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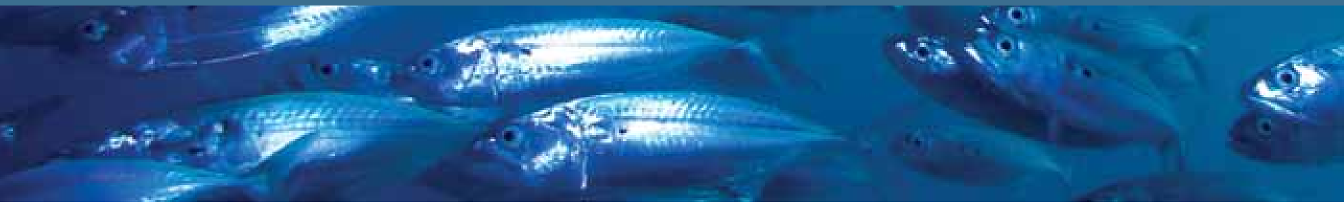

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From the Technical Editor

One hundred years ago, most non-seafaring people's experience of the ocean was aboard a passenger liner. These ships represented the pinnacle of technology. Massive structures moved at high speed across the world's oceans. These ships were one thousand feet long and travelled at 30 knots. They were symbols of power and prestige and given patriotic names. They made regular passages across the Atlantic and there was competition for the fastest crossing. They were the only way to travel and their accommodation reflected the social structure of the time. The *Queen Mary*, launched in 1936, carried over two thousand passengers divided between first class, tourist class, and third class. Each class had its own infrastructure within the ship. Although this system reflected a segregated society, it provided affordable passage to migrants escaping economic hardship and old social structures.

Skip ahead to the present and the great liners of the past have become obsolete due to the airplane. The last liners were built in the 1960s even though it was clear that the airplane was the new (and more egalitarian) standard in long-distance travel. The new standard in ocean passenger transport became the cruise ship. Recent statistics show that the cruise industry continues to grow, despite the recent recession. December 2009 saw the maiden voyage of the world's largest cruise ship *Oasis of the Seas* with accommodation for almost 6,300 passengers. The focus is now on luxury and entertainment rather than high-speed transportation. As a result, these ships have become floating resorts, with all kinds of entertainment for all ages. The ships still represent the pinnacle of ocean technology. There is less emphasis on high speed, but there is more emphasis on manoeuverability, to enable this large ship to dock. The ship is fitted with azimuthing podded propulsion systems and bow thrusters. The ship's hull is wide to provide a stable platform with a shallow draft. The power needed for the electric propulsion motors is 60 MW, which is a fraction of the total generating capacity of almost 96 MW. By contrast, the *Queen Mary* had a total power of 120 MW, most of which would have gone into driving the propellers. All this onboard entertainment comes with a cost.

Unfortunately, my own cruising experience has been at the other end of the spectrum, in small sailboats, with amenities little better than a dry tent. Coincidently this style of activity also started about 100 years ago, with people having more leisure time, sufficient disposable income, and a desire to explore the world for fun. I have been to some beautiful locations during my cruises, but sometimes I would trade it for fresh sushi that was not dependent on my limited skill with a fishing rod.

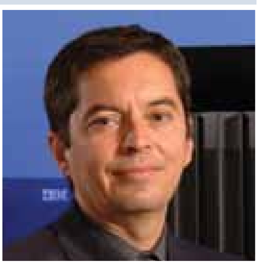
Dr. David Molyneux
Technical Editor

Sorry Joni - we really do know clouds

Justin R. Davis

Renato J. Figueiredo

Y. Peter Sheng



José Fortes

Davis, Figueiredo, Sheng, Fortes, Ganguly, Paramygin, Wolinsky, Zhang, and Tutak describe ways to enhance the use of cyberinfrastructure (distributed computing via the Internet) by the coastal and estuarine modeling community.

Who should read this paper?

Researchers and educators with an interest in complex modeling and visualization of coastal and estuarine processes.

Why is it important?

Complex, process-based, integrated modeling systems are more commonly being used to predict the future state of coastal and estuarine systems, but they can be difficult to use, cumbersome to modify, and typically come with heavy computational requirements. In this paper, the authors discuss the techniques used and lessons learned building coastal and estuarine science applications using emerging cyberinfrastructure technologies. These technologies allow for the complete encapsulation of all necessary libraries, models, and visualization tools into a single package which can be tailored for various research, training, educational, and outreach activities. Through a simple and practical software system, the authors demonstrate how robust coastal and estuarine science research and educational tools can be developed and easily shared, making the results more accessible to all concerned.

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Justin R. Davis is a Research Assistant Scientist at the University of Florida. His research focuses on the development and application of integrated coastal and estuarine modeling systems using advanced cyberinfrastructure.

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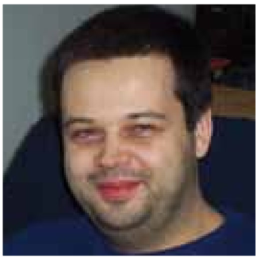
Arijit Ganguly



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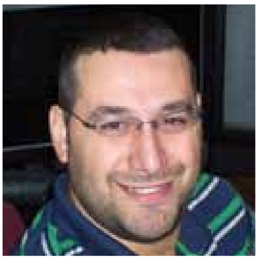
David Wolinsky

Jian Zhang



Bilge Tutak

APPLICATION OF EMERGING CYBERINFRASTRUCTURE TECHNOLOGIES TO AID IN THE EDUCATION AND TRAINING OF COASTAL AND ESTUARINE SCIENTISTS

Justin R. Davis, Renato J. Figueiredo, Y. Peter Sheng, José Fortes, Arijit Ganguly, Vladimir A. Paramygin, David Wolinsky, Jian Zhang, and Bilge Tutak

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ABSTRACT

While coastal and estuary simulation models are powerful tools, the effort which goes into learning how to setup, compile, configure and execute such models and their corresponding visualization and analysis tools can be significant. In addition, these models often require significant computational resources, particularly when ensemble calculations are performed or when a real-time event (e.g. forecasts of storm surge and inundation) demands a quick turn-around time. In this paper, several coastal and estuary science (CES) applications which have been developed to aid in the education and training of CES using emerging cyberinfrastructure (CI) technologies are discussed. These technologies allow for the complete encapsulation of all necessary libraries, models and visualization tools into virtual machines (VMs). Furthermore, these VMs automatically and securely connect to a "Grid" of computing resources enabling the user to seamlessly access remote computing resources. Beginning with the enabling In-VIGO virtualization CI technology and soon after by the Grid Appliance, CES applications which used these underlying technologies are presented. The In-VIGO applications, using a web portal interface, focus on simulations of hydrodynamics in the lower St. Johns River and Charlotte Harbor, Florida. These applications emphasize the ease with which unmodified applications can be integrated into the system. In addition, the ability to integrate Linux applications with Microsoft Windows visualization as well as the simplicity by which ensembles can be handled is also presented. Finally, an entire Grid Appliance has been developed which allows coastal simulation models, visualization tools, and Grid computing middleware to be packaged and made available to users. These capabilities are demonstrated through an application which focuses on hydrodynamics and species transport in the Guana-Tolomato-Matanzas National Estuarine Research Reserve.

