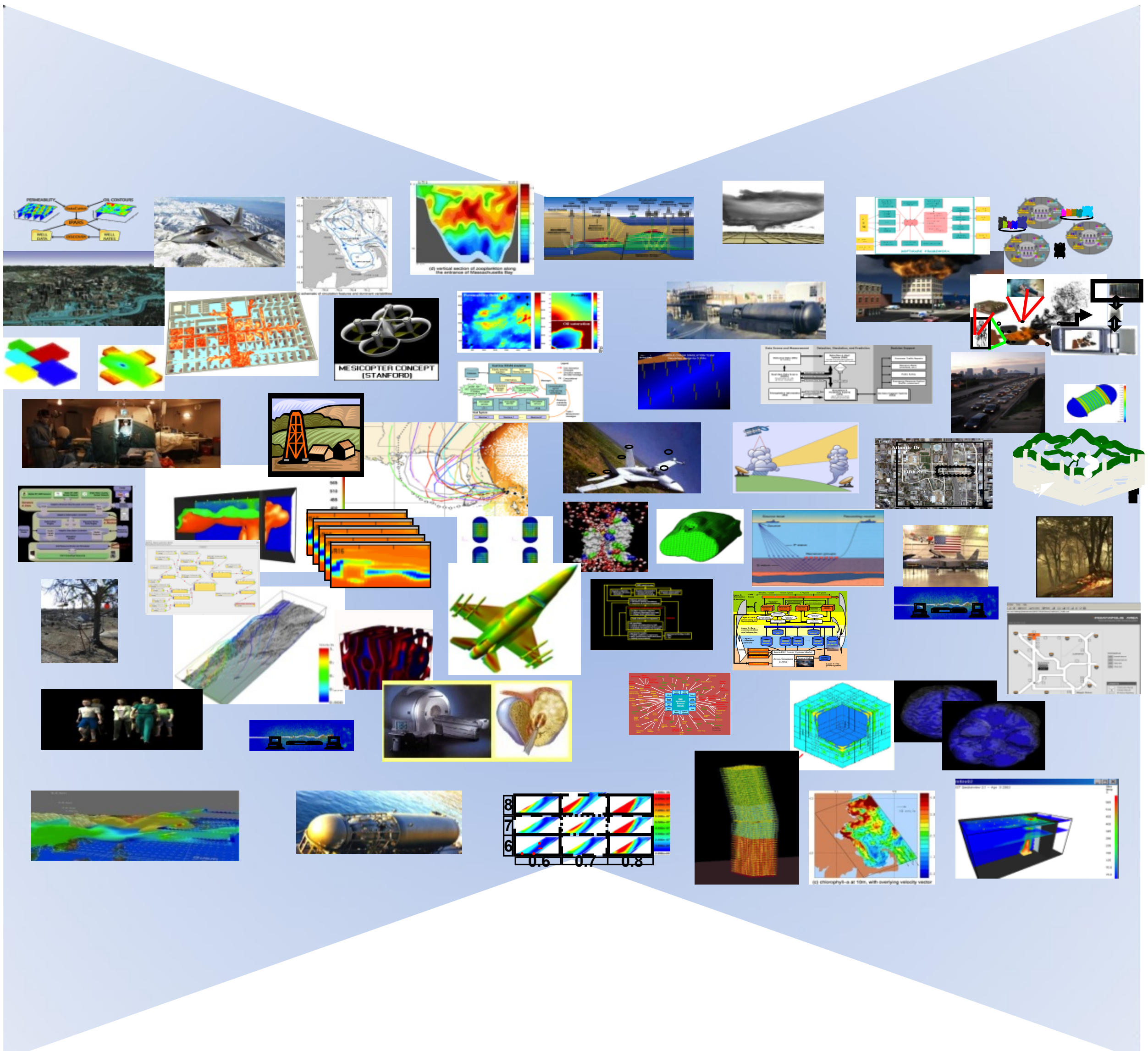
Report of the

August 2010 Multi-Agency Workshop on

InfoSymbiotics/DDDAS

The Power of Dynamic Data Driven Applications Systems



Workshop Sponsored by:
Air Force Office of Scientific Research
and
National Science Foundation

Workshop Co-Chairs

Craig Douglas, University of Wyoming

Abani Patra, University at Buffalo, SUNY

Principal Sponsoring Agency Liaisons

Frederica Darema, AFOSR

H. Edward Seidel, NSF

Working Group Leads

Gabrielle Allen, LSU; George Biros, Georgia Tech; Janice Coen, NCAR; Alok Chaturvedi, Purdue; Shantenu Jha, Rutgers; Bani Mallick, Texas A&M; Dinesh Manocha, NCSU; Adrian Sandhu, Virginia Tech; Srinidhi Varadarajan, Virginia Tech; Dongbin Xiu, Purdue

Workshop Award Contract Managers

Robert Bonneau, AFOSR

Manish Parashar, NSF

Cross-Agencies Committee

DOD/AFOSR:
F. Darema
R. Bonneau
F. Fahroo
K. Reinhardt
D. Stargel
DOD/ONR: Ralph Wachter
DOD/ARL/CIS: Ananthram Swami
DOD/DTRA: Kiki Ikossi

NASA: Michael Seablom

NSF:
H. E. Seidel (MPS)
J. Cherniavsky (EHR)
T. Henderson (CISE)
L. Jameson (MPS)
G. Maracas (ENG)
M. Parashar (OCI)

NIH:
Milt Corn (NLM),
Peter Lyster (NIGMS)

Acknowledgements

Gratefully acknowledge support by
the Air Force Office of Scientific Research under Contract no. FA9550-10-1-0477
and the National Science Foundation under Award number OCI-1057753*.*
Sincerely appreciate administrative support by the SUNY-Buffalo Center for Computational Research.

Report Editors

Frederica Darema, Craig Douglas, and Abani Patra

Executive Summary

InfoSymbioticSystems/InfoSymbiotics embody the power of the Dynamic Data Driven Applications Systems (DDDAS) paradigm, where data are dynamically integrated into an executing simulation to augment or complement the application model, and, where conversely the executing simulation steers the measurement (instrumentation and control) processes of the application system. In essence, the InfoSymbiotics/DDDAS control loop unifies complex computational models of a system with the real-time data-acquisition and control aspects of the system, and engenders transformative advances in computational modeling of applications and in instrumentation and control systems, and in particular those that represent dynamic, complex systems. Initial work on DDDAS has accomplished much towards demonstrating its potential and broad impact. The concept is recognized as key to important new capabilities, critical in many societal, commercial, and national and international priorities and initiatives, identified in important studies, blue ribbon-panels and other notable reports. The 2005 NSF Blue Ribbon Panel on Simulation Based Engineering Science characterized DDDAS as visionary and revolutionary concept. Recently published scientific and technological roadmaps such as the NSF CyberInfrastructure Framework for the 21st Century (CIF21) and the Air Force Technology Horizons 2010 Report highlight the need for advances requiring the integration of simulation, observation and actuation, as envisioned in the InfoSymbiotics/DDDAS concept. InfoSymbiotics/DDDAS has transitioned from being a concept to becoming an area, one may say a new field, driving future research and technology directions towards new capabilities. The present report outlines a research agenda, integrating the multidisciplinary research scope of DDDAS with opportunities motivated by the referenced roadmaps and recent technological advances, and transmits the research community's call for systematic support of such a research agenda.

A confluence of needs and recent technological advances render InfoSymbiotics/DDDAS approaches more opportune than ever. Systems of today and those foreseen in the future, be they natural, engineered or societal, will provide unprecedented opportunities for new capabilities, but with concomitant increased scales of complexity and interconnectivity. The ensuing "systems of systems", exhibit increased fragility where even small failures in a subset of any of the component systems have the potential of cascading effects across the entire set of systems. These new realities call for more advanced methods of systems analysis and management. The methods needed go beyond the static modeling and simulation methods of the past, to new methods, such as InfoSymbiotics/DDDAS which augment and enhance the system models through continually updated information from monitoring and control/feedback aspects of the system. Moreover, the need for autonomic capabilities and optimized management of dynamic and heterogeneous resources in complex systems makes ever more urgent the need for DDDAS approaches, not only at the design stage, but also for managing the operational cycle of such systems. Together with these driving needs of emerging systems, several technological and methodological advances over the last decade have produced added opportunities and impetus for DDDAS approaches. These include: multi-scale/multi-modal modeling; ubiquitous sensoring and networks of large collections of heterogeneous sensors and actuators; increased networking capabilities for streaming large data volumes; multicore-based transformational computational capabilities at the high-end, and the real-time data acquisition and control systems.

Capitalizing on the promise of the DDDAS concept and the successes of precedent initial research efforts, a multi-agency workshop, cosponsored by AFOSR and NSF, was convened on August 30-31, 2010, in Arlington VA, and attended by over 100 representatives from academia, industry and government, to address further opportunities that can be pursued and derived from InfoSymbiotics/DDDAS approaches and advances, and in the context of the changed landscape of underlying technologies and drivers referenced above. The scope of relevant efforts spans several dimensions, and requires multidisciplinary thinking and multidisciplinary research, for innovations in the entire hierarchy: from instrumentation for sensing and control, to the systems software, to the algorithms, to the applications built using them. The report identifies needs in each of these areas as well as critical science and technology challenges that must be met, and calls for synergistic research: • in *applications* (for new methods where simulations are dynamically integrated with real-time data acquisition and control, and where application models are dynamically invoked); • in *algorithms* (tolerant in their stability properties to perturbations from streamed data, and algorithmic methods for uncertainty quantification and for efficient estimation of error propagation across dynamically invoked application models; • in *systems software* supporting applications that exhibit dynamic execution requirements (where models of the application are dynamically invoked, and where the application computational load, across the high-end platform and the sensors or controllers side, shifts across these platforms, during execution-time, depending on the DDDAS application's dynamic requirements, and on resource availability); • in *instrumentation systems and "big-data" management* (dynamic, adaptive, optimized management of instruments and heterogeneous collections of networks of sensors and/or networked controllers); and • in *cyberinfrastructures* of unified computational and instrumentation platforms and their environments. These, are not only opportunities for highly innovative research advances, but also opportunities that can bridge academia and industry, inducing new and innovative directions in industry and developing a globally competitive workforce.

InfoSymbiotics/DDDAS is a well-defined concept, and a well-defined research agenda has been articulated through this and previous workshops and reports, and a multi-agency program solicitation in 2005. Advances made thus far through InfoSymbiotics/DDDAS add to this promise, albeit they have been achieved through limited and fragmented support. A diverse community of DDDAS researchers has been established over the years, drawing from multiple disciplines, and spanning academe, industry research and governmental laboratories, in the US and internationally. As was resoundingly expressed in the August 2010 Workshop, these research communities are highly energized, by the success thus far and by the wealth of ideas in confluence with other recent technological advances, all of which provide added stimulus for increasing research and development efforts around the DDDAS concept. All these, make timely a call for action for systematic support of research and technology development, necessary to nurture furthering knowledge, and bring these advances to the levels of maturity needed for enabling the transformative impact recognized as ensuing from InfoSymbiotics/DDDAS.

Report Outline

1. Introduction - InfoSymbiotics/DDDAS Systems

InfoSymbiotics/DDDAS is a paradigm in which on-line or archival data are used for updating an executing simulation and, conversely, the simulation steers the instrumentation process… … integration/unification of application simulation models with the real-time data-acquisition and control

InfoSymbioticSystems[1]/DDDAS embody the power of the Dynamic Data Driven Applications Systems (DDDAS) paradigm, where data are dynamically integrated into an executing simulation to augment or complement the application model, and, where conversely the executing simulation steers the measurement (instrumentation and control) processes of the application system. In essence, the DDDAS control loop unifies complex computational models of an application system with the real-time data-acquisition and control aspects of the application system. The core ideas of the vision engendered by the DDDAS concept have been well articulated and illustrated in two previous NSF Workshop Reports in 2000 and in 2006[1,2] as well as presentations and papers of research projects in a series of International DDDAS Workshops inaugurated in 2003 [3], and a 2005 multi-agency Program [4]. Initial work on DDDAS has accomplished much towards demonstrating the potential and broad impact of the DDDAS paradigm. A confluence of several technological and methodological advances in the last decade has produced added opportunities and impetus for integrating simulation with observation and actuation as envisioned in InfoSymbiotics/DDDAS, in ways that can transform many more areas where information systems touch-on, be it natural, engineered, societal, or other environments. Such advances include: the increasing emphasis in complex systems multi-scale/multi-modal modeling and algorithmic methods; the recent emphasis and advances towards ubiquitous sensoring and networks of large collections of heterogeneous sensors and actuators; the increase in networking capabilities for streaming large data volumes remotely; and the emerging multicore-based transformational computational capabilities at the high-end and the real-time data acquisition and control systems. All this changing landscape of underlying technologies makes it more than ever timely the impetus to increase research efforts around the InfoSymbiotics/DDDAS concept.

