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A Paradigm for Digital Twins to Safeguard the Planet

Big Idea. Develop a multi-fidelity, scalable, long-lived open-source platform which consists of protocols, such as quantification and analysis of dynamic uncertainty, that enables systematic analysis of Earth system processes. From this platform, scientists will be able to build problem-specific digital twins. The problem-specific digital twins would continuously adapt as new data is ingested; detect changes in the climate system; measure response to climate mitigation actions; integrate scientific understanding; inform policy decisions; and reduce risk by being uncertainty-aware.

Reasoning and Justification. Other open-source and "Digital Twin" initiatives are underway both within the US and outside. By using the latest developments in mathematics, statistics and computing, the US can supersede existing efforts by providing a systematic approach to continuous-adaptation and uncertainty quantification. Uncertainty-aware Digital Twins invert observed time-lapse data for the system's state using established techniques from simulation-based inference; differ from existing approaches by enabling systematic analysis of Earth system processes and include analysis of dynamic uncertainty; and update themselves as new data comes in, using current state to make predictions of future states according to different scenarios.

Requirements. The research collaboration and infrastructure needed to develop the platform for problem-specific digital twins on Earth system processes consist of:

- Interdisciplinary collaboration between mathematical modelers, biological, physical, chemical, social science domain experts, and software engineers
- contemporary open science practices such as adoption of FAIR (Findable, Accessible, Interoperable, and Reusable) guiding data principles and adoption of standards working with organizations e.g. Open Geospatial Consortium (OGC) and the Earth Science Information Partners (ESIP).
- Access to massive computational infrastructure (computer and storage)
- Long-term sustained investment in software and software maintenance

Value and Impact. The value and impact include the following and more:

- Mathematical and statistical methods to enable continuous adaptation for problem-specific dynamical systems
- Detect "change/tipping points" including social and ecological responses to climate mitigation measures
- Make policy decisions to start or optimize climate mitigating measures along with confidence levels
- Inter/multi/cross-disciplinary long-term effort spanning many disciplines
- Prototype model for global cooperation between the U.S. and other countries
- Potential for generating huge amounts of data for education and experimentation purposes while training the next generation workforce

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What Happens in the Arctic Does NOT Stay in the Arctic

Big Idea. From micro to macro in the Arctic climate system. Understanding signature indicators of planetary warming – the loss of sea ice and thawing of permafrost – at the micro level and building up from there will help to make better models and predictions of what's happening in the Arctic and enable us to better understand and respond to the cascading effects experienced both in the United States and globally. The small-scale effects that add up to control the larger scale mechanisms are not understood at the physical level for models in the Arctic. Multiscale hierarchical modeling offers an approach through the development of complex cross-scale models to transfer the critical information from microscales to the macro behavior. Upscaling can be physics-informed and data-driven where possible but may rest on mathematical constructs when the physics is not yet determined, and experimental data are not available.

Reasoning and Justification. Warming in the Arctic has led to rapid, precipitous declines in sea ice and to thawing of the permafrost, with both contributing to further warming on a global scale. These dramatic changes in the Arctic environment affect not only the climate, ecology, economics, infrastructure, transportation and human activities in the region, but also impact the rest of the world and the U.S. Significant, transformative advances are needed to rigorously compute effective material properties of sea ice and permafrost from information about the composite microstructure and microscale processes and build up hierarchically from there. Success of mathematical theories and computational frameworks, statistical mechanics, and rigorous homogenization methods in the theory of composite materials have helped trigger the widespread use of composites throughout today's technological world. The time is right to develop the next generation of sea ice and permafrost modeling which thoroughly leverages modern math, physics, and vast data sets, including those from the recent Arctic expedition, MOSAiC. NSF has the needed scale, the interdisciplinary culture, the resources, and stature to leverage additional support for all aspects of the program – to facilitate the success of the first sustained effort to establish a new multiscale paradigm, from micro to macro, for modeling sea ice, permafrost and complex Arctic systems. **It is time to bring these advances to Arctic research.**

Requirements.

- Create a community of interdisciplinary teams of researchers, engineers, and stakeholders to develop a new paradigm for sea ice and permafrost modeling.
- Funding for smaller and larger interdisciplinary and multi-institutional teams for pilot/exploratory studies, and research projects with 2-3 cycles of 3–5-year awards.
- Establish a center coordinating the various types of theoretical, computational, and experimental efforts over 10 years.
- Fund two dedicated expeditions to the Arctic region over 10 years to inform and validate models, and to "piggy-back" on other expeditions around the world.

