

January 2006 DDDAS Workshop Report

Introduction

“DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process.”

The DDDAS paradigm provides a vision that has novel intellectual focus and broad impact. Through the recent (FY05) DDDAS program solicitation (www.cise.nsf.gov/dddas) and the preceding seeding DDDAS efforts, primarily through the NSF sponsored Workshop in 2000 and the ITR (Information Technology Research Program, FY00-04), the technical community has begun to explore and realize the promise of DDDAS. The DDDAS solicitation provides the venue for systematic support of research and technology development that is needed to enable dynamic integration of computation and measurement capabilities. The solicitation articulates the DDDAS concept, its beneficial impact to many research and technology areas, the research and technology advances that can be enabled by DDDAS and those that are needed to enable DDDAS, the need for synergistic multidisciplinary work among several research and technology communities, and the opportunities of collaboration among multiple sectors: academia, industry, national laboratories, US government agencies, and international partners.

The ensuing DDDAS community that is being established brings together considerable skill and leadership. However, continued leadership in this program and full impact of these projects will depend critically on continued growth and expansion of these kinds multidisciplinary projects and collaborations, sustenance of existing newly developed communities, and further support and nurturing the expertise and expansion of emergent communities.

The Dynamic Data Driven Application System (DDDAS) program funds multi-disciplinary research to build applications, algorithms, measurement processes, and software components from which diverse computational environments can be developed on demand, by combining such components to solve problems of national and international interests. DDDAS fosters synergistically the knowledge and technology advancements that need to be made. The DDDAS program is enabling the emergence of a vibrant community from disciplines as diverse as natural and applied sciences, engineering and medicine, as well as economic, social and behavioral sciences, and liberal arts, all forming collaborations to address an ever-increasing breadth and depth of problem classes and approaches. The value of this synergism and diversity is that new computational and measurement methods, and corresponding environments, are being developed and deployed, which are not only breaking down discipline boundaries, but are enabling solutions and insights to problem classes that were previously unexplored, reaching broader research communities not previously involved in computational techniques benefiting from the DDDAS concept. The resulting advancements in capabilities and frameworks in addition to software repositories of applications and other software components are of great interest to industry and mission agencies, as well as international partners.

“...The value of this synergism and diversity is that new computational and measurement methods, and corresponding environments, are being developed and deployed, which are not only breaking down discipline boundaries, but are enabling solutions and insights to problem classes that were previously unexplored. ...”

The projects that were launched through the recent (FY05) DDDAS competition, and prior to that with DDDAS projects spawned through the broad NSF ITR program (FY2000-2004) include many areas of National and International priority, and span synergistic advances in four key technology frontiers: Applications, Systems Software, Mathematical and Statistical Algorithms, and Measurement Systems, and driven by aimed at enabling and applying the DDDAS concept.

The DDDAS research community is actively advancing the frontiers, developing a diverse set of technologies that involve: modeling of physical systems; engineering systems design, management and control; biological systems; environmental fluid mechanics; intense weather events identification and path prediction; near real-time assessment of critical events; image based analytics; spatial optimization models; agent based modeling; problem solving environments; identification of anomalous

Representative DDDAS Technology Areas

Fostering and nurturing research and technical communities to develop DDDAS capabilities begun a few years ago with the NSF DDDAS March 2000 Workshop (www.cise.nsf/dddas), and continued by seeding efforts on DDDAS through NSF's ITR program, and presently more systematically through the recent DDDAS program solicitation. Through these initial efforts, a wealth of new multidisciplinary research advances, as well as novel approaches and methods have begun to emerge, that push the boundaries of current technologies to enable DDDAS capabilities. While all these projects cover a wide scope of areas and technologies, many of the projects that have started have common and/or complementary approaches in enabling adaptivity of computations under dynamic data inputs or dynamic steering of the measurement process. The projects launched comprehensively integrate research in applications, systems, algorithms, and measurement, and involve multiple discipline domains within a single project. The areas these projects span are as diverse as the traditional science and engineering areas, as well as emerging areas like environmental modeling, biological systems, health and medical systems, and business, as well as social sciences and humanities.

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DDDAS research, complimented by other science and engineering domains in areas such as collaboratories, workflow management, computational modeling, software engineering, and data management, is clearly relevant to issues of important technological priority areas. However, in addition, there exist several unique aspects of the DDDAS community, that are *not* present in specialized domains that enable new capabilities of broad impact. Specifically, the broad range of computational challenges and real-time data requirements force new levels of research and development, and additionally inspire creativity and new opportunity in many fields, thereby revolutionizing research and development. Real-time data streaming and steering, data validation, extraction, and federation, decision-based (re)-sampling, data provenance tracking, and mechanisms to support data fusion and model creation and use, are particularly relevant and are areas where this community may drive DDDAS requirements and standards. Critical research and development areas that have the potential of involving experiments drawing data from instruments and/or thousands to millions of sensors and high-throughput data-streaming, are leading-edge drivers for new DDDAS capabilities.

In the following subsections (A-D) are challenges, opportunities, advances and impact within the representative DDDAS areas are discussed.

A. Applications

Many key research areas are being pursued within the scope of DDDAS supported projects that address National and International priorities, and with the notion of establishing leadership in multidisciplinary research going beyond the scope of existing programs. As exemplified within this document, and further in the Appendix, such examples span the disciplines of physical sciences, engineering, geo-sciences, bio- and medical sciences, social and economic sciences, and in a wide range of areas in: natural disaster and hazard prevention, mitigation and response; critical infrastructure systems and future capabilities; air, water and ground transportation of human and goods; energy and the environment, reliable/cost effective health care systems and support for large scale health issues; enterprise-wide decision making, next generation software methods and systems for computing, communications and data management.

“leadership in multidisciplinary research going beyond the scope of existing programs”

“...individual research programs and disciplines, acting in isolation, do not have the capacity to pursue the needed multidisciplinary research” driven by the DDDAS focus...”

A view that was been widely expressed by the participants of the 2006 Workshop is that individual research programs and disciplines, acting in isolation, do not have the capacity to pursue the needed multidisciplinary research driven by the DDDAS focus, with the level of capability and relevance attainable by the DDDAS program. Implicit in the DDDAS projects is the high level of coordinated integration across several disciplines needed to perform the synergistically directed research. For example, complex issues involving experimentation, real-time measurement, data handling, pre- and post-processing, real-time data streaming, model development

and refinement, measurement refocusing, visualization and knowledge generation can be addressed comprehensively within the rubric of DDDAS.

