PHYSICS-INFORMED MACHINE LEARNING AND GENERATIVE AI FOR SURROGATE MODELING IN SCIENCE AND INDUSTRY MIKE O'KEEFFE, SENIOR SOLUTIONS ARCHITECT, NVIDIA NEW YORK SCIENTIFIC DATA SUMMIT 2024: ADDRESSING DATA CHALLENGES IN DIGITAL TWINS

# **D**VDA



# SCIENTIFIC COMPUTING IS EVOLVING

NATIONAL Science ACADEMIES Medicine

COMPUTING PERVADES ALL aspects of society if ways once imagined by only a few. Within scie and engineering, computing has often been c the third paradigm, complementing theory a experiment, with big data and artificial intell experiment, with *Dig uata and artification* A Spani (AI) often called the fourth *paradigm*. Utilities data analysis and disciplinary and multidisc modeling, scientific computing systems hav ever larger and more complex, and today's e scientific computing systems rival global sc facilities in cost and complexity. However, a well in the land of scientific computing. In the initial decades of digital computin government investments and the insights designing and deploying supercomputers shaped the next generation of mainstream consumer computing products. VINICATIONS OF THE ACM | FEBRUARY 2023 | VOL. 55 | NO.3

BY DANIEL REED, DENNIS GANNON, AND JACK DONGA

DANIEL REED, DENNIS GANNON, COMPARIENCE OF COMPARIE

charting a Shifting T Geopoliti

Post-Exascale Com National Nuclear

Thought Leaders Map Out the Opportunity and Constraints Given Current Technology and Market Reality

August 21–23, 2019

Lawrence Berkeley



# TRANSITION TO POST EXASCALE ERA

	EXPERIMENTS SIMULATION Viz	EDGE
FEATURE	TERA THROUGH EXASCALE	
USAGE	BATCH & MOSTLY LOCAL TO A SITE	
WORKLOAD	SINGLE SIMULATION/ENSEMBLE	WORKFLOW COMPRI
EXPERIMENTS	<b>OFFLINE DATA ANALYSIS FOR EXPERIMENTS</b>	MIX OF RI
DIGITAL TWINS	<b>IN-SITU VISUALIZATION OFFLNE</b>	<b>INTERAC</b>
QUANTUM COMPUTING	SIMULATION	
PROGRAMMING MODELS	FORTRAN, C++, MPI, OPENMP	STANDARD PARA
SYSTEM CONFIGURATION	MONOLITHIC	
CLOUD	GRID	BURST CAPABILITIES



## POST EXASCALE

## **INTERACTIVE & DISTRIBUTED WITH MULTIPLE SITES**

## ISED OF SIMULATION ENSEMBLES, AI TRAINING AND INFERENCE, LIVE DATA ANALYTICS

## EAL-TIME ANALYSIS TIGHTLY COUPLED WITH OFFLINE

## TIVE\_VISUAL MODEL COUPLED WITH PHYSICAL ASSET

## SIMULATION PREPARING FOR A HYBRID MODEL

ALLELISM SUPPORT IN FORTRAN, C++, MPI, OPENMP, OPENACC, PYTHON, JULIA, PYTORCH, TENSORFLOW

## MODULAR

**5, FASTER REFRESH CYCLE, ACCESS TO LATEST TECHNOLOGY AT SCALE** 



# NATIONAL Sciences ACADEMIES Medicine

# Foundational Research Gaps and Future Directions for Digital Twins

A Relatively New Modeling Concept That is Being Adopted by the HPC Community in the Post Moore Era

The concept was first publicly introduced in 2002 by Michael Grieves, at a Society of Manufacturing Engineers conference as the conceptual model underlying Product Life Cycle Management

A digital twin is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems), is dynamically updated with data from its physical twin, has a predictive capability, and informs decisions that realize value.

The bidirectional interaction between the virtual and the physical is central to the digital twin.

## **DIGITAL TWIN FOR SCIENCE**







# NATIONAL Sciences ACADEMIES Medicine

# Foundational Research Gaps and Future Directions for Digital Twins



## A Digital Twin is More Than Just Simulation and Modeling





## Noel Crespi Adam T. Drobot Roberto Minerva Editors

## The Digital



Evolutio

Information

## CHAPTER: DIGITAL TWIN PAST, PRESENT **AND FUTURE**

Michael Grieves



https://www.brighttalk.com/webcast/18347/456987

- Executive Director Chief Scientist Digital Twin Institute
  - **Digital Twin Evolution**