InfoSymbiotics/DDDAS … …visionary and revolutionary concept
– Prof. Tinsley Oden

… DDDAS key for objectives in Technology Horizons
– Prof. Werner Dahm (former AF Chief Scientist)

Starting with the NSF 2000 DDDAS Workshop and the resulting report [1], research efforts for enabling the DDDAS vision have commenced under governmental support, in the beginning as seeding-level projects, and later with a larger set of projects initiated through the 2005 multi-agency Program Solicitation. Under this initial support, research advances have been made, together with the increasing recognition of the power of the DDDAS concept. The 2005 NSF Blue Ribbon Panel [5] characterized DDDAS as visionary and revolutionary concept. A Workshop on DDDAS convened in 2006 produced a report [2] which in its comprehensive scope covers scientific and technical advances needed to enable DDDAS capabilities, presents progress made towards addressing such challenges, and provides a wealth of examples of application areas where DDDAS has started making impact. Building upon a 2007 CF21 NSF Report [6] and several more recent TaskForces [7], the recently enunciated vision of the National Science Foundation CyberInfrastructure for the 21st Century (CIF21 - NSF 2010)[8], lays out "*a revolutionary new approach to scientific discovery in which advanced computational facilities (e.g., data systems, computing hardware, high speed networks) and instruments (e.g., telescopes, sensor networks, sequencers) are coupled to the development of quantifiable models, algorithms, software and other tools and services to provide unique insights into complex problems in science and engineering."* The InfoSymbiotics/DDDAS paradigm is well aligned with and enhances the CIF21 vision. The more recent TaskForces ([7]), set-up

[1] The term *InfoSymbiotics* or *InfoSymbioticSystem*s is meant to be tautonymous to DDDAS and was introduced in recent years by F. Darema, as an alternative to the more mathematical term Dynamic Data Driven Applications Systems (DDDAS) she introduced in 2000. To be noted though that "DDDAS" has become "part of the vernacular" and we will continue to use it in this report, interchangeably, or together with the terms InfoSymbiotics and InfoSymbioticSystems (as InfoSymbiotics/DDDAS or InfoSymbioticSystems/DDDAS). DDDAS is said to be creating a new field of *unification* of traditionally distinct aspects of an application, namely unification of the application computational model (or simulation) with the measurement-data (instrumentation & control) components of the application system, that is: "*Unification of the High-End Computing with the Real-Time Data-Acquisition and Control*"; the term InfoSymbiotics is used to denote this new field.

by NSF, have reported-back with recommendations reinforcing the need for this thrust, as do "14 Grand Challenges" posed by the National Academies of Engineering [9]. In a similar if more targeted and futuristic vision, the recent Technology Horizons 2010 Report [10] developed under the leadership of Dr. Werner Dahm, as Chief Scientist of the Air Force, declares that "*Highly adaptable, autonomous systems that can make intelligent decisions about their battle space capabilities … making greater use of autonomous systems, reasoning and processes ...developing new ways of letting systems learn about their situations to decide how they can adapt to best meet the operator's intent"* are among the technologies that will transform the Air Force in the next 20 years. Dr. Dahm has specifically called-out DDDAS as key concept in many of the objectives set in Technology Horizons. Thus, InfoSymbiotics/DDDAS has transitioned from being a concept, to becoming an area, one may say a new field, driving future research and technology directions towards new capabilities. Therefore more than ever, it's now timely to increase the emphasis for research in the fundamentals and in technology development to create a well-developed body of knowledge around InfoSymbiotics/DDDAS as well as the ensuing new capabilities.

Thus, InfoSymbotics/DDDAS has transitioned from being a concept to becoming an area, one may say a new field, driving future research and technology directions towards new capabilities.

Capitalizing on the promise of the DDDAS concept and the precedent initial research efforts, on August 30-31, 2010, a multi-agency Workshop was convened to address further opportunities that can be pursued and derived from InfoSymbiotics/DDDASs approaches and advances. The Workshop, co-sponsored by the Air Force Office of Scientific Research and the National Science Foundation, was attended by over 100 representatives from academia, government and industry, and explored these issues. The Workshop opened with remarks by Dr. Werner Dahm, and Senior Leadership of the co-sponsoring agencies[14]. The remainder of the Workshop was organized into Plenary Presentations, Working Group Sessions, and out-briefs of the Working Groups [Appendix 0 – *Agenda*]. The plenary keynote presentations [14], by a distinguished set of speakers [Appendix1- *Bios of Keynotes*], addressed several key application areas, discussed the need and the impact of new capabilities enabled through DDDAS, and showcased progress that has been made in advancing fundamental knowledge and technologies contributing towards enabling DDDAS capabilities in important application areas. Prior to the workshop, a number of questions had been developed by the workshop co-chairs together with the working groups co-chairs and participating agencies program officials, and posed to the attendees [Appendix-2 – *List of Participants;* and Appendix-3 - *WG Charges*]. The working groups addressed these questions, as well as other topics brought-up during break-out and plenary discussions.

The main science and technology challenges discussed in the August2010 Workshop have also been well articulated in previous DDDAS workshops and their reports [1,2], as well as the 2005 DDDAS program solicitation. Therefore in the present report, discussions whose conclusions and recommendations have already been presented in the previous two reports are referred to synoptically here and the reader is referred to these previous documents for further details. The present report, in summarizing deliberations of the recent workshop, focuses on selected topics that are complementary to and add substantially to the previous reports in the context of recent advances and drivers. The 2nd Chapter of the present report provides a synopsis of the broad science and technology components that have also been identified in the previous reports and in the solicitation. In the 3rd Chapter are addressed key elements of new drivers and new opportunities, together with challenges and impacts in increasing synergistic research efforts on InfoSymbiotics/DDDAS. Subsequent chapters and subsections are organized around questions posed to the participants of the workshop, but addressing more specific issues related to more recent research directions and new opportunities, as they relate to InfoSymbiotics/DDDAS; specifically: a) applications modeling and algorithms, such as multiscale modeling, dynamic data assimilation, uncertainty quantification, b) ubiquitous data management, c) systems software for seamlessly integrated high-end with data acquisition and control systems taking advantage of emerging multicore processing directions, and d) the wealth of new CyberInfrastructure projects serving as laboratories and testbeds of a diverse set of science and engineering discovery efforts, and where InfoSymbiotics/DDDAS can have transformative impact.

2. InfoSymbioticSystems/DDDAS Multidisciplinary Research

The InfoSymbioticSystems/DDDAS paradigm engenders transformative advances in computational modeling of applications and in instrumentation and control systems (and in particular those that represent dynamic systems). Enabling DDDAS capabilities involves advances, through individual research efforts but mostly through synergistic multidisciplinary research, in four key science and technology frontiers: applications modeling, mathematical and statistical algorithms, systems software, and measurement (instrumentation and control) systems. Multidisciplinary thinking and multidisciplinary research are imperative, and specifically through synergistic and systematic collaborations among researchers in application domains, in mathematics and statistics, in computer sciences, as well as those involved in the design/implementation of measurement and control systems (instruments and instrumentation methods, and other sensors and embedded controllers). Cyberinfrastructure is the collective set of technologies spanning "*computing systems, data, information sources, networking, digitally enabled-sensors, instruments, virtual organizations, and observatories, along with interoperable suite of software services and tools*" [6]. InfoSymbiotics/DDDAS environments push these sets of technologies and their collective interoperability to new levels, and require architectural software frameworks, comprehensively representing the corresponding cyberinfrastructures, and at the same time require advanced testbeds that will allow experimentation on the new capabilities sought.

InfoSymbiotics/DDDAS requires synergistic, multidisciplinary thinking and multidisciplinary research along four science and technology frontiers: applications modeling, algorithms, computer and information sciences, and instrumentation systems

Challenges and opportunities for individual and multidisciplinary research, technology development, and software-hardware frameworks requisite for InfoSymbioticSystems/DDDAS-related Cyberinfrastructures are summarized below, along these four key frontiers:

- Applications modeling: In InfoSymbiotics/DDDAS implementations, an application/simulation must be able to accept data at execution time and be dynamically steered by such dynamic data inputs. The approach results into more accurate modeling and ability to speed-up the simulation (by augmenting and complementing the application model or replacing targeted parts of the computation by the measurement data), thus improving analysis and prediction capabilities of the application model and yielding decision support systems with the accuracy of full-scale simulations; in addition, application-driven instrumentation capabilities in DDDAS enable more efficient and effective instrumentation and control processes. This requires research advances in application models, including: methods that allow incorporating dynamic data inputs into the models, and augmenting and/or complementing computed data with actual data, or replacing parts of the computation with actual data in selected regions of the phase-space of the problem; models describing the application system at different levels of detail and modalities (multi-scale/multi-level, multi-modal modeling) and ability to dynamically invoke appropriate models as induced by data dynamically injected into the executing application; and interfaces of applications to measurements and other instrumentation systems. A key point is that DDDAS leads to an integration of (large-scale) simulation modeling with traditional controls systems methods, thus providing impetus for new directions to traditional controls approaches.
- Mathematical and Statistical Algorithms: InfoSymbiotics/DDDAS require algorithms with stable and robust convergence properties under perturbations induced by dynamic data inputs: algorithmic stability under

dynamic data injection/streaming; algorithmic tolerance to data perturbations; multiple scales and model reduction; enhanced asynchronous algorithms with stable convergence properties; uncertainty quantification and uncertainty propagation in the presence of multiscale, multimodal modeling, and in particular in cases where the multiple scales of models are invoked dynamically, and there is thus need for fast methods of uncertainty quantification and uncertainty propagation across these dynamically invoked models. Such aspects push to new levels the traditional challenges of computational mathematical and statistical approaches.

- Application Measurement Systems and Methods InfoSymbiotics require innovations in the entire hierarchy of instrumentation for sensing and data acquisition and control, systems software, algorithms and applications built using them. In each of these areas there are critical science and technology challenges that must be met, improvements in the means and methods for collecting data, focusing in a region of relevant measurements, controlling sampling rates, multiplexing, multisource information fusion, and determining the interconnectivity and overall architecture of these systems of heterogeneous and distributed sensor networks and/or networks of embedded controllers. Advances through InfoSymbioticSystems/DDDAS will create improvements and innovations in instrumentation platforms, and will create new instrumentation and control systems capabilities, including powerful methods for dynamic and adaptive utilization of resource monitoring and control, such as collections of large number of heterogeneous (networked) sets of sensors and/or controllers.
- Advances in Systems Software runtime support and infrastructures, to support the execution of applications whose computational resource requirements are adaptively dependent on dynamically changing data inputs, and include: adaptive mapping (and re-mapping) of applications (as their requirements and underlying resources change at execution time) through new capabilities, such as compiler-embedded-in-the-runtime (runtime-compiler) approaches; dynamic selection at runtime of application components embodying algorithms suitable for the kinds of solution approaches depending on the streamed data, and depending on the underlying resources, dynamic workflow driven systems, coupling domain specific workflow for interoperation with computational software, general execution workflow, and software engineering techniques. Software Infrastructures and other systems software (OS, data-management systems and other middleware) services to address the "real time" coupling of data and computations across a wide area heterogeneous dynamic resources and associated adaptations while ensuring application correctness and consistency, and satisfying time and policy constraints. Other capabilities needed include the ability to process large-volumes and high-rate data from different sources including sensor systems, archives, other computations, instruments, etc.; interfaces to physical devices (including sensor systems and actuators), and dynamic data management requirements. The systems software environments required are those that can support execution in dynamically integrated platforms ranging from the high-end to the real-time data acquisition and control - cross-systems integrated.

InfoSymbiotics/DDDAS Enables decision support systems with accuracy of full scale simulations…
… creates powerful methods for dynamic and adaptive utilization of resource monitoring and control, such as collections of large number of heterogeneous (networked) sets of sensors and/or controllers…

Research that has been conducted thus far has already started making progress in addressing a number of these challenges and across multiple domains as discussed above. Not only there is progress to be made along the traditional S-curve in each of these domains, but in essence there is need for coordinated progress across multiple S-curves. That is challenging indeed. However, based on fundamental knowledge advances made thus far, the recognition of the transformative capabilities of the DDDAS concept, and other emerging methodological and technological advances (discussed next), all these are fueling the interest to increase efforts and systematic support for InfoSymbiotics/DDDAS.

3. Timeliness for Fostering InfoSymbiotics/DDDAS Research

3.1 Scale/Complexity of Natural, Engineered and Societal Systems

Today not only such systems are becoming increasingly more complex, but also we deal with environments which involve "systems-of-systems", of multiple combined engineered systems, of engineered systems interacting with natural systems, engineered systems with humans-in-the-loop; such as for example are: all types of complex platforms, communication systems, wide-area manufacturing systems, large national infrastructure systems ("smart grids", such as electric power delivery systems), and threat and defense systems.

systems are becoming increasingly more complex…

…"systems-of-systems"…

…today's complex systems are InfoSymbiotics/DDDAS in nature

The increase in both complexity and degree of interconnectivity in such systems, provides unprecedented opportunities for new capabilities, and at the same time drives the need for more advanced methods for understanding, building, and managing such systems in autonomic ways. Furthermore, this complexity has added to the fragility of such systems. As the interconnectivity across multiple systems has increased tremendously, so has the impact of cascading effects across the entire set of systems, for even small failures in a subset of any of the component systems.

These new realities have led to the need for more adaptive analysis of systems, with methods that go beyond the static modeling and simulation methods of the past, to new methods, such as InfoSymbiotics/DDDAS, which augment and enhance the system models through continually updated information from monitoring and control/feedback aspects of the system. Moreover, the need for capabilities of optimized management of dynamic and heterogeneous resources in complex systems makes ever more urgent the need for DDDAS approaches, not only at the design stage, but also for managing the operational cycle of such systems.

This report takes the thesis that most of today's complex systems are InfoSymbiotics/DDDAS in nature. Preliminary efforts in DDDAS, such as those spawned through the comprehensive multiagency DDDAS Program Solicitation in 2005, created an impetus for advances in DDDAS techniques in several application areas, including for example management and fault-tolerant electric power-grids (this and many other examples cited in the earlier 2006 DDDAS Report [2]). Moreover, there are many other systems that have complexity and dynamicity in their state space, making the use of InfoSymbiotics/DDDAS approaches not only essential but imperative.

3.2 Applications' Modeling and Algorithmic Advances

A second factor that favors renewed and coordinated investment now, are the rapid advances in a number of algorithmic methods relevant for creating DDDAS capabilities. In fact, together with increased research emphasis in multi-scale modeling and new algorithmic methods, for dynamic systems DDDAS drives further the capabilities and the needs for new capabilities in multimodal and multiscale modeling and algorithms, both numeric and non-numeric, and where these multiple levels and modalities are invoked dynamically. Such new advances that can be exploited in the context of DDDAS include non-parametric statistics allowing inference for non-Gaussian systems, faster methods for uncertainty quantification (UQ) and uncertainty propagation, as well as advances in the numerics of stochastic differential equations (SDEs), parallel forward/inverse/adjoint solvers, and smarter data assimilation, (that is: dynamic assimilation of data with feed-back control to the observation and actuation system), hybrid modeling systems and math-based programming languages.

Simulations of a system are becoming synergistic partners with observation and control (the "measurement" aspects of a system). It was highlighted at the workshop that creating DDDAS brings together the application modeling and simulation research communities with the controls communities, on synergistic research efforts to create these new applications and their environments, where the (often high-end) simulations modeling is dynamically integrated with the real-time data acquisition and control components of the application. Workshop participants, representatives of the controls communities (and several of them principal investigators of projects that have commenced under the DDDAS rubric) highlighted the fact that DDDAS opens new domains for controls research.