NOMENCLATURE

CES	=	coastal and estuary science
CHIMP	=	Chesapeake Interactive Modeling Project
CI	=	cyberinfrastructure
CI-TEAM	=	Cyberinfrastructure Training, Education, Advancement, and Mentoring of Our 21st Century Workforce
GTM NERR	=	Guana-Tolomato-Matanzas National Estuarine Research Reserve
GUI	=	graphical user interface
IaaS	=	infrastructure-as-a-service
IMS	=	integrated modeling system
IOOS	=	integrated ocean observing system

LAN	=	local area network	SJRWMD	=	St. Johns River Water Management District
LSJR	=	lower St. Johns River	SURA	=	Southeastern Universities Research Association
LSU	=	Louisiana State University	UF	=	University of Florida
MOM	=	maximum of maximum	VDFS	=	virtual distributed file system
ORNL	=	Oak Ridge National Laboratory	VIMS	=	Virginia Institute of Marine Science
P2P	=	peer-to-peer	VM	=	virtual machine
ROMS	=	Regional Ocean Modeling System	WFS	=	web feature service
SOAP	=	simple object access protocol	WMS	=	web mapping service
SCOOP	=	SURA Coastal Ocean Observing and Prediction			

INTRODUCTION

To enhance the education and training of coastal and estuarine science (CES), as well as to aid in estuarine ecosystem management and restoration, scientists, engineers and educators need effective modeling tools. These tools can range from the use of local knowledge, to statistically-based probabilistic estimates determined from years of measured data, to fully three-dimensional process-based integrated modeling systems such as CH3D-IMS [Sheng et al., 2002; Sheng, 2003; Sheng and Kim, 2009]. As such tools are improved to better represent the underlying physical processes, their ability to accurately predict the future state of the system improves greatly. While complex, process-based, integrated modeling systems are more commonly being used to predict the future state of the coastal and estuarine systems [Sheng, 2003], they can be difficult to use, cumbersome to modify, and typically come with a heavy computational cost.

The availability of a cyberinfrastructure (CI) that supports modeling/simulation of coastal and estuarine processes is poised to have a profound impact on the ability of coastal and estuarine scientists and engineers to address the aforementioned challenges, using quantitative analyses to improve efforts in ecosystem-based water quality and resource management, emergency preparedness and response, and planned development, among others. This paper describes capacity building activities which address the challenge of lowering the barriers of entry that exist in the adoption of CI in the coastal and estuarine modeling community. In this context, the meaning of "capacity building" is to assist the community to identify and address issues and gain the insights, knowledge and experience needed to solve problems and implement changes in operations or management by using CI.

CH3D, the model used in this study, is a Curvilinear-grid Hydrodynamic 3D model originally developed by Sheng [1987; 1990; and 1998]. CH3D uses a horizontally boundary-fitted curvilinear grid and a vertically sigma grid, and hence is suitable for application to coastal and nearshore waters with complex shoreline and bathymetry. A fully Integrated Modeling System CH3D-IMS [Sheng, 2000; 2003; and Sheng et al., 2002] has been developed and applied to several

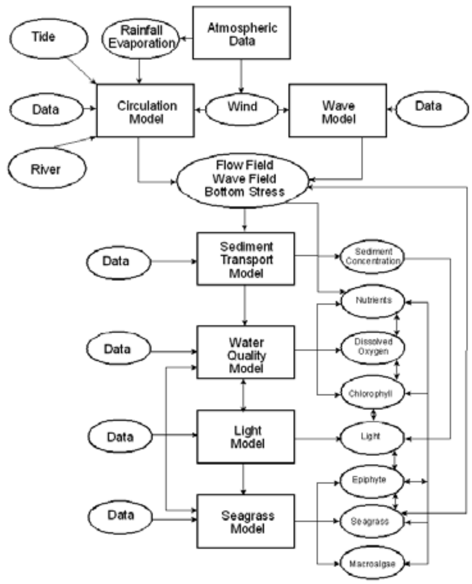

Figure 1: Block diagram of CH3D Integrated Modeling System (IMS).

estuarine systems including the Indian River Lagoon, Tampa Bay, and Charlotte Harbor. Recent applications of CH3D and CH3D-IMS to integrated-scale and integrated-process modeling of large coastal and estuarine waters are summarized in Sheng et al. [2004] and Sheng and Kim [2009]. CH3D-IMS includes circulation (CH3D), wave, sediment transport (CH3D-SED3D), water quality (CH3D-WQ3D), light attenuation (CH3D-LA), and seagrass models (CH3D-SAV) (Figure 1). Currently, as part of the Southeastern Universities Research Association (SURA) Coastal Ocean Observing and Prediction (SCOOP) Program, a CH3D-based real-time forecasting system of storm surge and coastal flooding, CH3D-SSMS (http://ch3d-ssms.coastal.ufl.edu), is being developed for several Florida coastal regions: East Florida Coast, Tampa Bay, Charlotte Harbor, and the northern Gulf of Mexico.

While models such as CH3D are powerful, the effort which goes into learning how to setup, compile, configure and execute such models and their corresponding visualization and analysis tools can be significant. In addition, these models often require significant computational resources, particularly when ensemble calculations are performed or when a real-time event (e.g. forecasts of storm surge and inundation) demands a quick turn-around time.

In this paper, we discuss the techniques used and lessons learned building CES applications with In-VIGO and Grid Appliances. These technologies allow for the complete encapsulation of all necessary libraries, models and visualization tools into a virtual machine (VM). Furthermore, this VM automatically and securely connects to a "Grid" (Grid computing is defined as "flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources [Foster et al., 2001]) of computing resources enabling the user to gain access to significantly more computing power than typically available with their own resources.

A related effort to bring a simple interface to lay users is the Chesapeake Interactive Modeling Project (CHIMP) developed at the University of Minnesota, Duluth [Austin et al., 2006]. CHIMP consists of a graphical front end to a ROMS (Regional Ocean Modeling System) [Shchepetkin and McWilliams, 2005] simulation of the Chesapeake Bay located along the mid-Atlantic U.S. coastline. Targeting science museums, K-20 education and resource managers, users can alter fresh water runoff, wind speed and direction, etc. as the simulation is running to investigate how hydrodynamic and salinity transport vary in the Bay. While CHIMP has the benefit of being installable without any supporting infrastructure and is similar to the applications presented herein in its ease-of-use, it is significantly different in several ways: it is limited to running in a Microsoft Windows-based environment; parameters such as model resolution are limited to what the graphical user interface provides; only a single simulation can be performed at a time; and there is no ability to access distributed computing resources.

EMERGING CI TECHNOLOGIES

A universal CI for coastal and estuarine scientists must support a diverse set of tools and users, as well as those who develop and/or maintain the tools. Tools are diverse with respect to how they are designed and programmed beyond the fact that they can be written in different programming languages. Some codes are sequential in nature while others are parallel. Some tools are open-source research-grade codes often developed in universities and research labs for an initially restricted set of users. In contrast, other tools are commercial codes – for which only binaries might be available – with a large user base. Tool interfaces and usage modes also vary greatly – from command-line oriented with numeric and/or text-like inputs and outputs, to sophisticated graphical user interfaces (GUIs).

Users are diverse with respect to how they interact with simulation tools. Many users will be interested in conducting research by using simulation tools, whereas other users might only be interested in demonstration runs for evaluation and for educational purposes. In some cases tool usage for educational and research purposes requires interactive access to resources whereas in other cases it uses batch execution. Tool usage may require extensive resources and execution times or may only use a few computational cycles on a single machine. An important class of users consists of those who develop, modify or compose existing tools in order to maintain them, experiment with new models or adapt existing ones to specific needs. The following sections describe some of these emerging CI technologies.