In the following, some specific examples are presented to motivate and convey the kinds of requirements, challenges and capabilities developed within the scope of the funded DDDAS projects.

“the project illustrates the kind of synergistic research and technology advances that are needed for accurate and timely predictions of... the actual events that occurred ...”

A project (*General DDDAS Framework with Coast and Environment Modeling Applications*) funded under the recent DDDAS solicitation, deals with environmental situations such as those that occurred with the recent Katrina hurricane and its effects therein. The scope of this project illustrates many of the challenges that arise when applying and enabling DDDAS capabilities. Additionally, the project illustrates the kind of synergistic research and technology advances that are needed for accurate and timely predictions of the course of the hurricane, the water surge, the resulting toppling of the levees. In some ways, the actual events that occurred as a consequence of Katrina had been speculated. However, because of the inaccuracies of the traditional modeling approaches, the power of definite and concrete predictions was lacking, with an ensuing strategy of “wait and see” that was adopted, with respect to the evacuation of the population, followed by “ad-hoc” emergency response afterwards, with the disastrous consequences that ensued. Traditional methods that employ models driven only by static input data in isolation, are completely inadequate for providing realistic, real-time forecasts, essential for complex phenomena analysis, and, in this specific example, for decision making and response to the subsequent actual emergency.

“... powerful new methods for more accurate analysis and decision support systems, which can be deployed to accurately predict the onset of such critical events and guide decision making ...”

This example and other critical events such as tornadic events, coastal oil spills, contaminant transport in the atmosphere, are application areas that are studied in projects investigated/pursued under the DDDAS rubric. The dynamic modeling capability enabled with the DDDAS concept, is able to provide powerful new methods for more accurate analysis and decision support systems, which can be deployed to accurately predict the onset of such critical events and guide decision making in taking appropriate mitigation actions. In the funded project, which is dealing with events such as Katrina, the hurricane is continually monitored by: radar, satellites, aircraft, as well as other sensors, all of which provide rich and continuous streams of data. This project develops capabilities so that such data are dynamically fed into sophisticated simulation codes (that have been developed to model and forecast the intensity, wind speed, etc.) in order to more accurately predict the projected paths of the storms themselves, their interaction with the oceans underneath, the developing storm surge that ensues, the waves that develop, the interaction of surge and waves with the wetlands and rivers, stresses on levees and other structural analysis aspects, and floods that may develop. Each simulation code uses the dynamically input data to resolve unique and specific features at very different scales, involving different physical processes, and so on. In the DDDAS funded project application-modeling methods and systems software are developed to enable combining these data streams and simulation codes in a comprehensive and dynamic way, thereby enabling to adaptively refine forecasts, invoke appropriate algorithms needed if the hurricane is projected to pass over different types of terrain, or to request, additional data, to refine the simulations or to incorporate in the simulation new or modified data streams as the storm is forecasted to move over different locations.

“...project encompasses synergistic research in all areas critical to DDDAS: applications, systems, software, measurement, and algorithms ...”

Such a project encompasses synergistic research in all areas critical to DDDAS: applications, systems, software, measurement, and algorithms. For example algorithms are developed to distill voluminous data streams into appropriate dynamic inputs to the simulation codes, ability to dynamically invoke the appropriate simulation models, request and discover appropriate computational and other resources on which can accommodate the varying computational requirements based on the streamed data, or to execute appropriate ensembles of models. Other capabilities needed are ability to preempt nonessential jobs executing on critical resources; assemble the results from the various models and compare it with ongoing and up-to-date observations. Based on this information, the best performing models can be updated with new conditions, and the cycle is repeated, in a dynamic

control loop between the on-line acquired (or archival) measurements and the executing simulations. Simultaneously, output from storm tracking models can be fed into storm surge models, which in turn can be fed into wave models, and subsequently to local levee and flooding models. Each of these models execute on different time and length scales, contain different physical aspects of the system, and involve different mathematical algorithms and error properties. Based on the analysis and predictions from the ensemble of models, sensors and other instruments can be steered to acquire more accurate and relevant real-time data that are streamed back to appropriate applications to further improve the accuracy of the predictions. Such information, provided by a fully developed DDDAS process, can then be fed directly to emergency response agencies, providing a valuable tool for determining where and how to respond, which areas to evacuate, which highways to open or close, or where to place supplies or station red cross workers.

As shown in the list of the supported projects, the scope includes a wealth of many other projects dealing with physical systems, and additional examples are elaborated-on in the other subsection.

“Eventually the suite of the technologies developed under these projects can be put together to enable end-to-end, prediction, impact, response and mitigation for critical events.”

In addition, other projects funded under the DDDAS umbrella deal with process planning management, critical infrastructure, emergency response and emergency medical services (e.g. *Synthetic Environment for Continuous Experimentation*,; *Hourglass: An Infrastructure for Sensor Networks*; *Dynamic, Simulation-Based Management of Surface Transportation Systems*; *Dynamic Real-Time Order Promising and Fulfillment for Global Make-to-Order Supply Chains*; *A Data Driven Environment for Multi-physics Applications*; *Data Dynamic Simulation for Disaster Management (Fire Propagation)*; *Building Structural Integrity*; *An Adaptive Cyberinfrastructure for Threat Management in Urban Water Distribution Systems*). These projects are motivated through different application areas. However the capabilities and inputs developed in these kinds of projects are relevant to decision support systems such as for emergency response and mitigation, and as such they can also be deployed for events like Katrina. Eventually the suite of the technologies developed under these projects can be put together to enable end-to-end, prediction, impact, response and mitigation for critical events, like natural and man-made disasters.

