Cyberinfrastructure, Cloud Computing, Science Gateways, Visualization, and Cyberinfrastructure Ease of Use

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INTRODUCTION

Computers accelerate our ability to achieve scientific breakthroughs. As technology evolves and new research needs come to light, the role for cyberinfrastructure as "knowledge" infrastructure continues to expand. In essence, cyberinfrastructure can be thought of as the integration of supercomputers, data resources, visualization, and people that extends the impact and utility of information technology. This article defines and discusses cyberinfrastructure and the related topics of science gateways and campus bridging, identifies future challenges in cyberinfrastructure, and discusses challenges and opportunities related to the evolution of cyberinfrastructure and cloud computing.

BACKGROUND

Today's US national cyberinfrastructure ecosystem grew out from the National Science Foundation-funded supercomputer centers program of the 1980s (National Science Foundation, 2006). Four centers provided supercomputers and support for their use by the US research community. Researchers generally accessed one supercomputer at a time, sometimes logging into a front-end interface. At this time, the focus of the research computing community was centered on supercomputers – traditionally defined as computers that are among the fastest in existence. Over time there have been several different supercomputer architectures, but the key points were that supercomputers were monolithic systems that were among the fastest in the world. At present we can think of supercomputers as being a subset of the more general term high performance computer (HPC) – where HPC means that many computer processors work together, in concert, to solve large computational

challenges and where the computer processors communicate via very fast, networks internal to the HPC system. HPC focuses on computing problems where a high degree of communication is needed among the processors working together on a particular problem. HPC is a more general term than supercomputers because there are many HPC systems that are modest in total processing capacity relative to the fastest supercomputers in the world (cf. Top500.Org, 2016).

In the early days of supercomputing, using multiple supercomputers in concert was not possible. In the late 1980s, the National Research and Education Network initiative created several testbeds for distributed computing, including the CASA testbed which linked geographically distributed supercomputers to solve large-scale scientific challenges (U.S. Congress Office of Technology Assessment, 1993). A turning point in distributed high performance computing was the I-WAY project – a short-term demonstration of innovative science enabled by linking multiple supercomputers with high performance networks (Korab & Brown, 1995). It demonstrated the possibilities to advance science and engineering by linking supercomputers using high-speed networks.

In the late 1990s, the NASA Information Power Grid provided a production grid of multiple supercomputers connected by a high-speed network (Johnston, Gannon, & Nitzberg, 1999). Around this time began also the concept of high throughput computing (HTC) with a software system called Condor (Litzkow, Livny, & Mutka, 1988). HTC takes the approach of breaking a problem up into small pieces of work and distributing them to multiple CPUs over network connections that may be relatively slow. HTC best suits problems where relatively little communication is needed among the processors working together on a particular problem or simulation. Because HTC applications can operate relatively efficiently on processors with little communication among the processors, HTC applications have always fit naturally into a distributed computing environment (Thain,

Tannenbaum, & Livny, 2005). Today, a popular framework for distributed storage and processing of large data sets is Apache Hadoop (The Apache Software Foundation, 2006).

Over time, distributed computing evolved into 'grids,' with grids emerging as a commonly used term in the late 1990s. Typically, computational grids are the hardware and software infrastructure which provides access to the computational capabilities (Foster & Kesselman, 1998, 2004). *Middleware* is a key software component of cyberinfrastructure, enabling the disparate components of cyberinfrastructure to work together. In effect, middleware manages complex interactions between resources which allows for the development of new networked applications (National Science Foundation, 2004). Around the turn of the century, the US government funded two major grid projects – TeraGrid and the Open Science Grid. In 2001, the NSF funded an experimental computational, storage, and visualization resource called TeraGrid, which developed grid capabilities for supercomputer centers (National Science Foundation, 2006). The Open Science Grid (OSG) (Livny et al., 2006; Open Science Grid, 2015), first funded with that name in 2006, grew out of three projects that developed HTC grids for the purpose of analyzing data from physics experiments (Avery, 2007).

Tying geographically distributed computing systems together into grids to create a whole greater than the sum of its parts was widespread around the turn of the century. However, the term grid computing was becoming laden with sometimes competing definitions. In addition to computing and data grids, other terms such as collaboration, semantic, and peer-to-peer grids emerged, distinguished by the characteristics of the protocols and interactions between components (Fox, 2006). The potential for confusion and competing definitions of different types of grids led Dr. Ruzena Bajcsy, then NSF assistant director of the Computer and Information Science and Engineering Directorate, to use the term cyberinfrastructure when charging a new advisory group to offer advice to

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