Exascale Computing Systems, Methodologies, and Applications

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Summary. Exascale computing architecture, system software, and applications are to be cooperatively developed to deliver unprecedented efficiency and scalability that will enable breakthrough advances in science and engineering and empower economic and social progress in Indiana and the US.

Abstract. This interdisciplinary inter-institutional grand challenge proposes to develop the necessary innovations in algorithms, computer architecture, programming models, and system software to enable unprecedented computing capability, up to and including exascale (notionally, 10^{18} operations per second). This achievement will require a fundamental paradigm shift, which is further complicated by the recent emergence of data analytics as a computational tool. A strongly interdisciplinary effort, it requires close association of the computational domains including scientific, engineering, commerce, and societal problems. Although computing technology has exhibited growth of more than ten trillion in a single lifetime, it is nonetheless approaching stagnation. As a result, real-world efficiencies are declining, fewer problems are able to fully exploit system scale, and applications have become much harder to program. Reversing this crisis as high-performance computing progresses towards exascale constitutes a Grand Challenge of the first order. IU is uniquely positioned to address such a challenge because of its combined world-class strengths in advanced HPC systems research, its strong infrastructure hardware and software support, the emerging focused academic program in the new Department of Intelligent Systems Engineering, and the breadth of computational science disciplines throughout the university. To create the necessary paradigm shift in HPC, specific goals of this project include formal specification for the theoretical foundations our approach, design of key hardware architecture components, implementation and deployment of a full exascale-ready software stack, development of key applications, support for partner Grand Challenge projects, transfer of our technology to external organizations, and enhancement of disciplinary and cross-disciplinary educational programs.

1. The Grand Challenge

Computing is well-established as the third pillar of scientific investigation and supercomputing in particular has enabled enormous breakthroughs in science and engineering. In almost any technical endeavor, carrying out experiments with computational models, rather than with physical infrastructure, is faster, cheaper, and safer. Moreover, entirely new types of investigation are now being enabled due to the ability of supercomputers to rapidly analyze massive amounts of data. In a sense, supercomputing allows us to explain the past, control the present, and, in certain limited ways, predict the future. Although computing performance has exhibited unprecedented growth (more than a factor of ten trillion in a single human lifetime), it is nonetheless approaching stagnation, forcing a brute force approach of ever-increasing number of processor cores per system for sustained performance increases. As a result, real-world efficiencies are declining, fewer problems are able to exploit full system scale, and applications have become much harder to program. Reversing this crisis as high performance computing (HPC) progresses towards exascale (notionally, 10^{18} operations per second) constitutes a Grand Challenge of the first order. The principal goal of this grand challenge project is to develop essential HPC architecture, system software, programming technologies, and high-impact applications to enable breakthroughs in science, engineering, and societal domains that increasingly rely on supercomputing for their advancement. Working with tech transfer and economic development partners, this proposed grand challenge will create substantial economic opportunities for Indiana and its residents and US global competitiveness.

2. Goals and Objectives

Goals and objectives for this project fall into three categories: technology research and development, technology transfer and commercialization, and education.

1. The technology research and development goal is to create a paradigm shift and to develop enabling technology for accelerating progress in applied fields. The objectives for the core computer technology research and development are to:
   a. Further refine innovation in **execution models** to guide the development of new system component layers and govern their interoperability in support of extreme scale application computing;
   b. Fully structure an advanced introspective dynamic adaptive **runtime system** for guided computing, resource management and task scheduling that uses system and application runtime information for continued operational optimization through high efficiency and parallelism discovery;
   c. Devise **programming interfaces** that expose powerful semantic constructs for exposure and exploitation of parallelism as well as interoperability with other program modules, and legacy codes;
   d. Design hardware **architectur**e components to accelerate runtime mechanisms for greater efficiency and scalability and implement these designs at IU and with industrial partners.
2. The objectives for the application technology research and development are to:
   a. Cooperatively develop a select set of extreme-scale **applications** that will enable breakthroughs in strategic leading-edge fields – both to drive exascale advances and to demonstrate potential end-user achievement through future innovative exascale computing;
   b. Support **other IU Grand Challenge projects** that may heavily rely on and benefit from exascale computing to better achieve their goals.
3. The technology transfer and commercialization goal is to accelerate adoption of the technology in the marketplace and to bring economic benefits to IU, Bloomington, and the state of Indiana. The objectives are to:

