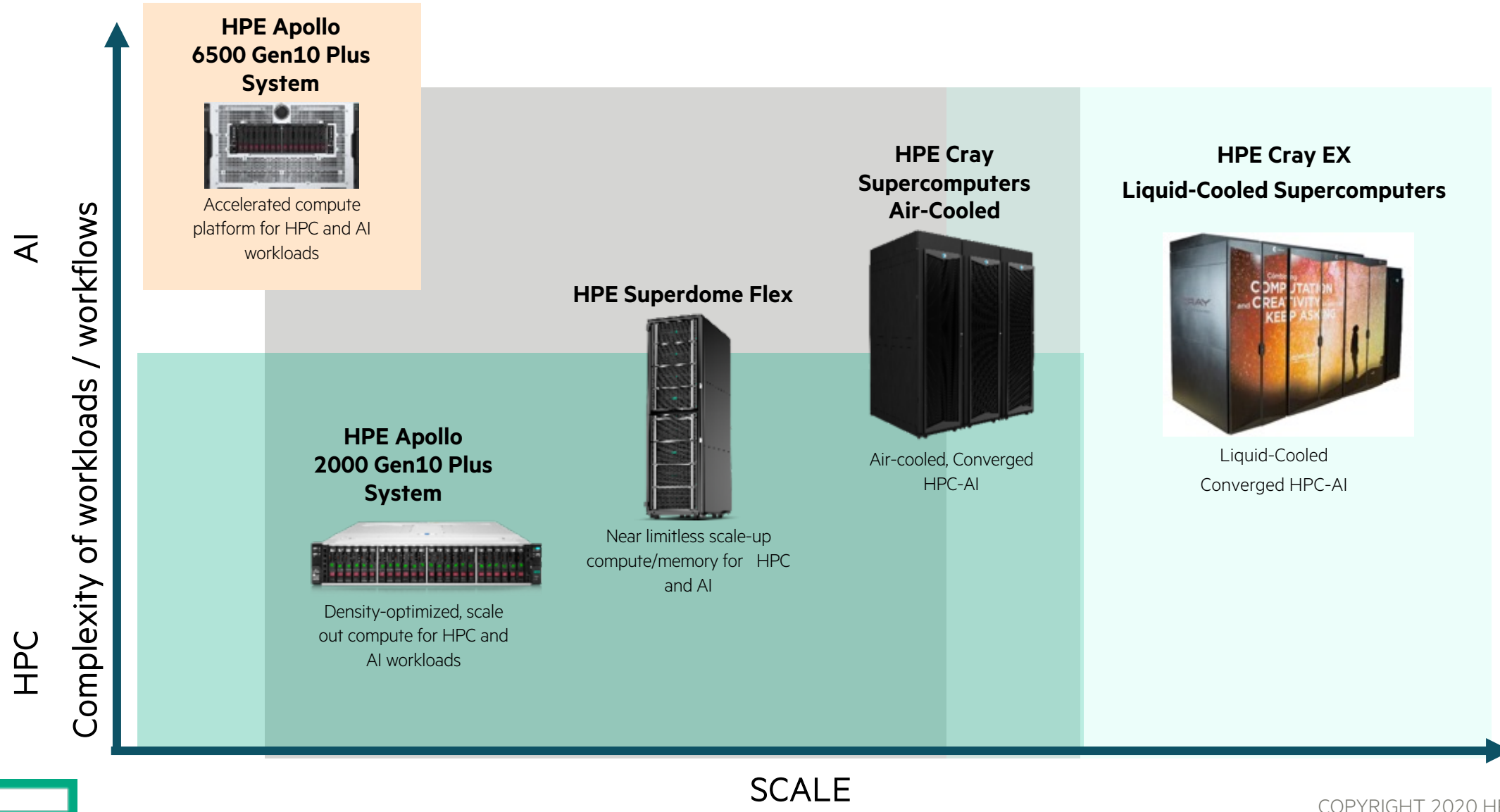
BIG DATA ANALYTICS X ARTIFICIAL INTELLIGENCE X MODELING & SIMULATION

RUNNING ON ONE MACHINE IN MISSION-CRITICAL WORKFLOWS

EXASCALE ERA


PERFORMS LIKE A SUPERCOMPUTER
RUNS LIKE A CLOUD

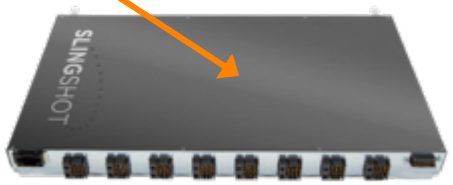
HPE PURPOSE BUILT HPC/AI SYSTEMS



HPE SLINGSHOT IS HPC ETHERNET OPTIMIZED FOR UNIFIED INFRASTRUCTURE

HPE Slingshot switch ASIC

HPE Slingshot top of rack switch



HPE Slingshot integrated blade switch

- Breakthrough congestion management
- 100 GbE and 200 GbE interfaces
- 1.2 billion messages/s
- 25.6 Tb/s aggregate bandwidth
- Scalability to > 250,000 host ports

High-performance switch microarchitecture	Ethernet standards and open APIs	Efficient congestion management	Low, uniform latency	Adaptive routing and quality of service
64 ports at 200 Gb/s Ethernet edge or optimized fabric functionality in each port High packet throughput with reduced packet overhead in network fabric	Easy connectivity to data centers and third-party storage Standard Ethernet protocol support Open RESTful management API's	Workload performance isolation Outperforms data center Ethernet (DCN) and InfiniBand Switch hardware tracks all packets across the network to identify congestion and apply stiff back pressure to the source	Focuses on tail latency, because real apps synchronize Collective engine with low-latency barrier, reduce, all-reduce, and broadcast Built into the microarchitecture of the switch	Improves network performance by 20% to 40% for a variety of traffic patterns Over 90% utilization at scale using system wide QoS classes Guaranteed packet delivery for mixed workloads

