DIFFERENTIATE— Design Intelligence Fostering Formidable Energy Reduction (and) Enabling Novel Totally Impactful Advanced Technology Enhancements

PROJECT DESCRIPTIONS

National Renewable Energy Laboratory – Golden, CO

End-to-End Optimization for Battery Materials and Molecules by Combining Graph Neural Networks and Reinforcement Learning - $538,618

The National Renewable Energy Laboratory (NREL) will develop a machine learning-enhanced approach to the design of new battery materials. Currently, such materials are designed in part via numerous expensive high-fidelity computational simulations that predict the performance of a given composition. However, at present, humans must sift through the vast amounts of data generated and manually identify new compositions. To accelerate this process, NREL plans to develop a machine learning enhanced prediction tool that uses existing simulation data to predict the performance of new material compositions at high fidelity but lower cost. NREL plans to combine this tool with reinforcement learning techniques to automate the identification of new candidate compositions. It is expected that these design tools will enable the identification of new battery materials faster and thereby accelerate the rate at which battery performance is improving.

National Renewable Energy Laboratory – Golden, CO

INTEGRATE – Inverse Network Transformations for Efficient Generation of Robust Airfoil and Turbine Enhancements - $507,878

The National Renewable Energy Laboratory (NREL) will develop a novel wind turbine design capability that enables designers to explore advanced technology concepts at a lower cost. This capability will harness the power of a deep neural network (DNN)-based inverse design methodology. To overcome challenges in with the use of traditional DNNs in this application, NREL will develop innovative techniques to sparsify the neural network using active subspaces that will ensure that the model is invertible and can quickly zoom in on relevant designs at minimal cost. The models will be trained using data from computational fluid dynamics simulations, running on NREL's supercomputers, which in turn use machine learning assisted turbulence models to predict flow separation and stall observed in wind turbine flows.

Northwestern University – Evanston, IL

Adaptive Discovery and Mixed-Variable Optimization of Next Generation Synthesizable Microelectronic Materials - $570,712

Northwestern University will develop a machine learning-enhanced mixed-variable conceptual design optimization framework to construct new functional materials. The team will use natural language processing (NLP) and physics-based machine learning (ML) to more efficiently guide the autonomous search for materials. The project will deliver a series of new ML techniques using NLP, conditional variational autoencoders, active learning, latent-variable Gaussian processes, and reinforcement learning in Bayesian optimization. Northwestern University's project leverages functional and promising materials exhibiting metal-insulation transitions, a set of materials that can revolutionize microelectronics science to provide energy-saving solutions.

Iowa State University – Ames, Iowa

Context-Aware Learning for Inverse Design in Photovoltaics - $607,138

Iowa State University will develop novel machine learning tools to accelerate the inverse design of new microstructures in photovoltaics. The team will create a new deep generative model called bi-directional inverse design networks to combat challenges in real-world inverse design problems. The proposed inverse design tools, if successful, will produce novel, manufacturable material microstructures with improved electromagnetic properties relative to existing technology.

Massachusetts Institute of Technology – Cambridge, MA

Machine Learning Assisted Models for Understanding and Optimizing Boiling Heat Transfer on Scalable Random Surfaces - $521,602

The Massachusetts Institute of Technology (MIT) will develop a machine learning (ML) approach to optimize surfaces for boiling heat transfer and improve energy efficiency for applications ranging from nuclear power plants to industrial process steam generation. Predicting and enhancing boiling heat transfer presently relies on empirical correlations and experimental observations. MIT’s technology will use supervised ML models based on Gaussian processes and convolutional neural networks to identify important features and designs that contribute to heat transfer enhancement autonomously. If successful, MIT’s designs will lead to more readily adopted scalable surfaces in energy applications, enhancing performance and shortening deployment timetables.

Massachusetts Institute of Technology – Cambridge, MA

Global Optimization of Multicomponent Oxide Catalysts for OER/ORR - $1,268,183

The Massachusetts Institute of Technology (MIT) will develop machine learning (ML) enhanced tools to accelerate the development of catalysts that promote the oxygen evolution reaction (OER) or the oxygen reduction reaction (ORR). These reactions are critical to the cost-effective generation (OER) or oxidation (ORR) of hydrogen. Available catalysts for promoting these reactions include scarce and costly precious metals like platinum. Hence, their practical applications are limited by high cost and low abundance in addition to moderate stability. The MIT team will tailor the chemical composition of non-platinum-group transition metal oxides to improve their catalytic performance and reduce the number of potential combinations required for testing. MIT’s ML approach will integrate literature, simulations, synthesis, lab-scale testing, and industrial prototyping to yield a catalyst design methodology that is faster and more efficient than traditional trial-and-error or serial experimentation based approaches. The ML techniques to be employed are expected to include generative models and message-passing neural networks for materials as well as convolutional neural networks for machine vision to characterize catalysts.