a. Derive plans for intellectual property stewardship and **technology transfer** from our results to industrial, commercial, academic, and government customers and implement these plans to yield market and licensing revenue;

b. Provide **professional facilities** to support and deploy IU exascale hardware and software products, leveraging established UITS capabilities, procedures, staff, and infrastructure management.

4. The education goal is to disseminate results of the research and development and further increase IU's reputation as a premier academic institution. The objectives are to:

a. Enhance IU education across a **diversity of disciplines** with scientific computing;

b. Support the nascent **Intelligent System Engineering Department** for graduate and undergraduate curriculum and research, so that it emerges as a leading program of its kind;

c. Provide cutting edge research opportunities for **undergraduates from regional campuses**.

3. Proposed Research and its Impact

The research agenda for this grand challenge integrates three focus areas: exascale computing, applications, and impacts. It reflects an exciting program of research and application and will contribute to IU's preeminence in supercomputing (systems and applications) on the national and international stages. A unique practical aspect of this project from the business perspective is the investigation of technology transfer mechanisms as a research topic in its own right.

Exascale Computing Systems Frontiers and Strategy

Delivering exascale performance will require fundamental advances in multiple inter-related technology areas, from hardware architecture through application software design. Figure 1 illustrates the exascale technology stack. To make this a well-integrated stack, it is essential that the component technologies be unified by a defined intellectual framework (an "execution model"). Key aspects of the technology stack are described below.

The **ParalleX execution model** provides the conceptual framework for the cross-cutting design and operation of future exascale computing systems and in particular addresses the technical challenges described above through dynamic adaptive mechanisms and semantics. ParalleX incorporates and integrates the elements of local dataflow execution, distributed contexts, message-driven computation, global name spaces, and powerful synchronization mechanisms. It can support heterogeneous system architectures including GPUs and expose and exploit diverse parallel forms for scalability and adaptive load balancing.

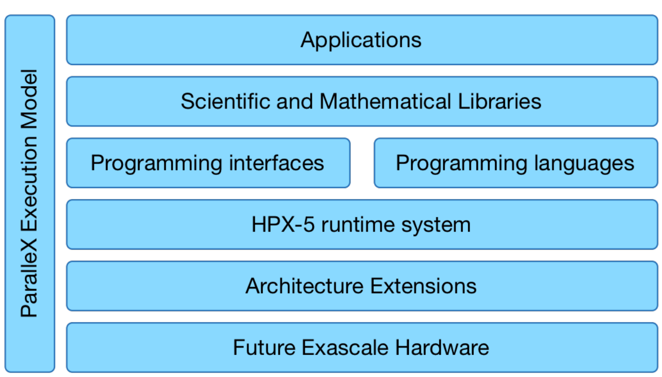

Figure 1: The exascale grand challenge technology stack extends from the domain applications down to the exascale hardware platform and is conceptually integrated by the ParalleX execution model.

The **HPX-5 runtime system** is a reduction to practice of the ParalleX concepts and delivers many of its benefits to large-scale conventional systems and provides a template for future advanced exascale computer architectures for reduced overheads and increased scaling.

Programming interfaces and languages. Access to runtime system capabilities will be provided directly through defined interfaces (similar to OS system calls) as well as through programming language extensions. The programming interfaces expose capabilities of the HPX-5 runtime system, whereas the programming language extensions make these capabilities first-class entities in the host programming language (C and/or C++). Full support for the programming language will require toolchain development, including compilers, utility libraries, debuggers, and performance monitoring infrastructure.

