Integrated-Process and Integrated-Scale Modeling of Large Coastal and Estuarine Areas

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ABSTRACT

To predict the response of coastal and estuarine ecosystems to anthropogenic and natural changes, it is necessary to conduct integrated-process and integrated-scale modeling of large coastal and estuarine areas. This paper presents an integrated modeling system, CH3D-IMS (http://ch3d.coastal.ufl.edu/), which includes models of circulation, wave, particle trajectory, sediment transport, water quality dynamics, light attenuation, and seagrass dynamics. The CH3D-IMS has been and continues to be validated with data from various estuaries in Florida. A 3-D variable-density groundwater flow model and a fishery model are being coupled to the CH3D-IMS. We present example applications of the CH3D-IMS including: (a) simulation of the Indian River Lagoon and trajectory of Shuttle *Columbia* debris in North and Central Florida Atlantic Coastal water, (b) simulation of storm surge in Tampa Bay, Sarasota Bay and adjacent Gulf of Mexico, and (c) simulation of circulation in Charlotte Harbor and adjacent Gulf of Mexico water. As the integrated modeling system continues to be applied to ever more complex problems over increasingly larger coastal areas, it requires more computational resources and disciplinary expertises which are often unavailable in any single institution. To facilitate integrated-process and integrated-scale modeling by multiple institutions, the development of an infrastructure - a regional modeling "grid"- is proposed.

INTRODUCTION

More than 50% of the U.S. and world population live within 100 miles from the coastline. By 2025, it is expected that more than 75% of the population will live in the coastal zone. Changes in estuarine and coastal ecosystems have occurred due to anthropogenic and natural causes. On the one hand, increased pollutant loadings have led to deteriorated water quality, increased incidences of harmful algal bloom, and loss of fishery habitat. On the other hand, climatic change and episodic storms have affected ecosystems. To protect and restore ecosystems and to mitigate storm-induced damages, it is essential to be able to predict the response of coastal ecosystems to anthropogenic and natural climatic changes. To this end, integrated modeling systems that include a variety of physical and biogeochemical processes and cover a wide range of spatial (from boundary layers to basin/global scale) and temporal (from turbulence to decadal) scales are needed. A calibrated and validated integrated modeling system, e.g., the CH3D-IMS (Sheng et al., 2002) can be used by resource management agencies to set science-based loading limits, e.g., pollutant load reduction goal (PLRG), total maximum daily load (TMDL), and minimum flow and level (MFL) criteria, to a water body. Similarly, a validated integrated storm surge modeling system can be used to quantitatively delineate flood zones and guide hurricane evacuation.

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Sheng (2000) presented the framework of an integrated modeling system, CH3D-IMS (Figure 1). Earlier versions of the CH3D-IMS were developed to study the effect of reduced nitrogen loading to Roberts Bay and upper Little Sarasota Bay in Florida (Sheng et al., 1996a), the effect of nitrogen load reduction on hypoxia and seagrass in Tampa Bay (Sheng and Yassuda, 1996b; Yassuda and Sheng, 1998), and the preliminary effect of nutrient load reduction on Indian River Lagoon (Sheng, 1997). Sheng et al. (2002) presented the validation CH3D-IMS using extensive data from the Indian River Lagoon collected during 1998. In this paper, we first present the continued development of CH3D-IMS, followed by some recent applications of CH3D-IMS to several Florida coastal and estuarine ecosystems of Florida (Figure 2). We then discuss two difficult issues related to the computational and interdisciplinary aspects of integrated modeling systems, followed by a proposal for the development of a regional "grid" (Foster et al., 2001) to facilitate integrated-process and integrated-scale modeling by multiple institutions.