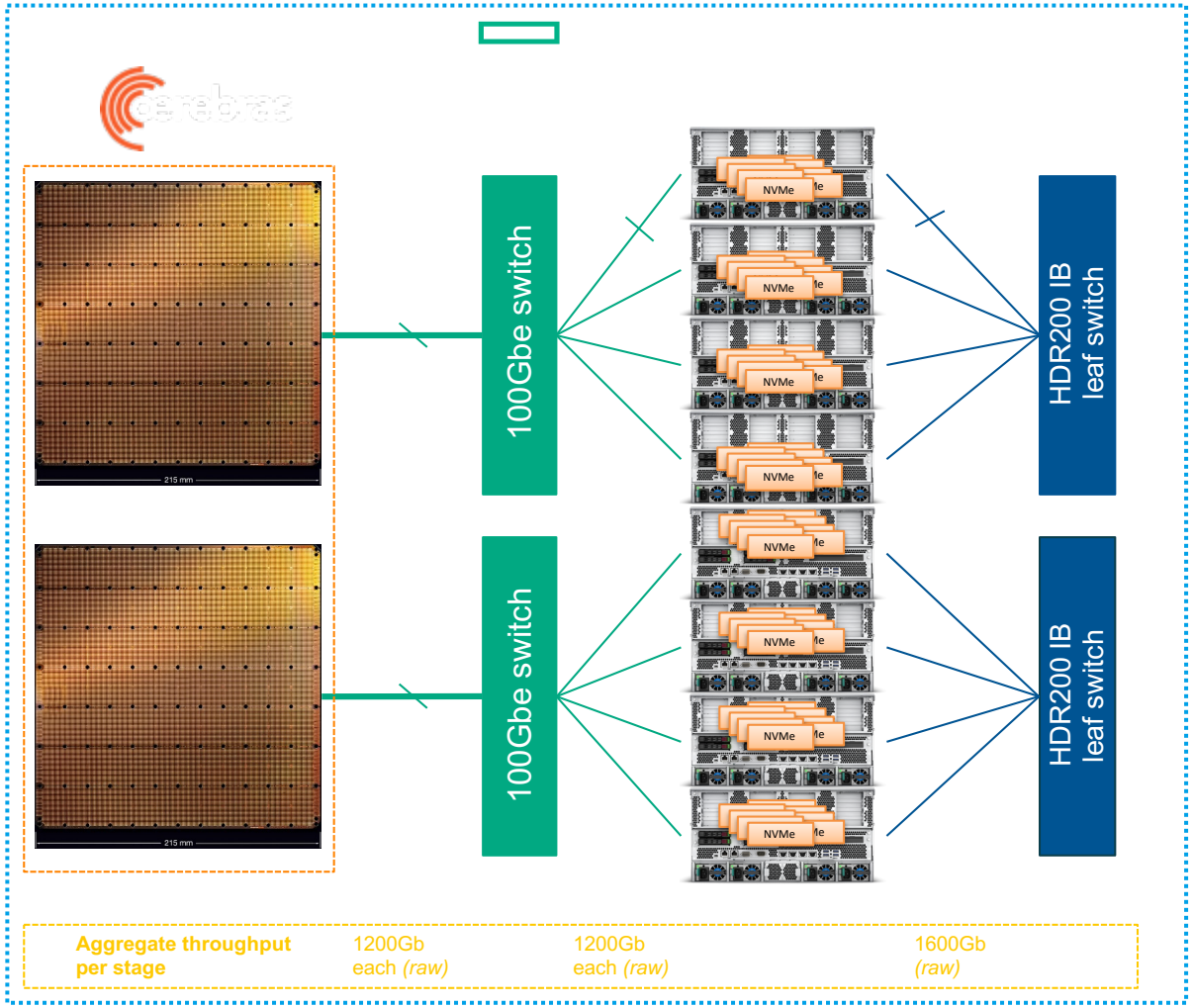
COMPLEX WORKFLOWS

PITTSBURGH SUPERCOMPUTING CENTER

PSC's Neocortex system

- 2x Cerebras CS-1, with each:
  - 400,000 sparce linear algebra "cores"
  - 18 GB SRAM on-chip Memory
  - 9.6 PB/s memory bandwidth
  - 100 Pb/sec on-chip interconnect bandwidth
  - 1.2 Tb/s I/O bandwidth
  - 15 RU
- HPE Superdome Flex
  - 32 Xeon "Cascade Lake" CPUs
  - 24.5 TB System Memory
  - 200 TB NVMe local storage
  - 2 x 12 x 100G Ethernet (to 2x CS-1)
  - 16 x 100G HDR100 to Bridges-II and Lustre FS

Neocortex



Courtesy of Nick Nystrom, PSC – http://psc.edu

INTRODUCING CRAY CLUSTERSTOR E1000

Parallel HPC storage system purpose-engineered to solve the typical HPC storage challenges of the new era

- **Unprecedented performance:** Up to 80 GB/sec from just two rack units via Slingshot, Infiniband or Ethernet
- **Unprecedented efficiency:** With media support of NVMe SSD or HDD
- **Benefits of open source file system:** No license per TB or storage drive
- **Enterprise-grade customer support from HPE Pointnext Services:** Including the open source file system through Lustre R&D team
- **Multiple configuration options:** Including all-Flash, all-HDD and Hybrid