“... new methods and technological infrastructure, including a prototype disaster response test bed which combines an actual evolving crisis event in-tandem with a simulation framework where the on-going event data are continually and dynamically integrated with the on-line simulations. Agent-Based Modeling and Simulations approaches are a core approach for these kinds of simulations..... ”

For example, the project (*Synthetic Environment for Continuous Experimentation*) develops new methods and technological infrastructure, including a prototype disaster response test bed which combines an actual evolving crisis event in-tandem with a simulation framework where the on-going event data are continually and dynamically integrated with the on-line simulations. In eventually deploying such systems will provide the ability for decision support and crisis management of real situations as well as more effective training of first-responders. The computational aspects of the framework developed under this project are built using peer-reviewed published models, driven and validated by real world data. The framework encompasses data and models from public domain, such as Census data, GIS data (street networks, buildings, topography, surrounding farm lands, etc.) from geospatial databases, fire-models, models for blast-explosives-impact dynamics and structural failure, models of building structures under stress, and models of wind and other environmental influences, models for radiological transport and health-economic consequence risk assessments. Real-time sensor data, video streams, and human inputs from the actual or exercise scenarios can be bridged to the virtual environment. Agent-based emergency response simulations can dynamically invoke models, such as the above, to represent a given scenario and also they encompass agent modeling of model human behavior including cultural and other region (or sector) specific characteristics. All this information and data - real-time, historical, and computed/synthetic - may be transmitted to first responders, local, state, and federal government agencies, industry, non-governmental organizations, citizens, and the media coordinate a comprehensive plan for responding to the crises, minimizing this event's impact, and assisting in the recovery from a crisis event.

Furthermore such approaches have relevance to other areas. *Agent-Based Modeling and Simulations (ABMS)* approaches which are a core approach in the above

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referenced example, are well suited for social science objectives such as how interactions among multiple individual entities generate macro-level outcomes, in ways discussed hereby. ABMS is the computational study of complex systems comprising multiple interacting agents. The agents are software entities whose behavior is determined in part by internal rules and in part by external forces. The agents can represent any persistent real-world entities. For example, agents might represent people (consumers, producers, voters), social groupings (firms, families, communities, nations), institutions (legal systems, governments), biological entities (crops, forests), or physical entities (highway systems, transmission grids, or weather). ABM could potentially embody DDAS principles in two respects, "in the small" and "in the large." First, agents in ABM social science applications can be configured to have cognitive capabilities enabling learning based on internal deliberations and external observations. Such agents are effectively DDAS agents "in the small," in the sense that they can deliberately change their measurement and observation modes on the basis of new information received. Any ABM application incorporating such cognitive agents is intrinsically a DDAS. Second, an ABM agent can be configured with the particular attributes and behavioral methods of a real-world referent. (For example, an ABM stock trader can embody the trading strategies of an actual stock trader as determined by empirical or laboratory observations; and an ABM stock market can be designed to embody the salient features of an actual stock market.) The ABM agent then becomes, in effect, the virtual embodiment of this real-world referent. Alternatively, the real-world referent can literally replace the ABM agent through an appropriately designed graphical user interface, thus permitting this real-world referent to act within the virtual world as the world develops over time. These ABM capabilities thus permit data streaming within an ABM application through either the virtual or literal embodiment of real-world processes. The connection with DDAS "in the large" arises if these ABM capabilities are used in support of an *Iterative Participatory Modeling (IPM)* process, thus permitting the form of this data streaming to adapt over time. This process involves the repeated looping through four stages of analysis: Field study and data collection; role-playing games; agent-based model development; and intensive computational experiments. "Role playing games" refers precisely to the two kinds of data streaming previously outlined: application stakeholders can participate in the design of their modeled counterparts; and application stakeholders can participate actively and dynamically in model simulations through immersion by means of an appropriately designed graphical user interface. The repeated looping aspect of IPM then helps to ensure that input from both application stakeholders and researchers will be used in iterative and interactive fashion to revise the data-collection process as well as the form of the model.

“...funded projects ... which originated independently, have a number of common research technology areas... in application models involved, ... in application composition technologies, in data management, in systems software, in user interfaces systems... “

The two examples of funded projects that are elaborated above and which originated independently, have a number of common research technology areas; for example in application models involved, but also in application composition technologies, in data management, in systems software, in user interfaces systems. Furthermore the capabilities developed can be deployed in tandem thus increasing the impact of the work developed in the individual projects. This last aspect is also the case for many other projects, and the workshop provided opportunity for such discussions to commence among various researchers.

Supporting the runtime of such dynamically invoked computations requires advanced systems software that seamlessly integrates heterogeneous platforms: from the real-time data acquisition, and data mining of archival data, to computational grids and other high-end and low-end workstations, to hand-held end-user devices. Runtime technologies needed range from optimized partitioning and mapping of the various component models of the application, depending on the underlying platforms and other resources (like bandwidth, storage, etc), data processing, transfer and management systems, and software frameworks that coherently support such complex environments. More details on the challenges, opportunities, and research efforts pursued under the presently launched projects are discussed in a subsequent subsection. While the discussion above was centered in the two examples of projects, many of the projects mentioned in the beginning of this section and other projects pursue similar frameworks.

"...DDDAS... .. goes beyond the previous approaches... DDDAS concept is more general and extends well beyond methods such as data assimilation "

DDDAS represents an important nexus between models and data. The dynamic interaction between measurements and application models, with the objective on one hand of making the application modeling processes more accurate, and on the other hand, making the measurement process more effective, goes beyond the previous approaches. For example, the DDDAS concept is more general and extends well beyond methods such as data assimilation, which have been around for some time. DDDAS can be applied in a number of important ways in modeling, and one of the compelling features of DDDAS is that it provides an effective and systematic means of dynamically incorporating data into the executing simulation. In addition the measurement steering component is a key aspect of DDDAS and a major advance in measurement methods and in data management. The data measurement steering component is a unique feature of DDDAS systems and further research and technology development is required to enable such capabilities.

"...Instruments, sensors, databases, human inputs and other devices for taking measurements; data quality assessment, data formatting, and feature extraction; and data measurement steering. In DDDAS environments these ... are ... linked with numerous feedback loops,.."

The measurement system consists of several components: Instruments, sensors, databases, human inputs and other devices for taking measurements; data quality assessment, data formatting, and feature extraction; and data measurement steering. In DDDAS environments these components are all closely linked with numerous feedback loops, and they are all strongly impacted by the underlying application, system software, and algorithms. In DDDAS environments, data challenges will be driven by the need for the capability to perform dynamic data measurement as well as dynamic data inputs to models, and ability to incorporate measurement data from completely new data sources. Important issues to address in such systems include: on-demand data collection and management, data streaming into the simulation, data representation, data models and congruence of data, real-time constraints, data processing/preprocessing, data collection rates, consumption rates, available bandwidths and other resources and how to discover, obtain, establish the authenticity and correctness and how to maintain an audit trail.