University of Michigan-Dearborn – Dearborn, Michigan

ML-ACCEPT: Machine-Learning-enhanced Automated Circuit Configuration and Evaluation of Power Converters – $658,321

The University of Michigan-Dearborn will develop a machine learning-enhanced design tool for the automated architectural configuration and performance evaluation of electrical power converters. This tool will help engineers consider a wider range of innovative concepts when developing new converters than would be possible via traditional approaches. This tool is expected to leverage a number of ML techniques—including decision trees, supervised learning and reinforcement learning—and is expected to reduce the cost and time required to develop new ultra-efficient power-converter designs.

Carnegie Mellon University – Pittsburgh, PA

Predicting Catalyst Surface Stability under Reaction Conditions Using Deep Reinforcement Learning and Machine Learning Potentials - $500,675

Carnegie Mellon University will use deep reinforcement learning and atomistic machine learning potentials to predict catalyst surface stability under reaction conditions. Current methods for determining the metastability of bifunctional and complex surfaces undergoing reaction are difficult and expensive. Carnegie Mellon's technology will enable stability analysis in both traditional catalysts and new classes of materials, including those used in tribology, corrosion-resistant alloys, additive manufacturing, and battery materials.

Julia Computing, Inc. – Cambridge, MA

Accelerating Coupled HVAC-Building Simulation with a Neural Component Architecture - $1,125,679

Julia Computing, Inc. will develop a neural component machine learning tool to reduce the total energy consumption of heating, ventilation, and air conditioning (HVAC) systems in buildings. As of 2012, buildings consume 40 percent of the nation's primary energy, with HVAC systems comprising a significant portion of this consumption. It has been demonstrated that the use of modeling and simulation tools in the design of a building can yield significant energy savings—up to 27 percent of total energy consumption. However, these simulation tools are still too slow to be practically useful. Julia Computing seeks to improve upon these tools using the latest computing and mathematical technologies in differentiable programming and composable software to enhance the ability of engineers to design more energy efficient buildings.

University of Maryland – College Park, MD

Invertible Design Manifolds for Heat Transfer Surfaces (INVERT) - $426,647

The University of Maryland (UMD) will develop inverse design tools for the development of enhanced heat transfer surfaces at reduced computational cost. Heat transfer surfaces are used to increase the efficiency of many energy conversion systems, but they are currently designed in a slow, iterative fashion. UMD will use a direct inverse design method map from given environments and performance metrics to design variables or materials. The project will make use of generative adversarial networks, statistical connections between optimization and dynamical systems, and active learning to achieve its goals. The team will test its tools on turbine blade components and heat exchangers.

Los Alamos National Laboratory – Los Alamos, New Mexico

Machine Learning based Well Design to Enhance Unconventional Energy Production—$897,577

Los Alamos National Laboratory (LANL) seeks to increase the efficiency with which oil and gas are extracted from unconventional reservoirs while reducing the environmental impact of such processes. Current hydrofracturing-enabled extraction efficiencies are only 5 to 10%. LANL seeks to improve upon these levels by developing physics-informed machine learning (ML) based models from field data to discover effective well design characteristics. LANL will use its ML framework, which is based on recent advances in ML, differentiable programming, and cloud computing, to extract actionable information to enhance energy production while mitigating its environmental impact. Current baseline well design testing takes about 4 years and costs more than $6M per well. LANL predicts that if completely deployed, it is expected that the proposed framework will reduce the time and cost of well design by 40% and energy extraction can be tripled.

The University of Texas at Austin—Austin, Texas

Learning Optimal Aerodynamic Designs—$655,410

The University of Texas at Austin proposes to create efficient, accurate, and scalable deep neural network (DNN) representations of design optimization problem solutions. The inputs to these DNN representations will be the vector of design requirement parameters, the outputs will be the optimal design variables, and the goal is to learn the map from inputs to outputs (i.e., the inverse design map). The team will focus on the problem of the optimal shape design of aerodynamic lifting surfaces —in particular aircraft wings– using Reynolds-Average Navier Stokes models for minimal drag. The inverse design map for such problems is very complex and high-dimensional, involving inputs and outputs on the order of 1000s. Instead, the team will use the inverse design map to construct parsimonious DNN architectures trained with multifidelity methods. The resulting methodology will accurately and automatically design optimal and energy-efficient aerodynamic lifting surfaces at interactive speeds.