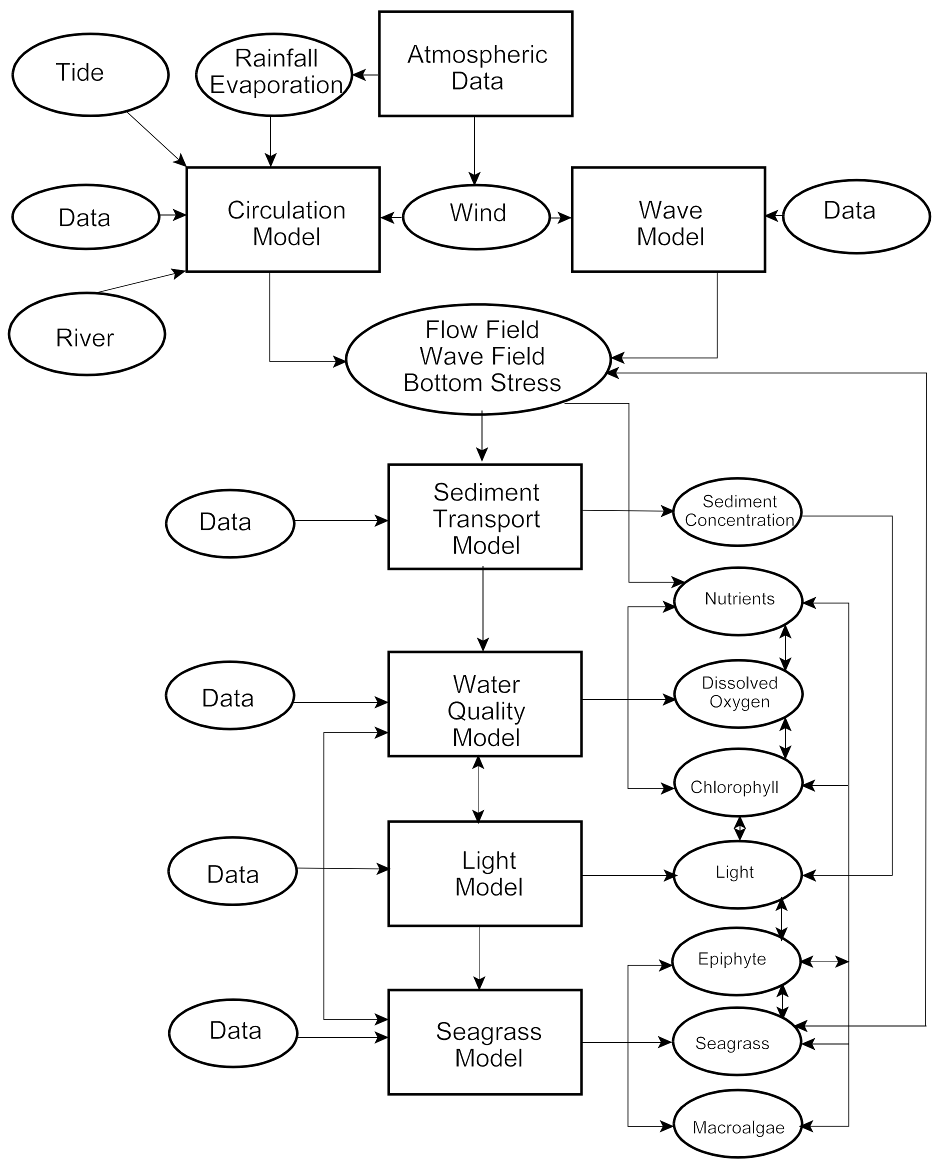


Figure 2. Central and South Florida with several estuarine and coastal ecosystems: Tampa Bay, Sarasota Bay, and Charlotte Harbor on the West coast, Indian River Lagoon on the East coast, and Florida Bay and Biscayne Bay on the South coast.