Value and Impact.

- Educate new generations of scientists on the basics of interdisciplinary math and science, developing their ability to build and use advanced models.
- Develop new multiscale methodologies, computational tools, data collection, storage, and imaging technologies suited to multiscale analysis for complex Arctic systems.
- Connect the broader public to the goals of climate research and specific deliverables, exciting research and field experiments in one of the most extreme environments on Earth.

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Transforming Education to Address Complex Futures

Big Idea. The world is facing challenges of increasing complexity at an accelerating pace. Mathematics, modeling, data science, and systems analysis are central to researching and developing solutions for complex problems. However, today's students often find it difficult to place coursework into a broader context and synthesize subject areas. A collaborative approach to curricula, classes, and pedagogy should be designed to cross boundaries among STEM, social science, and other disciplines and graduate thinkers who can contribute professionally and personally to solutions for society's Grand Challenges (e.g., climate, human health, food security, national security).

Reasoning and Justification. Work to prepare for complex futures is timely, given the recent, global examples of extreme weather, clean energy and its role in energy security, the global pandemic, and supply chain challenges. There is a need to ensure that students in all majors eventually develop an increased awareness of these problems through interdisciplinary courses and project work so they understand their role as a citizen and professional, and have the capacity and skills to develop and contribute to solutions. NSF is in the unique position at the interface of scientific advancement and education, with expertise across disciplines and focused on far-reaching efforts that advance society to develop this improved workforce. NSF also has experience with funding award structures that could be applicable to this topic, making implementation more straightforward.

Requirements. Implementation of this idea requires a shift toward a collaborative, less siloed mindset within academia and between academia, industry, and government. Three steps are envisioned to get there: (1) A 3–5-year pilot period, when multiple institutions develop and test transformative strategies for curriculum design and pedagogy. (2) An assessment period, where successful strategies are identified and refined. (3) A broad promulgation of lessons learned through replication and continued innovation. At all stages, stakeholders – including students, faculty, university leadership, industry, non-profit organizations, and government – should be consulted to ensure that disparate needs and ideas are being addressed.

Value and Impact. The adoption of revised educational paradigms can meet the needs of both students and industry. Integrating industrial partners into the education pipeline will (1) offer new insights into the pedagogical process; (2) attract new students into STEM associated fields and improve retention rates; (3) enhance workforce readiness and align degree programs more closely with emerging societal needs. The approach outlined will result in innovations including, but not limited to:

- Pedagogical practices that promote more active and engaged learning through incorporation of relevant issues and context into lessons
- Adoption of curricula that are adaptable to university strengths while promoting interdisciplinary work
- Disruption of academic silos and traditional academic reward systems to improve inter/transdisciplinary education and/or research collaboration teams
- Improved U.S. leadership and economic competitiveness through greater capacity for innovation
- General increase in public awareness of issues surrounding complex problems, for example sustainability and climate
- Improved general numeracy as K-12 and community learning are implemented

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Extreme Learning

Big Idea. Extreme weather events are the visible effects of a changing climate. We propose to develop and apply novel mathematical and statistical techniques to capture, characterize and predict extreme events. We need: (1) more data on extreme meteorological events; (2) input from meteorological subject matter experts to identify particular types of extremes; and (3) new mathematical algorithms that can quantify the likelihood of particular extremes given a non-stationary background.

Reasoning and Justification. Adapting our infrastructure to extreme weather events of ever-increasing severity and frequency requires a much better understanding of the statistics and dynamics surrounding them. We have limited data on past and current extremes and an incomplete representation of the climate system within which extremes form. We lack mathematical approaches that can incorporate and account for a non-stationary (or unstable) climate from which extremes can develop, as well as ways to describe and measure extremes that would occur after a climate has reached a tipping point. Advances in these areas require investigations along multiple pathways: (1) loss functions that better match predictions with observed extreme behavior; (2) improved stochastic optimization techniques; (3) new approaches to bypass the 1/p number of samples required by brute-force numerical simulations; (4) new statistical models that account for a lack of stationarity in space and time as well as the fat-tail behavior of the marginal distributions; and (5) new research in copula approaches informed by machine learning.

