Sudhakar Pamidighantam

Senior Research Scientist, National Center for Supercomputing Applications

University of Illinois at Urbana-Champaign

spamidig@ncsa.illinois.edu

Topics of Interest

1. Programming Models for the Cloud
2. Cloud Inter-operability and Standardization

Current Research.

Current research interests are in cyberenvironments for science and engineering research, education and training. We are in production with a computational chemistry science gateway (GridChem.org) and we are close to deploying a workflow based cyberinfrastructure for parameter optimization Gateway for molecular sciences (ParamChem.org) both supported by NSF. A training cyberinfrastructure is in the planning to be deployed for engineering applications this year supported by EU funding under LinkSceem2 project. As part of comprehensive cyberenvironments we are interested in hybrid environments with heterogeneous resources including clouds as the services should be able to exploit heterogeneous resources depending on optimal service levels for each type. The clouds are particularly relevant for addressing on demand computing needs, training needs and certain education needs. Certain class of high throughput computing needs for research can also be fulfilled by cloud resources and can be used in hybrid settings and for individual tasks in workflows for the above mentioned types of computations.

Future Research

Cloud cyberinfrastructures(CI) are of current interest in providing and extending high performance computational resources for scientific and engineering research, education and other services. We propose to provide this extension for two Cyberenvironments, an integrated set of tools and services, to illustrate a spectrum of scientific workflows and usage scenarios that can exploit coherently and opportunistically a hybrid CI eco-system consisting of Clouds (e.g., Microsoft Windows Azure, NCSA private cloud), TeraGrid/XD, Future Grid and other resources. These cyberenvironments are GridChem[gridchem.org], a production Science Gateway, ParamChem, A Paramaterization Gateway and Discovery Environments for Science and Engineering Research and Training (DESERT) for multiphysics multiscale simulation research and training and provide logistics for other sensor driven decision support systems such as RT-GeoSWAVE[Liu et al., 2010]. Common integration modalities for engaging Cloud computing resources and inherent services, obtain requirements for productive utilization of the hybrid CI resources, and analyze the conditions for the optimal utilization for both computing and data/meta-data management needs. The Clouds fulfill an unmet need for *on demand* resources for the Cyberenvironments. This investigation of diverse use cases will establish the utility and need for the hybrid CI with Clouds in solving complex scientific and engineering computational and data management issues. We will also provide important metrics for an end-to-end integration and utilization of "Clouds" in production, and establish benchmarks for setting future standards of services for hybrid CI-based Cyberenvironments. This project will advance the state-of-the-art of using hybrid-CI for E-Science in general and Science and Engineering Discovery Environments for research, training and Decision Support in particular. Domain-specific computational codes and workflow patterns will be explored to opportunistically use Clouds (Microsoft Azure) and other computing resources. The services that will be developed could be deployed in other E-Science Hybrid CI environments. Data management and provenance tracking in such a hybrid CI eco-system will be experimentally explored to reveal the usage patterns and underlying challenges. Benchmarks with production scientific research codes and workflows will advance the understanding of the role played by Clouds in hybrid CI environments and how they are supported. The production environment that the services will be deployed advances production related management beyond simple test bed models and provide a complete end to end deployment strategy for Hybrid-CI and results in direct impact for scientific and engineering research, computational science education and allied services to diverse communities. Such comprehensive cyberenvironments would also be deployed experimentally for private sector under the NCSA private sector program that may help US competitiveness for manufacturing sector by reducing the costs of prototyping and making product development cycles more efficient.