SURAgrid Applications
(As of 3/15/07)

Applications Under Active Deployment

UNC/SCOOP: Storm-Surge Modeling with ADCIRC – ADCIRC is a finite element method shallow water model for computing tidal and storm surge water level and depth-averaged currents associated with these phenomena. Grid environments such as SURAgrid are ideal for the ensembles in applications like ADCIRC, which is one of a set included under SCOOP (SURA Coastal Ocean Observing and Prediction) program that is focused on improving predictions of coastal phenomena. Project Partners: University of North Carolina Marine Science, Renaissance Computing Institute (RENCI), MCNC, SAIC.

LSU/SCOOP: Wave Modeling with Wave Watch 3 – WAVEWATCH 3 solves the spectral action density balance equation for wave number-direction spectra. Grids such as SURAgrid have the potential to greatly improve the ability to distribute Event Driven Wave Watch 3 instances across geographical domains and take advantage of supercomputing resources to process wave model for Hurricane events. Project Partners: Center for Computation and Technology (CCT), Louisiana State University; SCOOP; Bedford Institute of Oceanography.

UFL/SCOOP: CH3D Storm Surge Monitoring System with Grid Appliance – The Curvilinear Hydrodynamics in Three Dimensions (CH3D) application is used to model physical processes in bays, rivers, lakes, and estuaries. CH3D is a circulation model that aids storm surge forecasting and is one of a set of applications included under the SCOOP program. On SURAgrid, CH3D is implemented in combination with the Grid Appliance application, which is a self-configuring virtual machine that contains the IPOP virtual networking package and the NSF/NMI Condor middleware. The retrospective analysis the application duo is used for requires high-throughput, is computationally intensive, and can thus take advantage of the resources available on SURAgrid.

LSU: UCoMs Petroleum Reservoir Simulation via Task Farming – UCoMS (the Ubiquitous Computing and Monitoring System) is a DOE-funded project that addresses key research issues to arrive at appropriate technical solutions in the areas of wireless networked systems, grid computing, and application software. In order to optimize the return on investment for a given reservoir, this project uses task farming and ResGrid, a grid-enabled reservoir simulation framework, to conduct massive reservoir simulations on grids such as SURAgrid to generate both good estimates of reservoir parameters and reliable predictions of oil production. Project Partners: CCT at LSU; Department of Petroleum Engineering, LSU; Center for Advanced Computer Studies, University of Louisiana at Lafayette; Department of Computer Science, Southern University and A&M College, Baton Rouge.

NCSU: EPANET Simulation-Optimization for Threat Management in Urban Water Systems – This application incorporates dynamic demand data, in real-time, into a simulation-optimization process for contamination threat management in drinking water distribution systems. The nature of this work is highly compute-intensive and requires multi-level parallel processing via computer clusters and high-performance computing architectures such as SURAgrid. Simulation-Optimization with EPANET is part of a multi-disciplinary, three-year NSF-funded DDDAS (Dynamic Data-Driven Application Systems) research project to develop a cyberinfrastructure system that will both adapt to and control changing needs in data, models, computer resources and management choices facilitated by a dynamic workflow design. Project Partners: North Carolina State University; University of Chicago; University of Cincinnati; University of South Carolina.

TTU: Grid-enabled ENDyne (Grid implementation of electron nuclear dynamics (END) theory) – The ENDyne application is used in simulations, such as calculating the trajectories of molecules, in areas such

as Computational Chemistry. Environments like SURAgrid offer the grid-enabled version of ENDYNE access to the large number of CPUs required to do timely trajectory calculations, thus SURAgrid can aid the user in carrying out more efficient research.

ODU: Bio-electric Simulator for Whole Body Tissues – This application is designed to simulate the response of a "whole body tissue" model to potential/current stimulus through direct electrode contact. The Electrical and Computer Engineering and Office of Computing and Communications Services departments at Old Dominion University are using SURAgrid to grid-enable this application to utilize concepts such as work-flow and virtual data methods. The Bio-electric Simulator, which is both computation and data intensive, has been demonstrated to scale with the number of processors and can thus benefit from the accessibility to the additional computational resources of SURAgrid.

GSU: Multiple Genome Sequencing & Alignment – This multiple sequence alignment algorithm application takes a number of genome sequences as input and gives an aligned sequence based on their structure by using a pairwise alignment algorithm. When run on grids like SURAgrid, carefully designed and grid-enabled algorithms like this, which implement a memory efficient method for computation and are also parallelized efficiently so that the workload is well distributed on grids, afford bioinformatics users a performance comparable to cluster environments while giving them added flexibility and scalability.

UAB: Grid-Enabled Distributed BLAST – BLAST is a database search application for matching protein and nucleotide sequences. Maximizing the throughput of searches is key to improving research results. This distributed implementation of BLAST uses the DynamicBLAST Meta-scheduler to select appropriate grid resources for select query strings. Globus is used for job staging, submission and retrieval. ncbiBLAST performs the computations. Jobs are submitted using a web-based interface that leverages campus identity credentials via Pubcookie and manages grid authentication on behalf of the user via MyProxy, providing a simplified user authentication experience.

Applications under Consideration

SURA: SURAgrid Teaching Environment -The SURAgrid Teaching Environment is a multi-organization project that is addressing the development of teaching grid technology and teaching with grids. Effective teaching about grids, within Computer Science as well as other disciplines, is greatly enhanced by students and instructors having hands-on access to a stable grid environment. Through coordinated commitment, operation and support across a subset of SURAgrid resources, SURAgrid is developing a predictable, secure and reliable grid-based teaching facility for use by SURAgrid sites in their grid course development and/or delivery. Basic grid access for students to supplement theory taught in an HPC course at Old Dominion University is being provided for spring 2007 semester.

Hampton University Tokamak Divertor Map – Hampton University's Center for Fusion Research and Training (CFRT) main area of research is mathematical maps to calculate trajectories of magnetic field lines in divertor tokamaks. The purpose is to calculate the footprint of magnetic field lines on collector plates of tokamaks. Mathematical maps preserve topological invariants, and have the advantage of computational efficiency. We take a large number of initial positions of field lines and calculate their trajectories for a long time. Evolution of each field line is independent of other field lines. So, each processor can independently calculate trajectory (or path) of one field line. When paths of all field lines are calculated, their accumulative statistical behavior can then be determined. So our research on maps is ideally suited to run on a large number of processors in a parallel fashion.