Architecture extensions. For sufficient performance, some capabilities provided by the runtime system require direct support by the underlying hardware. Support mechanisms can be realized directly using FPGAs (as standalone, integrated with network hardware, or integrated with processing cores), a technology specifically for hardware prototyping. In some cases, it may be necessary to incorporate hardware support mechanisms into the processor core, which will require vendor participation. Runtime system capabilities that are expected to benefit from hardware acceleration include thread and message scheduling, active global address translation, and fine-grained synchronization.

Proposed Selected Applications

The development of exascale system software and architecture will be guided by a co-design process including key parallel applications, emphasizing both importance and intellectual content. These driver applications represent areas of brain science, machine learning for data analytics, materials and manufacturing, mesoscale meteorological phenomena, and computational science. In addition, this project will be relevant to and informed by other IU Grand Challenges.

Brain science. We are entering a golden age of data collection and computational modeling in neuroscience, which presents numerous opportunities for exascale computing. Data from instrumented neurons must be processed in order to understand the spatial and temporal relationships in the neuronal network. Inferring functional connections between only 500 neurons based on the time series data of their spikes might take 10-20 hours on a supercomputer like IU's Quarry. Future experiments will require rapid data analysis so that spike identification and functional network structure can be obtained within minutes. With this kind of rapid data analysis, a first draft of network connectivity can be completed while the tissue is still viable, which can serve as a model to guide stimulation in maximally informative ways, allowing the model to be updated and refined. Additional variables like sensory input, motor output and behavioral state, could also be added. To develop and refine predictive models of the brain, experiments of the future will involve a rapid loop between millions of neurons and an actively behaving animal.

Deep machine learning. The ecosystem surrounding "Big Data" includes a number of high-productivity systems that unfortunately suffer from performance limitations. Careful analysis of application characteristics has enabled us to develop systems that provide the "best of both worlds" – a high-performance runtime combined with the programmability of (e.g.) MapReduce. The IU Digital Science Center (DSC) has worked with NSF funding to look at multiple application communities such as biomolecular simulations, network science and computational social science, computational epidemiology, computer vision, deep learning, et al. and so is well prepared to support a wide variety of IU needs. First, we will develop a high-performance "Infrastructure as a Service" that allows the same code to be deployed on cloud environments as well as HPC clusters. The systems to be built are insensitive to underlying technology change and allow trade-offs to be made regarding performance, cost, security and ease of use. Second, we will integrate our exascale runtime into streaming and batch programming models to allow a full range of data analytics to run with scalable performance. Third, we will develop the Scalable Parallel Interoperable Data Analytics Library with core machine learning libraries combining parallel database backends and high-performance runtimes.

Severe Weather Prediction. Numerical weather prediction (NWP) exploits the cutting edge of supercomputing, yielding steadily improving forecasts of large-scale weather patterns on timescales of days to weeks. Through HPC, researchers have continually increased the resolution of NWP models, such that they can now resolve individual thunderstorms (on the order of 10 km or less) and produce useful forecasts on timescales of minutes to hours, even real-time operational forecasting unheard of 15 years ago. Severe thunderstorms cause numerous deaths, injuries, and property damage from flooding, hail, lightning, high winds, and tornadoes. Tornadoes constitute a particularly challenging problem due to their inherently small size and short duration while exhibiting extremes of wind force. There is a great need to meet this challenge, due to the high threat for tornadoes--which is maximized in the Plains and Midwest. Current operational NWP models can only resolve the larger scale mesocyclone circulations within the thunderstorms that spawn tornadoes. The ability to reliably resolve tornado-scale circulations in near real-time would require exascale supercomputing technology with many fundamentally unsolved scientific problems surrounding the development and behavior of tornadoes still remaining.