Requirements. There are three main requirements: (1) more data for extreme weather events; (2) stakeholder input to identify particular types of extreme events; and (3) new mathematical algorithms that can quantify the likelihood of particular extremes (or tail events) given a non-stationary background. This research thrust will determine data sources and needs for future data collection efforts and assess the quality of existing data. This program requires stakeholder meetings, including with infrastructure planners and operators, to identify initial types of extremes for focus. The program requires fundamental advances in mathematics and statistics that accurately predict extremes - averages as well as variances - under a non-stationary background. Computing and data storage needs will be significant for the project. Transdisciplinary collaborations between climate scientists, meteorologists, mathematicians, statisticians, and computer scientists and with users of extreme weather forecasts - industry, state and local decision makers, engineers, and social scientists.

Value and Impact.

- Tools and approaches will be developed to map out climate scenarios in greater detail, focusing on rare but powerful events that have the largest impact on human wellbeing and on ecosystems.
- Interdisciplinary training in mathematics, various domain sciences, computer science, computational science and engineering, data science, and statistics, including aspects of business, economics, social science, political science, architecture, information science, etc.
- Climate extremes are global, fostering cooperation with researchers outside the U.S. is essential. Partnerships with industry should be encouraged.
- With accurate predictions of alternative scenarios and anticipated catastrophic events and possible cascading effects, decision making and intervention at multiple scales can be prioritized.

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The End of Fossil Fuels

Big Idea. Save the planet for future generations by ending the use of fossil fuels. It is time for science to speak up and push for a moon-shot program of decarbonization. We have overstepped the planetary boundaries and treated the planet without regard for the consequences. Scientists had raised the alarm long ago but failed to motivate decision makers to prepare for action.

Reasoning and Justification. NSF has the intellectual standing to propose a science-based approach to decarbonization and can do its part by supporting the basic research needed to accelerate a national effort to eliminate the need for fossil fuels. New analytical and computational techniques need to be developed to improve the efficiency of green energy production processes, to improve storage capabilities of batteries and fuel cells, to discover new materials that enable energy production and conversion processes, to incorporate large numbers of renewable energy generators into the power grid, to design green buildings that consume less energy, etc.

Requirements. This is an ambitious goal that requires progress on many levels. Needed in particular are:

- The formation of multidisciplinary teams that bring together scientists, engineers, social scientists, and industry
- Coordinated support from multiple funding agencies and, within NSF, multiple divisions.
- A timeline of 25 years:
  - 5 years to start up, identify topics, recruit teams, and begin implementation.
  - 10 years until first significant results provide accelerated progress towards a net-zero carbon economy
  - 25 years to complete implementation of a net-zero vision.

Value and Impact.

- Reduce energy consumption and increase energy efficiency
- Electrify what can be electrified and develop renewables for what cannot be electrified
  - Biofuels, hydrogen, methanol, etc. - from methanol and some biofuels, other fuels such as kerosine (for jet fuel) or diesel (for ships or long-distance trucking) can be obtained in a carbon-neutral fashion, producing only as much CO2 released as was extracted before from the atmosphere
  - Enable the production of plastics without use of fossil fuels.
- Manage the transition to a fossil-free state.

From this effort, numerous other and diverse impacts will result, for example,

- Dramatic reduction of carbon emissions
- Significant improvements in quality of life, health, and environment.
- Creation of green jobs
- Independence from oil and gas
- Increased geopolitical stability
- Localized energy production ("power to the people")
- Reduced transportation costs.

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ACED: Accelerated Circular Economy Development

Big Idea. The world must more rapidly pursue the circular use of extracted minerals and manufactured products (aka "the circular economy"), and it must create new materials and innovative advanced processes from which replacement, non-petroleum-derived products can be produced. Rapid innovation-aimed at reducing waste and eliminating waste streams, reusing, repairing, remanufacturing, reprocessing, recycling, repurposing what is already available, and replacing systems, norms, products that are petroleum-reliant and/or petroleum-derived-is a necessary approach given finite global resources. Important aspects include novel lifecycle models (accounting, simulation), independently operated system optimizations, planning and investment processes linked by prices of shared inputs and outputs, research on shifting consumer behavior, strategic communications and engagement, and expedited shifts to a circular materials system, or a circular economy.

Reasoning and Justification. Economic policies and societal norms have enabled the dominance of fossil fuels and other resource extractions for energy and material needs. The linear economy based on these dominating industries has led to the massive accumulation of waste worldwide that threatens all forms of life. The overproduction of plastics and other petroleum-derived products is expected to increase and is not responding to environmental and public health threats. The current extraction of resources is not sustainable; fossil fuels and other extracted assets from the earth are non-renewable. A system-wide approach for materials recovery and reuse is required for global supplies of resources for safe and comfortable lifestyles and technological advances.