3.3 <u>Ubiquitous Sensors</u>

A third factor is the increasing ubiquity of sensors – low cost, distributed intelligent sensors have become the norm in many systems and environments, which include: terrestrial, airspace and outer-space, underwater and underground. Major investments in satellites, manned and unmanned aerial vehicles equipped with multitudes of sensors, and other observation systems are now coming online; in the subsequent section a wealth of examples are overviewed, drawn from the CIF21, the TechHorizons, the 2006 DDDAS Reports, and other sources. Examples range from environmental observation systems, to phone geo-location information and instruments in automobiles, are already in place, collecting and/or transmitting data, even without the user's knowledge or involvement.

ubiquitous, heterogeneous collections of networked sensors and controllers … … managing … in static and ad-hoc ways inadequate… InfoSymbiotics/DDDAS allows adaptive, optimized management of these heterogeneous resources…

Static or ad-hoc ways of managing such collection of data, in general produces very large volumes of data that need to be filtered, transferred to applications that require the data, and possibly partially archived. Given the ubiquity of sensors and other instrumentation systems, and the ubiquity and data volumes, tradeoffs need to made, for example between which data are collected and bandwidth available. Architecting and managing large numbers and heterogeneous resources cannot be done in the ad-hoc and static ways pursued thus far, it's woefully inadequate. DDDAS provides a powerful methodology for exploiting this opportunity of ubiquitous sensoring, through the DDDAS-intrinsic notion of having the executing application-model control and dynamically schedule and manage these heterogeneous resources of sensors (and actuators or controllers).

In fact, in DDDAS, the application model becomes unified and seamlessly integral with the real-time data-acquisition and control application-components executing on the sensors and the actuators. Moreover, as is discussed later in the systems software section, it becomes variable as to what parts of the application model execute on the higher-end platforms, versus what may execute at the sensor or the controller side, and such variability in execution requirements depends for example on bandwidth and other resource limitations, which will dictate that data preprocessing, compression, and combining, may need to happen at the sensor or controller side. Thus, how to architect these networks of sensors and sets controllers, and how to dynamically schedule and utilize these heterogeneous resources is guided by the executing simulation model, as this is a fundamental premise in DDDAS.

3.4 <u>Transformational Computational and Networking Capabilities</u>

A fourth factor is the dramatic transformation of the computing and networking environment. The advent of multicore/manycore chips as well as heterogeneous architectures like GPUs, create revolutionary advances in heterogeneous distributed computing and in embedded computing. All these new directions are leading to unparalleled levels of increased computing capabilities and at reduced cost. In the midst of this transformation – many technologies that were exclusively HPC (e.g. massively parallel processing) can now used at all scales from high end machines to desktop and embedded systems.

Recent years have seen a continuous movement towards embracing dynamic data throughout all areas of computing. For example, as HPC applications look towards exascale computing with billion-fold concurrency, applications will need to be fundamentally aware of their environment and able to react dynamically to self optimize or self heal. The emergence of Cloud computing is elevating the demand and expectations for on-demand computing. As data becomes pervasive across scientific disciplines supercomputer centers are recognizing and embracing data intensive needs. Data availability is catalyzing new computational disciplines across the arts and humanities. New mobile platforms are leading to an explosion in web 2.0 and social networking technologies which are intrinsically data driven and location aware. The time is right to leverage the decade of experience in academia of grid computing and distributed applications to steer a path that integrates agencies and industry to support dynamic data driven applications.

At the same time, network bandwidths have also undergone transformative advances – for example, the DOE/ESNET network expects to have the ability to transfer 1TB in less than 8 hours [10], allowing transfer of large volumes of data from distributed sources, such as remote instruments and other sensors, and also ability of remote on-line control of networks of such sensors and controllers. Commercial networks expect to provide 100Gbps in the near future. Together with increasing bandwidth capabilities at the wired and wireless domains, the ramping-up adoption of IPv6 increase opportunities of exploiting further the ubiquitous interconnectivity, across multitudes of heterogeneous devices with increased transmission rates. Such capabilities create interconnectivity across peta- and exa-scale capacity platforms, connecting them at the same time also to instrumentation systems (networks of sensors and networks of controllers).

… MPUs populating the range of computational and instrumentation platforms … from the high-end to the real-time data acquisition and control…
… opportune to exploit in InfoSymbiotics/DDDAS

DDDAS entails unification across the large-scale computing (simulations/modeling) and the real-time data-acquisition and control. Commensurately, in DDDAS environments, the respective range of supporting platforms are also becoming a unified platform, from the high-end to the sensors and controllers. These new environments require significant advances in systems software to support the dynamic integration and a highly heterogeneous runtime across this range of platforms. While this is a formidable software challenge, the advent of multicores is an aspect that somewhat simplifies one dimension of this challenge, as it will be the same kinds of multicores (MPUs – Multicore Processing Unit) populating the high-end platforms as well as the instrumentation systems.

Thus, the increasing emergence of ubiquitous sensing, high bandwidth networking, and the unprecedented levels and range of multicore-based computing that are becoming available, all these are timely advances, providing impetus for exploiting DDDAS to create new capabilities in numerous critical applications and application areas.

4. InfoSymbiotics/DDDAS and National/International Challenges

In the 2006 DDDAS Report [2], over 60 projects are listed. It is discussed there how these projects are advancing the capabilities, through DDDAS approaches, and are impacting in a wide set of areas, all key and critical in the civilian, commercial, and defense sectors. Specifically: in Physical, Chemical, Biological, Engineering Systems (e.g.: chemical pollution transport - atmosphere, aquatic, subsurface, in ecological systems, protein folding, molecular bionetworks,…); in Critical Infrastructure Systems (e.g.: communications systems, electric power generation and distribution systems, water supply systems, transportation networks, and vehicles -air, ground, underwater, space; monitoring conditions, prevention, mitigation of adverse effects, recovery, …); in Environmental (e.g.: prevention, mitigation, and response, for earthquakes, hurricanes, tornados, wildfires, floods, landslides, tsunamis, terrorist attacks); in Manufacturing (e.g.: planning and control); in Medical and Health Systems (e.g.: MRI imaging, cancer treatment, control of brain seizures, …); in Homeland Security (e.g.: terrorist attacks, emergency response); and, in a boot-strapping way, in Dynamic Adaptive Systems-Software (e.g.: robust and dependable large-scale systems; large-scale computational environments).

In addressing the future AirForce, the Technology Horizons Report has called for revolutionary new directions in complex systems, that apply beyond the domains of interest to the AirForce, to systems which have corresponding analogues in the civilian, commercial sectors, for example in manufacturing and environmental concerns. As articulated in Technology Horizons, these dozen directions are:

- *From* (design of customized) *Platforms ...To* (design for) *Capabilities; From … Fixed* (specialized purpose systems) ...To … *Agile* (adaptive); *From … Integrated ...To … Fractionated* (to allow plug-and-play adaptability - leverage and reuse); *From … Preplanned ...To … Composable* (to meet evolving needs); *From … Long System Life ...To … Faster Refresh*
- *From … Control ...To … Autonomy; From … Manned* (operator-based) ...To … *Remote-Piloted* (remote human or autonomic); *From … Single-Domain ...To … Cross-Domain* (to account for interoperability – systems-of-systems)
- *From … Sensor* (data collection) ...To … *Information* (dynamically processed data); *From … Permissive* (passive) ...To … *Contested* (active and changing situations)
- *From … Cyber Defense (fire walls) ...To … Cyber Resilience (fault-tolerance, recovery)*; *From … Strike (corrective action) ...To … Dissuasion/Deterrence* (prevention, mitigation).

InfoSymbiotics/DDDAS… key for autonomic systems, collaborative/cooperative control… ad-hoc networks… sensor based processing… agile, composable, … …cyber resilient…

To address such challenges, a number of core scientific and technological capabilities are also emphasized in the TechHorizons Report. The identified key areas are: autonomous systems; autonomous reasoning and learning; resilient autonomy; complex adaptive systems; V&V for complex adaptive systems; collaborative/cooperative control; autonomous mission planning; ad-hoc networks; polymorphic networks; agile networks; multi-scale simulation technologies; coupled multi-physics simulations; embedded diagnostics; decision support tools; automated software generation; sensor-based processing; behavior prediction and anticipation; cognitive modeling; cognitive performance augmentation; human-machine interfaces. As articulated by Dr. Dahm in his remarks at the 2010 Workshop, InfoSymbioticSystems/DDDAS play a major role in all these.

The 2007 NSF CF21 Report [6] provides a wealth of new science and engineering research frontiers and their corresponding cyberinfrastrure collaboratories. Nearly sixty examples of such major projects are listed in that report (cf. pp.50-55 CIF21 ibid). The projects are exploring phenomena and systems ranging across many dimensions, scales and domains of natural, human, and engineered systems, and interactions there-of: from the nanoscale to the terascale; from subatomic and molecular to the black-hole dynamics of galaxies; from understanding the dynamics of the inner mantle of the earth, to the atmospheric events, weather, climate, to outer space weather; from the molecular levels of biological systems, the proteomics and genomics, to the organismal, ecological and environmental systems; from the interplay among genes, microbes, microbial communities to interactions with earth and space systems - from the bio-sphere to the oceans, atmosphere, cryo-sphere; from individualized models of humans to behaviors and complex social networks.

InfoSymbioticSystems/DDDAS are relevant to a multitude of the projects cited in the CIF21 Report.

Keynote presentations at the August2010 DDDAS Workshop (some by principal investigators in cyberinfrastructure projects referenced in CIF21) spoke about the major role InfoSymbioticSystems/DDDAS plays in such efforts. InfoSymbiotics/DDDAS-based advancements in several application areas, environmental, civil-infrastructures, and health, were highlighted by the speakers, and specifically: in weather forecasting and advancing the modeling methods for climate analysis; in environmental monitoring and in water management; in resource management in urban environments, in health monitoring of complex airborne platforms; in the medical and pharmaceutical application areas, where examples range from medical diagnosis and intervention, like cancer treatment and advanced surgical procedure capabilities, to genomics and proteomics, and customized drug delivery and release in the human-body.

The 14 NAE Grand Challenges cover a range of important topics: *Make solar energy economical; Provide energy from fusion; Develop carbon sequestration methods; Manage the nitrogen cycle; Provide access to clean water; Restore and improve urban infrastructure; Prevent nuclear terror; Engineer better medicines; Advance health informatics; Reverse-engineer the brain; Enhance virtual reality; Secure cyberspace; Advance personalized learning; Engineer the tools of scientific discovery*.

…research is needed at the fundamental levels and in technologies,
… in order to climb along the steep part of multiple innovation S-curves, and create robust InfoSymbiotics/DDDAS capabilities and concomitant CyberInfratructures

While all these challenges and the related research directions and drivers have been called by in principle different stakeholders and communities, it should be noted that there is a remarkable affinity in the basic research areas and advances needed spanning across the NAE Challenges, and those that are articulated in the TechHorizons, in CIF21, in the invited keynotes and other applications discussed at the August2010 DDDAS Workshop, and related DDDAS reports. Many other examples were discussed during the Working Groups discussions. A sample is provided here:

a) The role of DDDAS in energy: from designing and operating smarter power plants and other power generation sources, like solar, water, and wind renewable energy power sources; effectively managing the power distribution from such sources, and addressing current and foreseen problems with the power grid, such as optimized management of resources, addressing the powergrid fragility by predicting the onset of failures, and stemming-off and mitigating cascading failures and limiting their impact (see also 2006 DDDAS Report on existing energy-related DDDAS projects with respect to that [2]).
b) In national security and defense applications, DDDAS can play a major role in homeland security and in addressing decision-making, in battlefield settings. For example, actual battlefields are cluttered with dense numbers of fixed and moving objects, myriads of many types of sensors (radar, EO/IR, acoustic, ELINT, HUMINT etc.), and all their data need to be fused in real-time. This deluge of data includes video-data which need to be correlated with radar, SIGNIT, HUMINT and other non-optical data. Lt. Gen. Deptula stated "(we are) swimming in sensors and drowning in data''. Moreover, these data are incomplete, include errors, and need to be optimally processed to produce unambiguous and target state vectors, including time-dependent effects.
c) With respect to specific examples in civilian critical infrastructure environments, already DDDAS projects included in the 2006 DDDAS Report have covered incidents like: the 2005 Hurricane Katrina event in New Orleans [2], and using DDDAS to monitor and predict the propagation of oil spills (e.g. Douglas et al [2], Patrikalakis et al [2]). The recent Macondo oil spill in the Gulf of Mexico showed the need for better predictions of the spread of the oil in order to take more effective mitigating actions. Moreover, in the aftermath of this disastrous event, the problem of

determining the residual oil and its locations, called for the advancing the kind of work that had started through some small DDDAS efforts on oil-spill propagation. Observations involve tracking the residual oil from a large set of heterogeneous sources of data, such from satellites and visual inspection, ocean water sampling, tracking winds and oceanic currents, and air and water temperature measurements, all of which are in nature multimodal, dynamic and involve multiple scales, requiring fusion of such heterogeneous sets of data. Moreover all these data need to be integrated on-line with coupled models of wind and oceanic circulation models in a DDDAS-loop. These are research endeavors which the above referenced research projects started to pursue. However, further research is needed at the fundamental levels and in technologies, in order to climb along the steep part of multiple innovation S-curves, and to create the robust DDDAS cyberinfrastructure frameworks that would allow such analysis to be done at the scale needed for a Macondo-like event.

5. Science and Technology Challenges discussed in the Workshop

Successful DDDAS require innovations in the entire hierarchy: from instrumentation for sensing and control, to the systems software, to the algorithms and application models, and the cyberinfrastructure software frameworks encompassing this integrated hierarchy. In each of these areas there are critical science and technology challenges that must be met.

InfoSymbiotics/DDDAS entails invoking multiple modalities and model scales… dynamically at run-time… driven by dynamic data inputs … observability, identifiability, tractability and dynamic and continuous validation and verification (V&V)

The 2006 DDDAS Report [2] discusses advances and open issues in applications modeling, algorithms, runtime systems discussed in that report include the need to go beyond traditional approaches to develop application models able to interface and be steered by real-time data streamed into the model, dynamic model selection, and multiscale and multimodal modeling methods where the multiple scales and modalities of models are dynamically invoked based on the streamed data for dynamic-data driven, on-demand scaling and resolution capabilities; uncertainly quantification and uncertainty propagation across dynamically invoked models; self-organization of measurement systems, application workflows; observability, identifiability, tractability and dynamic and continuous validation and verification (V&V) of models, algorithms, and systems. That report also includes discussions on methods related to computational model feedback on the instrumentation data and control system relevant advances such as instrumentation control, data relevance assessment, noise quantification and qualification, and robust dynamic optimization, sensor and actuator steering. In mathematical and statistical algorithms the 2006 Report discusses progress and open issues on methods related to the measurement/data-feedback on the computational model that requires algorithms tolerant and stable under perturbations from streamed data, dynamic data assimilation methods, stochastic estimation for incomplete, possibly out of time-order data, and fast error estimation. In the area of systems software the 2006 DDDAS Report provides an extensive discussion on the requirements and systems services for dynamic adaptive runtime and end-to-end support for DDDAS environments, and namely support the applications' data- and knowledge-driven-, and adaptive composition and time- constrained execution and feedback-control with instrumentation systems.