"...basic enhancements in the design, efficiency and sensitivity of measurement instrumentation as a result of technology or a result of the learning process of the DDDAS functioning system, are continually sought..."

The measurement devices collect raw data from a variety of sources. Because of the nature of measurement instrumentation, unexpected failures due to mechanical problems or human intervention are possible. Likewise, basic enhancements in the design, efficiency and sensitivity of measurement instrumentation as a result of technology or a result of the learning process of the DDDAS functioning system, are continually sought. One primary area concerns issues of power. If the measurement device runs on battery, for example, limitations such as battery lifetime, bandwidth, battery draw as a function of load, and reliable function in extreme conditions, are all targets of errors, uncertainties in measurements, and/or failure. Overall cost of the measurement device can also become an issue depending on the nature of the device, and the number and density required.

The next component of the measurement system is central to the state of the raw data that is collected directly from a measurement device. While the data could in principle be of the correct form for modeling, in many cases, due to a variety of experimental limitations and established collection procedures, some pre-processing may be necessary. Several data conditions need to be considered here, including:

- Uniformity: data collections from different instruments will show variances.
- Format: collections taken across different instrument types can range in format and units.
- Noise: percentage of noise in data collections can vary across measurement devices.
- Time stamps: relevance tags and error bars need to be associated with measured data.
- Failure: diagnostics must be in place to establish instrument/measurement failures.

The measurement steering strategy must be tailored to both the application and the measurements available, which can be categorized as static, dynamic, and adaptive control of instruments and sensor networks. For static networks, for example sensing steering can be used to change key sensor properties to trade off the rate that the environment is observed by a network of sensors vs. the power consumed

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(*Dynamic Sensor Networks - Enabling the Measurement, Modeling, and Prediction of Biophysical Change in a Landscape*); and the direction that distributed arrays of telescopes are pointed to track transient astrophysical sources (*Real-Time Astronomy with a Rapid-Response Telescope Grid*); or the phased radar arrays can be steered by the executing simulation model to monitor specific aspects and areas tornadic activity. Mobile sensor platforms linked by communication networks can be used to change the location and temporal/length scales over which measurements are taken. The DDDAS framework enables observational probes (stationary and mobile) such as UAVs, AUVs, and buoys, to form self-organizing reactive observing systems that enable distributed on-demand sensing (several projects have started addressing such issues). Examples include using the DDDAS framework to (1) tighten the coupling between the weather forecasting and the design of the aircraft sensor flight plans by reducing the timescales and embedding the data-driven decision making onboard the vehicles (*Coordinated Control of Multiple Mobile Observing Platforms for Weather Forecast Improvement*); (2) actively deploy a combination of fixed and floating sensors to rapidly identify micro-organisms to predict the onset of algal blooms (*A Generic Multi-scale Modeling Framework for Reactive Observing Systems*); and (3) direct the measurements from AUVs to more accurately predict the ocean state and uncertainties in real-time (*Multiscale Data-Driven POD-Based Prediction of the Ocean*). Adaptive networks can be used to change the types of measurements taken, such as in case of CCD-based imaging systems adaptively focus the analysis of a image to different regions depending on the camera CCD imaging substrate, or using adaptive optics to directly modify a mirror such as those deployed in today's state-of-the-art large astronomical telescopes, multicue tracking of objects with many degrees of freedom (*Stochastic Multicue Tracking of Objects with Many Degrees of Freedom*). DDDAS enables new applications, such as updating (during surgery) 3D in-situ MRIs in real-time (*A Novel Grid Architecture Integrating Real-Time Data and Intervention During Image Guided Therapy*), and adaptively changing the measurement grid (NEXRAD and phased radar arrays) to track the severe local weather patterns over CONUS (*Linked Environments for Atmospheric Discovery (LEAD)*).

Measurement steering must determine what, where, and how to obtain the data; this is a real-time resource allocation problem, that also requires performing a cost/benefit analysis. Data collection steering must directly determine what data to collect from the available sources, which in turn requires the ability to assess the relative value of the measurements and information available. For complex large-scale systems, this can be a very indirect process because it is often difficult to determine what needs to be measured, and how to relate the information extracted from the available sensors to the system dynamics of interest; the dynamicity involved may require invoking appropriate models of how the sensors interact with the system. DDDAS extends the state of the art by tightly integrating the data requirements and the application-level models into this decision making process.

“...DDDAS can have major impact on the development and support of instrumentation infrastructure efforts, ...”

DDDAS can have major impact on the development and support of instrumentation infrastructure efforts, as for example the (*Dynamic Sensor Networks - Enabling the Measurement, Modeling, and Prediction of Biophysical Change in a Landscape*) project can provide insights on the proposed NEON infrastructure. Another new potential opportunity is in the context of the DANSE (Distributed Data Analysis for Neutron Scattering Experiments) neutron scattering facility providing measurement infrastructure to numerous communities, ranging from biological to basic physics and materials. Specifically for DANSE provides the infrastructure for neutron scattering research. This involves the production of neutron beams at large national facilities, while experiments are performed by small teams who bring their own samples to these facilities for a few days or weeks of beam-time. This research community spans from biology through basic physics, and includes numerous science subfields. From data acquisition through data analysis and identification of trends, computing is an important part of all this neutron scattering research, and advances in computing will elevate the level of science in neutron scattering research. This aspect has been recognized in setting-up the DANSE infrastructure. The underlying technology of DANSE is a runtime framework with interchangeable software components -- an architecture that is well suited for developing and implementing DDDAS applications.

Opportunities for DDDAS have been identified both in data acquisition and in data analysis. Most obvious are applications for real-time control of data acquisition, where data are used to optimize a physical model, and predictions of this model are used to tune neutron instrumentation or experimental parameters. Today this feedback is obtained after an experiment is complete, and an optimized measurement often occurs months, or even years later. For data analysis, many of the tasks in the DANSE project are based on optimizing physical models, and can benefit from DDDAS. Refinements of physical models based on experimental data are widely used today. The next step will be developments in the automated selection of optimizer packages, or data-driven selection of physical models that follow the emerging features in experimental data. Algorithms that perform computations on data streams would enable new DDDAS applications, and algorithms that identify features in the data need development as these features are used to steer computations. There are also needs to understand better the robustness of data-driven computations, and the best approaches for validation, verification, and certification by neutron facilities. Some of these issues are best addressed by prototyping DDDAS applications. The DANSE project is a fertile ground for application and runtime software systems that can benefit from DDDAS, in collaboration with the neutron-physics community and the neutron facilities. For the neutron scattering community, the time is right for testing DDDAS ideas and developing new concepts.