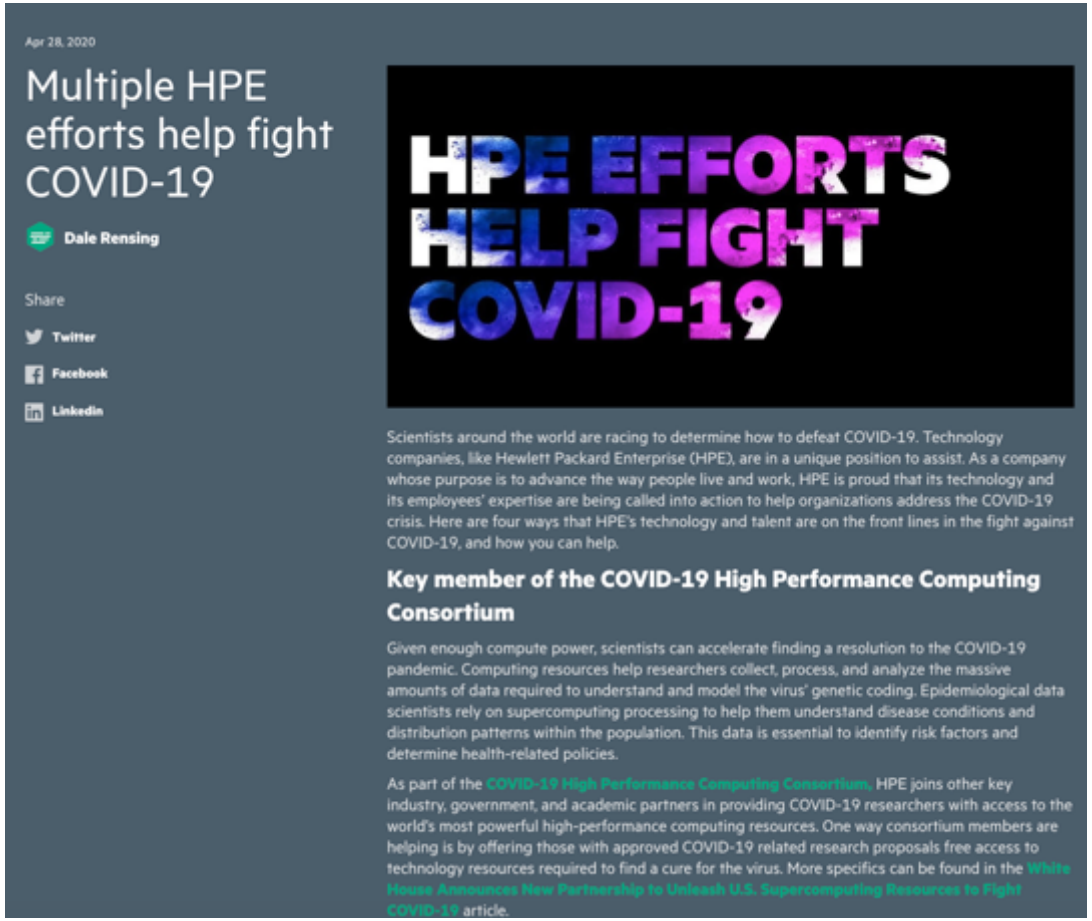
COVID-19 AND HPE EFFORTS

HPE opens its patents to fight COVID-19

APRIL 20, 2020 • BLOG POST • BRETT ALTEN, CHIEF INTELLECTUAL PROPERTY COUNSEL, HEWLETT PACKARD ENTERPRISE

HPE Is Using Its $1.3 Billion Cray Acquisition To Support COVID-19 Research

Hewlett Packard Enterprise is arming COVID-19 researchers with the high-performance computing and artificial intelligence capabilities necessary to make scientific breakthroughs on new treatments and vaccines — two fields that are "more critical than ever," according to the vendor's top HPC executive.



Apr 28, 2020

Multiple HPE efforts help fight COVID-19

Dale Rensing

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Scientists around the world are racing to determine how to defeat COVID-19. Technology companies, like Hewlett Packard Enterprise (HPE), are in a unique position to assist. As a company whose purpose is to advance the way people live and work, HPE is proud that its technology and its employees' expertise are being called into action to help organizations address the COVID-19 crisis. Here are four ways that HPE's technology and talent are on the front lines in the fight against COVID-19, and how you can help.

Key member of the COVID-19 High Performance Computing Consortium

Given enough compute power, scientists can accelerate finding a resolution to the COVID-19 pandemic. Computing resources help researchers collect, process, and analyze the massive amounts of data required to understand and model the virus' genetic coding. Epidemiological data scientists rely on supercomputing processing to help them understand disease conditions and distribution patterns within the population. This data is essential to identify risk factors and determine health-related policies.