These research and technology challenges and the need for systematic support and concerted multidisciplinary research efforts were also overviewed during the present workshop, and the participants reaffirmed the content and the recommendations of the 2006 DDDAS Report. In the sections following here, are discussed additional opportunities, identified by the participants of the present workshop, and salient points are made in the context of emerging underlying methodological and technological drivers and advances in modeling and sensoring, and in computational and networking capabilities, as well as cyberinfrastructure collaboratories and other testbeds recently available.

5.1 Algorithms, Uncertainty Quantification, Multiscale Modeling

DDDAS environments, where new data are streamed into the computation at execution time and where application models can be invoked dynamically, stress further the traditional requirements in terms of quantification of error in data and uncertainty propagation not only within a model but across models invoked dynamically at execution time. In DDDAS environments one is tasked with uncertainty fusion of both simulation and observational data in dynamic systems, design of low-dimensional and/or reduced order models for online computing, decision-making and model selection under dynamic uncertainty. In the broader context of UQ, one of the persistent challenges is the issue of long-term integration. This refers to the fact that stochastic simulations over long-term may produce results with large variations that require finer resolution and produce larger error bounds. Though none of the existing techniques is able to address the issue in a general manner, it is possible to apply the DDDAS concept of augmenting the model through on-line additional data injected into targeted aspects of the phase-space of the model, in-order to reduce the solution uncertainty by utilizing selected measurement data.

InfoSymbiotics/DDDAS … requires new, faster methods for uncertainty quantification & propagation across multiple scales of dynamically invoked models...

To address these challenges, in the DDDAS context, new ideas need to be explored, that either take advantage or further advances in existing methods in UQ and multi-scale modeling. Notable approaches include: generalized polynomial chaos methodology for UQ, Bayesian analysis for statistical inference and parameter estimation (particularly to develop efficient sampling methods as standard Markov-Chain Monte-Carlo (MCMC) does not work in real time), filtering methods (ensemble Kalman filter, particle filter, etc) for data assimilation, equation-free, multi-scale finite element methods, scale-bridging methods for multi-scale modeling, sensitivity analysis for reduction of the complexity of stochastic systems, etc. These methods have been attempted but their capabilities need to either be extended to the DDDAS domain, or new methods and tools for UQ and multi-scale modeling be developed which can satisfy the stringent dynamic DDDAS requirements. For example, methods for adaptive control of complex stochastic and multi-scale systems, efficient means to predict rare events and maximize model fidelity, methods for resource allocation in dynamic settings, tools to reduce uncertainty (if possible) and mitigate its impact.

Key challenges emerge in DDDAS for integrating the loop from measurements to predictions and feedback for highly complex applications with incomplete and possibly low quality data. Novel assimilation for categorical/uncertain data (graphical models, SVMs) must be developed. These advances can be coupled to recent advances in large-scale computational statistics and high-dimensional signal analysis to enabling tackling of complex uncertainty estimation problems. Algorithms for model analysis and selection (model error, model verification and validation, model reduction for highly-nonlinear forward problems, data-driven models) still need further research to create application independent formulations. New algorithms in large-scale kernel density estimation algorithms, on reduced order models and model reduction, interpolation on high-dimensional manifolds, multiscale interpolation, and manifold discovery for large sample sizes are examples of major breakthroughs in the last decade that can be furthered in the context of InfoSymbiotics/DDDASs to create the new levels of capabilities enabled through the DDDAS concept.

In another dimension, all these new algorithmic approaches need to be addressed and exploit the new computational platform architectures, multicore-based MPUs and specialized accelerators like GP-GPUs, populating embedded sensors and controllers, and Peta- and Exascale-scale HPC platforms, Grids and Clouds, etc. These environments on one hand translate to a need for distributed/parallel, fault-tolerant resource aware/resource adaptive versions of the referenced algorithms, and on the other hand provide new opportunities for powerful analysis schemes based on algorithmic approaches as discussed above.

5.2 Large, Complex, and Streaming Data

Key advances over the recent years in data management but also increasing challenges from the "data deluge" make evermore timely the role of the DDDAS paradigm, both in creating InfoSymbiotics/DDDAS capabilities and at the same time pushing the present advances in data management to new dimensions for more effective and efficient management processes. There have been impressive recent advances in commercial and academic support infrastructures for what is often termed the "Big Data" problem [13]. Efficient, scalable, robust, general-purpose infrastructure for DDDAS will addresses the Big Data problem in the context of the "Dynamic Data" entailed in the DDDAS paradigm – characterized by either (i) spatial-temporal specific information, (ii) varying distribution, or (iii) data that can be changed in dynamic ways, e.g., either operated upon in-transit or by the destination of data so that the load can be changed for advanced scheduling purposes. While Grids and Clouds have attempted to address the core connectivity and remote data-access issues between producers and consumers of data, DDDAS creates new levels of requirements and engenders new levels of capabilities not addressed or present in current state-of-the-art. The interoperability capabilities fostered within the Grids model are important for DDDAS environments. On the other hand, it's an open question how the ubiquitous and remote streaming data capabilities encountered in DDDAS environments can be accommodated within the Cloud model, which thus far is not addressing ubiquitous interoperability

"Big Data" problem…
"we are swimming in sensors and drowning is data"…
- ***Lt. Gen Deptula***

InfoSymbiotics/DDDAS concept is key to the ability for collecting data in targeted ways rather than ubiquitously

One consequence of the "Big Data" problem is a need for reducing the data set to that which is essential and carries the most information. DDDAS has the intrinsic ability to help prioritize data collection to the most critical areas as opposed to indiscriminate uniform acquisition, thereby greatly reducing the volume of data needed to support prediction/decision making. In DDDAS, the executing application model guides what data are really needed to improve the application analysis; this notion is key to collecting data in targeted ways rather than ubiquitously. Also, in DDDAS, parts of the computation can be replaced by the actual data, thus reducing the scaling of the computational cost of the simulation model, but at the same time such methods also pose unique requirements in managing data acquisition and ensuring QoS. Likewise, DDDAS methods can also render more accurate reduced order modeling methods, by using the actual and targeted data to construct the manifold of extrapolation or interpolation among full-scale solutions, thus creating decision support systems having the accuracy of full-scale models for many critical applications. To enable these capabilities, formal methodologies need to be developed, and software specifications as to what data is important and what is important in data (i.e., data pattern recognition through templates or some other system) and what to do when something important is found along with a measure of uncertainty, thus reducing redundancy and describing data by reduced order representations (e.g. features) instead of quantity, aspects that are essential.

Typical algorithms today deal with persistent data, but not streaming data. New algorithms and software are needed for supporting streaming data in the DDDAS context, allowing on-the-fly, situation-driven decisions about what data are needed at a given time and to reconfigure the data collection from sensors in real-time, to push or pull-in more useful data. Rather than just "pull-in more data ubiquitously", as are the present static and ad-hoc approaches of today, in DDDAS scheduling and correlating scheduling of multiple heterogeneous sets of sensors is determined dynamically by the executing application. Data collection, and scheduling data collection resources, is done adaptively, and aspects like granularity, modality, and field of view, all these are selectively targeted. Searching and discovering sensors and data must be expressed through some functional representation, both algorithmically and by software. Data collection and scheduling data collection resources is done adaptively, and aspects like granularity, modality, and field of view, all these are selectively targeted.

New strategies are needed for sensor, computing, and network scheduling. Scheduling maybe be quasi-optimal, intelligent and automatic, to support the needs of DDDAS environment. Need to evaluate which data and results are critical for the executing application and which are not, and prioritize which data to collect: "when and how", "now or later". Where, when, and how to do the processing must be decided on-the-fly, so that data can be delivered and reconfigured, models changed, and symbiotically make the DDDAS work. Where and how include locally, centrally, (geographically) distributed through networks, or some combination thereof. Methods and new tools are needed to disambiguate semantic non-orthogonality in data and models (time, space, resolution, fidelity, science, etc.). The gap needs to be bridged, between the differential rates of innovation in data capture, computation, bandwidth, and hardware.

Methods for fusing data from multiple sensors and models dynamically will have to be developed that are on demand, context dependent, actionable, and fast. Likewise, data mining in DDDAS requires similar advances, and must be addressed in the dynamic and adaptive ways that are intrinsic to DDDAS. Data security and privacy issues frequently arise in the data collection and must be addressed in the DDDAS context where the data are acquired and streamed into the models dynamically, therefore assessment of their integrity and provenance must be done in real-time, and new mechanisms are needed to support such capabilities. Smart data collection means faster results that are useful. Such methods are expected to be general and applicable across a range of applications and thus it is expected that multiple stakeholders would benefit from the ability to detect content on-the-fly and to couple sensor data with domain knowledge.

InfoSymbiotics/DDDAS require seamlessly integrated runtime support for environments spanning from the high-end to the real-time data-acquisition and control… support dynamic mapping of the application across this range and under dynamic computational and other resource

5.3 <u>Autonomic Runtime Support in InfoSymbiotics/DDDAS</u>

In DDDAS, the application environments consist of simulation models which are dynamically integrated with the instrumentation components of the application. These application components execute on a collection of platforms which may span a wide range: from the high-end, mid-range, workstation-level and the hand-held, to measurement systems, instruments, sensors and actuators or embedded controllers (and networks thereof). That is, DDDAS environments entail dynamic integration of the traditionally distinct application simulation and real-time control domains, and where the application platform becomes the unified collection of computational and instrumentation platforms for the diverse range referenced above. Consequently the application program will likely encompass heterogeneity of programming models commensurate to the computational and real-time application components, and likely have requirements that are typically changing during execution time.

Thus, DDDAS imply application execution requirements that are highly dynamic. Not only the computational requirements of the simulation may change at execution time depending on the data streamed into the simulation model, but also at execution time additional models of the application maybe invoked, depending on dynamic data inputs. Such changing computation-needs require dynamic discovery of resources, and dynamic mapping (and remapping, as needed) of the application/simulation program on these resources. Moreover, depending on the rates of the streamed data and depending on network resources availability, it may be that the parts of the application executing at the instrumentation (sensors or controllers) side, they may also change. For example, if there are limitations in bandwidth to transmit all data collected from a sensor (or sensors) then some of the data preprocessing and analysis may be performed at the sensors side, or combining operations may be performed across a group of sensors, etc.

In the context of DDDAS, systems software involves specification languages, programming abstractions and environments, software platforms, and execution environments, including runtimes that stitch together dynamically reconfigurable applications. Given the vast diversity of DDDAS application areas, platforms of interest encompass the range from distributed and parallel systems to mobile and/or energy efficient platforms that assimilate sensors inputs. Core DDDAS components by definition have evolved from executing on static platforms with fixed inputs to executing on heterogeneous platforms with widely varying capabilities fed by real-time sensing. Algorithms and platforms must evolve symbiotically to effectively utilize each other's capabilities. Algorithmically, we need to develop along three axes in a complementary manner: specification languages that can be used to define the performance characteristics of algorithms; methodologies for algorithms to adapt to changing resource availability or heterogeneity resource availability; and methodologies for algorithms to change behavior predictably, based on data and control inputs. Similarly, advances are need in execution platforms to support dynamically adapting applications. Platforms capabilities and interfaces need to be extended to include: interfaces to define and specify the performance characteristics of the underlying execution platforms; ability to reallocate resources in response to the changing needs of algorithms. DDDAS algorithms stress dynamicity – symbiotically; DDDAS platforms should expose interfaces that enable applications to sense and respond to resource availability, and interfaces that expose control inputs and monitoring of the DDDAS application behavior, to ensure their observability and controllability.

Novel directions to support dynamic &adaptive runtime: "compiler-embedded-in-runtime"
… interfaces to define and specify performance characteristics of the underlying execution platforms; ability to reallocate resources in response to the changing needs of algorithms…

To support these highly dynamic and heterogeneous execution requirements, new runtime systems methods are needed providing capabilities for dynamic adaptation of the application program, encompassing the heterogeneity of high-end computational models and real-time components. The runtime needs to support adaptive mapping of such heterogeneous programs across multiple levels of platform heterogeneity with commensurate heterogeneity in the respective operating systems, seamlessly integrated. The runtime must manage these heterogeneous resources and satisfy at the same time the goal of achieving a desired application level quality of service (QoS), under stringent conditions of high-end computations coordinated with the real-time nature of data-acquisition and control aspects. Novel directions for such capabilities include "compiler-embedded-in-the-runtime", which have *shown* promise. Capabilities needed include new methods and application interfaces for determining available resources requesting resources, supporting program adaptivity, and at multiple levels of granularity, and defining and determining level of quality of service.

Such requirements for autonomic runtime, and characteristics and capabilities needed for such runtime systems, and the challenges to create such capabilities have been discussed in 2006 DDDAS Report, and the reader is referred to that report for further details. Since that time, the role of multicore technologies as core engines in computational platforms has become more prevalent. Multicore-based processors (MPUs- Multicore Processing Units) will populate the high-end and mid-range platforms, and will also be the processing engines in instrumentation systems, sensors and embedded controllers. This aspect is very important for DDDAS environments. The systems software needed to support dynamic and adaptive mapping of DDDAS applications and dynamic runtime support requirements entail unprecedented levels of challenges. However, there is a simplification along one dimension of this complex software challenge, by the fact that the same kinds of basic processors (MPUs) will populate the entire range of platforms; that is, the same kinds of multicores (MPUs) will populate the high-end, and will be the computational engines for the sensors and controllers in the instrumentation components of a DDDAS application. For example, ideas, like "compiler-embedded-in-the-runtime" can now be examined in the context of multicores being the unifying engines across the wide array of computational and instrumentation platforms.