In-VIGO

In-VIGO [Adabala et al., 2005; Fortes et al., 2005] is a Grid middleware system that differentiates from related approaches with respect to its extensive reliance on virtualization techniques, including logical user accounts [Adabala et al., 2004], virtual machines [Figueiredo et al., 2003; Zhao et al., 2004], virtual file systems [Zhao et al., 2005], virtual networks [Sundararaj and Dinda, 2004] and virtual applications (Figure 2). In-VIGO enables the installation and service of unmodified applications with a user-friendly front-end that provides to the user a Web-based interface for the configuration and steering of simulation tools – both batch-oriented and interactive graphical user interface tools that can reach a broader user base. Finally, In-VIGO can run on any resources (virtual or physical) that have interfaces available to control the instantiation of virtual machines. By supporting a broad user and application base, In-VIGO middleware can be used to create science gateways for diverse communities – nanoelectronics, computer architecture and coastal and estuarine sciences being representative examples. The first use of In-VIGO for CES was an application which simulated the release and movement of discrete

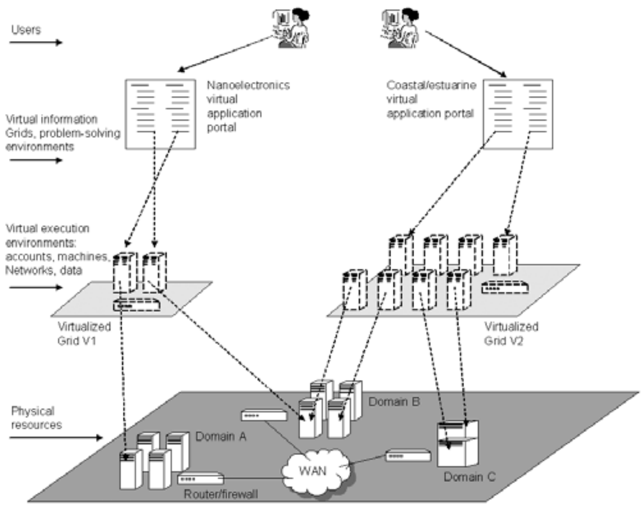

Figure 2: In-VIGO middleware uses virtualized resources to create virtualized grid execution environments that support unmodified programs. Application portals tailored to different science/engineering domains can be deployed. Users interact with grid resources through "virtual applications" accessible via Web browsers. Users do not have accounts on physical resources – rather, they authenticate to In-VIGO logical user accounts through a login/password pair, while In-VIGO's user and resource management middleware interfaces dynamically broker resources on the user's behalf. In-VIGO can interface with several grid and cluster-based middleware for job submission (e.g. PKI-SSH, Globus GRAM, Condor-G, and PBS).

particles in Florida Bay, FL [Davis et al., 2004]. The CH3D hydrodynamics model was dynamically coupled with particle tracking and visualization models. Coupling of the models was achieved through the use of a Grid-enabled version of MPI, MPICH-G2 and then executed on a small Local Area Network (LAN)-based Grid. The coupled system was then used to simulate the trajectories of 2000 particles with concurrent visualization of particle movement provided through the In-VIGO web portal. Although the resource pool was relatively small, this initial application demonstrated the relative ease of converting an existing coupled modeling system into a dynamically coupled system running in a Grid environment.

With the initial success of the particle tracking application, three additional In-VIGO applications were then developed for a prototype Wide Area Network (WAN) Grid deployed by the SURA SCOOP Program. This Grid consisted of identical pools of resources deployed at the University of Florida (UF), the Virginia Institute of Marine Science (VIMS), and Louisiana State University (LSU). Resources included two Dell Dimension 4600, one Dell PowerEdge 2600, and one Dell PowerEdge 6600. In total, 24 processor elements were available for use. These applications included a distributed file system used to share files between the sites and two additional applications based on the CH3D model.
In the following sections, several coastal and estuarine science applications based on the In-VIGO infrastructure are presented: a Virtual Distributed File System and several CH1D/CH3D models.

Virtual Distributed File System

To facilitate the exchange of files and low level distributed modeling coupling between SURA SCOOP Program resources (UF, VIMS and LSU), a virtual distributed file system (VDFS) was deployed connecting resources at these sites using the In-VIGO middleware (Figure 3). Network connectivity between the sites was made through *ssh* tunneling, thus providing a secure and reliable connection to transfer data. Access to the file system was achieved through a local loopback mount and made available via Microsoft Windows

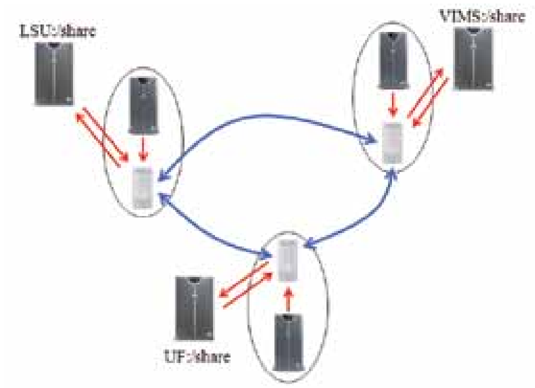

Figure 3: The virtual distributed file system connecting UF, VIMS and LSU.

through Samba, through command line-level server access or through the web portal interface. Samba is a freely available software suite that provides file service interoperability between Unix and Microsoft Windows clients (http://www.samba.org). The benefits of the VDFS approach are that: 1) data transfer is secure; 2) data resources can be added / removed on demand; and 3) access to both local and remote data occurs through simple file read/writes with no special libraries (e.g. MPI) and that both local and remote data access can occur at any level. Depending on network connectivity, the VDFS can potentially be slow; however, a previous study which coupled coastal and estuarine models running at UF, VIMS and LSU using the VDFS showed only a 13% increase in wall clock time [Davis et al., 2006].

CH1D Application

Dispersion in estuarine and riverine environments is influenced by circulation and mixing which are caused by tides, wind, and density gradients created by freshwater from the rivers and salt water from the ocean. Estuarine and riverine circulation is also significantly affected by the complex bathymetry and geometry. To demonstrate some of these concepts, an application was deployed based on a simple one-dimensional estuary/river transport and dispersion model developed for the Oak Ridge National Laboratory (ORNL) [Sheng and Davis, 2004a and 2004b] to study the lower St. Johns River (LSJR), Florida. The model, CH1D (1D version of CH3D), was based on an enhanced version of the one-dimensional model originally developed by Sheng et al. [1990] for the Indian River Lagoon, Florida. The rationale for using a one-dimensional model in this application is that it is very efficient and thus many different scenarios can be demonstrated quickly.

Using observed initial and boundary condition data from 1998, the user selects a release time and location and begins the simulation (Figure 4). Observed data include water level, wind speed and direction, tributary discharge, precipitation and evaporation, etc. The application then uses CH1D to simulate the circulation and transport in the LSJR for the time period 30 days before until seven days after the release time. Simulated contours of species concentration are then provided to the

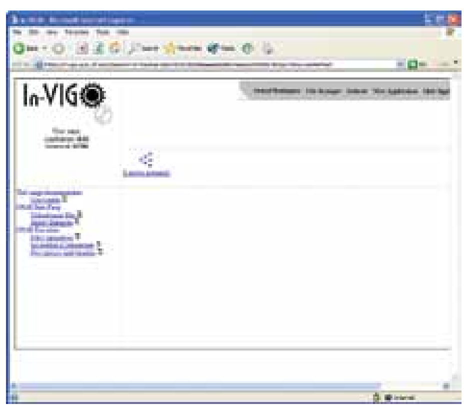

Figure 4: The In-VIGO CH1D application simulation setup interface.