Physical to Virtual Maturity









# ш

# **AI ENABLES DIGITAL TWINS FOR SCIENCE** Quantum Accuracy at Cost for Physical Scale Models



# Log computational cost

![](_page_6_Picture_7.jpeg)

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Exact solution

![](_page_6_Picture_9.jpeg)

![](_page_7_Figure_0.jpeg)

# **AI ENABLES DIGITAL TWINS FOR SCIENCE** Quantum Accuracy at Cost for Physical Scale Models

# Log computational cost

![](_page_7_Picture_3.jpeg)

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Exact solution

![](_page_7_Picture_5.jpeg)

![](_page_8_Figure_0.jpeg)

# AI INTRODUCES NEW USE CASES FOR SCIENCE AND ENGINEERING Al Bridges the Gap Between Simulation and Real-Time

# Log computational cost

![](_page_8_Picture_3.jpeg)

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![](_page_8_Picture_4.jpeg)

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![](_page_8_Picture_5.jpeg)

![](_page_8_Picture_6.jpeg)

![](_page_8_Picture_8.jpeg)

🧆 NVIDIA.

## DIGITAL TWIN POC SCIENCE EXAMPLES Collaborate with the Global Research Community to Pursue Science Discovery that Benefits Mankind

![](_page_9_Picture_1.jpeg)

## <u>Towards Real time Fusion Reactor Design</u> Generative AI to Predict Disruption

![](_page_9_Picture_3.jpeg)

Multi-Messenger Neutrino Detection

![](_page_9_Picture_5.jpeg)

## Earth 2 **Destination Earth**

![](_page_9_Figure_7.jpeg)

Earthquake Model with Machine Learning Earthquake Early Warning SCEC

![](_page_9_Picture_9.jpeg)

## Genome Scale LLMs for Covid Covid is Airborne

![](_page_9_Picture_11.jpeg)

Kubota For Earth For Life

![](_page_9_Picture_15.jpeg)

# DVDA -

![](_page_10_Picture_1.jpeg)

![](_page_11_Picture_1.jpeg)

## Accelerating NWP codes on GPU

## Earth-2 Program

Build the technology needed to create the digital twin of the earth's weather and climate systems

![](_page_11_Picture_6.jpeg)

## Al research and collaboration with the science community

Interactive Visualization – **Digital Twins** 

![](_page_11_Picture_10.jpeg)

**Operationalize using Cloud** Services

![](_page_11_Picture_13.jpeg)

![](_page_11_Picture_14.jpeg)

# AI ALGORITHMS EVOLVING AT UNPRECEDENTED PACE FourCastNet High Resolution for Data-Driven Weather Models

**Comparison of resolutions for** data-driven weather models since 2018 (Dueben & Bauer)

SOTA evolving rapidly Recent Pre-print Kang Chen et al (2023) extend forecast to 10 days with 0.25° resolution using "cross modal Transformer"

![](_page_12_Picture_3.jpeg)

![](_page_12_Picture_4.jpeg)

Weyn et al. (2019), 2.5° N.H only, 72x36, 2.6k pixels, ConvLSTM

WeatherBench, Rasp et al. (2020). 5.625°, 64x32, 2K pixels, CNN

Deuben & Bauer (2018), 6°, 60x30, 1.8K pixels, MLP

![](_page_12_Picture_9.jpeg)

![](_page_12_Picture_10.jpeg)

DLWP, Weyn et al. (2020). 2°, 16K pixels, Deep CNN on Cubesphere/(2021) ResNet

![](_page_12_Picture_13.jpeg)

FourCastNet, Pathak et al. (2022), 0.25°, ~1,000,000 Pixels, ViT+AFNO

GNN, Keisler et al. (2022), 1°, 64,000 Pixels, Graph Neural Networks

33

💌 NVIDIA,

## **REGIONAL FORECASTING VIA KM-SCALE SUPER-RESOLUTION** Generative AI - Diffusion models

- Case Study:
- Super-resolve 25-km Al weather models (SFNO, GraphCast, Pangu Weather) 12.5x super-resolution & channel synthesis using CorrDiff over Taiwan (25 km --> 2 km)
- Sample diversity from Gen-AI of equivalently plausible fine-scale atmospheric conditions.
- IOOOx Faster, 3000x more Energy Efficient, 200x Data Compression relative to WRF on CPU (Numerical Model)

![](_page_13_Figure_5.jpeg)

![](_page_14_Picture_0.jpeg)

## Data Sources

## EARTH-2

## Connecting Complex Simulation, Data and AI Workflows

![](_page_14_Picture_7.jpeg)

## **NVIDIA MODULUS Open-Source Platform for Developing Physics-Based Machine Learning**

## Training Neural Networks Using Both Data And The Governing Equations

![](_page_15_Figure_2.jpeg)

![](_page_15_Picture_3.jpeg)

Renewable Energy Siemens Gamesa: 4000X Faster wind turbine wake optimization

![](_page_15_Picture_5.jpeg)

Climate Change 45,000X Faster extreme weather prediction with FourCastNet

![](_page_15_Picture_7.jpeg)

Healthcare

![](_page_15_Figure_9.jpeg)

Science and Engineering Teaching Kit available now.