D. Systems Software

As demonstrated in the sections A-C above, the DDDAS paradigm is enabling a new generation of end-to-end multidisciplinary applications that are based on seamless aggregation of and dynamic interactions between computations, measurement systems and other data and computational resources. These environments include scientific and engineering simulations of complex physical phenomena that symbiotically and opportunistically combine computations, experiments, observations, and real-time data, and can provide important insights into complex physical, engineering, and process management systems, such as crisis management applications that use pervasive conventional and non-conventional information for crisis prevention and response, medical applications that use in-vivo and in-vitro sensors and actuators for patient treatment, and business applications that use anytime-anywhere information access to optimize profits.

To illustrate the systems software and the DDDAS software frameworks required and developed by several projects, we consider two example projects funded under the DDDAS rubric: the *Instrumented Oil-Field of the Future* and the *Dynamic Data-driven treatment of Cancer* projects.

The *Instrumented Oil-Field* project investigates data-driven efficient and robust control and management of diverse subsurface and near subsurface geo-systems. The specific goal of this project is to enable a new generation of data-driven strategies for subsurface characterization and reservoir management based on completing the symbiotic feedback loop between measured data and the computational models. These strategies can provide more efficient, cost-effective and environmentally safer production of oil reservoirs, which can result in enormous strategic and economic benefits. Accurate and timely characterization and manipulation of the hydrological and biogeochemical state of the subsurface is critical for a broad range of applications, including CO2 sequestration, contaminated site cleanup, bio-landfill optimization, aquifer management and fossil fuel production. The recent development of low cost, reliable, in situ hydrological, physical and geophysical sensors has resulted in densely instrumented field sites providing continuous streams of heterogeneous data. These have enabled continuously evolving quantitative estimates of subsurface properties and their uncertainty, and such estimates will provide the information needed for optimized oil field exploration, recovery and management, and such technologies can also find applicability in other areas, like making strategic decisions regarding increasing demands for clean water, energy supply and homeland security.

“... the DDDAS paradigm is enabling a new generation of end-to-end multidisciplinary applications ...”

“... enable a new generation of data-driven strategies for management based on completing the symbiotic feedback loop between measured data and the computational models...”

“...support dynamic assimilation of data and from varying numbers and classes of sensors... dynamically compose simulation components, ... dynamic composition ... involve metadata management schemes, ... semantic functional and performance oriented data service interfaces ... workflow scheduling and management schemes...”

“...unique requirements ... vertically integrated application domain knowledge-based software system as well as horizontal software technologies ...”

“... adaptive real time response (hard- or soft-, or both, ...)...Systems software ... needs to be able to address aspects of performance prediction, performance negotiation, and performance guarantees. system level quality of service guarantees...”

“...Application components need to be designed with “hooks” ... allow middleware to answer hypothetical questions about functionality and response time characteristics...”

The project investigating laser cancer treatment is similar in many ways. In that project online patient information, including MRIs and tissue data (tumor properties, cell damage data, HSP kinetic data, nano-shell data, etc.) are used along with finite elements models to predict temperature, HPS expression and cell damage, to form a distributed adaptive control system to manage pre-treatment planning, for dynamic real-time control during laser surgery and for post-treatment monitoring.

DDDAS applications frequently involve the dynamic choice of algorithms. Different physical, engineering, biological, economic or social science models may be employed and the ability to dynamically compose and couple different components is a common theme in DDDAS applications. Another related common theme is the need to support dynamic assimilation of data and from varying numbers and classes of sensors. The need for and ability to dynamically compose simulation components, to support dynamic choice between different simulation models and on-demand real-time sensor data assimilation requirements pose substantial systems software challenges. Approaches to dynamic composition are likely to involve metadata management schemes, development of schemes for supporting semantic functional and performance oriented data service interfaces along with workflow scheduling and management schemes.

DDDAS environments present unique requirements and core research challenges from the systems software perspective, as articulated in the solicitation. Further, these projects have already led to the development of a number of solutions, including vertically integrated application domain knowledge-based software system as well as horizontal software technologies that can support a broader class of DDDAS environments, and have started developing some the software technologies to enable and support such environments. Such challenges are articulated in the solicitation, and the following discussion puts them in the context of some of the funded efforts and outlines some of the technologies that are either pursued within the funded projects or were articulated by the current investigators as further research challenges and opportunities:

Application Driven DDDAS System Software Requirements: DDDAS applications pose a number of unique system software and middleware support requirements. These applications involve an element of adaptive real time response (hard- or soft-, or both, depending on the control task or application phase). Systems software (also referred to as Middleware) used to support DDDAS therefore needs to be able to address aspects of performance prediction, performance negotiation, and performance guarantees. Furthermore, DDDAS environments require system level quality of service guarantees. DDDAS applications typically require multiple computational inputs within sometimes predictable, and sometimes unpredictable, periods of time. The timescales differ from application to application, and possibly for different stages and tasks of a given application. For example, applications involving aerodynamic stabilization and neural control may require millisecond level responses while oil reservoir management may require responses in seconds, hours, days or weeks depending on the nature of the control task. In all of these cases, DDDAS software stacks need to be able to support predictable temporal response to such varying characteristics.

The need for predictable temporal response behavior has many implications on system software design. Application components need to be designed with “hooks” (sensors and actuators) that allow middleware to answer hypothetical questions about functionality and response time characteristics. For instance, an adaptive multipole-expansion or unstructured mesh -based application component might contain hooks that control the refinement factor, the refinement mechanisms, the problem partitioning granularity, or the partitioning strategy. An application that processes electrical system sensor data might have a hook that controls the choice of the dynamical system model used for modeling network transient characteristics.

System software middleware stacks need to be able to use predicted and measured application/system behaviors and response time characteristics to generate overall performance predictions and to make strategic decisions based on these estimates.

“...DDDAS system software stack should also incorporate application knowledge-based solutions that can enable domain-specific selections and adaptations...”