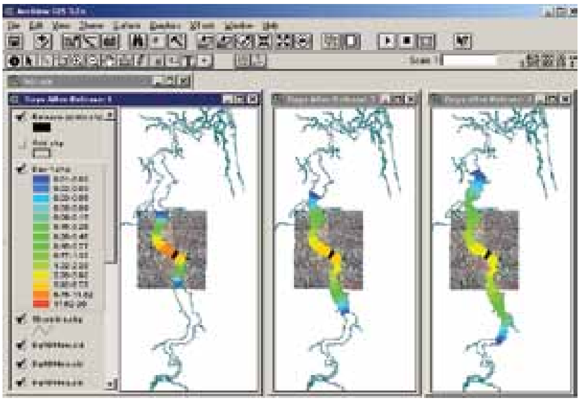

Figure 5: The concentration of the conservative tracer species one, three, and seven days after release.

user through an integrated Microsoft Windows-based ESRI ArcGIS 3.2 interface at one, three, and seven days after the initial release time days (Figure 5).

The CH1D model was compiled on an external Linux machine using the Intel Fortran Compiler and then uploaded into an In-VIGO Linux VM. No modification of the model was needed. An In-VIGO application rule was created allowing for two web interfaces to the CH1D application: 1) Basic: The user selects simulation parameters through a series of drop down menus; and 2) Advanced: The user selects simulation parameters by uploading their own input or boundary condition files. The job submission process for the CH1D application is shown in Figure 6.

The relatively simple CH1D application demonstrated: 1) using the In-VIGO web portal for job configuration, instantiation, and visualization for a CES application; 2) coupling between Linux and Microsoft Windows applications on the Grid; and 3) how Grid-based modeling can be performed without model user/developer needing to know Grid details.

CH1D Ensemble Application

A typical application of CES models is to perform an ensemble of simulations to represent errors within the system. These simulations are typically first performed independently and then combined to produce a single overall product. This type of application is ideally suited to In-VIGO where the system can schedule and submit jobs to numerous Grid resources automatically. Thus, to demonstrate this capability, a CH1D ensemble application was created which expands the previous application to include an ensemble parameter.

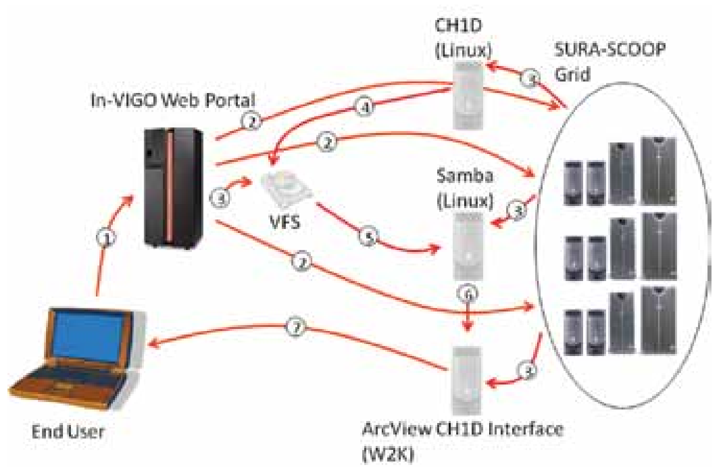

Figure 6: The job submission process for the CH1D application: 1) Login into the In-VIGO Portal; 2) Select the CH1D application and input parameters and then start the job; 3) In-VIGO then stages the necessary input and output files on the virtual file system (VFS) and sets up the output interface. In-VIGO schedules and submits jobs to available grid resources and notifies user when complete; 4) As the model runs, output is written back to the VFS; 5) Once completed, output data is made available to Microsoft Windows clients using Samba; 6) Output data is then loaded by the ArcView GUI and plotted; 7) The In-VIGO ArcView application is started and the results viewed.

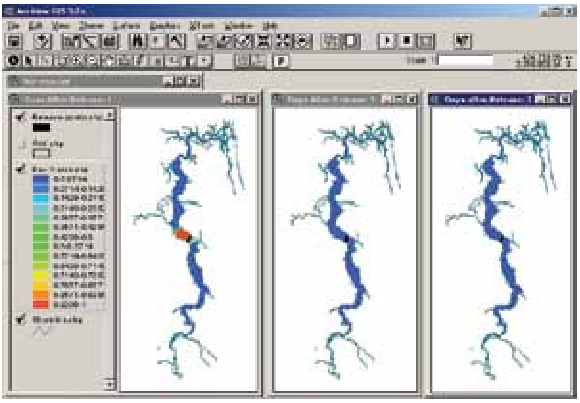

Figure 7: The probability that the conservative tracer exceeds a critical value one, three, and seven days after release.

For purposes of estuary modeling, river discharge data is one of the least accurate datasets used as a boundary condition. For example, daily discharge collected by the U.S. Geological Society is only accurate to within 5-10% (e.g. see [Boning, 1992]) and considered "good" if the values are within only 10% of the actual value. Thus, the CH1D ensemble application uses discharge error as the ensemble parameter. Assuming a normal distribution of errors (mean=0, std. dev=1) at each discharge location, flow values are allowed to vary (e.g. within a range of +-10%). The user selects the number of simulations to perform and then begins the ensemble. Once all the simulations have been completed, an additional post-processing step is performed which aggregates all the simulations to produce an ensemble mean and an ensemble standard deviation. In addition, using a specified critical value of concentration, the probability that the simulated concentration exceeds this value can be determined. Again, an ArcGIS GUI is made available to the user which allows for viewing of these three products. An example of a probability of exceedance plot is shown in Figure 7.

The CH1D ensemble application demonstrated how In-VIGO can be used to setup, execute and post-process a typical ensemble application used for CES.

CH3D Ensemble Application

Another typical CES application is the simulation of storm surge and inundation. Using virtualization techniques, the advanced CH3D Storm Surge Modeling System (SSMS) [Sheng et al., 2006; 2008] is Grid-enabled through the In-VIGO web portal and Grid middleware. Again, virtualization allows the model to be Grid-enabled without modification of the source codes in any way, thus requiring minimal IT expertise by the modeler. A more detailed description of this application can be found in Davis et al. [2006].

Using the prototype Grid resources, an ensemble is created to demonstrate the response of Tampa Bay, FL, to various hypothetical tracks of Hurricane Charley (2004). Although more advanced probabilistic methods could be used (e.g. [Davis et al., 2008a, 2008b, and 2010]), for this application, these tracks are obtained through simple clockwise or counter clockwise rotation of the best track data [Pasch et al., 2005]. Wind fields are then created from the tracks using a simple parametric wind model [Holland, 1980]. Similar to the other applications, the user selects a start time for the simulation and defines the ensemble: minimum rotation angle, maximum rotation angle and the number of simulations to perform. The user then begins the simulation at which time In-VIGO creates storm tracks by evenly dividing the number of simulations between rotation angle extents. Simulations are then distributed for computation on Grid resources.