Materials by Design for Advanced Manufacturing. A revolution in manufacturing is occurring through additive fabrication commonly referred to as "3D printing". Now being used as structural components in complex systems like motors, engines, product bodies, and even human replacement elements, this core methodology demands rapid simulation of strength, thermal, stress-strain, electrical, and other mechanical properties some of which are uniquely caused by the fabrication process itself. With each printed object custom made, complex simulation is in the critical path and therefore cost of production. Advances in HPC including exascale will become increasingly important to the success of additive manufacturing and the emerging industries based on it. These related applications will support the nascent Intelligent Systems Engineering (ISE) program at IUB. It arises from and will extend the successful large-scale Indiana collaboration among IU, Notre Dame and Purdue to design a complete solution to shock-wave production of cubic boron nitride. Building on this existing capability, the proposed exascale application will present a unique opportunity that will significantly enhance the attractiveness of the new engineering program at IU as well as lay the foundation for new opportunities in Indiana's industrial base and skill force.

Computational Materials, Biology, and Energy Science: Much of molecular science is based on a detailed understanding of quantum mechanics, dictated by the probabilistic interpretation of nature as expounded by Schrödinger's equations. A detailed understanding of these fundamental processes is critical for (a) designing artificial energy sources that use and store solar power through photosynthesis, (b) cancer research and vaccine design through the action of certain biological enzymes, (c) the design of new materials that will have impact on information technology through "quantum enabled" chips, and (d) impact air pollution and climate change. Detailed understanding of these processes is a major challenge of computational science and applied mathematics. Solving such problems is extremely compute-intensive (NP-hard), requiring new heuristic-based algorithms, software frameworks, and exascale power to solve.

Impacts

The technical, societal, and commercial impacts of this project are broad and deep for IU, Indiana, and the nation. The technical impacts will dramatically advance the field of HPC and the application domains associated with this project. The infrastructure, tools, and methodologies will fundamentally change HPC and thus enable and accelerate discovery in other fields, which discoveries we can only imagine. Equally important will be the direct impact on Indiana economic prosperity, including industrial and skill-force development. Just as Silicon Valley was catalyzed by university research, our emphasis on technology transfer will create new wealth and attract new talent to Indiana. Licensing of intellectual property will provide new revenue streams to the university and the state. IU will fulfill its objective of being the national leader in HPC through the combined capabilities of CREST, DSC, and UITS. The timing of this project is ideal to stimulate and engage the new ISE Department both directly in computer engineering and cyber-physical systems areas as well as emphasizing interdisciplinary fields with COAS. Finally, this project contributes to the health and well-being of Indiana residents through brain science simulation, resource management through machine learning, industrial base through materials simulation for additive manufacturing, natural resource and agricultural stewardship through weather prediction, jobs through industrial expansion and spin-offs, and improved education in engineering and computational sciences.

Research Plan

Based on prior research at IU in both advanced HPC and end-discipline sciences, the Exascale Grand Challenge will undertake simultaneous determination of computational science demands while characterizing the highly disparate regime of data analytics represented by machine learning. Our HPX runtime system prototype will be employed as a source of quantified costs and compared with application requirements restructured to incorporate new knowledge and innovations by CREST. UITS will refine this code to ensure industrial-grade quality and manage dissemination, documentation, customer reporting, and porting. All partners will contribute to evaluation of critical mechanisms to establish efficiency and scalability. The results from these crucial explorations will drive invention of architecture advances initially with FPGAs to be implemented by CREST at UITS' test-beds. Further architecture developments will be simulated and shared with industrial partners including Intel and Micron among others. A plan will be formulated by Kelley and IURTC for licensing of IP through patents as well as commercialization through one or more startups in Indiana will be pursued for enhanced local economic prosperity growth. The new Department of ISE will be expanded by faculty through this grand challenge project to enhance IU capability in computer architecture and systems, build a strong computational science program in conjunction with COAS, and position IU as a leader in computer engineering.