InfoSymbiotics/DDDAS push the collective sets of technologies constituting CyberInfrastructures to new levels … to support the required interoperability software and hardware SuperGrids … New generations of CyberInfrastructure Collaboratories

5.4 <u>InfoSymbiotics/DDDAS CyberInfrastructure Testbeds</u>

DDDAS connects real-time measurement devices and special purpose data processing systems with distributed applications executing on a range of resources, from mobile devices operating in ad-hoc networks to high-end platforms connected to national and international high-speed networks. Supporting infrastructure for these environments must go beyond present, static computational grids and include integrated and autonomous components that ingest data and drive adaption at all levels. Here components can be for example sensors, actuators, resource providers or decision makers; data can be real time, historical, filtered, fused or metadata; adaption can be applied at all levels such as choosing resources or mediating between data sources. DDDAS capabilities require software and hardware cyberinfrastructures supporting SuperGrids[12] of computational platforms dynamically integrated with the instrumentation platforms, and where such cyberinfrastructures embody applications and systems software architectural frameworks that support seamlessly the integration of this range of platforms, from the high-end to the real-time data acquisition and control. These software frameworks need to vertically integrate the systems' layers, from the applications to the hardware layers, and across computational and instrumentation components (including sensors and controllers, and networks thereof). Moreover, there is need to leverage horizontally (across different application examples or areas) advances made on such software frameworks.

In thinking about future DDDAS infrastructures we observe that the existing landscape provides a rich set of computational, networking and data systems infrastructures. Broadly speaking DDDAS applications can be seen as exploiting these capabilities but also posing high and differing demands in existing computational infrastructures. High-performance computing resources, such as for example the NSF TeraGrid and the planned XD and Blue Waters facilities, they are targeted to support high-end users, with application models exhibiting the highest levels of concurrency. There are many DDDAS applications with such characteristics and needs for high-performance capabilities. However, policy restrictions in resource management in these high-performance systems have traditionally hindered the broad and regular use of shared HPC environments for DDDAS applications, because these facilities use for example static batch queues, not suitable for the dynamic and interactive requirements of DDDAS High-throughput computing resources, such as for example the Open Science Grid which support interoperability across heterogeneous platforms, are possible computational infrastructures to be explored in DDDAS environments.

DDDAS connects real-time measurement devices and special purpose data processing systems with distributed applications executing on a range of resources, from mobile devices operating in ad-hoc networks to high-end platforms connected to national and international high-speed networks…
… require software and hardware cyberinfrastructures … computational, networking … data systems infrastructures

In Section 4 of the present report, application examples and cyberinfrastructure collaboratories are provided that are potential candidates as testbeds for DDDAS. Other such cyberinfrastructure frameworks are being created by several of DDDAS-supported projects, such as for example adverse weather prediction (Droegemeier in [2]), in environmental monitoring and critical infrastructures cited elsewhere in this report, and also examples of industry applications, such as for example in seismic migration and inverse problems which deal in addition with "big data". The advances in DDDAS applications modeling, in algorithms, and understanding errors and uncertainty invoke additional requirements for robust and efficient infrastructure support, for example operating at diverse time-scales, with concomitant increase in potential for failures at all levels and fail-safe implementation requirements.

For InfoSymbiotics/DDDAS environments, infrastructure will need to address myriad issues arising from diverse, dynamic data from different sources.

Integrating sensors into the DDDAS infrastructure will necessitate rethinking network architectures to support new protocols for push-based data, and two way communications to configure sensors based. Data in the DDDAS infrastructure will be stored and accessed in new hierarchies based on locality, filtering, quality control and other features. Experimental environments to support DDDAS computing are available at different levels of production use. The NSF sponsored Global Environment for Network Innovations (GENI) [17] provides exploratory environments for research and innovation in emerging global networks, and the NSF EAVIV [16] project provides a dynamically configurable network testbed for high speed end-to-end connectivity with TeraGrid resources. More recently, the NSF Future Grid [18] is being deployed to allow researchers to tackle complex research challenges in computer science related to the use and security of grids and clouds. Cloud computing is an emerging infrastructure that builds upon recent advances in virtualization and data-centers at scale to provide an on-demand capability. There are both commercial clouds (EC2, Azure, IBM Deep-Cloud) and academic clouds (DoE Science-Cloud, NSF Future Grid) that are viable infrastructure for DDDAS applications. They provide different models for data-transfer, localization and data-affinity. Consequently, exploring how the different data capabilities in conjunction with the on-demand compute Clouds can be used, and in combination with "traditional" grids to collectively support DDDAS applications, are important open questions.

The underlying hardware platforms need to be elastic and able respond to dynamic requirements. Persistent national infrastructure is envisioned as needed as well as infrastructure that is portable and able to be quickly deployed in the field to support medical, military and other application scenarios. End-user connectivity must be addressed, connecting national infrastructure to researchers in academic laboratories as well as to mobile users and devices in the field. Infrastructure itself thus needs to be dynamically configurable. A fundamental need for end resources supporting DDDAS, whether storage, compute, network or data collecting, is that they support dynamic provisioning which is flexible, adaptive and fine grained. This issue involves both technical developments (e.g. such as the ION dynamic network protocols [19]) along with appropriate policies to allow dynamic use of resources. Production resources focused on CPU utilization have the technologies to provide dynamic use, but their usage models do not typically allow for dynamic usage policies.

***InfoSymbiotics/DDDAS require new cyberinfrastructures supporting resource aware and resource adaptive methodologies… include capabilities for application software evolution and maintenance, repositories of application models and repositories of data, knowledge-based systems for application characterization, application analytics, application models validation, and verification* and testing…**

5.5 <u>InfoSymbiotics/DDDAS CyberInfrastructure Software Frameworks</u>

InfoSymbioticSystems/DDDAS environments embody dynamic integration of computational and instrumentation aspects of the application support system, and in fact DDDAS imply a unified computational-instrumentation platform for an application, rather than traditional infrastructure approaches where the computational platforms, while integrated with the archival data repositories, they are viewed as distinct from the instrumentation platforms. Integration of sensing, modeling and feedback, is the primary challenge in constructing DDDAS capabilities; that is: integrating the loop from measurements to predictions and feedback for highly complex systems, dealing with large, often unstructured and streaming data. Thus, InfoSymbiotics/DDDAS require new cyberinfrastructures supporting resource aware and resource adaptive methodologies. Systems-software frameworks of interest here include application programming environments, runtime, application composition and problem solving environments. Application software frameworks for InfoSymbiotics/DDDAS raise the level of requirements needed to include capabilities for application software evolution and maintenance, repositories of application models and repositories of data, knowledge-based systems for application characterization, application analytics, application models validation, and verification and testing.

Once dynamic behavior is provided at all levels of the infrastructure the question becomes how can resources be provisioned and used by applications and middleware. A common definition is needed to describe the quality of service (QoS) provided by the resource. This description needs to include the capabilities provided by the resource (e.g. bandwidth, memory, available storage) along with usage characteristics (e.g. cost, security, reliability, performance). Requirements for DDDAS systems overlap with known needs for many complex end-to-end scientific applications. However, additional and fundamental requirements are introduced to support dynamic data scenarios, such as the ability to handle events, and the integration of temporal and spatial awareness into the system at all levels necessary to support decision making. Systems need to react swiftly and reliably to deal with faults and failure to provide a guaranteed quality of service.

Autonomic capabilities are important at all levels to respond to the content of dynamic data or changing environments. The need for autonomic capabilities arise at many levels of DDDAS, for example, wherever dynamic execution and adaptivity is required – models and algorithms, the software and systems services, infrastructure capabilities; autonomic capabilities (such as behaviors based upon planning & policy) provide an effective approach to manage the adaptations and mechanics of dynamical behavior. In many DDDAS scenarios, application workflows need to be dynamically composed and enacted based on real-time data and changing objectives. An example includes an instrumented hurricane modeling, which can achieve efficient and robust control and management of diverse model by dynamically completing the symbiotic feedback loop between measured data and a set of computational models.

DDDAS connects real-time measurement devices and special purpose data processing systems with distributed applications executing on a range of resources, from mobile devices operating in ad-hoc networks to high-end platforms connected to national and international high-speed networks…
… require software and hardware cyberinfrastructures
… computational, networking
… data systems infrastructures

Multiple coordination strategies in DDDAS infrastructures are essential to ensure meeting the highly stringent and dynamic requirements of such environments. DDDAS infrastructures need to support complex, intelligent applications using new programming abstractions and environments able to ingest and react to dynamic data. Initially, different infrastructures may be needed for different application types, but the expectation is that there will be convergence and leverage of methods and technologies, if not universally across all application areas, at least among classes of such application areas. With respect to testbed efforts, national, persistent DDDAS infrastructures connecting new Petascale-range compute resources via 100 Gbps networks to special purpose data devices could serve as testbed for a range of important and critical applications. Researchers operating in university and national or industrial laboratories will require DDDAS testbeds that reliably and securely connect external data sources to institutional and distributed resources with QoS guarantees and fault tolerance. Easily deployable and reliable systems will be needed architected and implemented in the field over ad-hoc networks to explore new DDDAS-based capabilities supporting medical, military, and other applications, operating in special conditions.

Research opportunities are presented to provide persistent and fully featured infrastructure, integrating frameworks, programming abstractions and deployment methods into an overall architecture, developing common
APIs and schemas around which powerful tools can be provided, providing methods for decomposing applications to take advantage of emerging environments such as Clouds or GPUs in an integrated infrastructure, and deploying persistent DDDAS infrastructure for research and production use. Specific research challenges include: • Architecture: Application scenarios, characteristics and canonical problems to drive infrastructure research and development; Network architectures to support new protocols for sensor data (push, pull, subscribe); Architecture of data hierarchy for dynamic data processing and access; Integration of location and time awareness; • Tools: Dynamic workflow tools building on above capabilities (unique demands: run time environment, with changing services, events controlled workflows, resource discovery, ...); Visualization, analysis and steering of large and

dynamic data (haptics, ...) for closed loop scenarios, real-time data, changing characteristics, ... ; Security issues for sensors and autonomy, security issues generally for new software; Execution environment supporting collaboration and decision making (social networking), crowd-sourcing, citizen engineering,... ; • Integration and Interoperability: How to define, carry and operate on provenance information; Generalized interoperability, collaboration and negotiation in decentralized decision making; Generalization of allocation across different resources (networks, data ...), new methodologies of allocation, ...; Negotiation mechanisms between applications and infrastructure; Description for QoS (includes cost, availability, security, performance, reliability, ...); More effective integration of computable semantics throughout the infrastructure (e.g. tradeoff between simplicity and expressiveness); Policies/cost models for dynamic resource allocation, resource contention (e.g. for different applications); Integration with cloud computing to take advantage of business model and scalability and collaboration, virtualization, mutual collaboration between cloud computing and DDDAS

Developing DDDAS infrastructure is challenging, bringing issues related to dynamic data that reach beyond those addressed in traditional grids that require new and flexible policies along with comprehensive and integrated services. The capabilities needed for the infrastructure are diverse, and many facets have already been addressed in a diverse set of projects across the different agencies which should be adopted where possible to leverage knowledge advances and prevent duplication and/or re-invention. Funding mechanisms need to be put in place that provide and support complete, integrated, production infrastructure for broad DDDAS across international and agency borders. Expectations for this infrastructure need to be carefully thought out, so that appropriate outcomes are evaluated rather than traditional metrics of utilization.

6. Learning and Workforce Development

InfoSymbiotics/DDDAS creates exciting multidisciplinary training opportunities …

… developing a globally competitive workforce …

InfoSymbiotics/DDDAS creates exciting multidisciplinary research opportunities for undergraduate, graduate, and postdoctoral education and training. Given the recognition of InfoSymbiotics/DDDAS as a key scientific and technological direction, and perhaps a new field, this presents a high potential for inspiring students and attracting them into the many science and technology in individual disciplines and in multidisciplinary experience involved in developing DDDAS capabilities. The required research and technology efforts can bridge academia and industry, providing more broadly trained academic and industry workforce, or workforce in other parts of the private sector, as well as the public sector. The industry sector has expressed interest in DDDAS, and already partnerships between academe and research in industry have been established for several DDDAS research projects. Also, the industry sector has expressed the need for multidisciplinary educational experience as a key element for their workforce. Research in the context of InfoSymbiotics/DDDAS can create new alliances within and across departments, as well as cross-institutional connections across academe, national laboratories, and industry, nurturing relationships, enduring as students graduate and transition into the workforce.

7. Multi-Sector, Multi-Agency Co-operation

InfoSymbiotics/DDDAS has engendered multidisciplinary research and technology development across disciplines and in multi-institutional and multi-sector, and multi-national collaborations. Such activities emerged initially as seeding activities within broad agency programs, but the required synergism was more systematically cultivated through the 2005 multi-agency program solicitation which included co-operation from the EU-PF7 (Information Society

Technologies) Program and the UK e-Sciences Program. From early-on DDDAS attracted the interest of the international community, and such collaborations were encouraged and nurtured both in the projects that were created under the DDDAS rubric but also through a broader community activities, including the International DDDAS Workshop Series that have taken place yearly since 2003 (DDDAS/ICCS – www.dddas.org). The interest by industry is also evident in the many projects which have created connections with industry, especially the research arms of the industry sector. Overall, multidisciplinary research and systematic support of multidisciplinary research, and in particular under the umbrella of multi-agency collaborations, and connections with research in industry, behoove consideration from several perspectives as we move forward, and these are discussed in the case of InfoSymbiotics/DDDAS.

… systematic support of multidisciplinary research, and in particular under the umbrella of multi-agency collaborations, and connections with research in industry, behoove consideration from several perspectives…

In the US, DDDAS enticed interest and support from multiple stakeholders within a given agency as well as across agencies. The 2005 solicitation was under the co-sponsorship of all NSF Directorates and the NSF International and Small Business Offices, but also brought participation of NIH, NOAA, and AFOSR, as well as international collaborations. The January 2006 DDDAS Workshop that followed, included participation by several agencies: DHS, DOD (OSD, JFCOM-J9, ONR, NRL, AFOSR), DOE (several National Laboratories), NASA, NIH, NOAA, CIA, and NIST. The present workshop in addition to the two co-sponsors, AFOSR and NSF, had participation from other parts of DOD (AFRL, ARO, ARL, ONR, and NRL), DOE (Labs) DTRA, NASA, and NIH.