IBM Research—Yorktown Heights, NY

Model-based Reinforcement Learning with Active Learning for Efficient Electrical Power Converter Design—$407,057

IBM Research will develop a reinforcement learning (RL)-based electrical power converter design tool. Such converters are widely used and critically important in many applications. Designing a specific converter is a lengthy and expensive process that involves multiple manual steps—selecting and configuring the correct components and topologies; evaluating the design performance via simulations; and iteratively optimizing the design while satisfying resource, technology, and cost constraints. In this project, the design problem will be formulated as mixed integer optimization to be intelligently and automatically solved using an RL-based optimizer. Because the physics-based simulation models used for design are computationally expensive and time-consuming, IBM's framework will use surrogate models with similar fidelity but lower computation cost and query the physics-based models only infrequently via intelligent strategies. The proposed RL-enhanced automated design can explore the design space much more effectively, decreasing development time and cost without compromising performance.

Carnegie Mellon University—Pittsburgh, PA

High-fidelity Accelerated Design of High-performance Electrochemical Systems—$600,152

Carnegie Mellon University and team will develop an integrated machine learning-accelerated design and optimization workflow that will reduce the time and cost required to develop functional energy materials in devices. The core innovation pairs machine learning based filtering of candidate materials with accelerated high-fidelity modeling to efficiently search a large design space for high-performance materials under realistic operating conditions. The team will create detailed designs for (1) catalyst systems for electrochemical reactions that convert electrical energy into carbon-neutral chemicals and fuels and (2) electrolyte systems for next-generation batteries. Designing electrochemical systems capable of high turnover and efficiency is a challenge to enable the cost-effective production of carbon-neutral chemicals and fuels. Designing liquid electrolytes for next-generation batteries will provide an alternative transportation fuel to petroleum by improving energy density, thus enabling long-range electric vehicles. In particular, the project will develop software and hardware-accelerated methods for high-fidelity objective function evaluation, and an efficient global optimization approach using sequential learning and design of experiments to achieve its goals.

Stanford University—Stanford, CA

Energy efficient integrated photonic systems based on inverse design—$405,000

Stanford University will develop a machine-learning enhanced framework for the design of optical communications components that will enable them to operate at their physical performance limits. Information processing and communications systems use a significant fraction of total global energy. Data centers alone consume more than 70 billion kilowatt-hours per year. Much of this energy usage is intrinsic to electronic wiring. However, optical-based technologies offer a promising option to reduce energy consumption. Stanford's design platform is intended to enable optical technologies to serve in the next generation of information processing hardware with ultra-low energy footprints. The proposed framework will use generative neural networks for global optimization of nanophotonic components, machine learning to accelerate the solving of electromagnetic field calculations, and advanced optimization concepts to calculate the upper limits in photonic device performance.

University of Missouri—Columbia, MO

Deep Learning Prediction of Protein Complex Structures—$167,797

The University of Missouri will develop deep learning methods to predict inter-protein amino acid interactions and build three-dimensional structures of protein complexes, which are useful for designing and engineering protein molecules important for renewable bioenergy production. Proteins in cells interact and form complexes to carry out various biological functions such as catalyzing biochemical reactions. The team will use the deep learning methods it develops to construct green algae protein complexes that play important roles in biomass and biodiesel production. The technology and predicted structures of protein complexes will become valuable tools and resources for advancing U.S. bioenergy production and research.

United Technologies Research Center – East Hartford, CT

LENS: Learning Enabled Network Synthesis—$697,094

The United Technologies Research Center (UTRC) will develop an AI-accelerated search technique, LENS, to quickly discover new design concepts for energy applications. The project will combine the strengths of the two pillars of AI—logical inference and statistical learning—to achieve this task by using constraint programming, generative models, reduced order models, active learning, and rule discovery. The end goal is to accelerate the design of power converters, which have a significant impact on energy savings. UTRC's project will aim to address key challenges in power converter design by identifying the most suitable circuit topologies and simultaneously optimizing the design of power-converter components. LENS will enable exploration of very large design spaces of circuit topologies and components by addressing the limitations of the conventional process for design of non-linear, high switching speed, and multi-dimensional power converters.