4. Resources

IU is almost ideally positioned to lead the nation in future generations of supercomputing and strategic applications. The proposed grand challenge draws on significant IU strengths in advanced HPC systems (CREST), data analytics and machine learning (DSC), strong infrastructure hardware and software support (UITS), the emerging Department of ISE, the breadth and quality of computational science disciplines throughout the university, excellence of Kelley School of business, and experience of IURTC that fosters collaborations between IU stakeholders and industry at all stages of engagement. Additional resources required to achieve the goals of this project include the following:

Strategic hires. This project provides a vital means for attracting high-quality faculty to the new ISE program. We anticipate requiring 6 tenure track faculty in Intelligent Systems Engineering in the areas of advanced materials, metallurgy, advanced manufacturing, embedded systems, computer architecture, and computational engineering and 4 tenure track faculty in COAS in computational science.

Senior Professionals. Accomplishing the necessary development aspects of this project will require a cadre of research scientists and professional scientific programmers (3 and 2, respectively).

Post-docs and PhD students. We expect one or more post-docs and three or more PhD students assigned to each major technical task in this project (15 post-docs and 45 grad students).

Deployment. To facilitate deployment of our work to local (and other) computing resources, we anticipate 2-3 FTEs assigned to UITS.

Hardware. We will require a capable test bed cluster to support our FPGA development work.

5. Team

This project will be directed by Andrew Lumsdaine and Thomas Sterling, who each have decades of experience managing and collaborating on complex projects.

Point of Contact and PI - Andrew Lumsdaine: Lumsdaine is the Associate Dean for Research and a Professor of Computer Science in the School of Informatics and Computing, and Director of the Center for Research in Extreme Scale Technologies (CREST). As the Director of the center, he has managed growth of 20 to 70 employees over a 5-year period and a portfolio of over $18 million.

Chief Scientist - Thomas Sterling: Sterling holds the position of Professor in the Department of Intelligent System Engineering at the School of Informatics and Computing and serves as Chief Scientist of CREST. Dr. Sterling has a key role in guiding the design of the exascale computing system, as well as interfacing and overseeing the applications and collaborations with global industry and academic partners.

Two specific examples of multi-discipline and multi-institutional leadership include the XPRESS and C-SWARM projects. In 2012, Lumsdaine and Sterling were awarded $1.1 million as part of a project involving seven institutions titled, "eXascale PRogramming Environment and System Software". In 2014, DOE funded a $10 million center (at ND) titled, "Center for Shock Wave-processing of Advanced Reactive Materials", for which IU leads the exascale research.

The following key team members of this project are highly-respected experts in their specific fields and have conducted influential research nationally and internationally.

- Geoffrey Fox, Chair of Intelligent Systems Engineering and Director of Digital Science Center – data intensive and machine learning applications
- John Beggs, Associate Professor, Department of Physics – neuroscience application
- Siri Terjesen, Assistant Professor of Strategic Management and International Business – examine pragmatic and effective means of transferring a new radical technology into the real world market
- Srinivasan S. Iyengar, Associate Professor, Department of Chemistry – computational science
- Dan Dawson, Assistant Professor, Department of Earth, Atmospheric, and Planetary Sciences, Purdue University – numerical meteorology (tornadoes) application
- Engineering faculty member (to be hired) – additive manufacturing application
- Tony Armstrong, President and CEO, IURTC and Associate VP for Engagement – IP and partnership management
- Craig Stewart, RT UITS – artifact management and deployment

6. Sustainability

The proposed grand challenge project is well-aligned with important large-scale national and international initiatives. Because our proposed work will be pushing the boundaries of supercomputing and related application areas, we will be ideally positioned to maintain leadership in these areas as major participants. Grand challenge investment at this time will give IU a competitive advantage and greatly enhance our position for future support as important new funding opportunities come on line.