## Advancing Scientific Discovery With Modulus

## Industrial HPC NETL: 10,000X Faster build of high-fidelity surrogate models

![](_page_15_Picture_13.jpeg)

![](_page_15_Picture_16.jpeg)

# Generative AI making headway into Biology and Drug Discovery

AI Published Papers

![](_page_16_Figure_2.jpeg)

Source: arXiv.org Q-bio: AI, ML, DL, NN

![](_page_16_Picture_5.jpeg)

Lab Automation: Sensors & Robotics

![](_page_16_Picture_7.jpeg)

GensLMs Genome-scale language models reveal SARS-CoV-2 Evolutionary Dynamics

![](_page_16_Figure_9.jpeg)

In Silico Drug Discovery: AI & Computing

![](_page_16_Picture_14.jpeg)

Nucleotide Transformer Building and Evaluating Robust Foundation Models for Human Genomics

MolMIM Improving Small Molecule Generation using Mutual Information Machine

![](_page_16_Picture_17.jpeg)

NeuralPlexer Dynamic-Backbone Protein-Ligand Structure Prediction with Multiscale Generative Diffusion Models

![](_page_16_Picture_21.jpeg)

![](_page_16_Picture_23.jpeg)

## DRUG DISCOVERY IS AT AN INFLECTION POINT Computer Aided Drug Discovery is Expanding Exponentially

## CHARMM DFT & Force Fields X-Ray Protein Structures

Large Scale Simulation High Throughput Screening

1980

1985

1990

![](_page_17_Figure_7.jpeg)

![](_page_17_Picture_8.jpeg)

AlphaFold **AI Structure Prediction** Multi-Scale Omics

![](_page_17_Picture_15.jpeg)

## **GENERATIVE AI DRY LABS ARE ACCELERATING DRUG DISCOVERY** 3 Years Faster | 100s of Millions Cheaper

![](_page_18_Picture_1.jpeg)

![](_page_18_Picture_3.jpeg)

![](_page_19_Figure_1.jpeg)

## **NVIDIA BioNeMo** Build, Optimize and Deploy Foundation Models for Computer-Aided Drug Discovery

Microsoft Azure

![](_page_19_Picture_5.jpeg)

![](_page_19_Picture_8.jpeg)

## **BioNeMo Framework Supports Optimized Biomolecular Models** Proteins | Small Molecules | Genomics

![](_page_20_Picture_1.jpeg)

ESM-1 | ESM-2 Protein LLMs

![](_page_20_Picture_3.jpeg)

**NEW:** OpenFold **3D Protein Structure Prediction** 

![](_page_20_Picture_5.jpeg)

![](_page_20_Picture_6.jpeg)

MegaMolBART Generative Chemistry Model

ProtT5 Protein Sequence Generation

![](_page_20_Picture_9.jpeg)

**NEW: DNABERT DNA Sequence Model** 

![](_page_20_Picture_11.jpeg)

COMING SOON: MolMIM Molecular Generation

**NEW:** DiffDock | EquiDock Docking Prediction

![](_page_20_Picture_14.jpeg)

**COMING SOON:** Single Cell BERT Single Cell Expression Model

![](_page_20_Picture_17.jpeg)

## Build Generative AI Virtual Screening Workflows with NVIDIA NIM Use composable NVIDIA NIMS to build workflows for CADD applications

![](_page_21_Picture_2.jpeg)

![](_page_21_Figure_3.jpeg)

![](_page_21_Picture_4.jpeg)

DiffDock

![](_page_21_Picture_7.jpeg)

## NVIDIA PLATFORM EVOLVING TO MEET THE CHALLENGE SIMULATION

**EXPERIMENTS/ SENSORS** 

**VIRTUAL DESIGN** AND CONTROL

![](_page_22_Figure_4.jpeg)

HPC\*AI

![](_page_22_Picture_7.jpeg)

# THANK YOU

![](_page_23_Picture_1.jpeg)

# 

![](_page_23_Picture_3.jpeg)