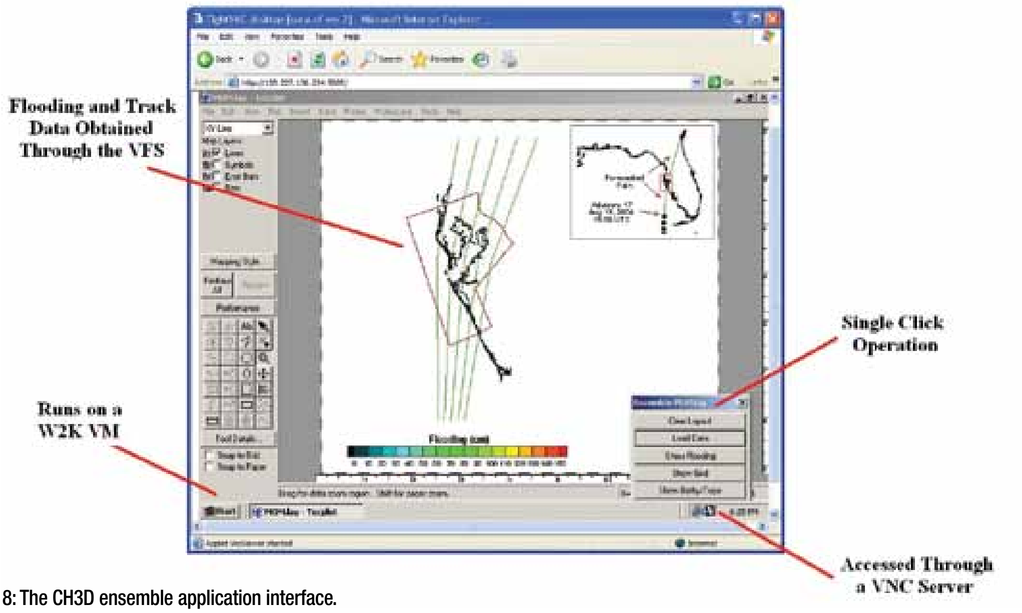

Figure 8: The CH3D ensemble application interface.

Once complete, a post-processing routine calculates the water level Maximum of Maximum (MOM) for all the simulations. A water level MOM is a useful tool for emergency managers who wish to see the "worst case" scenario for a given storm. The MOM simulated using Grid resources is identical to the MOM simulated on a single host with the advantage that the Grid computations can be performed in parallel across the regional Grid's resources. A small 1% increase in wall clock time is observed when solving the simulations on different Grid resources. The user is then presented with a Microsoft Windows-based Tecplot visualization tool (integrated into In-VIGO) which displays the water level MOM (Figure 8).

As with the previous application, the CH3D ensemble application demonstrates how an ensemble application can be performed, albeit with a more advanced model.

Grid Appliance

The Grid Appliance builds upon the core virtualization technologies of In-VIGO, and packages them in a way that facilitates dissemination to end users. While In-VIGO provides a Web-based portal interface to its users, essentially giving them access to a remote infrastructure, the Grid appliance allows users to run part of the middleware on their own personal computer. The appliance is then used to educate scientists, engineers and students on three key aspects of such environments: application development and deployment on science gateways (for model developers); user, resource and application management (for CI technical personnel); and simulation-based experimentation on science gateways (for end users in research and education).

The Grid Appliance is a self-configuring Virtual Machine appliance that is used to create ad-hoc pools of computer resources both within a local-area and across wide-area networks [Wolinsky et al., 2006]. Although the appliance focus has been on executing high-throughput, long-running jobs, it has also proven successful in performing real-time, forecasting simulations. Appliances are connected to each other through a peer-to-peer (P2P) virtual network using private IP addresses called IPOP [Ganguly et al., 2006]. Upon starting an appliance, it is automatically connected to a pool of resources and is capable of submitting and executing jobs using the Condor Grid scheduler. Currently, a public infrastructure for bootstrapping such pools is running on PlanetLab (http://www.planet-lab.org); deployments on private resource pools are also supported. For example, pools are currently in place for researchers working on a National Oceanic and Atmospheric Administration (NOAA) integrated ocean observing system (IOOS) program funded surge and inundation Testbed (http://ioos.coastal.ufl.edu) as well as for the SURA SCOOP Program.

The Grid Appliance approach is fully compatible with cloud-provided "Infrastructure-as-a-Service" (IaaS) resources such as Amazon EC2. This is one of the main advantages of virtual appliance packaging and the use of virtual networks; that is, a user can run an appliance on local resources, on cloud-provided resources, or both. Amazon EC2 provides an infrastructure where to run appliances; what the Grid Appliance provides in this context is an environment that is tailored to the coastal/estuarine science community, in particular educators.

In the following section, a Grid-enabled application, CH3D-GTM, which applies the robust shallow water estuarine model CH3D to the Guana-Tolomato-Matanzas National Estuarine Research Reserve (GTM NERR), is described.

CI-TEAM APPLICATION

The goal of the CI-TEAM application is to deploy a CES model which will enable users to learn about CES and CI concepts through an interactive virtual application. To this end, a Grid-enabled application, CH3D-GTM, which applies CH3D to the GTM, has been deployed as a virtual application in a CI-TEAMS web portal.

The application is centred on the release of a conservative tracer species in the GTM NERR that is located on the northeast coast of Florida, U.S. (Figure 9). The waters of the GTM NERR reside within the St. Johns River Water Management District (SJRWMD) jurisdiction. Portions of these waters are currently being studied by the SJRWMD as part of the Northern Coastal Basin Program [SJRWMD 2003a; 2003b]. The release of tracer species is often used in CES to study the movement of non-native species in a region to better understand their source. For example, the GTM is currently being threatened by the arrival of green mussels (*Perna viridis*). These mussels are bivalve mollusks which are native to the Indo-Pacific [Sidall, 1980], but have now spread throughout the world. In Florida, they were first observed on the west coast in Tampa Bay (1999) [TBNEP, 2000; Benson et al., 2001]. Within several years, they were seen as far south on the west coast as the Ten Thousand Islands region (2002) as well as on the east coast between Daytona (2002) and Jacksonville (2003) Beaches [Baker et al., 2007].

The CH3D-GTM virtual application is based on an existing CH3D model of the GTM [Sheng et al., 2008]. This model has been validated with tidal constituent data available at nearly 20 locations (including Pablo Creek, Oak Landing, Palm Valley, Vilano Bridge, St. Augustine, Anastasia Island, Ft. Matanzas, Matanzas Inlet, Flagler and Ormond Beach,