The most relevant initiative to the core research in this grand challenge proposal is the National Strategic Computing Initiative (NSCI), which was recently created by executive order from the President of the United States. The executive order identified the following priorities:

- Accelerate delivery of exascale machine (100X power of todays fastest machines)
- Increase coherence between computational modeling and data analytics
- Establish a path forward for post Moore's Law era
- Increase capacity and capability of enduring national infrastructure
- Enrich public-private collaborations

These priority areas are key and explicit research topics in our proposal. The lead agencies for this initiative are the Department of Energy, Department of Defense, and the National Science Foundation, with which the PIs and participating faculty have a strong track record of securing research funding. Also significantly, PI Sterling regularly participates in the program development process with DOE, thereby strongly influencing its research direction.

In addition to the NSCI, the President also recently directed the creation of a ten-year plan for "Brain 2025: A Scientific Vision" for the NIH's portion of the Brain Research through Advancing Innovative Neurotechnologies (BRAIN) initiative. Application work in this proposal coordinates well with the BRAIN initiative. The co-design process in this project between exascale computing capabilities and brain modeling will place IU's work at the leading edge, making the work an attractive funding target.

Since the proposed work contributes directly to the development and delivery of an exascale machine (as well as follow-on post Moore's law technologies), the products of the proposed research and development will have significant appeal to the vendors that will be delivering future HPC platforms. Coupled with the strong existing connections that the PIs have to industry leaders, support will also be sought from these sources. Potential commercial funding sources include Intel, Micron, Qualcomm, Cray, IBM, Broadcom, and others. We will work with IU's existing development offices, from the level of individual schools to IU Foundation, to secure and further explore these non-traditional sources of funding.

Educational activities engendered from the proposed grand challenge will be eligible for their own funding. For FY2016, the NSF Research Traineeship Program announced two new priority areas for Traineeship Track, one of which is Understanding the Brain (UtB). For FY2016, UtB persists as one of three priority areas for the program. NSF NRT is dedicated to effective training of STEM graduate students in high priority interdisciplinary research through the use of innovative training models. The proposed grand challenge will constitute a foundation upon which an attractive traineeship program can be built.

7. Partners

We are proud to partner with institutions locally, nationally, and internationally to facilitate advances in exascale computing around the world. Indiana state partners include IURTC and IUF (for tech transfer, licensing, and fund-raising), as well as Purdue for collaboration on the weather simulation application. Existing relationships with a number of industrial partners will be fostered for collaborative research as well as tech transfer. Industrial partners include Intel, Micron, Data Vortex, Cray, and Qualcomm. In addition, CREST will be an inaugural member of the Open HPC consortium, a new organization founded by Intel for dissemination of HPC technologies and software. Existing collaborations with international research partners include EPFL (Switzerland), A*STAR (Singapore), Moscow State University, Center for HPC (South Africa), and the Swiss National Supercomputer Center. The support of these collaborative efforts and affiliations with a network of government agencies, national labs, academic universities, industry partners, and community organizations will enable this project to reach its highest potential worldwide.

8. Metrics

Tracking progress and evaluating success for this grand challenge project will depend on a set of qualitative and quantitative metrics at several levels. The three levels will be 1) technical, 2) application discipline capability, and 3) Indiana prosperity impact. The most detailed and highest frequency factors relate to the technical advances in terms of the fundamentals of time, energy, computing work, and resources. Such parameters include efficiency, scalability, time to solution, accuracy, cost, generality, and user productivity. Together, this ensemble of detailed measures will quantify the improvement of execution capability. The second level of metrics is the empowerment of expanded range of applications in science, engineering, and societal areas and the new performance regimes in which they can be engaged. These metrics will use as controls the selected problem domains of brain science, mesoscale meteorology, industrial materials for additive manufacturing, computational science, and data analysis through machine learning. Additional problem areas will be taken from other IU Grand Challenge problems that can benefit from advances in HPC including exascale. The third level of metrics will evaluate the direct impact on Indiana, its economy, and its quality of life. While less precise than the other measures, key indicators can nonetheless be observed that will make clear the value of this work. These will include but not be limited to: a) new jobs created, b) number of industrial concerns employing the new technologies and applications, c) startup ventures within the state, d) improved quality of life from enabled applications such as tornado prediction, brain diagnosis, or manufacturing, and e) enhanced educational opportunities for Indiana students. Other measures include grants awarded and adoption of Indiana technologies by major US industrial corporations. Finally, we will track the international communities and markets to monitor worldwide impact and improvement of IU ranking.