Requirements. To embark on a comprehensive, rapid-paced conversion to a circular economy, a cross-disciplinary approach is needed and broad engagement across multiple political and social scales, guided by social science methodologies is a prerequisite. This effort will require expertise from a variety of disciplines, including the quantitative sciences (computing, data, statistics, and mathematical modeling), various aspects of engineering (systems, industrial, mechanical, control), physical and life sciences, economics, behavioral/social sciences, political science, communications, education, industry and manufacturing, and business/management/accounting/finance. The resultant models, strategies, and tactics will reflect a new way to view and handle materials; their development guided by input from entities across industrial supply chains and consumer groups. Frequent and consistent communication with stakeholders, including industrial leaders, elected officials and politicians, and numerous other communities. It will be imperative to include nonprofit organizations (e.g., Ellen MacArthur Foundation), NGOs, national laboratories, global finance organizations (e.g., The World Bank), and U.S. government agencies and the local, state, and federal levels already engaged within the existing circular economy orbit.

Value and Impact. Numerous positive impacts are expected as a result of the comprehensive circular economy approach; for example: (1) increasing the sustainability of resources at the local, national and global levels, (2) improving economic equity for underserved and under resourced populations, (3) reducing waste and its related undesired social, economic and environmental problems, (4) emergence of new technologies and creative solutions in multiple parts and sectors of the economy, (5) reducing reliance and dependence on petroleum and its derivatives, and (5) tackling looming climate change disasters.

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Sustainable Smart Water Systems (aka Sustainable Water Grid)

Big Idea. We recommend investment in new research and development of a multiscale framework that transforms water management in the U.S. through more efficient resource distribution and use. Our aging water infrastructure and management practices have not kept pace with the demands of a growing population and are at significant risk due to the emerging impacts of climate change. To address these challenges within this complex system, we require technological, industrial, and social innovations that go well beyond business-as-usual. We need a nation-wide Smart Water Grid — a holistic, coordinated, multidisciplinary research framework that transforms the U.S. water infrastructure and management practices into a system that is sustainable, resilient, and will get us through the next century.

Reasoning and Justification. Due to climate change and climate variability — e.g., El Niño and La Niña abnormal weather patterns — the temporal variability and spatial distribution of water availability has been dramatically changing. On the other hand, demand for fresh water — i.e., water for agriculture, water for the energy sector, water for industry as well as drinking water — has increased and will continue to increase, driven by population growth, industrialization, and globalization. Indeed, a significant fraction of the global population is located in areas or regions of high or extremely high freshwater supply risk, while other regions face the problems related to overwhelming amounts of water. The development of a comprehensive multiscale water management framework could facilitate the adaptation to climate change and climate variability impacts related to changing levels of water resources.

Requirements. To enable this, each framework must co-design and integrate advances from mathematics, computing, engineering, chemistry, economics, environmental sustainability, and social science to make resource use more efficient, sustainable, adaptable, and equitably accessible. The applications that these frameworks enable should include those for decision support, inference, modeling, and prediction, data analysis and visualization, and intelligent automation that span multiple temporal and spatial scales.

Value and Impact. The first-order impacts are (i) more efficient resource use through better water management, and (ii) a system that is more resilient to the extreme events induced by climate change. The second-order impacts include improved leak detection (e.g., smart water meters, remote sensing, GeoAI to detect and localize leaks) for consumers (inside, outside of residences) as well as for municipal water utilities. (Note that approximately one-third of municipal water is lost as the result of leaks due to aging pipes, running toilets, etc.). We foresee benefits in terms of science informed policy and gap identification (industry opportunities) in terms of technologies that impede understanding of system behavior and pricing as well as in terms of advances that inform the next of strategic investments, e.g., water storage and transport, desalination, etc.

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Unraveling the Climate Vulnerability Web: Integration of Physical, Biological, Social, and Economic Models in Time and Space

Big Idea. We recommend a community-focused research effort to develop and integrate high resolution models of climate, social, ecological, and economic systems to identify vulnerabilities in human and ecological systems — and use that information to manage and reduce climate risks and increase resiliency. The effort will be carried out by teams who work in concert with community stakeholders, so decision makers and stakeholders can develop recommendations and policies to adapt to and mitigate climate change vulnerabilities in their affected communities.