For example, a DDDAS application involving laser prostate surgery will need to carry out intra-operative estimates of temperature distribution. These estimates need to be available while surgery proceeds. Furthermore, the application may have several algorithms used to generate temperature distribution estimates. In addition, the algorithm runtime environment may depend on patient specific data as well as on current state of the computational environment. In this and many other cases a DDDAS application would dynamically choose an algorithm (or choose a parameter such as degree of mesh refinement) based on performance estimates. Finally, the DDDAS system software stack should also incorporate application knowledge-based solutions that can enable domain-specific selections and adaptations; for example knowledge-based systems of application models and application algorithms may be used to enable the dynamic (at runtime) selection of appropriate models and algorithms that are suitable to the available underlying computing, communications and data resources, and that will satisfy potential hard and soft real time constraints of the application requirements or the controlled measurement system.

“...Programming environments and runtime support systems ... support development of application components ... dynamically choose between different simulation models ... dynamically compose models....”

A complex system software stack consisting of middleware and application support components needs to have predictable temporal response characteristics. Programming models, runtime support and application development frameworks need to be constructed to allow support for accurate behavior and performance prediction and need to be constructed to allow programmers to develop, integrate and compose temporally predictable components. Programming environments and runtime support systems need to support development of application components that can interoperate in a manner that allows DDDAS applications to dynamically choose between different simulation models and to dynamically compose models. Composition and interoperability is challenging as models describing the same system may differ in time, and /or space-scales or in computational technique.

Programming models and abstractions need to be able to describe adaptation policy, sensing and actuating hooks and adaptation policies and constraints. While there are limited precedents for this in various communities (e.g. past work in data parallel compilers that support language constructs that allow choice of parameterized data-partitioners, frameworks for computational interactive monitoring and steering), the DDDAS requirements are much broader and more general than current high-performance and grid computing requirements. While efforts exist (e.g. NGS, CSR, NMI, referenced in the DDDAS solicitation), this state of the art needs to be pushed further. Current middleware/systems software cannot robustly support the dynamic requirements of DDDAS environments.

The need to dynamically compose applications as required in DDDAS environments, and to characterize behaviors and predict performance of complex system software and application components, will also drive the development of DDDAS metadata schemas. DDDAS applications will benefit from systematic methods of describing performance and functional information arising from middleware and application components. Descriptions of how function and performance related "hooks" are embedded in applications and manipulated by the system should also be standardized using appropriate metadata schemas.

“ ... research challenges that penetrate all the layers for the software systems stack...”

DDDAS environments are multidisciplinary and holistic, and are inherently complex, highly dynamic in their behaviors and interactions, involve uncertainty, and enforce time and space constraints on data and resource availability, data transport, computation, and data-driven response. Furthermore, the underlying Grid computing environment is similarly large, complex, heterogeneous and dynamic, globally aggregating large numbers of independent computing and communication resources, data stores and sensor networks. Together, these characteristics lead to unique requirements and associated research challenges that penetrate all the layers for the software systems stack from programming systems to system services and that are not adequately satisfied by existing solutions. Traditional models, technologies and software components have to be extended to address the unique end-to-end application-centric requirements of DDDAS application to allow them to access, assimilate, analyze and process and respond to dynamic data within

the ability to process large volume, high rate data from different sources including sensor systems, archives, other computations, instruments, etc. – the processing has to be dynamically scheduled at the sources, destinations, in-the-network or a combination of these; (2) the ability to deal with dynamic resource requirements and support dynamic allocations, scheduling, instantiation and deployments. (3) support for accessing and visualizing at runtime, computational, measured and sensed data using a variety of portals ranging from high end visualization system, to pervasive handheld devices; (4) support for handling system/application/data unreliability and uncertainty; (5) support for specifying, validating and enforcing adaptation and coupling policies including detecting and resolving conflicts; (6) support for detection of errors and instabilities (e.g., oscillations and infinite loops) and for end-to-end debugging to detect these behaviors.

*“ ... extend Grid services
...virtualize the integration of
multiple distributed Grids, ...
computational Grids, data
Grids, information Grids,
sensors Grids, instrument
Grids,...”*

System services: System services for DDDAS applications need to extend Grid services to virtualize the integration of multiple distributed Grids, including computational Grids, data Grids, information Grids, sensors Grids, instrument Grids, etc. These services include those that support immediate “just-in-time” dynamic resource co-allocation and co-scheduling, real-time event/data transport, data coupling, event/data logging, system wide time-synchronization, content based notification, communication and coordination mechanisms, element probing and monitoring, policy specification, evaluation and enforcement, specifying, evaluating and verifying quality and provenance of computation and data components, and dynamic time constrained security and trust.

*“ ... autonomic self-adapting
software stack ...”*

Funded DDDAS projects have proposed and implemented innovative system software architectures including both vertically integrated end-to-end environments as well as core crosscutting services. For example, the Instrumented Oil Field project has proposed an autonomic self-adapting software stack that includes a programming system for self-managing DDDAS applications, an autonomic Grid-based execution engine that supports self-optimizing, dynamically adaptive applications based on sophisticated numerical techniques, distributed data management services for real-time data access, exploration and coupling, and self-managing middleware services for seamless discovery, access, interactions and compositions of components, services and data on the Grid. Similarly, the (*Linked Environments for Atmospheric Discovery (LEAD)*) the (*Auto-Steered Information-Decision Processes for Electric System Asset Management*), the (*A Generic Multi-scale Modeling Framework for Reactive Observing Systems*) and other projects are developing similar layered service-oriented architecture frameworks with crosscutting Grid services at the lower layers and domain specific services at the higher levels.

Implications, Outreach and Outlook

The specific goals of the DDDAS program, as stated in the solicitation, are threefold:

- Advancement and propagation of the emerging field of dynamic data-driven applications system research,
- Training of a new generation of interdisciplinary specialists in DDDAS systems, and
- Broad outreach to other relevant sectors so as to create unique opportunities for the sharing of essential knowledge

*“... DDDAS approaches are a
novel pursuit both in
fundamental research and in
technology development...”*

In contrast to other research and development areas, DDDAS approaches are a novel pursuit both in fundamental research and in technology development. Standard simulation practices typically employ static notions of data infusion and relatively sequential processes, repeated when and if necessary for the scientific endeavor. DDDAS approaches, as illustrative in this document, demonstrate clear benefit over traditional approaches and provide the inspiration for new approaches to complex problems. In addition, many new communities would greatly benefit from DDDAS approaches. Pursuing multidisciplinary research and creating multidisciplinary projects, is a challenge; the setup, execution, and analysis involved in many computational arenas, in particular when they involve more than one

community to span multiple computational models and approaches, are still challenging. Furthermore, not all communities are at the same stages of development. The DDDAS community that has been established is a valuable resource. A target for the DDDAS community is thus to provide opportunity and links from established efforts towards these new communities.