AN INTEGRATED MODELING SYSTEM: CH3D-IMS

The cornerstone of the CH3D-IMS is the 3-D Curvilinear-grid Hydrodynamic (CH3D) circulation model originally developed by Sheng (1987; 1990) and significantly enhanced during the past 17 years at the University of Florida. The CH3D model at the University of Florida now includes such features as wetting-and-drying, non-hydrostatic pressure distribution, current-wave interaction, vegetation canopies, and a GIS-based graphic user interface. In addition to CH3D (Sheng and Davis, 2002), the CH3D-IMS now includes a wave model, a 3-D sediment transport model CH3D-SED3D (Sheng et al., 2002a), a 3-D water quality model CH3D-WQ3D (Sheng et al., 2002b), a light attenuation model CH3D-LA (Sheng et al., 2002c, Christian and Sheng, 2003), and a seagrass model CH3D-SAV (Fong et al., 1997; Sheng et al., 2003).

The integrated modeling system is comprehensive and uses the same curvilinear grid and time step for all component models. The boundary-fitted grid does not have to be orthogonal, and hence can fit the complex coastal and estuarine boundaries more accurately than orthogonal grid models. The circulation model CH3D simulates the circulation due to wind, tide, wave, and density gradients. The sediment transport model simulates the transport, mixing, deposition, and resuspension of both fine and coarse grained sediments. The model includes resuspension of sediments by both slowly varying currents and wave-induced oscillatory currents. The water quality model includes a nitrogen model, a phosphorus model, a dissolved oxygen (DO) model, a phytoplankton model, and a zooplankton model. A carbon model, a silica model, and a 3-species phytoplankton model have recently been added to the water quality model. The water quality model includes a fully 3-D model for the water column, plus a vertical two-layer model for the sediment column: an aerobic layer on top of an anaerobic layer. The light model includes the absorption of light by water, chlorophyll, non-algal particulate matter (tripton), and dissolved organic matter, as well as scattering by tripton. The seagrass model includes the influence of light, nutrients, temperature, and salinity on the biomass of several relevant species in Florida (*Thallasia, Halodule,* and *Serongodium*), plus epiphyte and macroalgae.

The component models of CH3D-IMS have been completely integrated for operation on one computer system. Both one-way and two-way interactions exist among the various component models. For example, the sediment transport model includes computation of bottom shear stress generated by currents (computed by CH3D) and wave-orbital currents (computed by the wave model). Suspended sediments near the sediment-water interface may cause large density gradients which can significantly affect the bottom shear stresses. Sediment resuspension and deposition fluxes at the sediment-water interface, computed by the sediment transport model, are fed into the water quality model to allow calculation of the nutrient fluxes at the sediment-water interface. The light attenuation model calculates the light attenuation due to water, chlorophyll (calculated by the water quality model), non-algal particulate matter (calculated by the sediment transport model and water quality model), and dissolved organic matter (based on data). The light attenuation in turn affects the algal growth rate in the water quality model. The seagrass biomass is influenced by light (calculated by the light model), nutrients (calculated by the water quality model), temperature and salinity (calculated by the circulation model). The integrated modeling system uses the same curvilinear grid/spacing and time step for all component models, thus eliminating the need for any spatial and temporal averaging of fine-scale component model results to be used as input for other coarse component model(s), which tend to result in violation of mass conservation and loss of information from the fine scale component model.

To facilitate model improvement and model comparison, the CH3D-IMS has been made modular such that every module (i.e., component model) can be readily replaced by a newly improved version of the same module or a model developed by another research group. To improve the computational efficiency, the CH3D-IMS has been made flexible by using numerous *macros* and *cpp's* (C-preprocessors) to allow flexible execution of one or more component models that a user chooses (Davis and Sheng, 2000; 2002). To allow efficient simulations, the CH3D-IMS has been parallelized by using *OpenMP* for shared memory computers (Davis and Sheng, 2002) and *MPI* (Davis and Sheng, 2002; 200) for Beowulf clusters.

Sheng et al. (2002) presented the validation of the CH3D-IMS using 1998 data from the Indian River Lagoon. In the following, we present some further validations and applications of the CH3D-IMS to Indian River Lagoon (IRL), Tampa Bay (TB), and Charlotte Harbor (CH), Florida, and adjoining coastal ocean waters.