Key team members and their roles

Geoffrey Fox, Chair of Department of Intelligent Systems Engineering and Director of Digital Science Center

Geoffrey Fox received a Ph.D. in Theoretical Physics from Cambridge University and is now distinguished professor of Informatics and Computing, and Physics at Indiana University where he is director of the Digital Science Center, Chair of Department of Intelligent Systems Engineering and Director of the Data Science program at the School of Informatics and Computing. He previously held positions at Caltech, Syracuse University and Florida State University after being a postdoc at the Institute of Advanced Study at Princeton, Lawrence Berkeley Laboratory and Peterhouse College Cambridge. He has supervised the PhD of 68 students and published around 1200 papers in physics and computer science with an hindex of 70 and over 26000 citations.

He currently works in applying computer science from infrastructure to analytics in Biology, Pathology, Sensor Clouds, Earthquake and Ice-sheet Science, Image processing, Deep Learning, Manufacturing, Network Science and Particle Physics. The infrastructure work is built around Software Defined Systems on Clouds and Clusters. The analytics focuses on scalable parallelism. He is involved in several projects to enhance the capabilities of Minority Serving Institutions. He has experience in online education and its use in MOOCs for areas like Data and Computational Science. He is a Fellow of APS (Physics) and ACM (Computing). Dr. Fox will lead the data intensive and machine learning applications.

John Beggs, Associate Professor, Department of Physics, College of Arts and Sciences

John Beggs is an Associate Professor of Biophysics. He obtained his BS and MEng degrees in applied physics from Cornell and his PhD in neuroscience from Yale. The Beggs lab uses high-density microelectrode arrays to study the emergent properties of networks of hundreds of neurons. His group has published highly cited papers on neuronal avalanches and functional network structure. They have received consistent support from NSF over the past 12 years, and in the past two years won a major research instrumentation grant for a 512 microelectrode array for stimulation and recording. Another NSF grant awarded this year will allow the Beggs group to apply this 512 array to study how local cortical networks perform computations. Dr. Beggs will lead the neuroscience application.

Siri Terjesen, Assistant Professor of Strategic Management and International Business, Kelley School of Business

Siri Terjesen is an Assistant Professor in the Department of Management and Entrepreneurship in the Kelley School of Business at Indiana University as well as a Visiting Professor in the Department of Strategy and Management at the Norwegian School of Economics (NHH) in Bergen, Norway. She is an Associate Editor of three leading international journals of entrepreneurship, innovation, and education, and has published over 55 articles, 2 books, and 5 teaching cases. Some of her work explores the role of open innovation in commercializing technologies, and has examined a case of a NASA-developed technology which was recently commercialized for the consumer market. Her role on the project will involve examining pragmatic and effective means of transferring a new radical technology into the real world market.

Srinivasan S. Iyengar, Associate Professor, Department of Chemistry, College of Arts and Sciences

Dr. Iyengar holds joint appointments as an Associate Professor in Department of Chemistry and Adjunct Professor in Department of Physics. Research efforts in the Iyengar group are on the interface of chemistry, computational physics and applied mathematics. They deal with the development of new theoretical methods and the subsequent implementation of these into efficient computational models.

Dr. Iyengar has been the recipient of the Camille and Henry Dreyfus young faculty award and the Arnold and Mabel Beckman young investigator award. His research program has been funded through the NSF, NIH and ACS-PRF grants. Dr. Iyengar will lead the efforts related to the exascale scientific computing application, specifically methods for the analysis of the quantum many-electron system.

