Integrating Clouds and Cyberinfrastructure for CDS&E: Research Challenges

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**I. Introduction**

Cloud computing has revolutionized the procurement, use, and the overall economics of compute and data resources. It provides viable ways for users to acquire resources on an operational pay-as-you go basis rather than making an up-front capital investment: a factor that has significantly accelerated the pathway from concept to execution for many businesses and other users of IT. Given their penetration, it is very likely that cloud computing will join traditional research cyberinfrastructure (CI) components, such as high-performance computing (HPC) systems, clusters, and Grids in supporting scientific exploration and discovery.

Cloud computing has the potential for having a similar revolutionary impact on Computational and Data-Enabled Science and Engineering (CDS&E)[[1]](#footnote-1),[[2]](#footnote-2) in multiple ways by enabling new paradigms and practices. For example, clouds can increase overall productivity, provide resources for applications when local infrastructure is not available, supplement local infrastructure with additional capacity or complementary capabilities to meet dynamic needs, or provide resilience by moving execution to alternative resources when a failures occur. The ability to scale resources up and down is important when dealing with increased demand for resources in response to unexpected application needs, in support of ongoing experiments and new insights, to deal increased activity after important discoveries are made, when concluding research in preparation for sharing at a collaborative forum, or simply to support activity growth in an efficient manner. Similarly, the ability to seamlessly move computation to alternative resources is critical when providing continuous computational services required by many observatories. Finally, cloud computing is a disruption that may impact science in ways that we have not yet discovered.

However, before CDS&E can fully realize the potential benefits of cyberinfrastructure that integrates cloud services, important research challenges need to be addressed. In 2011/2012, the NITRD MAGIC[[3]](#footnote-3) subcommittee (chaired by Gabrielle Allen, NSF and Rich Carlson, DOE/SC) discussed and documented those challenges. This report summarizes these findings.

**II. Findings**

The NIRTD MAGIC subcommittee discussions in September 2011 (led by K. Keahey) focused on *applicability to science* and in April and May 2012 (led by M. Parashar[[4]](#footnote-4)) focused on the *Challenges and Opportunities of Integrating Clouds with Cyberinfrastructure*. During these calls the committee discussed experiences from projects such as FutureGrid, Open Science Data Cloud, Magellan, XSEDE and GENI, as well as core research challenges. An overall observation of the committee was that research in cloud computing remains challenging due to the lack of targeted funding opportunities, which handicaps major intellectual investments needed to realize the promise of clouds for science. The research challenges identified were grouped into 6 rough categories: (1) Algorithms and Application Formulations for Clouds, (2) Programming Models, Abstractions and Systems, (3) Middleware Stacks and Services, Management Services, (4) Data Management in the Cloud, (5) Security Policies and Mechanisms, and (6) Deployment/Transition to Practice. These categories and associated research challenges are presented below. Note that the discussions below are from the CDS&E perspective and are complementary to more general cloud research challenges.

**(1) Algorithms and Application Formulations for Clouds**

Cloud computing promotes abstractions, usage patterns and execution behaviors that are different form traditional CI platforms, and it is important to understand these differences and their impact on how algorithms are developed and applications are formulated. For example, only applications capable of dynamically integrating new resources can leverage on-demand availability of infrastructure clouds. Key research challenges in this category include exploring application formulations that can effectively utilize cloud computing and addressing, at the algorithmic level, implications of cloud characteristics such as elasticity, on-demand provisioning, virtualization, multi-tenancy, and failure. Furthermore, specific science/engineering applications classes lead to specific challenges, such as, for example, privacy in case of bio- and medical-informatics applications and bursty data streams in case of sensor-actuator applications.

**(2) Programming Models, Abstractions and Systems**

A key research challenge is developing appropriate programming models and systems that can enable CDS&E applications to take advantage clouds. These include developing programming abstractions and tools to support the federation of clouds (with the associated issues of interoperability and fungibility through multiple levels of the infrastructure) and CI and elastic access to cloud services, extending existing cloud programming models and platforms, e.g., MapReduce and BigTable, to support scientific computing, as well as exporting entire applications, applications patterns and kernels, optimized libraries, and/or specialized middleware as a service. Research addressing tools for application debugging, validation management and performance engineering is critical.

