THE WRF PORTAL EFFORT

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1. INTRODUCTION

Scientific computing involves much more than program execution. Research also includes data preparation, code configuration, parameter definition, job submission, monitoring, and data analysis, visualization, and archival. For larger problems or large numbers of jobs, this "overhead" can take a disproportionate amount of time, even while the need to access, thoroughly interrogate, and understand the results remains unchanged.

Atmospheric scientists using WRF are working with scientific portal specialists in what is becoming a new paradigm for large-scale scientific computing. The "WRF Portal" described here includes development at the National Center for Supercomputing Applications (NCSA) and at the University of Oklahoma. The promise of portal technologies includes:

1. The ability to readily carry out computationally intensive tasks across multiple (e.g. PACI) sites or multiple machines at a single site
2. A sophisticated software infrastructure for job and data management using Grid services (GridFTP, remote job submission, etc.)
3. Improved graphical user interfaces (GUIs) for job preparation, execution and monitoring
4. The end-to-end workflow needed to manage large numbers of simulations.

2. DEVELOPMENT AND USE WITH WRF

Scientific portal efforts using WRF are underway at the University of Illinois (NCSA, in collaboration with the Atmospheric Sciences Department) and at the University of Oklahoma in consort with the MEAD expedition at NCSA and LEAD², a multi-organization project funded by NSF as a large ITR. Extensive research on portals is also taking place at Indiana University², and is planned at the Forecast Systems Laboratory. This portal development is directed toward a greatly enhanced computational capability, one that makes possible extensive modeling at, and across, the participating computational centers.

The ability to execute applications locally as well as across the network - "without becoming experts in Grid technology" (Gannon et al. 2004) - means computationally intensive problems can be distributed at runtime based on availability of resources as well as those best suited for the problem. Carrying out large sets of simulations, such as those in parameter or sensitivity studies or ensemble modeling, then becomes tractable. For the scientific user, an interface and infrastructure is needed in which scientific applications may be "plugged in" to portal services.

At Oklahoma, the web-based MEAD Portal Interface (MEAD-PI) includes the ability to prepare initial data and WRF configuration settings (Fig. 1). As part of this capability, the recently released ARPS2WRF package provides integration with, and through MEAD-PI the ability to execute WRF from, the ARPS Data Analysis System (Carpenter et al. 2004).

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At NCSA, the Java-based Grid Computing Environment for Applications has been designed to deliver "upper middleware tools enabling scientific applications to take advantage of distributed computational and data resources." This includes the job management system OGRE\(^5\), the Open Grid Computing Environments (GCE) Runtime Engine. The NCSA system also includes the GridDesktop interface that allows specification of input parameters and data, and the remote execution and monitoring of applications on local resources or distant Grid machines, using OGRE.

Examples of early use of this system for running WRF appear in Fig. 2. Shown are examples of a WRF job series (Fig. 2A), preparing new WRF input parameters (B), following the progress of individual job execution (C) and post-processing (D), and images derived from model output (E). Rather than being a template of what is possible, all of the elements in Fig. 2 have been tested and implemented. The NCSA team has carried out storm simulations with WRF v1.3 on computing systems at NCSA, San Diego and the California Institute of Technology, entirely through the portal engine. A new Java web start interface has been developed, and the system is being extended for input parameters of multiple jobs, making submission and monitoring of large sets of simulations possible. The use of this software will be discussed further at the Workshop.

The software and distributed job execution and management abilities described here will be incorporated into work on LEAD (see article by Wilhelmson et al., this volume), and is a glimpse of how future scientific computation will be done.

3. REFERENCES


4. ACKNOWLEDGMENTS

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\(^5\) http://otfrid.ncsa.uiuc.edu/ogre