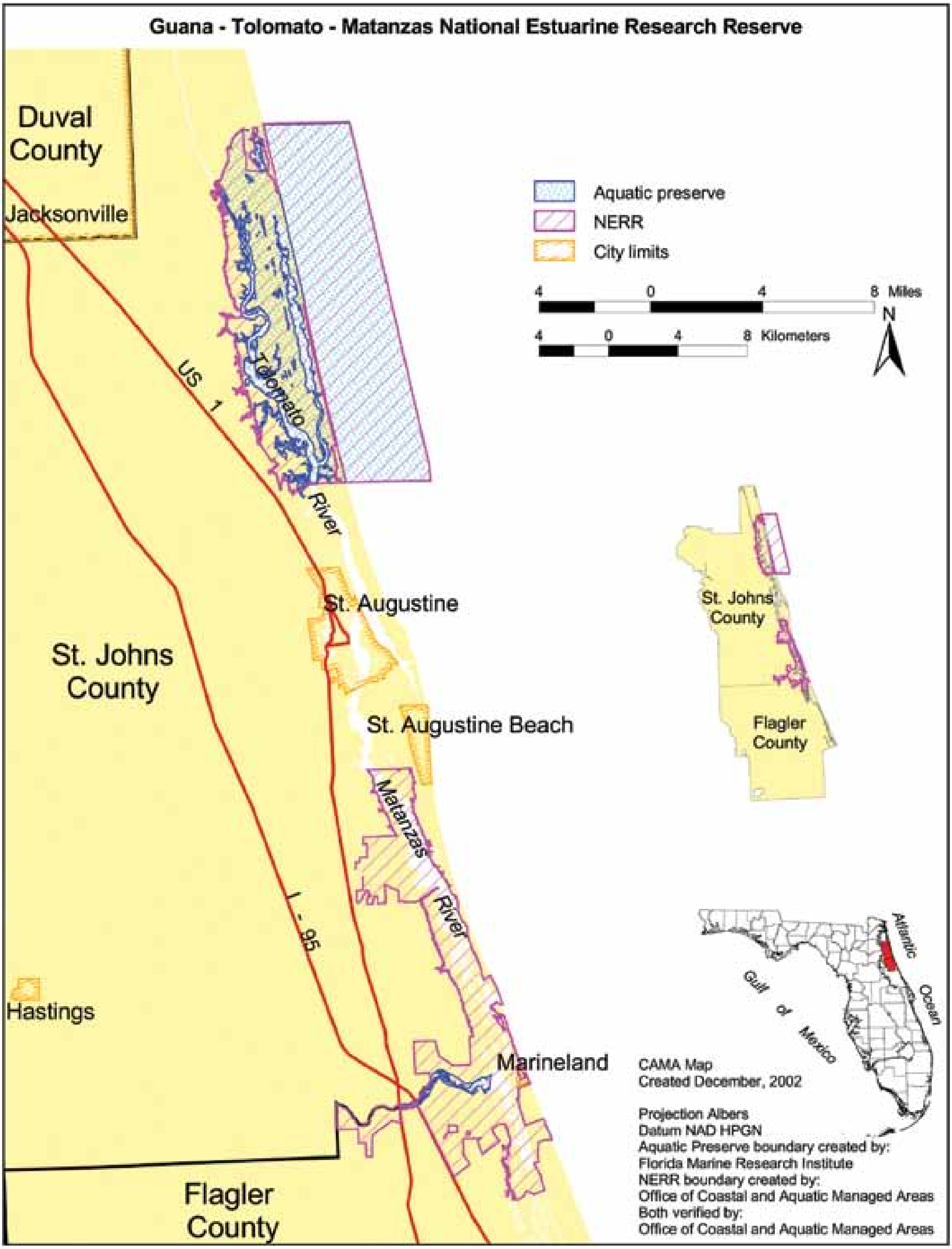

Figure 9: Boundaries of the GTM NERR. The Reserve is divided by the city of St. Augustine and extends approximately 48 kilometres (30 miles) north and 48 kilometres (30 miles) south of the city.

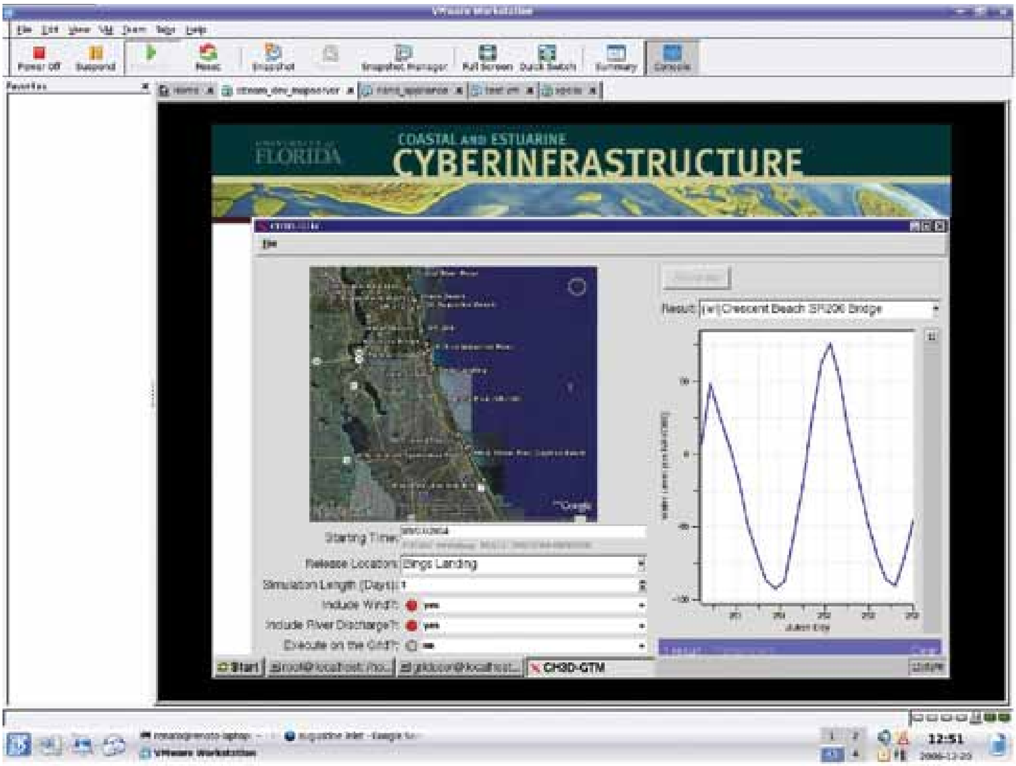

Figure 10: The first generation CI-TEAM Grid Appliance GUI for the CH3D-GTM Application.

Halifax River, and Ponce de Leon), water level and salinity data at four water-quality monitoring stations (Fort Matanzas, Pellicer Creek, Pine Island, and San Sebastian) as well as other NERR, U.S. Geological Society, NOAA, and SJRWMD data.

Two GUIs have been developed to interface with the CH3D-GTM application. The first generation GUI (Figure 10) is a stand-alone application developed using the Rappture Toolkit (http://www.rappture.org). Rappture is a C++ toolkit which has additional bindings that let it be used in various applications (e.g. C, Fortran, Perl, and Tcl). A series of simple dialog boxes and drop down menus was designed for the user to configure the simulation. As Rappture does not support geo-referenced coordinate systems, simulated spatial fields (e.g. water level or concentration) within the interface were obtained by including a static image plotted by MapServer (http://mapserver.gis.umn.edu). Time series of simulated parameters were plotted using native Rappture graphics routines. After surveying users of the first generation interface, several key capabilities were found to be lacking: the ability to zoom-in and zoom out, the ability to incorporate external geo-referenced datasets (e.g. aerial photos), and the ability to extract values from time series plots. Based on this feedback, development on a second GUI was begun.

