1 Strategic Plan

Since its inception the Open Science Grid (OSG) partnership has evolved into a world-class distributed computing facility enabling scientific discovery across a broad range of disciplines. Building on novel software and shared hardware capabilities the OSG has been offering an unprecedented capacity of High Throughput Computing (HTC) capabilities to a growing number of science communities. The proposed Institute for Distributed HTC (InDHTC) brings together a diverse and accomplished group of Computer and Computational scientists who will enhance and expand the impact of HTC on DOE science through novel frameworks, advanced technologies, state-of-the-art tools and close interdisciplinary collaborations.

The InDHTC will be organized in five research areas – *Data*, *Security*, *Systems*, *Tools* and *Workflows* - and will work synergistically with the OSG project. The two entities will have the same PI and key OSG personnel (Associate Executive Director, Security area lead and Technology area lead) who will be directly involved in the daily activities of the institute. Indeed, the InDHTC team of two DOE national labs and five universities builds on the cumulative experience of a unique partnership that cuts across science disciplines, technical expertise and institutions, while preserving local autonomy and encouraging self-resilience. Co-funded by the DOE (SciDAC-2) and NSF, the OSG partnership has evolved from the Particle Physics Data Grid (SciDAC-1) project and the Grid Physics Network and the International Virtual Data Grid Laboratory (NSF ITR) projects. The leadership of the InDHTC has been working together since the formation of these early interdisciplinary projects more than a decade ago.

Each research areas will provide a 'docking point' for DOE application communities and SciDAC institutions, where a community or an institute can interface through several docking points. The team leaders bring a rich history of collaborative computer and computational science research that was translated into widely adopted technologies and scientific tools. By building bidirectional and mutually beneficial collaborations through these research areas, the ten FTEs of the InDHTC will *provide the intellectual resources, expertise, and solutions needed to advance the computing throughput of DOE science through the wide adoption and enhancement of DHTC technologies.* Activities across areas will be coordinated by the associate director of the institute. The institute director, who also serves as the technical director of the OSG, will be responsible for setting directions and managing the research agenda. Impact on application communities will be closely monitored by each area lead and evaluated by the institute leadership.

Through the OSG the proposed institute will work closely with a world-class DHTC facility that supports more than half a million jobs and sustained data transfers of more than a quarter of a petabyte daily, across more than sixty universities and DOE laboratories. On average, 50% of OSG is used for event simulation, detector modeling and data analysis for the Large Hadron Collider collaborations, 30% supports activities by eight other high energy, nuclear and gravitational wave collaborations, and 20% is harnessed by non-physics groups spanning structural biology, climate modeling and computational chemistry.

The five research areas of the InDHTC will act as an anchor for a diverse community of researchers, software developers and operators of computing facilities ranging from small laboratories to large computing centers. The institute researchers and their collaborators will use the computing and storage resources offered by the OSG to test and evaluate at-scale novel distributed computing frameworks and technologies. Following a long and established tradition of experimental computer science in the context of end-to-end computational problems, they will work closely with members of application communities on translating innovative algorithms and methods into deployable scientific computing capabilities. These collaborations will bring DHTC solutions across DOE science that can benefit from these technologies, including transparent access to leadership class computing facilities and will enable computer scientists to see their research and innovations contribute "on the ground" to transform the science it enables.

Leveraging the already established lasting and mutually beneficial partnerships across organizational and disciplinary boundaries, the InDHTC team will bring collaborative experience and knowhow to the SciDAC-3 community. Beyond ongoing relationships and explicit docking points with the OSG partnership, the InDHTC is committed to collaborate with other institutes on active outreach and engagement with the DOE application communities through publications, scheduled workshops and focused ad-hoc meetings.

2 Research Plan

We define DHTC to be the shared use of autonomous resources toward a common goal, where all the elements are optimized for maximizing computational throughput. Sharing of such resources requires a framework of mutual trust whereas maximizing throughput requires dependable access to as much processing and storage capacity as possible. The inherent stress between these requirements underpins the challenges that the DHTC community faces in developing frameworks and tools that translate the potential of distributed computing into high throughput capabilities. The five research teams of the InDHTC will jointly address these challenges by following a framework that is based on four underlying principles: ***Resource Diversity*****:** Maximizing throughput requires flexibility to accept many types of resources and the integration of multiple layers of software and services. ***Dependability*****:** Throughput must be tolerant to faults since the scale and distributed nature of HTC environments means some service or resource will always be unavailable. ***Autonomy:*** Enable users and resource providers from different domains and organizations to pool and share resources while preserving their local autonomy to set policies and select technologies. ***Mutual Trust:*** The formulation and delivery of a common goal through sharing requires a web of trust relationships that crosses the boundaries of organizations as well as software tools.

While each research area will work autonomously, the shared end-to-end focus of the institute will require close coordination between the five teams. This will be accomplished through crosscutting activities. Examples are developing a conceptual blueprint of application community needs, and assisting those communities in developing, selecting, modifying, or constructing solutions to interoperate within this model. Other such activities include technology evaluation and understanding the HTC needs of DOE scientists.

The *Data* area will focus on the different steps involved in interfacing processing and data in a DHTC environment. This involves job submission, hierarchical storage, cache management, wide area data movement, temporary file systems, and the co-scheduling of different resources. In current practice, each of these steps presents a problem of some kind: staging areas overflow; networks become overcommitted; caches are thrashed; and failures abound. These problems are currently managed manually by application communities with significant effort and lost throughput. We have identified resource allocation of networked storage and I/O capacity, dynamic deployment of support services and matchmaking for data access and storage resources as the initial technical foci for this area.

Software assurance, risk management and identity management are the cornerstones of dependable DHTC infrastructure. The *security* area will work along three threads of research that will address these challenges. One thread will focus on developing a trust framework for secure software development and integration. By creating a standard framework for describing both what software provides and expects of its environment regarding policy enforcement, security and privacy, a deployed set of software can be analyzed for gaps. Such gaps can lead to vulnerabilities and unintended interactions during integration of the software with other components and the operational environment. The other two threads of the security area will be to develop a framework for risk assessment and mitigation for distributed open science, and to establish a trust model as a framework for reasoning about identity management.

The *systems* area will address the impact of fast changing technologies for virtualization, multi-core, GPU and networking on DHTC. Working closely with the *tools* team this area will study the impact of such developments on DHTC scheduling, resource management and software deployment algorithms and tools. Guided by the DHTC blueprint and principals this area will serve as a conduit for research results into DHTC production infrastructures such as the OSG, by integrating technologies along two dimensions: across the institute research areas and according to application communities needs.

Researchers using DHTC do not run a single workflow for a single experiment; rather, they run workflow ensembles. Managing complex interrelated ensembles of jobs and their data products is a growing challenge for the DHTC community. The *workflow* area will address this challenge by developing methods for workflow lifecycle automation and for managing workflow ensembles. This will require novel approaches to the debugging and monitoring of long running distributed workflows.