United Technologies Research Center – East Hartford, CT

MULTI-LEADER: MULTI-source LEarning-Accelerated Design of high-Efficiency multi-stage compRessor—$564,188

The United Technologies Research Center (UTRC) will work to accelerate the design of high-efficiency multi-stage compressors, via machine learning (ML), with considerations of aerodynamics, structures and additive manufacturability through their framework, MULTI-LEADER. The framework addresses four design challenges in current industrial practices: (1) concurrent optimization of multiple stages under non-linear constraints; (2) evaluation of high-fidelity and expensive solvers and their gradients during optimization convergence in high-dimensional design spaces; (3) multi-disciplinary design to maximize aerodynamic performance while guaranteeing structural integrity and additive manufacturability; and (4) use of multiple fidelity of solvers with disparate parameterization and modeling assumptions. MULTI-LEADER has the potential to cut design costs by 80% while generating more energy-efficient designs of multi-stage compressors through faster and fewer design iterations, improved empiricism and performance evaluation, and quicker concurrent design processes. The proposed framework will deploy novel machine learning algorithms for multi-source learning of universal surrogate, physics-constrained data augmented modeling, generative manifold embedding, and budget-constrained fidelity-adaptive sampling to achieve the project goals.

GE Research – Niskayuna, NY

IMPACT: Design of Integrated Multi-physics Producible Additive Components for Turbomachinery—$1,365,066

GE Research will develop design optimization tools for the laser powder bed fusion based additive manufacturing of turbomachinery components. The team will integrate the latest advances in multi-physics topology optimization with fast machine learning-based producibility evaluations extracted from large training datasets comprising high-fidelity physics-based simulations and experimental validation studies. The integrated methodology will be used to demonstrate simultaneous improvements in the producibility and thermodynamic efficiency of a multi-physics turbomachinery component. Improved turbomachinery efficiency is a competitive advantage for U.S. industry and will help ensure the nation's energy security. The proposed manufacturing producibility-aware, multi-physics detailed design optimization tools will advance the use of additive manufacturing within the U.S.

GE Research – Niskayuna, NY

Pro-ML IDeAS: Probabilistic Machine Learning for Inverse Design of Aerodynamic Systems—$853,708

GE Research will develop a probabilistic inverse design machine learning (ML) framework, Pro-ML IDeAS, to take performance and requirements as input and provide engineering designs as output. Pro-ML IDeAS will calculate the design explicitly without iteration and overcome the challenges of ill-posed inverse problems. Pro-ML IDeAS will use GE's Bayesian hybrid modeling with multi-fidelity intelligent design and analysis of computer experiments and a novel probabilistic invertible neural network (INN). The proposed framework can be applied to general complex design problems. The designs of interest are turbomachinery components, applicable to not only industrial gas turbines (IGT), but also aviation turbine engines, aero derivative engines, wind turbines, and hydro turbines.

Princeton University – Princeton, NJ

MLSPICE: Machine Learning based SPICE Modeling Platform for Power Magnetics—$290,383

The Princeton University team will use machine learning-enabled methods to transform the modeling and design methods of power magnetics and catalyze disruptive improvements to power electronics design tools. They will develop a highly automated, open-source, machine learning-based magnetics design platform to greatly accelerate the design process, cut the error rate in half, and provide new insights to magnetic material and geometry design. Princeton's Simulation Program with Integrated Circuit Emphasis-based, or SPICE-based modeling platform, will utilize a highly automated data acquisition testbed capable of measuring a large number of magnetic cores with a wide range of electrical circuit excitations, a machine-learning trained modeling method for modeling the core loss and saturation effects of magnetic materials for arbitrary excitation waveforms, and a computer-aided-design tool which can synthesize the SPICE netlist for planar magnetics.

Lawrence Berkeley National Laboratory – Berkley, CA

Deep Learning and Natural Language Processing for Accelerated Inverse Design of Optical Materials - $803,730

Lawrence Berkley National Laboratory (LBNL) will develop an optical metamaterial design tool to increase energy efficiency and reduce national primary energy consumption. Besides creating high-quality datasets, LBNL will train physics-informed generative adversarial networks that automatically suggest candidate structures to produce desired optical properties within the constraints of cost of materials and manufacturing. Currently, finding an optimal design can take years and is based mostly on intuition and iteration. The team's machine learning tool will be 10,000 to 100,000 times faster than existing technology.

Pacific Northwest National Laboratory – Richland, WA

Machine Learning for Natural Gas to Electric Power System Design - $401,734

Pacific Northwest National Laboratory (PNNL) will apply multiple machine learning tools to develop next-generation natural gas to electric power conversion system designs. The project leverages a physics-informed machine learning tool for automated reduced order model (ROM) construction to significantly reduce prediction errors compared to traditional approaches as well as superstructure-based mathematical optimization tools combined with reinforcement learning and graph network methods to explore and optimize component connections in fuel to electric power conversion systems.