Reasoning and Justification. Today, communities worldwide are struggling with the complex interaction of environmental threats, economic development, and societal inequity. These threats also impact the ecosystems on which these communities rely. Both human and ecological communities face interconnected risks that necessitate the use of data collection and an approach that can assess these impacts through a holistic lens. Existing integrated models are at a coarse scale, and frequently neglect important aspects of social and natural systems—such as social and ecological feedback and ecosystem responses—in the model development and analysis in favor of focusing on aggregated economic outcomes. NSF is uniquely positioned to bring together interdisciplinary teams due to its broad funding scope. Further, NSF has a successful history of programs that transcend the standard funding mechanisms of PI-driven funding, with the GLOBEC program a particular example. This type of funding structure is uniquely possible at NSF and is needed to leverage the expertise of STEM and social science researchers and community stakeholders. When these diverse teams co-produce the research questions, analysis and output, they will build the foundations of a new transdisciplinary approach to identify climate risks and mitigate vulnerabilities.

Requirements. Expertise from multiple mathematical sub-disciplines (dynamical systems, numerical analysis, simulation, machine learning, statistics, uncertainty quantification), and other STEM (computer science, environmental science and ecology, atmospheric, land, sea ice and ocean science, agricultural science) and social science disciplines (economics, behavioral science, and political science) is required, as well as input from stakeholders (local and regional government officials, community educators, policymakers, NGOs, and entities in the private sector). Typical funding structures break grants up, passing the pieces on to individual teams that pursue parts of the project and will not lead to the required interconnections among the different teams. This will inhibit the kind of integrated multi-disciplinarity required for the projects recommended. We recommend the development of an innovative and appropriate funding and governance mechanism for the overall research effort.

Value and Impact. In closing the distance between models and metrics for vulnerability assessment, we form a (far more) complete picture of attribution pathways from computational and mathematical modeling decisions, ecosystem services, social vulnerabilities, and human consequences. From this, comprehensive quantified uncertainty in forecasts (that can be attributed to processes covered by modeling) may be captured. Knowledge of uncertainty can lead to targeting resources to key aspects of model development, and targeted data acquisition, which leads to quantifiable uncertainty reduction for assessments. Such developments build greater scientific understanding on climate change vulnerability.

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Change the Conversation at the Local Level

Big Idea. The discussion of climate change needs to be brought home to the local level. To achieve this goal, we propose the creation of a research program that focuses on (i) the development of a framework for evaluating novel metrics of data streams, and (ii) building community-level networks of local decision makers and leaders to evaluate how these new metrics can inform the development of appropriate incentives to improve climate mitigation behaviors. Such a program requires the combined efforts of mathematical, computational, and social, behavioral, and political scientists working collaboratively at multiple interdisciplinary centers.

Reasoning and Justification. With the growing threat of climate change, scientists and decision makers have proposed various policy options that may mitigate the causes of climate change. However, optimal climate change mitigation and adaptation are unlikely to occur through the introduction of scientific information and policy options alone. To enable behavioral change, a global effort to drive solutions at the local level is needed. Social behavior has both a rational and an irrational element; it is important to understand this mathematically to enable scientific recommendations for improvements to resiliency and sustainability in communities. By developing models that can explain the behavior at a local level, policy recommendations from scientific research can be transformed more efficiently into action.

Requirements. We conservatively request $125 million for the establishment of five Multidisciplinary Climate Change Research Centers across the United States. This fund will provide $5 million per center for 5 years. These centers aim to help scholars in various disciplines — including but not limited to mathematics, statistics, social science, and engineering — to collaborate effectively with local community stakeholders to better understand human behavior.

Value and Impact. The proposed establishment of five geographically diverse, interdisciplinary research centers that focus on developing mathematical models that foster sustainable communities will enable mathematicians, social scientists, community leaders and other stakeholders to jointly address complex societal issues. The development of novel mathematical models that are equitable and just will deliver trustworthy information, eliminate biases toward historically underserved vulnerable communities, and support community leaders and other stakeholders to make well-informed decisions that benefit the entire community. The novel models will ingest heterogeneous data from diverse sources, including but not limited to climate, transportation, energy, water, and food sectors, and will provide actionable information that will enable the creation of software platforms and other technologies that will overall increase sustainability and resilience of our communities.

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