Special Report

Recent HPC-centric AI Success Stories

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INTRODUCTION

Each year, Hyperion Research highlights and celebrates researchers, scientists, and engineers who are employing advanced computational technology to address real-world, contemporary problems. Acknowledging these success stories spreads awareness of the world's most pressing social issues and reveals the varied and concrete solutions made possible by cutting-edge technology.

In recent surveys, Hyperion Research has inquired site-runners, research-leads, and project managers around the world about their endeavors and the ways in which they are helpful to their communities and society. There are teams the world over innovating and creatively applying HPC-centric AI for the benefit of society, far too many to be included here. This document highlights several of those success stories which are particularly noteworthy or impactful.

EXEMPLAR SUCCESS STORIES

Cornell Chemical and Biological Engineering

Rong Yang, Assistant Professor of Chemical and Biological Engineering at Cornell University, is using a novel combination of AI and production techniques to revolutionize how polymer nanoparticles are manufactured. These nanoparticles have emerged as a powerful tool for delivering medicine with pinpoint accuracy and timing. AI is used to analyze and guide the production of these polymer nanoparticles in real time.

With this same method, Cornell engineers have simplified and reinforced models that accurately calculate the fine particle matter like soot, dust, and exhaust emitted by combustion engines contained in urban air pollution. Now, city planners and government health officials can obtain a more precise accounting of the well-being of the local air quality and the well-being of the local community.

The Data Management and Statistics Core (DMSC) at the International Neurodegenerative Disorders Research Center (INDRC)

This effort provides each project at the INDRC center with the digital infrastructure necessary for accurate data capture, secure storage, access to high-quality integrated datasets, and expert statistical consultation. Through these resources, the DMSC directly facilitates the INDRC goals of advancing the careers of junior investigators, expanding the neuroscience and research infrastructure of Nevada, and enhancing the understanding of neurodegenerative diseases. This endeavor also includes the aim of fostering new research collaborations, expanding, and extending their service provision to external researchers, and pursuing independent funding in order to broaden their collaborative network.

The social objectives of this project include:

- Care for patients with neurodegenerative disorders.
- Clinical research in neurodegenerative disorders such as Alzheimer's, Parkinson's, and ALS.
- Reduce the cost and increase the efficacy of drug discovery and physiological research.
- Improve the rationale for particular target and lead molecule selection.
- Enable the simulation studies for new ideas and concepts.
- Improve the value derived from large research investments.

UT Health San Antonio and Universidad Católica de Murcia (UCAM)

With the aid of artificial intelligence technology, researchers discovered, patented, and licensed a drug that is now in clinical trials. Imipramine, an anti-depressant, has been demonstrated to block the growth of certain breast cancers by inducing cell cycle arrest and blocking recombination and certain kinds of DNA repair activities.

Studies suggest that repurposing imipramine could enhance routine care for breast cancer patients. Now in clinical trials, this treatment could prove useful alone or in tandem with other established treatments of some of the most aggressive cancer types. More information about this development can be found here: https://pubmed.ncbi.nlm.nih.gov/35568265/

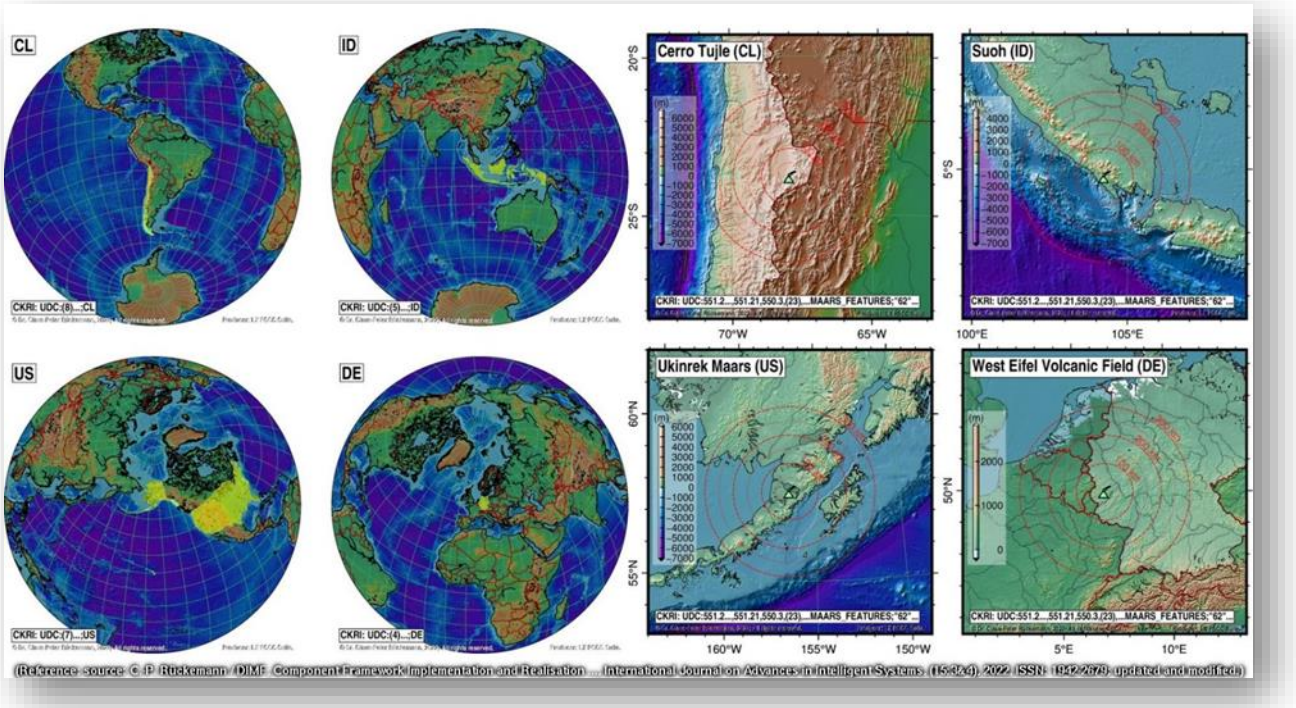
Claus-Peter Rückemann at the University of Münster:

Dr. Claus-Peter Rückemann at the University of Münster (WWU) created a Conceptual Knowledge Reference Implementation (CKRI) and a Component Reference Implementations (CRI) framework, which enable consistent multi-disciplinary conceptual knowledge contextualization, universal knowledge facets, method integration, flexible workflow definition, and parallelization on HPC resources. The reference implementations have had a positive impact on sustainable scientific research, innovative data strategies, industrial learning, and reuse of results and insight.

Results have been published as an outcome of the development and employment of these frameworks, notably several practical case studies of exemplary end user scenarios, e.g., automated "intelligent" object context discovery and contextualization for prehistory and archaeology and volcanological features, using advanced computation and visualization on supercomputing resources.

FIGURE 1

Generated symbolic representation result of object identification and contextualization based on CKRI and CRI framework, dynamically integrating multi-disciplinary resources



Source: C.-P. Rückemann, 2023

Additional information on these projects can be found in the appendix.

Centivax

Researchers at Centivax have used the AWS cloud to train and run machine learning models and data pipelines for vaccine development and antibody discovery. The effort is part of a push by the group to develop a universal influenza vaccine, with future programs to develop universal vaccines for other pathogens. The vaccine is currently in pre-clinical trials.

Their antibody programs target various diseases, including snakebite envenomation, a neglected tropical disease with substantial morbidity and mortality especially in the developing world. The same technology they have used to develop their broad-spectrum influenza vaccine is being applied to HIV and novel coronavirus strains. Broad spectrum vaccines for dengue, malaria, tuberculosis, herpes, RSV, and even the common cold will follow.

Georgia Polytechnical Institute

Combustion research, under the broader area of energy and power, traditionally leverages tremendous amounts of compute resources on modelling and simulation to understand the phenomena of practical power generation. This heavy compute load, which ultimately results in a more robust development of

fuel and emissions knowledge, has been lightened by AI methodologies including DNN and ML. With a basic data training set, researchers at Georgia Tech are reporting a massive reduction in time to solution paired with a 90-90% confidence of the emulations.

Endeavors like these can go a long way in the push towards cleaner, more responsible use of combustible fuels. Fuels often need rigorous testing for reliable and applicable results, and the use of AI platforms to cut that time down can bring positive impacts for the global cause of climate-change reduction as well as local amelioration of air pollutants.

Appendix

Additional information relating to Dr. Claus-Peter Rückemann's work can be found in these references:

1) Component Framework Implementation and Realisation for Development and Deployment of a Coherent Multi-disciplinary Conceptual Knowledge-based Holocene-prehistoric Inventory of Volcanological Features Groups and Faceting.

http://www.iariajournals.org/intelligent_systems/intsys_v15_n34_2022_paged.pdf

2) Faceting the Holocene-prehistoric Inventory of Volcanological Features Groups, Towards Sustainable Multi-disciplinary Context Integration in Prehistory and Archaeology Based on the Methodology of Coherent Conceptual Knowledge Contextualisation.

http://www.iariajournals.org/intelligent_systems/intsys_v15_n34_2022_paged.pdf

3) Coherent Knowledge Solutions From Prehistory to Future - Towards Coherent Multi-disciplinary Knowledge Reference Implementation Blueprints for Industrial Learning: Insight from Consistent Coherent Conceptual Integration of Prehistory, Archaeology, Natural Sciences, and Humanities, Machine Learning for Industry Forum 2021, Lawrence Livermore National Laboratory (LLNL).

https://ml4i.llnl.gov/file-download/download/public/301

About Hyperion Research, LLC

Hyperion Research provides data-driven research, analysis and recommendations for technologies, applications, and markets in high performance computing and emerging technology areas to help organizations worldwide make effective decisions and seize growth opportunities. Research includes market sizing and forecasting, share tracking, segmentation, technology, and related trend analysis, and both user & vendor analysis for multi-user technical server technology used for HPC and HPDA (high performance data analysis). We provide thought leadership and practical guidance for users, vendors and other members of the HPC community by focusing on key market and technology trends across government, industry, commerce, and academia.

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