Specifically, the groups of Raghavachari, Ortoleva and Iyengar, have great experience developing approximate computational methods to solve such problems. Some examples of recent developments from these groups that can address these problems are the "molecules-in-molecule" approach from Raghavachari, the multiscale factorization approach from Ortoleva and the introduction of deterministic sampling measures to ameliorate the exponential scaling problem of quantum dynamics from Iyengar at IU Chemistry. Such methodologies have great promise for addressing the computational challenges listed above by introducing novel algorithms which scale optimally on distributed and shared memory architectures. Dr. Iyengrar will lead the computation science application efforts.

Dan T. Dawson, Assistant Professor, Department of Earth, Atmospheric, and Planetary Sciences, Purdue University
Dan Dawson is an Assistant Professor at Purdue University affiliated with Clouds, Climate and Extreme Weather Research. His research interests include numerical prediction of severe convective storms and tornadoes, severe thunderstorm and tornado dynamics, cloud and precipitation microphysics, storm-scale EnKF radar data assimilation, and disdrometer and polarimetric radar observations. He has been the recipient of an NSF Postdoctoral Research Fellowship, is a member of the American Meteorological Society (AMS), and serves as Associate Editor of the AMS peer-reviewed journal *Monthly Weather Review*. Dr. Dawson has over a decade of experience with large-scale numerical weather simulations on shared- and distributed-memory architectures, and will lead the numerical meteorology (tornadoes) application.

Tony Armstrong, President and CEO, IU RTC and Associate Vice President for Engagement
Tony Armstrong supports our proposed grand challenge in a dual role reflective of his position of President and CEO of IU RTC and his appointment with OVPE.

IU RTC will be an important component of the proposed Grand Challenge from early on through the duration of the project. In the early stages IU RTC will help to broaden, and should the need arise, to establish partnership, and to formalize them by putting agreements in place (in conjunction with ORA). As the projects progress, IU RTC will secure proper treatment of IP, for example, patent applications, and handle commercialization, either by licensing or launching start-ups, as appropriate.

Additionally, Tony Armstrong will serve as a point of contact with the Office of Vice President for Engagement. The Office of Engagement serves as a gateway to the assets and expertise at Indiana University. By close collaboration with this office, our grand challenges efforts will be accessible to additional partners outside of Indiana University.

Craig Stewart, Associate Dean, RT UITS
Dr. Craig Stewart leads the Research Technologies division of University Information Technology Services (UITS), which serves IU's research and scholarship missions through computation, storage, and visualization facilities and support. UITS will play important roles in deployment and product management.

UITS will contribute to our efforts by operation of a cluster equipped with FPGAs for development purposes A modest cluster equipped with a high speed interconnect, current generation processors, and FPGAs is essential to the effective prosecution of the environment and application development plan. A dedicated cluster is required for proper (and publishable) performance tests. In addition, a cluster dedicated to HPX activities will foster and encourage development of applications that run with the benefit of this advanced computing environment.

Additionally, UITS will provide staff assistance for math library porting, specifically the BLAS Sparse linear algebra routines. The focus is on the BLAS partly because it is fundamental to other libraries, and partly because is has been so widely and effectively ported and optimized.

Moreover, UITS will deliver packaging, documentation, and application support such as: reading, tightening, and as needed commenting source code, writing documentation on installing and using software, and editing software installation routines. To aid in dissemination of our research results, UITS will be working with application scientists to encourage adoption of HPX, including proactively rewriting applications and doing performance tests.

Other collaborating faculty

Peter Ortoleva, Distinguished Professor of Chemistry, Department of Chemistry, IU Bloomington, nanoscience and bioanalytical data

Judy Qiu, Assistant Professor of Computer Science and Informatics, School of Informatics and Computing, IU Bloomington, data-intensive computing and life science applications

Krishnan Raghavachari, Professor of Chemistry, Department of Chemistry, IU Bloomington, computational quantum chemistry

Jeremy Siek, Associate Professor, School of Informatics and Computing, IU Bloomington, programming and programming languages

Martin Swany, Professor of Computer Science, School of Informatics and Computing, IU Bloomington, high-performance computing and networking