It's a key item that multidisciplinary research cannot be funded through fragmented and peripheral efforts. In recent years, there have been several initiatives from various funding agencies to support research related to various facets of DDDAS. The NSF ITR Program was a large 5-yr program with a general and broad scope, aspects that were used to seed some efforts on DDDAS, following the 2000 DDDASWorkshop. The more recent NSF Programs CDI (on general software methods) and CPS (focused on embedded systems) did not articulate the DDDAS vision to be considered by the community as viable support sources for DDDAS-related research. The DOE PSAAP Program, other recent DOE program calls on multi-scale research and Uncertainty Quantification (UQ), and the UQ MURI of AFOSR, as well as some the NIH RO1's, also have certain flavor of multi-scale and data-driven research. However, none of these programs has captured the full context of DDDAS and the comprehensive scope of synergistic and multidisciplinary research that was articulated and started with the 2005 multi-agency DDDAS Program Solicitation, and which resulted in a rich set of coherent projects. The solicitation inspired the community to embrace the DDDAS vision, and bring together the requisite representation from the applications areas, computer sciences, mathematics and statistics, and systems instrumentation, to open new frontiers in the fundamentals and in new capabilities. The progress that has resulted from these projects, as well as the increasingly wider realization of the value of DDDAS [10,14], make it ever more imperative for renewed programmatic efforts, and investments in DDDAS coordinated acros agencies through joint program solicitations.

Multidisciplinary programs, supported in coordinated ways with other agencies have been increasing in popularity, and have enticed overwhelming interest from the research community. On one hand the research communities have responded to cross-agency program calls on multidisciplinary research by initiating cross-disciplinary teams and producing innovative proposals. On the other hand it is known that multidisciplinary proposals and the ensuing projects require a longer gestation and incubation period, because not only it is challenging to bring together the multiple fields in the collaboration, but typically there is a ramp-up stage for each project to establish the communication and collaborative rapport across researchers from diverse fields. There has been a challenge to establish stable, long-term funding on a sustained basis. Several reports that have been produced over the recent years, each make these points.

InfoSymbiotics/DDDAS has excellent track-record of multistakeholder interest and support, multidisciplinary efforts...
…academe-industry-government…
higher impact results,…
well-defined problems, …
clarity, .. access to realistic data and infrastructures…
…ownership of results,

There are numerous benefits of coordination and joint efforts across agencies, nationally, and in supporting synergistically such efforts. Multiple agencies participating in coordinated and systematic efforts on DDDAS bring together different research and technology communities and a diverse set of stakeholders. Mission-oriented agencies can provide drivers and components, leading to higher impact results: well-defined problems, clarity on the specific decision information needed, feedback, access to key and realistic datasets and other infrastructure, and research personnel from agency-supported Research Laboratories that can participate in these interactions. Moreover, participation by several agencies as sponsors of a given project, leads to ownership of results and technology transfer of fundamental research. Finally, sponsorship across agencies, leverages individual funding and contributes to more continuity and stability of sustaining the research for longer term.

Likewise, involving the industrial sector in fundamental research engenders beneficial collaborations, brings to the research projects real-world data and infrastructure needed to validate the new ideas and research methods, and can expedite technology transfer. In addition to participation in joint workshops, joint research supported or catalyzed by government programs, and co-sponsored by industry support can lead to beneficial and varying forms of collaborations, driven by research efforts articulated in the preceding sections. Some example priority areas include partnerships in the energy sector, manufacturing, aerospace, telecommunications, medical, and information technology/computer industry.

The 2006 DDDAS [2] Report provides additional context and examples of benefits from cross-agencies and cross-sector joint efforts. The present workshop endorsed the findings of that report, and reaffirmed the value of coordinated efforts and including joint solicitations on InfoSymbiotics/DDDAS.

8. Summary

InfoSymbiotics/DDDAS provides the promise of new and exciting advances with transformative impact. The concept is recognized as key to important new capabilities, critical in many societal, commercial, and national and international priorities and initiatives, identified in important studies, blue ribbon-panels and other notable reports. The research required spans several dimensions, and requires synergistic multidisciplinary thinking and multidisciplinary research. Not only this is an opportunity of highly innovative advances, but also an opportunity for developing a globally competitive workforce. Advances made thus far, creating InfoSymbiotics/DDDAS capabilities, add to this promise, albeit they have been achieved, through limited and fragmented support. A diverse community of researchers has been established over the years, drawing from multiple disciplines, and spanning academe, industry research and governmental laboratories, in the US and internationally. These research communities are highly energized, by the success thus far, and by the wealth of ideas in confluence with other recent technological advances.

In summary, InfoSymbiotics/DDDAS related opportunities and challenges, involve synergistic multidisciplinary research in applications (for new methods where simulations are dynamically integrated with real-time data acquisition and control, and where application models are dynamically invoked), in algorithms (where algorithms tolerant in their stability properties to perturbations from streamed data, and algorithmic methods where uncertainty quantification and error propagation methods can support efficiently error propagation across dynamically invoked application models), in systems software supporting such applications that exhibit dynamic execution requirements (where models of the application are dynamically invoked, and where high-end application models are dynamically integrated with the real-time acquisition and control components of the application, and furthermore, where the parts of the application that execute on the high-end side versus those that execute at the sensors or controllers side, may vary during the execution of the application depending on dynamic requirements, and resource availability, e.g. data volume and bandwidth available). DDDAS drives these kinds of needs and technology advances, provides leapfrogging opportunities within the landscape of accelerating advances and emerging terrains in sensors and ubiquitous sensoring, in data collection and analysis, and in networking and computing. These advances create new platforms and environments for supporting the complex systems of interest in societal, commercial, industrial and national security settings, providing further motivation for embarking on comprehensive efforts for creating InfoSymbiotics/DDDAS capabilities.

InfoSymbiotics/DDDAS …
is a well-defined concept,
… new and exciting advances with transformative impact…
…well-defined research agenda…
research spans several dimensions…
…drawing from multiple disciplines,
research communities highly energized … wealth of ideas…
confluence with recent technological advances
… more than ever timely for

The present report, as well as precedent DDDAS reports and in particular the January2006 DDDAS Report, they provide to the research communities a wealth of science and technology challenges to be addressed in enabling InfoSymbiotics/DDDAS capabilities. The reports also provide examples of drivers and efforts on advances in a number of the challenges posed, such as on new methods and approaches that are needed in applications modeling methods, in mathematical and statistical algorithms, in systems software supporting seamless integration of high-end computing with the real-time data-acquisition and control systems, and in new instrumentation approaches and capabilities, as well as the software architectural frameworks that embody the DDDAS environments and the new kinds of cyberifrastructures that ensue, the testbeds that need to be put in place for the comprehensive development of the capabilities sought.

InfoSymbiotics/DDDAS is a well-defined concept, and a well-defined research agenda has been articulated through this and previous workshops and reports. All these, make timely the call for action, that was resoundingly expressed at the August2010 DDDAS Workshop, for systematic support to embark in pursuits for creating InfoSymbiotics/DDDAS capabilities, and to nurture the research as well as the technology development, necessary to bring these advances to the levels of maturity needed and enable the transformative impact recognized as ensuing from InfoSymbiotics/DDDAS.

BIBLIOGRAPHY

[1] F. Darema, C. Douglas, A. Deshmukh: DDDAS 2000 Workshop; in www.cise.nsf.gov/dddas

[2] G. Allen, K. Baldridge, G. Biros, A. Chaturvedi, C. C. Douglas, M. Parashar, J. How, J. Saltz, E. Seidel, A. Sussman - (Editor. F. Darema): DDDAS Workshop 2006 ; in www.cise.nsf.gov/dddas

[3] DDDAS/ICCS International Workshops Series www.dddas.org

[4] NSF Multiagency DDDAS Program Solicitation; in www.cise.nsf.gov/dddas

[5] Oden, J. T. ed., Simulation Based Engineering Science, Revolutionizing Engineering Science Through Simulation, Report of the Blue Ribbon Panel on Simulation Based Engineering Science: http://www.nsf.gov/pubs/reports/sbes_final_report.pdf

[6] NSF 07-28, CYBERINFRASTRUCTURE VISION FOR 21ST CENTURY DISCOVERY http://www.nsf.gov/pubs/2007/nsf0728/index.jsp?org=NSF

[7] National Science Foundation Vision for CyberInfrastructure for the 21st Century (CIF21), http://www.nsf.gov/about/budget/fy2012/pdf/40_fy2012.pdf

[8] NSF/ACCI Taskforces on CyberInfrastructure for 21st Century http://www.nsf.gov/od/oci/taskforces/index.jsp

[9] http://www.engineeringchallenges.org

[10] Technology Horizons - A Vision for Air Force Science & Technology During 2010-2030 http://www.af.mil/information/technologyhorizons.asp

[11] Dept. of Energy, ESnet Network Performance http://fasterdata.es.net

[12] F. Darema, SuperGrids, http://conferences.telecom-bretagne.eu/data/asn-symposium/actes/18_Keynote_Darema_Supergrids.pdf

[13] F. Berman ed. Sustainable Economics for a Digital Planet http://brtf.sdsc.edu/biblio/BRTF_Final_Report.pdf

[14] August2010DDDAS Workshop – Opening Remarks and Keynote Presentations, http://www.dddas.org/AFOSR-NSFworkshop2010-plenary.html

[16] Strategies for Remote Visualization on a Dynamically Configurable Testbed - The eaviv Project http://www.cct.lsu.edu/CCT-TR/CCT-TR-2009-18

[17] Global Environment for Network Innovations http://www.geni.net/?p=1984

[18] https://portal.futuregrid.org/

[19] http://www.internet2.edu/ion/

Appendix-0 Workshop Agenda

Day 1, Monday, August 30, 2010

7:30am - 8:15am	Registration and Refreshments
8:15am - 9:00am	Workshop Welcome *Opening Remarks* Dr. Werner Dahm, Chief Scientist, US Air Force *Introductory Remarks by AFOSR and NSF Leadership, and Co-Chairs* Dr. Frederica Darema, Director, Math, Info and LifeSciences Directorate, AFOSR Dr. Ed Seidel, Assistant Directorate, Math and Physical Sciences Directorate, NSF Prof. Craig Douglas, University of Wyoming Prof. Abani Patra, SUNY-Buffalo
9:15am - 12:30pm	Plenary Presentations
9:15am - 9:45 am	Prof. J. Tinsley Oden, Univ. of Texas, Austin *A Dynamic Data-Driven System for Optimized Laser Treatment of Prostate Cancer*
9:45am - 10:15am	Prof. Kelvin K. Droegemeier, Univ. of Oklahoma *DDDAS Applied to High-Impact Local Weather: The LEAD Project*
10:15am - 10:30am	Break
10:30am - 11:00am	Prof. Charbel Farhat, Stanford University and Dr. John Michopoulos, Naval Research Laboratory *DDDAS for Material Characterization, Health Monitoring, and Critical Event Prediction of Complex Structures*
11:00am - 11:30am	Prof. George E. Karniadakis, Brown University *Predictability and Uncertainty in DDDAS*
11:30am - 12:00pm	Dr. Sangtae Kim, Morgridge Institute of Research *Is Life a Dynamic Data Driven DNA Application System?*
12:00pm - 12:30pm	Prof. Patrick Jaillet, MIT *Data-Driven Optimization: Illustrations, Opportunities, Some Results, Key Challenges*
12:30pm - 1:30pm	Working Lunch
1:30pm - 2:00pm	Working Group Session
3:30pm - 3:45pm	Break
3:45pm - 5:00pm	Discussion of Summary Presentations
5:45pm	Adjourn for the day

Day 2, Tuesday, August 31, 2010

8:15am - 8:30am	Refreshments
8:30am - 10:00am	Working Group Session
10:00am - 10:15am	Break
10:15am - 12:00pm	Working Group Session
12:00pm - 1:00pm	Working Lunch
1:00pm - 3:00pm	Working Group Outbriefing
3:00pm - 3:30pm	Concluding Discussion
3:30pm	Workshop Ends
3:30 pm - 3:45pm	Break
3:45 pm - 5:00pm	Meeting Only with Working Group Chairs and Organizers

Day 3, Wednesday, September 1, 2010

Initial Write-up of the Report by Working Group Chairs and Organizer

<u>Appendix-1</u> Plenary Speakers

Professor Kelvin K. Droegemeier, University of Oklahoma
Professor Droegemeier is Vice President for Research, Regents' Professor of Meteorology, Weathernews Chair Emeritus in Applied Meteorology and Roger and Sherry Teigen Presidential Professor at the University of Oklahoma. In 2004, Dr. Droegemeier was appointed by President George W. Bush to a 6-year term on the National Science Board, the governing body of the National Science Foundation that also provides science policy guidance to the Congress and President. He presently chairs the Board's Committee on Programs and Plans. Dr. Droegemeier was co-founder in 1989 of the NSF Science and Technology Center (STC) for Analysis and Prediction of Storms (CAPS), and served for five years as its deputy director. He then directed CAPS from 1994 until 2006, and today CAPS is recognized around the world as the pioneer of storm-scale numerical weather prediction. He is also the Director of the Sasaki Institute, a non-profit organization that fosters the development and application of knowledge, policy, and advanced technology in the government, academic and private sectors. As director of the CAPS model development project for 5 years, he managed the creation of a multi-scale numerical prediction system that has helped pioneer the science of storm-scale numerical forecasting. This computer model was a fina list for the 1993 National Gordon Bell Prize in High Performance Computing. In 1997, Dr. Droegemeier received the Discover Magazine Award for Technology Innovation (computer software category), and also in 1997 CAPS was awarded the Computerworld Smithsonian Award (science category). Droegemeier also is a recipient of the NSF Pioneer Award and the Federal Aviation Administration's Excellence in Aviation Award. Dr. Droegemeier is a national leader in the creation of partnerships among academia, government and industry. He initiated and led a 3-year, $1M partnership with American Airlines to customize weather prediction technology for commercial aviation, and this resulted in him founding a private company, Weather Decision Technologies, Inc., located in Norman, that is commercializing advanced weather technology developed by the University of Oklahoma and other organizations. The success with American Airlines also played a role in the establishment in Oklahoma of the Aviation Services Division of Weathernews, the world's largest private weather company. Dr. Droegemeier led a $10.6M research alliance with Williams Energy Marketing and Trading Company in Tulsa, which is the largest such partnership between a university and a private company in the field of meteorolo gy. He initiated and led the Collaborative Radar Acquisition Field Test (CRAFT), a national project directed toward developing strategies for the real time delivery of NEXRAD radar data via the Internet. CRAFT won two awards from the National Oceanic and Atmospheric Administration, and its success led the National Weather Service to adopt its Internet data delivery strategy. As a follow-on to CRAFT, Droegemeier established Integrated Radar Data Services (IRaDS) at OU, which is a National Weather Service-designed top-tier provider of NEXRAD radar data to private industry. He has served as an associate editor for Mo nthly Weather Review for 6 years served on the UCAR University Relations Committee, the last two as chair. Elected to the UCAR Board of Trustees in 2002 and as its Vice Chairman in 2003, he became Chairman of the Board in 2004. Dr. Droegemeier has served as a consultant to Honeywell Corporation, American Airlines, the National Transportation Safety Board, and Climatological Consulting Corp. Dr. Droegemeier has graduated 27 students and served on the committees of numerous others. Dr. Droegemeier's research interests lie in thunderstorm dynamics and predictability, variational data assimilation, mesoscale dynamics, computational fluid dynamics, massively parallel computing, and aviation weather.