The second generation GUI (Figure 11) is web-based and was developed using JavaScript, the PHP scripting language (http://www.php.net), and OpenLayers (http://www.openlayers.org). Simulated parameters are made available

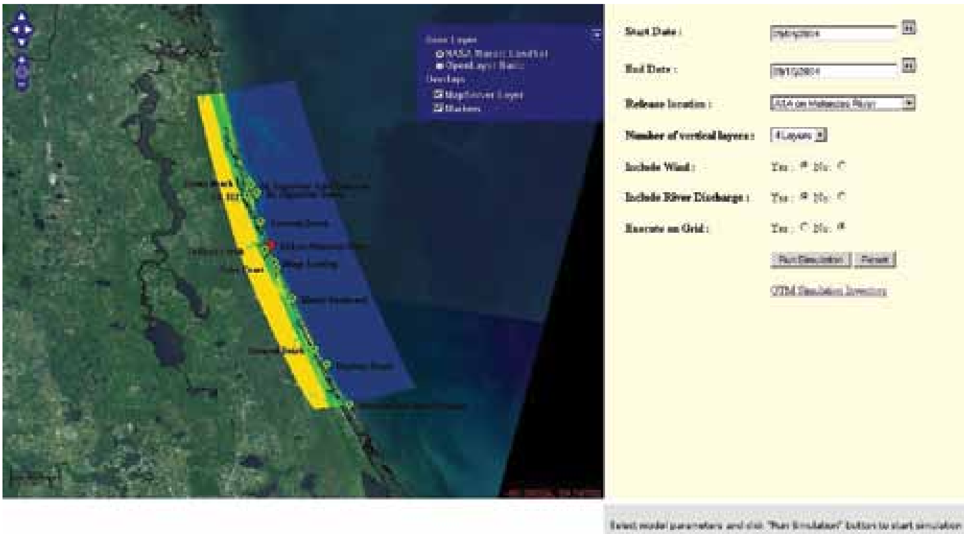

Figure 11: The second generation CI-TEAM Grid Appliance GUI for the CH3D-GTM Application developed using OpenLayers. Background layers consist of the OpenLayers basic global layer and NASA Mosaic Landsat 7 images.

as a Web Mapping Service (WMS) using MapServer's PHP MapScript and then plotted using OpenLayers. OpenLayers is a JavaScript library for displaying maps in web browsers capable of visualizing any WMS or Web Feature Service (WFS). The interface is accessed by connecting a web browser to an Apache HTTP web server (http://httpd.apache.org) running locally on the Appliance. For spatial reference, two sets of background images are accessible within the generated maps. These images are obtained through WMS requests to the following external sites: MetaCarta (http://www.metacarta.com) provides the OpenLayers basic global layer and Telascience (http://www.telascience.org) provides the NASA Mosaic Landsat 7 images. Shorelines and state boundaries are obtained from the U.S. Department of Transportation (http://www borderplanning.fhwa.dot.gov/data_gis.asp). By using WMS and OpenLayers, users can move around the region and zoom in and out without loss of viewing resolution (Figure 12). Time series plots of simulated water level (Figure 13) and conservative trace concentration (Figure 14) are displayed using the Flotr JavaScript plotting library (http://solutoire.com/flotr). Flotr supports "mouse tracking" extraction of values from plots using the flotr: mouseover event. The interface also supports temporal animation of spatial plots of water level and concentration.

Application scenarios used in the teaching processes include simulations of hydrodynamics and advection/diffusion of conservative tracer species (Eulerian/Lagrangian). These scenarios

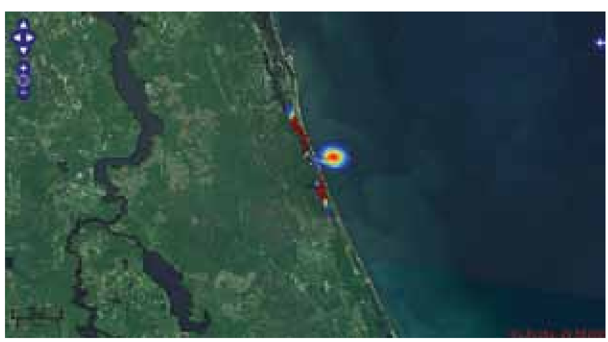

Figure 12: A zoomed-in snapshot of species concentration in the vicinity of Matanzas Inlet as viewed from the second generation GUI.

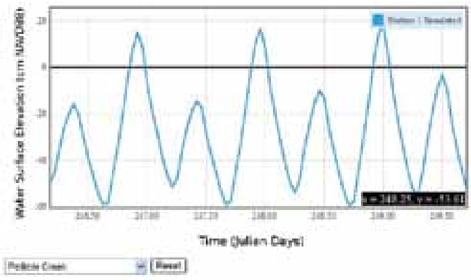

Figure 13: Simulated water level at Pellicer Creek as viewed from the second generation GUI. Mouse tracking values are shown in the bottom right.

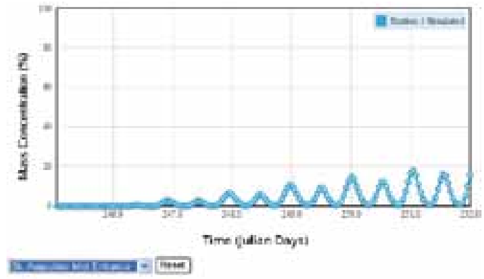

Figure 14: Simulated concentration of the tracer species at St. Augustine Inlet as viewed from the second generation GUI.

are based on variable simulation parameters which are available through the GUIs. A list of the variable simulation parameters for the first generation GUI is shown in Table 1. In the second generation GUI, the length of the simulation is replaced by the ending date and the number of vertical layers used by the model (4 or 8) can be specified.

OUTREACH

Along with making the CI-TEAM Grid Appliance and corresponding educational materials publicly available on the internet (http://www.grid-appliance.org), the CI-TEAM application has been targeted at several critical user groups: students and researchers, practicing scientists and engineers, and visitors to the GTM NERR.

Students and Researchers

The CI-TEAM appliance is currently being used as a teaching aide in several Coastal and Oceanographic and Electrical and Computer Engineering classes. It is being used as a teaching aide for both estuary hydrodynamics as well as CI. The appliance can also be used by researchers; for example, these models can be helpful for instrument placement for other studies currently being conducted in the GTM such as Dix et al. [2008]. Additionally, the base Grid appliance was used as an aid in teaching cluster/Grid computing concepts in a system services class at the University of Applied Sciences Northwestern Switzerland. Interestingly, the instructor of this class came across the appliance through the VMware appliance challenge where the Grid Appliance received an honourable mention.

Starting Time	MM/DD/YYYY			
Release Location	Pellicer Creek St. Aug. Airport Intl. Spd. Blvd. A1A on Mat. R. Vilano Bridge SR-206	Crescent Beach St. Aug. Inlet Ormond Beach Matanzas Bridge St. Aug. Light.	Guana R. Rd. Ponce de Leon Inlet Moody Blvd. Ft. Matanzas St. Aug. Beach	Bings Landing Main St. Pier Palm Coast Bridge of Lions SR-312
Simulation Length	days			
Include Wind?	yes or no			
Include River Discharge?	yes or no			
Execute on the Grid?	yes or no			

Table 1: Variable simulation parameters available within the first generation CI-TEAM GUI. The simulation period defined by the starting time and simulation time must be between Sep. 7, 2004, and Sep. 6, 2005.

Practicing Scientists and Engineers

Florida is divided into five Water Management Districts, which are dedicated to the preservation and management of Florida's precious water resources. The SJRWMD is responsible for managing ground and surface water supplies in all or part of 18 counties in northeast and east-central Florida. More than 700 dedicated staff members do this each day from offices in Palatka (Headquarters), Jacksonville, Altamonte Springs, and Palm Bay. Duties of the District include: issuing permits for various water use activities, buying land to preserve or restore vital wetlands and adjacent lands, conducting research about the quality and quantity of ground and surface water resources, mapping of ground and surface water resources, and conducting outreach and public education programs.

A hands-on CI education session at the SJRWMD, attended by District engineers and IT personnel, was conducted to demonstrate the CI-TEAM appliance. Using provided appliance software, the attendees installed the software themselves in the classroom PC desktops. The training session took a total of three hours, with a combination of a short presentation and hands-on experiments with Condor tutorial applications and the CH3D-GTM model. The sessions ran smoothly; all attendees were able to successfully install and use the software. Since then, engineers at the District started implementing a pilot program which is based on the use of VM appliances customized with their software for the execution of batch simulation jobs (Sun Microsystems Grid Engine) within their own domain.