As part of the COVID-19 High Performance Computing Consortium, HPE joins other key industry, government, and academic partners in providing COVID-19 researchers with access to the world's most powerful high-performance computing resources. One way consortium members are helping is by offering those with approved COVID-19 related research proposals free access to technology resources required to find a cure for the virus. More specifics can be found in the White House Announces New Partnership to Unleash U.S. Supercomputing Resources to Fight COVID-19 article.

COVID-19 AND HPE: COLLABORATION

MUSC, HPE make innovative drug discovery software publicly available in response to COVID-19 crisis

MAY 2, 2020

NEWS | UAH BOOSTS SEARCH FOR COVID-19 DRUGS USING HPE CRAY SENTINEL SUPERCOMPUTER

UAH boosts search for COVID-19 drugs using HPE Cray Sentinel supercomputer

MAY 05, 2020 | Jim Steele

LLNL uses a first-of-its-kind AI-driven modeling platform to design 20 initial antibody candidates among 10^{40} possibilities

We are incredibly proud to share that LLNL has already made significant progress narrowing down the number of potential antibody candidates from 10^{40} to an initial set of just 20! That's a dramatic process of elimination. On top of that, this inspiring breakthrough was achieved in just weeks, compared to a typical lead time of years using other approaches.

LLNL's COVID-19 response team, which includes researchers from various disciplines with deep expertise in vaccine and countermeasure development, used LLNL's Catalyst, an HPC cluster powered by HPE, to improve predictions and speed up this discovery process by using a first-of-its-kind modeling platform. The platform integrates important components to generate high-quality predictions, such as experimental data and structural biology data, with bioinformatics modeling, molecular simulations and machine learning algorithms.

FEATURE STORY | ARGONNE NATIONAL LABORATORY

Argonne's researchers and facilities playing a key role in the fight against COVID-19

BY JARED SAGOFF | APRIL 27, 2020

Argonne is bringing the power of its scientific leadership and state-of-the-art user facilities to bear in the global battle against COVID-19.

AN END-TO-END PIPELINE FOR ACCELERATED DRUG DISCOVERY

HPE + Community Efforts to Fight the Covid-19 Threat

Goal: Go from a 200,000-molecule database to a wet lab experiment in 2 days

Screening through 30+ Million Compounds to prioritize compounds for wet-lab testing

PharML.Bind | Molecular Docking

Chemical-structure discovery

Predicts enrichment factor between a virus protein and a potential drug molecule

Applying the AI-based drug discovery framework, PharML.Bind, to rank-order molecules using predicted binding potential

Simulates molecular dynamics between that "target" and "potential" for different confirmations

Using Cray supercomputers to perform molecular dynamics simulations, thus shortlisting molecules that bind to the target

Sifting through 30+ Million Publications to extract evidence-map from Knowledge Graph

Knowledge Graph | Question/Answering

Literature-based evidence discovery

Connects-the-dots across curated databases and reveal mechanisms for pharmacological response

HPE is currently working with researchers to use Cray Graph Engine, to host, query, and reason with a knowledge base of 100+ billion facts in a few seconds

Find bleeding edge content using natural language processing (NLP)

HPE has built a question-answering platform that can search through the CORD-19 corpus of 63,000 documents

SUMMARY

How can you engage with HPE on Covid-19 research?