Professor Charbel Farhat, Stanford University
Professor Farhat has been designated by the Institute for Science Information (ISI) as one of the most highly cited researchers in engineering. He is the recipient of numerous prestigious awards including the American Institute of Aeronautics and Astronautics (AIAA) Structures, Structural Dynamics and Materials Award (2010), the United States Association of Computational Mechanics (USACM) John von Neumann Medal (2009), the Institute of Electrical and Electronics Engineers (IEEE) Computer Society Gordon Bell Award (2002), the International Association of Computational Mechanics (IACM) Computational Mechanics Award (2002), the (AIAA) Rocky Mountain Section Engineer of the Year Award (2001), the Department of Defense Modeling and Simulation Award (2001), the USACM Medal of Computational and Applied Sciences (2001), the IACM Award in Computational Mechanics for Young Investigators (1998), the USACM R. H. Gallagher Special Achievement Award for Young Investigators (1997), the IEEE Computer Society Sidney Fernbach Award (1997), the IBM Sup'Prize Achievement Award (1995), the American Society of Mechanical Engineers (ASME) Aerospace Structures and Materials Best Paper Award (1994), the Society of Automotive Engineers (SAE) Arch T. Colwell Merit Award (1993), the CRAY Research Award (1990), a TRW fellowship (1989), the United States Presidential Young Investigator Award (1989), and the Control Data Corporation PACER Award (1987). He is a Fellow of the American Society of Mechanical Engineers (2003), Fellow of the International Association of Computational Mechanics (2002), Fellow of the World Innovation Foundation (2001), Fellow of the United States Association of Computational Mechanics (2001), and Fellow of the American Institute of Aeronautics and Astronautics (1999). He has been an AGARD lecturer on aeroelasticity and computational mechanics at several distinguished European institutions, and a keynote speaker at

numerous international scientific meetings. He serves as Editor of the International Journal for Numerical Methods in Engineering and serves on the editorial boards of eleven other international scientific journals. He also serves on the U.S. Bureau of Industry and Security's Emerging Technology and Research Advisory Committee (ETRAC) at the U.S. Department of Commerce, and on the technical assessment boards of several national research councils and foundations.

Professor Patrick Jaillet, MIT
Professor Patrick Jaillet is the Dugald C. Jackson Professor in the Department of Electrical Engineering and Computer Science and a member of the Laboratory for Information and Decision Systems at MIT. He is also Co-Director of the MIT Operations Research Center. He was Head of Civil and Environmental Engineering at MIT from 2002 to 2009, where he currently holds a courtesy appointment. From 1991 to 2002 he was a professor at the University of Texas in Austin, the last five years as the chair of the Department of Management Science and Information Systems. He co-founded and was director of UT's Center for Computational Finance. Before his appointment at UT Austin, he was a faculty and a member of the center for applied mathematics at the Ecole Nationale de Ponts et Chaussee in Paris. He received a Diplome d'Ingenieur from France (1981), then came to MIT where he received the SM in Transportation (1982) followed by a PhD in Operations Research (1985). Dr. Jaillet's research interests include on-line problems; real-time and dynamic optimization; network design and optimization; probabilistic combinatorial optimization; and financial engineering. His research has been funded by NSF, ONR, USDOT, and from private funds (e.g., UPS, Indosuez Bank). Professor Jaillet has taught courses in combinatorial optimization; network optimization; probabilistic methods in operations research; stochastic analysis; risk management; and mathematics in finance. Dr. Jaillet's consulting works include supply chain strategy, logistics and distribution optimization, electronic marketplace design, and development of optimization solutions in various industries, including automotive, financial and manufacturing. Dr. Jaillet was a Fulbright Scholar in 1990. He is a member of the Institute for Operations Research and Management Science Society (INFORMS) and of the Society for Industrial and Applied Mathematics (SIAM). He is currently an Associate Editor for Networks, Transportation Science, and Naval Research Logistics, and has been an Associate Editor for Operations Research from 1994 until 2005.

Professor George Em Karniadakis, Brown University
Professor George Karniadakis received his S.M. (1984) and Ph.D. (1987) from Massachusetts Institute of Technology. He was appointed Lecturer in the Department of Mechanical Engineering at MIT in 1987 and subsequently he joined the Center for Turbulence Research at Stanford / Nasa Ames. He joined Princeton University as Assistant Professor in the Department of Mechanical and Aerospace Engineering and as Associate Faculty in the Program of Applied and Computational Mathematics. He was a Visiting Professor at Caltech (1993) in the Aeronautics Department. He joined Brown University as Associate Professor of Applied Mathematics in the Center for Fluid Mechanics on January 1, 1994. He became a full professor on July 1, 1996. He has been a Visiting Professor and Senior Lecturer of Ocean/Mechanical Engineering at MIT since September 1, 2000. He was Visiting Professor at Peking University (Fall 2007). He is a Fellow of the Society for Industrial and Applied Mathematics (SIAM, 2010-), Fellow of the American Physical Society (APS, 2004-), Fellow of the American Society of Mechanical Engineers (ASME, 2003-) and Associate Fellow of the American Institute of Aeronautics and Astronautics (AIAA, 2006-). He received the CFD award (2007) by the US Association in Computational Mechanics. His research interests include diverse topics in computational science both on algorithms and applications. A main current thrust is stochastic simulations and multiscale modeling of physical and biological systems (especially the brain).

Professor Sangtae Kim, Morgridge Institute for Research
Dr. Kim is a member of the National Academy of Engineering and a fellow of the American Institute of Medical and Biological Engineers. His research citations include the 1993 Allan P. Colburn Award of the American Institute of Chemical Engineers, the 1992 Award for Initiatives in Research from the National Academy of Sciences and a Presidential Young Investigator award from NSF in 1985. His treatise, Microhydrodynamics, first published in 1991, is considered a classic in that field and was recently selected by Dover Publications for its reprint series. He has an active record of service on science and technology advisory boards of government agencies, the U.S. National Research Council and companies in IT-intensive industries. Despite significant administrative roles in public service, his research activities remain significant and lie at the intersection of applied mathematics, biological sciences, and informatics. One program exploits biomimetic, fluidic self assembly to contribute to the roadmap for the "one-cent" RFID tag. A second program leverages his leadership experiences in the pharmaceutical industry to help create the emerging discipline of pharmaceutical informatics and a pathway for the pharma industry to harvest the fruits of genomics. A third program combines his experiences in academic/industrial research, IT management, and public service, to create new information architectures (the cyberinfrastructure) for rapid-response manufacturing supply chains.

Dr. John Michopoulos, Naval Research Laboratory

Dr. Michopoulos is a Research Scientist/Engineer and director of Computational Multiphysics Systems Lab (CMSL) of the Center of Computational Materials Sciences at the Naval Research Laboratory (NRL), Dr. Michopoulos oversees multiphysics and information technology research and development, operations and initiatives. Current major initiatives include research and development of linking performance to material through dynamic data and specification driven methodologies, electromagnetic launcher dissipative mechanism modeling and simulation, heterogeneous integrated computational, sensing and communication grids via data-driven multidisciplinary and holistic approaches and environments, engineering sciences research, development and management in areas of computational, theoretical and experimental multiphysics, platform/structure simulation based design, mechatronic/robotic data-driven characterization of continua, automation of research, distributed supercomputing, and multiphysics design optimization. Dr. Michopoulos also currently serves as the vice-chair of the Computers and Information in Engineering Division of the American Society of Mechanical Engineers. He is an associate editor for the Journal of Computers and Information Science in Engineering and the Journal of Computational Sciences. He is a founding member and chair of the International Science and Technology Outreach Society and prior to joining NRL he has been a senior research scientist for Geo-Centers Inc and prior to that director of the Image Processing Laboratory of the Institute of Fracture and Solid Mechanics at Lehigh University. He has participated in several blue ribbon panels including the tri-services Workshop on SHM, November 17, 2008 b Thu, November 20, 2008, Austin TX. He has also consulted for various companies and research organizations and has authored and co-authored more than 210 publications and books and has been honored with more than 47 awards. Dr. Michopoulos holds an electrical and civil engineering degrees and a Ph.D. in Applied Mathematics and Theoretical Mechanics from the National Technical University of Athens, and has pursued post-doctoral studies at Lehigh University on computational multi-field modeling of continuum system.

Professor J. Tinsley Oden, University of Texas-Austin

Professor Oden is the Associate Vice President for Research, the Director of the Institute for Computational Engineering and Sciences, the Cockrell Family Regents' Chair in Engineering #2, the Peter O'Donnell Jr. Centennial Chair in Computing Systems, a Professor of Aerospace Engineering and Engineering Mechanics and a Professor of Mathematics at The University of Texas at Austin. Oden has been listed as an ISI Highly Cited Author in Engineering by the ISI Web of Knowledge, Thomson Scientific Company. His work was key to establishing computational mechanics as a new intellectually rich discipline that was built upon deep concepts in mathematics, computer sciences, physics, and mechanics. Computational Mechanics has since become a fundamentally important discipline throughout the world, taught in every major university, and the subject of continued research and intellectual activity. Dr. Oden is an Honorary Member of the American Society of Mechanical Engineers and is a Fellow of six international scientific/technical societies: IACM, AAM, ASME, ASCE, SES, and BMIA. He is a Fellow, founding member, and first President of the U.S. Association for Computational Mechanics and the International Association for Computational Mechanics. He is a Fellow and past President of both the American Academy of Mechanics and the Society of Engineering Science. Among the numerous awards he has received for his work, Dr. Oden was awarded the A. C. Eringen Medal, the Worcester Reed Warner Medal, the Lohmann Medal, the Theodore von Karman Medal, the John von Neumann medal, the Newton/Gauss Congress Medal, and the Stephan P. Timoshenko Medal. He was also knighted as "Chevalier des Palmes Academiques" by the French government and he holds four honorary doctorates, honoris causa, from universities in Portugal (Technical University of Lisbon), Belgium (Faculte Polytechnique), Poland (Cracow University of Technology), and the United States (Presidential Citation, The University of Texas at Austin). Dr. Oden is a member of the U.S. National Academy of Engineering and the National Academies of Engineering of Mexico and of Brazil. His current research focuses on the subject of multi-scale modeling and on new theories and methods his group has developed for what they refer to as adaptive modeling. The core of any computer simulation is the mathematical model used to study the physical system of interest. They have developed methods that estimate modeling error and adapt the choices of models to control error. This has proven to be a powerful approach for multi-scale problems. Applications include semiconductors manufacturing at the nanoscale. Dr. Oden, along with ICES researchers, is also working on adaptive control methods in laser treatment of cancer, particular prostate cancer. This work involves the use of dynamic-data-driven systems to predict and control the outcome of laser treatments using adaptive modeling strategies.

Appendix-2 List of Registered Participants

NON GOVERNMENT Partcipants

Adam Bojanczyk	Cornell University
Gabrielle Allen	Louisiana State University
Jeff Anderson	NCAR
Ron Askin	Arizona State University
Siva Banda	Air Force Research Laboratory
Kirstie Bellman	The Aerospace Corporation
Dennis Bernstein	University of Michigan Aerospace Eng. Dept
George Biros	Georgia Institute of Technology
Alok Chaturvedi	Purdue University
YangQuan Chen	Utah State University
Janice Coen	NCAR
Li Deng	University of Wyoming
Yu Ding	Texas A&M
Craig Douglas	University of Wyoming Mathematics Department
Kelvin Droegemeier	University of Oklahoma
Tony Drummond	Lawrence Berkeley National Lab
Johnny Evers	Flight Vehicle Integration, AFRL/RWAV
Yusheng Feng	University of Texas at San Antonio
Paul Flikkema	Northern Arizona University
Jose Fortes	University of Florida
David Fuentes	The University of Texas MD Anderson Cancer Center
Tryphon Georgiou	University of Minnesota
Omar Ghattas	University of Texas at Austin
Adom Giffin	Princeton University
Leana Golubchik	University of Southern California
Chuck Hansen	University of Utah
Salim Hariri	The University of Arizona
Don Hearn	University of Florida
Chris Hill	MIT
Vasant Honavar	Iowa State University
Jonathan How	MIT
Xiaolin Hu	Georgia State University
Marty Humphrey	Department of Computer Science, University of Virginia
Patrick Jaillet	MIT
Shantenu Jha	Louisiana State University
Geroge Karniadakis	Brown
Tim Kelley	North Carolina State University
Yannis Kevrekidis	Princeton University
Sang Kim	Morgridge Institute for Research
MJ Kramer	The Aerospace Corporation
Tahsin Kurc	Center for Comprehensive Informatics, Emory University
Craig Lee	The Aerospace Corporation

Gregory Madey	University of Notre Dame
Kumar Mahinthakumar	North Carolina State University
Amit Majumdar	San Diego Supercomputer Center
Bani Mallick	Texas A&M
William (Mac) McEneaney	UC San Diego
Dimitris Metaxas	Rutgers University
John Michopoulos	Naval Research Laboratory
Fairul Mohd-Zaid	711 Human Performance Wing, RHCV
Jarek Nabrzyski	Center for Research Computing
Lewis Ntaimo	Texas A&M
J. Tinsley Oden	University of Texas at Austin
Srini Parthasarathy	Ohio State University
Abani Patra	University at Buffalo
Jin-Song	University of Oklahoma, School of CEES
E. Bruce Pitman	University at Buffalo
Serge Prudhomme	ICES, UT Austin
Guan Qin	University of Wyoming
Anand Ranganathan	IBM TJ Watson Research Center
Sai Ravela	MIT
Joel Saltz	Emory University
Adrian Sandu	Virginia Tech
Puneet Singla	University at Buffalo
Young-Jun Son	The University of Arizona
Vaidy Sunderam	Emory University, Math & CS
Alex Szalay	Johns Hopkins University
Mario Sznaier	Northeastern University
Georgios Theodoropoulos	University of Birmingham
Carlos A. Varela	Rensselaer Polytechnic Institute
Anthony Vodacek	Rochester Institute of Technology
Gregor von Laszewski	Indiana Univerity, Pervasive Technology Institute
Tim Wildey	University of Texas at Austin - ICES
Dongbin (D.B.) Xiu	Purdue University
David Fuentes	University of Texas
Victor Giurgiutiu	University of South Carolina
Milton Halem	UMBC
Dinesh Manocha	UNC Chapel Hill
Andreas Terzis	Johns Hopkins University
Srinidhi Varadarajan	Virginia Tech
Jon Weissman	University of Minnesota