Visitors to the GTM NERR

A major goal of the NERR program is to improve coastal decision making by generating and transferring knowledge about coastal ecosystems. Reserve staff work with local communities and regional groups to address natural resource management issues, such as non-point source pollution, habitat restoration and invasive species. Through integrated research and education, the reserves help communities develop strategies to deal successfully with these coastal resource issues. Reserves provide adult audiences with training on estuarine issues of concern in their local communities through the NERRS coastal training programs. They offer classes for K-20 students and support teachers through professional development programs in marine education. Reserves also provide long-term water quality monitoring as well as the opportunities and infrastructure for both scientists and graduate students to conduct research in a “living laboratory.”

The GTM Environmental Educational Center is a new 21,000 square-foot facility that overlooks the Guana River Aquatic Preserve. Within the facility are exhibits, classrooms/auditoriums, laboratories and an outdoor amphitheater overlooking the Preserve. Educational programs are offered for school teachers, students, adults and environmental professionals. The Grid Appliance software is currently being made part of a Center exhibit.

FUTURE WORK

The coastal science applications presented herein represent only the beginnings of applications that can and will be incorporated into the virtualized CI. Additional work is ongoing in the following areas:

Additional Scenarios

While the hydrodynamic and transport simulations currently available as applications helped demonstrate some key estuarine physics concepts, more advanced scenarios are being developed and implemented. Currently the transport application is based on the advection / diffusion equations applied in an Eulerian framework. To further these types of applications, a transport application based on a Lagrangian framework is planned. Also known as particle modeling, the application will simulate the path of a "rubber ducky" set adrift in the domain. This application will also have the advantage of being more relatable to the K-5 grade levels that frequent the GTM NERR Educational Center. With the recent increase in the frequency and intensity of hurricanes in the region, an application based on the simulation of storm surge and inundation is also currently being developed (see *Integration with SCOOP* on page 56).

The current applications are barotropic thus implicitly ignoring the complex density gradient interactions that can occur in estuaries; hence, several baroclinic scenarios are planned. In 2003, a large scale coastal upwelling event occurred off Florida's NE coast [McCarthy, 2005]. During August and September of the following year, the region was affected by several hurricanes with heavy rainfall totals (e.g. see [Sheng et al., 2008]. Although each hurricane moved through the system quickly, it took nearly three months for the extremely low salinity values to recover to the pre-hurricane season values. Using results from global ocean models such as NCOM [Barron et al., 2005] or HYCOM [Bleck, 2002] for open boundary conditions, baroclinic applications based on these two events are planned.

Increased Functionality

To facilitate synthesis, additional analysis and visualization tools will be incorporated. Because of the flexibility of the infrastructure, both commercial and public domain tools can be included. Commercial tools, which require a purchased license, can be installed directly and configured to only allow certain users or certain domains access rights. In situations where installing the tool directly is problematic, the user can use a local copy of the tool and access data through the virtual file system using NFS or Samba. Useful commercial tools which may be added include: ArcGIS (http://www.esri.com), Matlab (http://www.matlab.com), and SAS (http://www.sas.com). Public domain tools which may be added include Arc Hydro (Maidment 2002), an Arc GIS data model, GRASS GIS (http://grass.itc.it), Scilab (http://www.scilab.org), and R (http://www.r-project.org). Rather than adding GIS packages such as these individually, using the freely available GIS Workstation VM: GISVM (http://gisvm.com) developed by R. Pinho, these packages can be added all at once using the appliance's stackable file system.

The CH3D applications developed so far have focused on the northeast coast of Florida. Additional applications are being planned based on other CH3D domains currently in use such as: Charlotte Harbor, FL; Tampa Bay, FL; Lake Okeechobee, FL; and the Northern Gulf of Mexico. Applications being planned revolve around hydrodynamics, storm surge and inundation, sediment transport and water quality. In addition, other modeling systems may be added such as

ADCCIRC and ELCIRC. By having additional models available, inter-model comparisons will be facilitated.

With the addition of new models, domains and tools, additional observed data will be needed for use as model boundary and initial conditions as well as for verification and validation. To facilitate obtaining these data, tools which data integrated through web services such as Hydroseek (http://www.hydroseek.org/search) (e.g. see [McKee and Graham, 2008]) will be incorporated.

Integration with SCOOP

SURA was established in 1980 and is a collaboration of over sixty universities working together to improve research in science and engineering. Some of their goals include: improve scientific research, strengthen scientific and technical capabilities of the southeast, and provide training and education for the generation to come. The SURA SCOOP Program provides information and technology that helps the community, especially coastal population, understand the science behind prediction. By combining scientists, internet resources, tools, and ideas great discoveries can be made. With this, it is very important to take the data and models and make them available to any type of user [Bogden et al., 2007].

A Grid Appliance application which incorporates the SCOOP tools and services into a single package is currently being developed. This application includes examples of how to: query the SCOOP catalog through publicly available Simple Object Access Protocol (SOAP) (http://scoop.sura.org/services/inventory.html) and web (http://scoop.sura.org/Catalog/) services [Conover et al., 2006; Graves et al., 2008]; download data from the SCOOP archives (e. g. [MacLaren et al., 2005; Huang et al., 2006]) (http://www.scoop.lsu.edu; http://scoop.tamu.edu); and visualize these data through various web mapping services tools. Additionally, several applications using CH3D-SSMS have been incorporated which use data in the SCOOP archive to simulate the storm surge and inundation response during several hurricane scenarios.

CONCLUSIONS

While models such as CH3D are very powerful, the effort which goes into learning how to setup, compile, configure and execute such models and their corresponding visualization and analysis tools can be quite significant. In addition, these models often require significant computational resources, particularly when ensemble calculations are performed or when a real-time event (e.g. forecasts of storm surge and inundation) demands a quick turn-around time.

In this paper, we have discussed how CES applications have been made available to scientists and educators using emerging CI technologies. These technologies allow for the complete encapsulation of all necessary libraries, models and visualization tools into a VM. Furthermore, this VM automatically connects securely to a Grid of computing resources providing the user with significantly more computing power.

Beginning with enabling CI technology In-VIGO and followed by the Grid Appliance, CES applications which used these underlying systems have been presented. The In-VIGO applications, using a web portal interface, focused on CH3D simulations of hydrodynamics in the LSJR and Charlotte Harbor, FL. These applications emphasized the ease of which applications can be integrated, unmodified into the system. In addition, the ability to integrate Linux applications with Microsoft Windows visualization as well as the simplicity by which ensembles can be handled was also presented.

The Grid Appliance allows an entire modeling, visualization and Grid computing system to be packaged and made available to users. These capabilities were demonstrated through the CES application which focused on hydrodynamics and species transport in the GTM NERR. Several users groups (students/ researchers, practicing engineers and the GTM NERR Educational Center) have been using the appliance to better understand the dynamics of the system. While the original goal of the appliance was to educate users on both elements of CES and CI, different types of users had slightly different outcomes. For example, practicing engineers, who are very experienced in CES, were more interested in using the virtualization technology to enhance their ability to perform pre-defined scenarios; while researchers at the GTM NERR, who are also very experienced in CES, were more interested in using the appliance for developing new scenarios. Ultimately, it is the flexibility of the appliance to be able to work with a variety of user groups who have a range of skill sets, which makes this technology so widely appealing to the CES community.

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