“...because of the nature of the projects, ... spanning multiple scientific and engineering cultures and technical backgrounds ... offer the opportunity to engage more strongly with these communities within the research and development efforts offered by DDDAS”

As important are the many examples of the efforts that have begun, where diverse communities are being engaged and which, because of the nature of the projects, are spanning multiple scientific and engineering cultures and technical backgrounds. Issues of social and economic impact of advancing these technological capabilities, become relevant as a result and offer the opportunity to engage more strongly with these communities within the research and development efforts offered by DDDAS. Participants at the Workshop from the fields of Social, Behavioral and Economic Sciences, felt that some of what has been started in their related areas provide good initial venues to expanded on by more involvement of their communities and provided additional example areas where DDDAS applies, for example in financial modeling and in dynamic detection and risk analysis of bubble collapse in financial and real estate markets. Also a web-forum maintained by one of the participants for their community will link to the DDDAS websites for facilitating and increasing the awareness of their community (<http://www.econ.iastate.edu/tesfatsi/abmread.htm>).

“...The DDDAS community that has started to build-up has already established venues to broaden outreach ...”

Developments in dynamic data-driven applications, and the communities that derive from these developments, will have profound impact on the delivery and accessibility of infrastructure of education in this arena. As such, in addition to the scientific advances made in this field, the accelerated growth of this field warrants revolutionary changes in the way we train young scientists desiring expertise at these interfaces. The DDDAS community that has started to build-up has already established venues to broaden outreach to other application areas and research communities (e.g. DDDAS Workshop series – see below). In particular, the working group viewed it beneficial to expand through such venues, connections of knowledge and synergy resulting from linkages among disciplines that view the world from different perspectives, and the profound relevance to the teaching and learning of science. Training of new scientists in this capacity is certainly a central mission of the DDDAS efforts. This has the capacity to be accomplished by the unique environment that is being brought together because of the multi-disciplinary nature of the program, and the students (undergraduate, graduate, and postdoctoral levels) supported in the DDDAS funded projects. Additional support for educational activities maybe enabled through already well established education programs that NSF and other agencies offer, and most notably the Research Education for Undergraduates (REU) program (see in addition numbered items below), as well as with many new outreach efforts that are being established as part of individual DDDAS projects. By bringing together the experts known to this field, the end users of the emerging research and technology, the up-and-coming generations of users and developers, and the institutions of universities, non-profit institutes, and private industry that are coupled to the utilization of the research, the resulting DDDAS efforts will create virtual working teams tied together by the very information-technology communication fabric that we are currently seeing being built in this program.

A. Community Outreach

From these observations, it is clear that an important directive of the DDDAS program is the sharing of knowledge and technology components, which can in turn enable further extension and opportunity for other communities. The existing DDDAS community has created and planned several important mechanisms for such sharing.

“... community web site... software repository... testbeds....”

- Community web site is key to providing new opportunities enabled by the DDDAS program to the broader community, the DDDAS groups have established of a functional web presence for the combined DDDAS efforts, through an NSF website (www.cise.nsf.gov/dddas). In addition a community web site, www.dddas.org, has been established to meet the needs of

and co-scheduling of resources; (2) real-time and soft real-time requirements for data acquisition, transport, injection, integration, coupling and actuation; (3) need for varied qualities of service requirements that are only known at runtime; (4) requirements for interactive (human in the loop) monitoring and control, remote runtime pervasive access (via display walls, workstations, laptops, PDAs and cellphones), and end-to-end adaptation; (5) dynamically synthesizing, composing and instantiating components and workflows on-the-fly; (6) automatically negotiated allocations and co-scheduling and possible predictive/anticipatory co-scheduling; (6) run time (possibly via proxies) authentication authorization and delegation of credentials and trust; (7) system services for monitoring, logging and error detection and localization, and application debugging and optimization. Test beds will integrate community hardware resources, software components, data, data models and data synthesizers (e.g., sensor simulators and emulators), knowledge repositories, workloads and benchmarks. Test beds provide a special opportunity for interaction and collaborations with the NSF Office of Cyberinfrastructure as well as efforts in other agencies, which have established operational testing facilities (see also below JFCOM example) – opportunity to coordinate in providing such an infrastructure.

D. Impact to Cyberinfrastructure

Many more specialized, computationally oriented environments are being spawned through specific NSF programs and other initiatives (many mentioned in the DDDAS solicitation), such as research involving modeling, simulations, research and infrastructure efforts on instrumentation, and general development and deployment of integrated and practical grid architecture for computational research. Such initiatives have resulted in technologies that are highly complementary to the DDDAS efforts. Additional examples include developments in middleware technologies, dynamic workflow driven systems, coupling domain specific workflow for interoperations with computational software, general execution workflow, software engineering techniques, biomedical infrastructure capabilities, and standards-oriented scientific capabilities. Most notably, efforts (referenced in the DDDAS solicitation) such as the NSF-Next Generation Software Program (1998-2004) and the successor the Computer Systems Research Program (2005-todate), together with the related infrastructure program NSF-National Middleware Initiative (2001-todate), the NIH-NCRR, and the DOE-SciDAC, to name a few, all support research and technology development for integrated frameworks for accessing grid resources that support research exploration, workflow capture and replay, and a dynamic services oriented architecture, with standards protocols. These efforts are complementary, but not tautological to DDDAS, and can clearly be leveraged for key aspects of the DDDAS project arena. The ability to effectively couple with these other agencies creates a higher level of impact than *cannot* be realized within single disciplinary programs, and often can enable areas of research and development, which will *not* be realized within individual disciplinary programs. Most importantly, DDDAS can influence the kinds of Cyberinfrastructure (CI) that needs to be created, and in turn leverage the CI supported infrastructure for test beds for testing and validation of the DDDAS related technologies.

“ ... DDDAS can influence the kinds of Cyber infrastructure (CI) that needs to be created...”

“ ... The ability to effectively couple with these other agencies creates a higher level of impact than cannot be realized within single disciplinary programs, and often can enable areas of research and development, which will not be realized within individual disciplinary programs....”