GOVERNMENT AGENCIES Participants

Van Blackwood	AFOSR
Bob Bonneau	AFOSR
Stephanie Bruce	AFOSR
Patrick Carrick	AFOSR
Milt Corn	NIH/NLM
Frederica Darema	AFOSR

Jason Davis	AFOSR
Maj Michelle Ewy	AFOSR
Fariba Fahroo	AFOSR
Jonathan Griffin	AFOSR
John Hannan	DTRA
Tom Henderson	NSF/CISE
Tom Hussey	AFOSR
Kiki Ikossi	DTRA
Suhada Jayasuriya	NSF
Scott Harper	ONR
Robert Kozma	AFRL/RYHE
Lee Jameson	NSF/MPS
David Luginbuhl	AFOSR
John Luginsland	AFOSR
Kim Luu	AFRL/RDSM
George Maracas	NSF/ENG
Peter McCartney	NSF/BIO
Joe Mook	NSF/OISE
Manish Parashar	NSF/OCI
Leonid Perlovsky	AFRL/RYHE
Kitt Reinhardt	AFOSR
Stan Rifkin	AFOSR
Steve Rogers	AFRL/RY
Janet Spoonamore	ARO
David Stargel	AFOSR
S. Ananthram	ARL
Ralph Wachter	ONR
H. E. Seidel	NSF/MPS
Kishan Baheti	NSF/ENG
Demetrios Kazakos	NSF/EHR
Terry Lyons	AFOSR
D. J. Mook	NSF/OISE
Tristan Nguyen	ONR
Michael Seablom	NASA
Doug Smith	NSF/ENG
Mitat Birkan	AFOSR

Appendix-3

All WGs - Common and overarching Issues
All WGs should address the following common and overarching issues:

- The scope of research challenges is clearly wide and in need of fundamental advances. Why is now the right time for fostering this kind of research?
- What are the Grand S&T Challenges in enabling DDDAS? What are ongoing research advances can be used as leverage and springboard to enable DDDAS?
  (*Each WG will address the research challenges and opportunities*)
- What kinds of processes, venues and mechanisms are optimal to facilitate the multidisciplinary nature of the research needed in enabling such capabilities?
- What past or existing initiatives can contribute, and what new ones should be created to systematically support such efforts?
- What are the benefits of coordination and joint efforts across agencies, nationally and in supporting synergistically such efforts?
- What kinds of connections with the industrial sector can be beneficial? How can these be fostered effectively to focus research efforts and expedite technology transfer?
- How these new research directions can be used to create exciting new opportunities for undergraduate, graduate and postdoctoral education and training?
- What novel and competitive workforce development opportunities can ensue?
- What National and International critical challenges are addressed through DDDAS capabilities?

WG1 – Algorithms and Data Assimilation
(Janice Coen and George Biros)
DDDAS environments require algorithms, mathematical and statistical, both numeric and non-numeric, that have good convergence properties under perturbations from streamed data into the executing application. DDDAS goes beyond the traditional data-assimilation approaches:

- What is the state-of-the-art and what are the challenges in the applications algorithms to enable such capabilities for the applications models/simulations?
- What algorithms' development is needed to enable application algorithms tolerant to perturbations from "on-line" input data, and with good stability properties?
- How can one select and incorporate dynamically appropriate algorithms as the application requirements and data sets change in the course of the simulation?
- What kinds of approaches, such as knowledge-based systems, can be employed, and what interfaces and applications assists are needed to allow such capabilities?
- What systems support is required to develop such environments?
- How do the existing methods and capabilities in the above need to be advanced?

WG2 - Uncertainty Quantification and MultiScale Modeling
(Bani Mallick, Dongbin Xiu)
DDDAS environments entail application models that can interface and dynamically interact with the measurement data systems (archival, real-time data acquisition and control systems). Such interaction entails dynamic application models and application components, at runtime, as dictated by the streamed data, and can include dynamic invocation of models at multiple scales – that is "dynamic multi-scale". Models, experiments and observations are all representations and discrete samples of behavior. Quantifying and managing the outcomes of application systems (predictions, control actions, …) must account for these uncertainties. Such situations ensue new and increased challenges, beyond the traditional multi-scale, and uncertainty quantification considerations.

- What are the overall opportunities and challenges in DDDAS applications modeling?
- What research and technologies are covered by the present projects?
- As DDDAS requirements are expected to be dynamic, what are the implied applications modeling technology advances that are need and what's the needed systems support?
- What is special if you have a multiscale/multiphysics system? How do you do deal with multimodal data?
- What methodologies from the emerging field of UQ are applicable here, and in particular in the case where models of other components of the application are dynamically invoked? Conversely what new developments are needed to enable the use of dynamic data and simulations especially for complex systems? What are the issues in data management, dynamic selection of application components, mapping, interfaces for request and allocation of systems resources so that quality of service is ensured for the applications?

- Provide applications examples that will benefit from the new paradigm, existing and potential new applications, challenges in developing such applications, multilevel and multimodal modeling, composition of such complex applications, data management and interfaces to experiments/field-data, computation, memory and I/O requirements.

WG3 - Large and Heterogeneous Data from Distributed Measurement & Control Systems
(Alok Chaturvedi, Adrian Sandhu)

DDDAS inherently involves large amounts of data that can result from heterogeneous and distributed sources, collected in differing time-scales and in different formats, and which need to be preprocessed before automatically integrating them to the executing applications that need use the new data.

- What is the state of the art in measurement systems and how are they integrated in DDDAS, where measurements from sensors, other instruments and data repositories are dynamically integrated with the application modeling to improve the application modeling?
- Conversely, what is the state of the art in on-line application control of the measurement instrument or process providing opportunity to improve the measurement process, guide the design and operational aspects of measurement instruments, and networks of distributed heterogeneous sensors and networks of embedded controllers?
- What are the methods that need to be developed to guide the architecture of sets of sensors and other instruments thus improving the effectiveness or efficiency of the measuring systems, and networks of distributed heterogeneous sensors and networks of embedded controllers?
- What are the challenges and opportunities in software and hardware technologies to enable such dynamic interfaces to such measurement and control systems, and their associated data sets? What improvements in the methods are expected, how are they going to be enabled?
- How the existing methods and capabilities in all the above need to be advanced?

WG4 - Building an Infrastructure for DDDAS
(Gabrielle Allen, Shantenu Jha)

DDDAS integrates real-time sensor and other measurement devices with special purpose data processing systems together with the parts of the application that execute in larger platforms and driving a seamless integration of stationary and mobile devices together with large high-end platforms, entailing grids that go beyond the present computational grids.

- What are the challenges in the infrastructure just described above?
- What are the challenges and opportunities in software and hardware technologies to enable such dynamic interfaces?
- What improvements in the measurement methods are expected and how are they going to be enabled?

WG5 - Systems Software
(Srinidhi Varadarajan, Dinesh Manocha)

Quality of service, program software environments, data massaging, network security, and availability of common libraries are all important to making a DDDAS work in a global manner.

- What is the state-of-the-art and what advances are needed in algorithms and software and what new capabilities need to be provided by the underlying systems and platforms on which these applications execute, so that quality of service is ensured?
- What are the software challenges in the programming environments for the development and runtime support, under conditions where the underlying resources as well as the applications requirements might be changing at execution time?
- What are the issues in data management, dynamic selection of components, dynamic invocation of components, mapping to underlying resources, interfaces for request, and allocation of systems resources so that quality of service is ensured for the applications?
- What are the additional capabilities that are needed in the application support and systems management services?
- How can these be fostered effectively to focus research efforts and expedite technology transfer

Projects Under the DDDAS Rubric

(1998- … precursor Next Generation Software Program)

SystemsSoftware - Runtime Compiler - Dynamic Composition - Performance Engineering

(2000 -Through NGS/ITR Program)

Pingali, Adaptive Software for Field-Driven Simulations

(2001 -Through ITR Program)

- Biegler - Real-Time Optimization for Data Assimilation and Control of Large Scale Dynamic Simulations
- Car - Novel Scalable Simulation Techniques for Chemistry, Materials Science and Biology
- Knight - Data Driven design Optimization in Engineering Using Concurrent Integrated Experiment and Simulation
- Lonsdale - The Low Frequency Array (LOFAR) - A Digital Radio Telescope
- McLaughlin - An Ensemble Approach for Data Assimilation in the Earth Sciences
- Patrikalakis - Poseidon - Rapid Real-Time Interdisciplinary Ocean Forecasting: Adaptive Sampling and Adaptive Modeling in a Distributed Environment
- Pierrehumbert- Flexible Environments for Grand-Challenge Climate Simulation
- Wheeler- Data Intense Challenge: The Instrumented Oil Field of the Future

(2002 -Through ITR Program)

Carmichael - Development of a general Computational Framework for the Optimal Integration of Atmospheric Chemical Transport Models and Measurements Using Adjoints

Douglas-Ewing-Johnson - Predictive Contaminant Tracking Using Dynamic Data Driven Application Simulation (DDDAS) Techniques

Evans - A Framework for Environment-Aware Massively Distributed Computing

Farhat - A Data Driven Environment for Multi-physics Applications

Guibas - Representations and Algorithms for Deformable Objects

Karniadakis - Generalized Polynomial Chaos: Parallel Algorithms for Modeling and Propagating Uncertainty in Physical and Biological Systems

Oden - Computational Infrastructure for Reliable Computer Simulations

Trafalis - A Real Time Mining of Integrated Weather Data

(2003 -Through ITR Program)

Baden - Asynchronous Execution for Scalable Simulation in Cell Physiology

Chaturvedi- Synthetic Environment for Continuous Experimentation (Crisis Management Applications)

Droegemeier-Linked Environments for Atmospheric Discovery (LEAD)

Kumar - Data Mining and Exploration Middleware for Grid and Distributed Computing

Machiraju - A Framework for Discovery, Exploration and Analysis of Evolutionary Data (DEAS)

Mandel - DDDAS: Data Dynamic Simulation for Disaster Management (Fire Propagation)

Metaxas- Stochastic Multicue Tracking of Objects with Many Degrees of Freedom

Sameh - Building Structural Integrity

{Sensors Program: Seltzer - Hourglass: An Infrastructure for Sensor Networks}

(2004 -Through ITR Program)

Brogan - Simulation Transformation for Dynamic, Data-Driven Application Systems (DDDAS)

Baldridge - A Novel Grid Architecture Integrating Real-Time Data and Intervention During Image Guided Therapy

Floudas-In Silico De Novo Protein Design: A Dynamically Data Driven, (DDDAS), Computational and Experimental Framework

Grimshaw: Dependable Grids

Laidlaw: Computational simulation, modeling, and visualization for understanding unsteady bioflows

Metaxas - DDDAS - Advances in recognition and interpretation of human motion: An Integrated Approach to ASL Recognition

Wheeler: Data Driven Simulation of the Subsurface: Optimization and Uncertainty Estimation

(2005 DDDAS Multi-Agency Program - NSF/NIH/NOAA/AFOSR)

Ghattas - MIPS: A Real-Time Measurement-Inversion-Prediction-Steering Framework for Hazardous Events

How - Coordinated Control of Multiple Mobile Observing Platforms for Weather Forecast Improvement

Bernstein - Targeted Data Assimilation for Disturbance-Driven Systems: Space weather Forecasting

McLaughlin - Data Assimilation by Field Alignment

Leiserson - Planet-in-a-Bottle: A Numerical Fluid-Laboratory

Chryssostomidis - Multiscale Data-Driven POD-Based Prediction of the Ocean

Ntaimo - Dynamic Data Driven Integrated Simulation and Stochastic Optimization for Wildland Fire Containment

Allen - DynaCode: A General DDDAS Framework with Coast and Environment Modeling Applications

Douglas - Adaptive Data-Driven Sensor Configuration, Modeling, and Deployment for Oil, Chemical, and Biological Contamination near Coastal Facilities

Clark - Dynamic Sensor Networks - Enabling the Measurement, Modeling, and Prediction of Biophysical Change in a Landscape

Golubchik - A Generic Multi-scale Modeling Framework for Reactive Observing Systems

Williams - Real-Time Astronomy with a Rapid-Response Telescope Grid

Gilbert - Optimizing Signal and Image Processing in a Dynamic, Data-Driven Application System

Liang - SEP: Intergrating Multipath Measurements with Site Specific RF Propagation Simulations

Chen - SEP: Optimal interlaced distributed control and distributed measurement with networked mobile actuators and sensors

Oden - Dynamic Data-Driven System for Laser Treatment of Cancer

Rabitz - Development of a closed-loop identification machine for bionetworks (CLIMB) and its application to nucleotide metabolism

Fortes - Dynamic Data-Driven Brain-Machine Interfaces

McCalley - Auto-Steered Information-Decision Processes for Electric System Asset Management

Downar - Autonomic Interconnected Systems: The National Energy Infrastructure

Sauer- Data-Driven Power System Operations

Ball - Dynamic Real-Time Order Promising and Fulfillment for Global Make-to-Order Supply Chains

Thiele - Robustness and Performance in Data-Driven Revenue Management

Son - Dynamically-Integrated Production Planning and Operational Control for the Distributed Enterprise

+…

* projects, funded through other sources and "retargeted by the researchers to incorporate DDDAS"

* ICCS/DDDAS Workshop Series, yearly 2003 - todate
- other workshops organized by the community…

- 2 Workshop Reports in 2000 and in 2006, in www.cise.nsf.gov/dddas & www.dddas.org

* www.dddas.org (maintained by Prof. Craig Douglas)

Projects Under the DDDAS Rubric