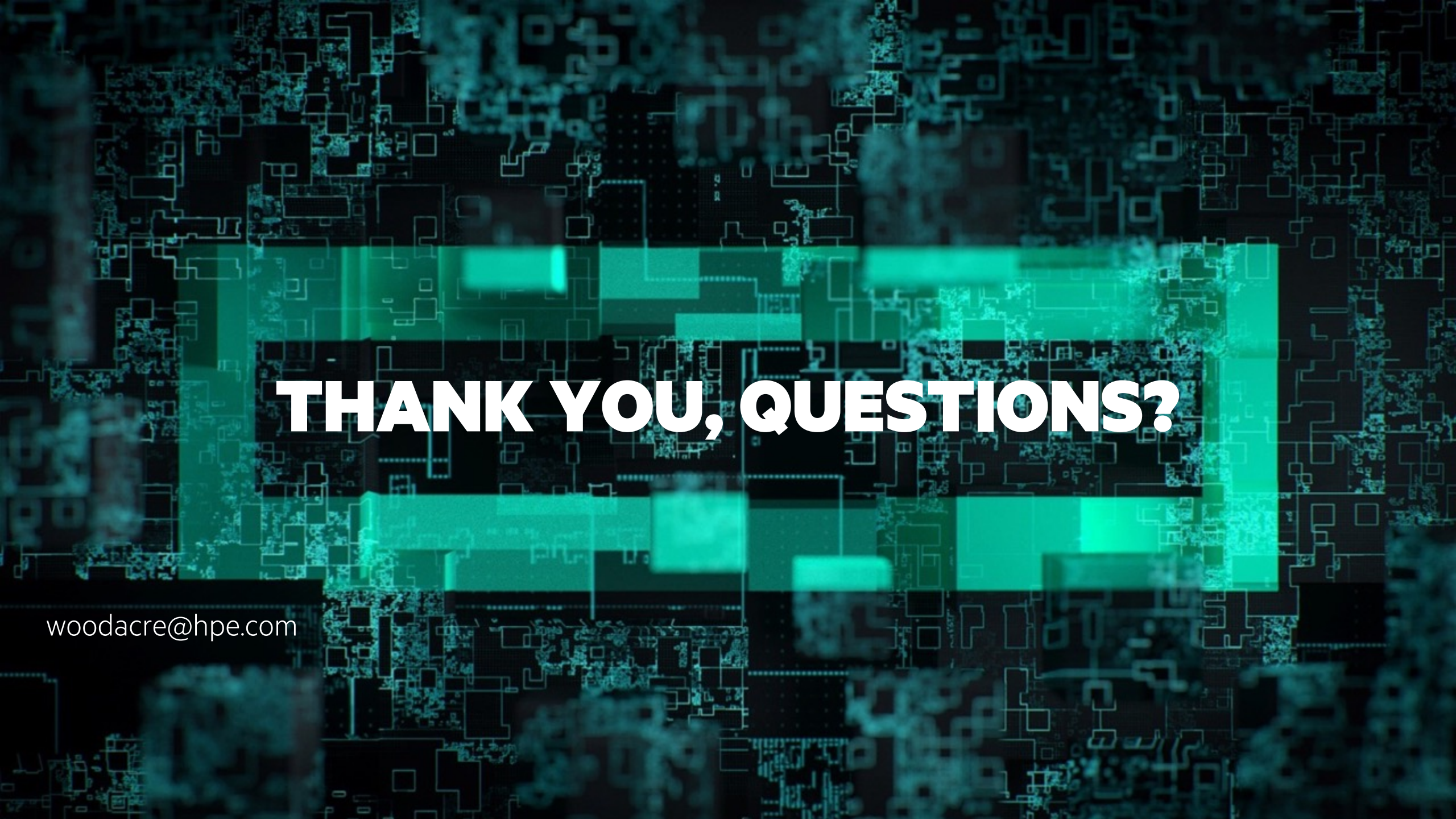
- Dedicated HPC
  - https://covid19-hpc-consortium.org/
- Cloud-based HPC via Azure Sentinel – Cray XC50
  - https://www.hpcwire.com/2020/05/05/cloud-based-supercomputer-accelerates-covid-19-drug-discovery/
- PharML – An AI approach to shortlist molecules
  - https://github.com/jbalma/pharml
- KnowledgeGraph hackathon
  - HPE is currently working with researchers to use HPE's Cray Graph Engine, to host, query, and reason with a knowledgebase of 150+ billion facts in a few seconds. The knowledge graph is an integrated dataset of Uniprot, Biosamples, Biomodels, DrugBank, ClinicalTrials, PubChem, ChemBL, Rhea These manually expert-curated datasets reveal "at-location", "process, "bio-synthesis equations" etc.

HPE HPC & AI PORTFOLIO LEADERSHIP

INDUSTRY LEADING CAPABILITIES

NEW EXASCALE ERA TECHNOLOGIES

DEPLOYED AND CONSUMED ANYWHERE



woodacre@hpe.com