**(3) Middleware Stacks and Services, Management Services**

There currently exists a significant gap between the capabilities provided by clouds and the scientific user’s ability to leverage them. This is because the existing scientific middleware was based on assumptions reflected by traditional CI models, which are not always true for cloud computing. Middleware stacks and service are needed to support CDS&E application formulations and hybrid usage modes that target a mix of traditional CI and cloud capabilities, including support for dynamic cloud bursting and infrastructure federation. Some of the key research challenges are: provisioning, scheduling, management and optimization (multiple objectives including performance, energy, cost, reliability, etc.), interoperability, and integration of science-specific cloud storage models and solutions. Developing and deploying cloud software stacks providing platforms for testing and research is a particularly promising application of cloud computing.

**(4) Data Management in the Cloud**

Data management research challenges are broadly due to different types of cloud storage solutions and the nature of cloud connectivity. For example, the need to enable efficient access to data recently promoted the development of relaxed consistency models. Specific research challenges include support for selecting between the large variety of storage options with varying service levels, networks architectures to support data transport needs and their interaction with cloud storage offerings, and the co-location of compute and data.

**(5) Security Policies and Mechanisms**

Outsourcing storage and compute resources means that user’s data can potentially be, at least theoretically, exposed to subversion by the resource provider and, in a multi-tenancy environment, also other users. As a result, ensuring data privacy is a central issue of security for cloud computing. Additional challenges specific to CDS&E include interoperability with broader CI security mechanisms and policies, such as for example, single sign-on, federated identify management (e.g., inCommon, cilogin, SCIM, etc.), and security policies and mechanisms for specific applications, e.g., differential privacy and data anonymization requirements for bio/medical informatics applications.

**(6) Cloud Research Ecosystem – Deployment/Transition to Practice**

An urgent and critical challenge is establishing a cloud ecosystem that can drive the discovery and deep understanding of the needs of scientific projects in the context of cloud computing, as well as an understanding of its potential impact on science. To do this we need to put in place mechanisms and experimental infrastructure that will overcome the transition barrier for scientific communities. Specific directions for addressing this challenge include the development of community testbeds, documentation of experiences and best practices, establishing support and advisory forums for science, and developing of curricula and training modules.

**III. Actions and Timelines**

The MAGIC committee discussions highlighted both short term and longer-term action items to address the research challenges outlined above. The **short term** activities are largely focused on the category 6 above and included:

(1) Development of strategic pilot projects to identify/highlight advantages as well as challenges in using clouds for science and education;

(2) Definition and prototyping of services bridging existing CI investments (e.g., XSEDE, OSG, FutureGrid) and cloud services (e.g., EC2, Azure, etc.) as well as designs for long-term co-existence and interoperability of these facilities;

(3) Fostering of community research and experimentation testbeds for cloud computing as well as establishment of benchmarks and common metrics;

(4) Development of processes for the translation of research innovation into software frameworks tools that can be used by applications;

(5) Creation of community forums for exchange of ideas and artifacts.

**Longer-term** activities include setting up programs to address the fundamental research challenges discussed above in categories 1-5, and incorporating resulting research innovations into sustainable software system that can be deployed and used by the community.

1. M. Parashar, M. AbdelBaky and I. Rodero, “Cloud Paradigms and Practices for CDS&E,” Technical Report, 2012, <http://cometcloud.org>, 2012. [↑](#footnote-ref-1)
2. G. Fox, D. Gannon, “Cloud Programming Paradigms for Technical Computing Applications,” Technical Report, <http://grids.ucs.indiana.edu/ptliupages/publications/Cloud%20Programming%20Paradigms.pdf>, 2012. [↑](#footnote-ref-2)
3. https://connect.nitrd.gov/nitrdgroups/index.php?title=Middleware\_And\_Grid\_Interagency\_Coordination\_(MAGIC) [↑](#footnote-ref-3)
4. Minutes of these meeting can be found at https://connect.nitrd.gov/nitrdgroups/index.php?title=MAGIC\_Meetings\_2012. [↑](#footnote-ref-4)