It is the hope of the workshop participants that continued efforts in this area will significantly improve on the coupling and interoperability with added resources, and providing a natural evolution into dynamically configurable user interfaces essential for the DDDAS application areas. Such a coupled capability for interactively steered and adaptive resource connection enables real-time construction of creative workflow strategies that under current disciplinary programs cannot be realized and perhaps not even be envisioned. Such prototyping environments should encompass new interactive application spaces, with yet unseen capabilities. Recent advances in grid infrastructure enable the pioneering of additional computational capability, but clearly a lot of work remains to be done specifically to realize impact for the DDDAS type application spaces, and will hopefully be further enabled by many agency initiatives working together. We have “only begun to scratch the surface” of the full potential and in addressing the full set of challenges. Further and sustained efforts are required to answer important questions of National and International importance,

Testament of the possibilities for collaboration and ensuing benefits can be gleaned from the following specific example of technology transfer of an NSF funded effort under the DDDAS rubric, which is now being transitioned to DOD/JFCOM. The project, Synthetic Environment for Analysis and Simulation -SEAS, has been nurtured by NSF through an initial seeding effort (starting in 2000) through a collaborative program between CISE and ENG, and subsequently expanded (in 2003) through an ITR DDDAS related project (Synthetic Environment for Continuous Experimentation). These successive efforts have conducted research that has transitioned the derived technology to Simulex (a Purdue University spin-off company that markets SEAS); SEAS was subsequently transitioned to Joint Forces Command in 2004 to provide joint context for combatant command sponsored war gaming exercises. In addition, another DOD organization, JPEO-CBD, provided (in 2004) funding in a complementary way, that enables the modeling methods and framework developed under the NSF funded project to be used for modeling chemio contaminant crisis-management events. Furthermore the simulation models and simulation framework developed under the NSF initiated project are now influencing the JFCOM's Sentient World Simulation (SWS) initiative. SWS will be developed in collaboration with Simulex, Joint Futures Lab, Joint Interagency Coordination Group (JIACG), the OakRidge National Laboratory, and IBM.

The above scenario provides an excellent example of academic research impacting broader technology development involving industrial and mission agency's interests, as well as an example of the value that can be derived through collaboration among agencies and among multiple sectors.

Summary

"...will need sustained nurturing of the kind of the synergistic emphasis fostered under the DDDAS program"

"... DDDAS provides an approach for improvements over the shortcomings of the traditional methods..."

" ... The DDDAS community needs to reach a critical mass both in terms of numbers of investigators, and in terms of the depth, breadth and maturity of constituent technologies..."

Clearly, the first wave of DDDAS projects demonstrated the potential impact and advances enabled by the DDDAS concept for tightly coupled end-to-end systems that can integrate data collection, instrumentation control, and sensor steering with computational simulations in a strongly symbiotic way. These projects also illustrate that, despite impressive projects that have begun under the DDDAS rubric with emerging advances in simulation, systems software and instrumentation technology, many pieces that guarantee DDDAS-level end-to-end performance are still missing and will need sustained nurturing of the kind of offered by the synergistic emphasis fostered under the DDDAS program. The algorithmic and software infrastructure for uncertainty estimation, fast multi-physics simulations, stochastic and fuzzy systems simulations, design of observation strategies, integration of multimodal simulation and data sources with real-time performance are examples of open problems. Real-time performance of the individual algorithmic components often requires sacrifices on the model fidelity, and currently there are no mature strategies on how to compensate for this loss of fidelity; DDDAS provides an approach for improvements over the shortcomings of the traditional methods. Moreover, the two DDDAS components (applications/simulations and measurements) have different needs from a mathematical and statistical methodological point of view and thus, traditionally, have been addressed separately by distinct research communities. In contrast, with the type of multidisciplinary projects emphasized in this solicitation, it is essentially within the DDDAS framework that end-to-end algorithmic challenges are exposed and can be successively addressed through innovative evolution, refinement or hardening of current approaches, or through development of totally different algorithmic approaches.

Close interaction of practicing scientists and engineers with information technology developers, iterative approaches to development and deployment, and mechanisms to share best practices were all seen as important aspects of developing new "dynamic data-driven research" capabilities that meet the needs of a diverse community. Many key research areas with National and International priority within funding agencies, and are being pursued with the notion of establishing leadership in research and computation beyond existing programs. The DDDAS community needs to reach a critical mass both in terms of numbers of investigators, and in terms of the depth, breadth and maturity of constituent technologies. The previous solicitation

“ ... the present work will inspire new advances and even more research and technology development to bring these efforts to a robust production-, operational- level for widespread use...”

“... There are beneficial outcomes from expanding the established multi-agency collaboration ...”

“...The basis for ... expansion is included within the scope of the present solicitation, and should be sustained and upheld though follow-up DDDAS proposal calls ...”

helped broaden the community by bringing investigators from many academic disciplines together, and through the projects started many advances in new algorithms, software, and applications will be enabled. Based on current investigations and breakthroughs, there will be the need to fund additional projects and generations of DDDAS research, as well foster existing strong efforts. Successive generations of DDDAS research hold promise to enable the capabilities envisioned by the DDDAS concept.

The first DDDAS call played a crucial role in identifying and crystallizing the need for the integration of measurement-application for complex systems, and creating the kinds of multidisciplinary endeavors that are needed to enable the sought capabilities. The field however is in its infancy and there remains a long promising future ahead for basic research and development, which will serve to materialize the envisioned technologies into mature tools. Furthermore, in many cases the present work inspires new advances and even more research and technology development to bring these efforts to a robust production-, operational- level for widespread use. Therefore, for research and development activities that will build-upon and expand the scope of projects started with the first DDDAS solicitation and sustenance of those efforts, the sustained and increased commitment to the DDDAS solicitation is urgently required. Additional resources must be committed, not only to strengthen academic research, but to encourage collaborations with the industry. Industrial participation at an early stage will ensure identification of the most important potential problems, and warrant immediate economic and societal rewards from the DDDAS initiative. Moreover, additional research resources should continue, to expand support of education and training of the scientific community, and collaboration with international institutions. There are beneficial outcomes from expanding the established multi-agency collaboration, together with expanding support on additional critical application areas within the scope of the DDDAS framework. Additional benefits and increased impact will be enabled by additional projects created through follow-up proposal calls under the DDDAS solicitation. The basis for such expansion is included within the scope of the present solicitation, and should be sustained and upheld though follow-up DDDAS proposal calls.