Indian River Lagoon and Atlantic Ocean

Validation of Hydrodynamic, Sediment, and Water Quality Models

Sheng et al. (2002) used the horizontal numerical grid with a total of 20988 (477x44) cells (Figure 3) and 4 to 8 vertical layers for the entire IRL. Validation of the circulation model, sediment transport model, and water quality model were presented. Basically, circulation in the IRL is driven by tides from Ponce, Sebastian, Ft. Pierce, and St. Lucie inlets, as well as wind and evaporation/precipitation. In the northern IRL and Banana River, where tides are negligible, circulation is driven by wind and evaporation/precipitation. Based on comparison with long-term data at 10 stations inside the IRL, simulated water levels are within 5% of the measured data, and simulated salinity values are within 10-25% of measured data. Based on measured currents during storms and within inlets, simulated currents are within 10-20% of observed values. During storm events and spring/fall/winter, sediments are readily resuspended by the combined action of slowly varying currents and high frequency wave-induced orbital currents. These resuspension events are often followed by release of nutrients from particulate phase into the water column. The sediment transport model simulates the sediment concentration during storm events and one year cycle with 30-50% error, due to lack of complete understanding and uncertainty in some model parameters and boundary/initial conditions. The water quality model simulates the annual variability of dissolved oxygen and dissolved nutrients with 10-35% error and particulate nutrients with 30-70% error, due to uncertainties associated with the sediment and nutrient processes.

Validation of Light and SAV Models and Ecological Forecasting

Since 2002, we have further validated the light attenuation model (Sheng et al., 2002c; Christian and Sheng, 2003) and the SAV model (Sheng et al., 2003), using the same numerical grid shown in Figure 3. Figure 4 shows the simulated light (Photosynthetically Available Radiance) at the bottom of water column, epiphyte biomass, and *Halodule* biomass in the IRL on June 30, 1998. The simulated Halodule biomass compares qualitatively well with the seagrass map produced from aerial photographs (SJRWMD, 2002). Using the validated CH3D-IMS for the IRL, we conducted ecological forecasting, i.e., predicting the response of the IRL ecosystem to various changes in pollutant (nutrients and total suspended solids, i.e., TSS) loading and hydrological structures (e.g., removal of causeways). For example, Figure 5 shows the *Halodule* distribution in the IRL on June 30, 1998 with and without loadings of nutrients and TSS. While the impact of load reduction on seagrass distribution appears to be rather insignificant for the most part of IRL, there is some appreciable changes in the vicinity of major tributaries. The impact of pollutant load reduction is expected to be more significant over periods longer than six months. Simulations of 5-20 years are being planned.

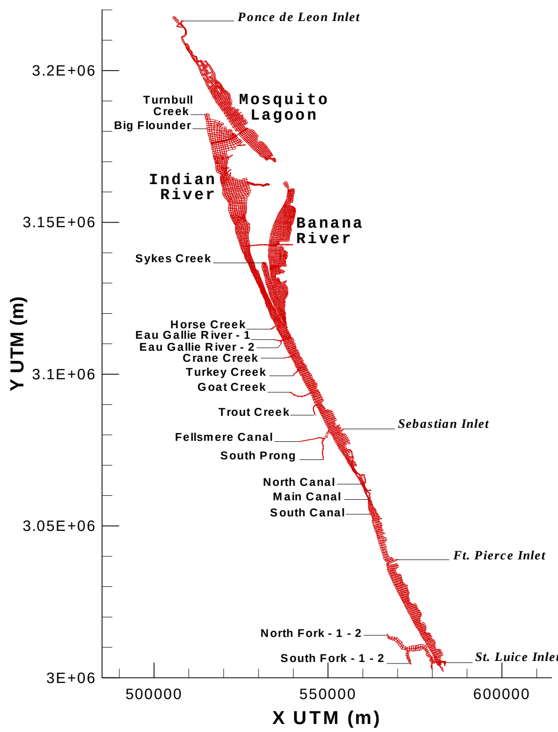


Figure 3. A numerical grid for IRL.

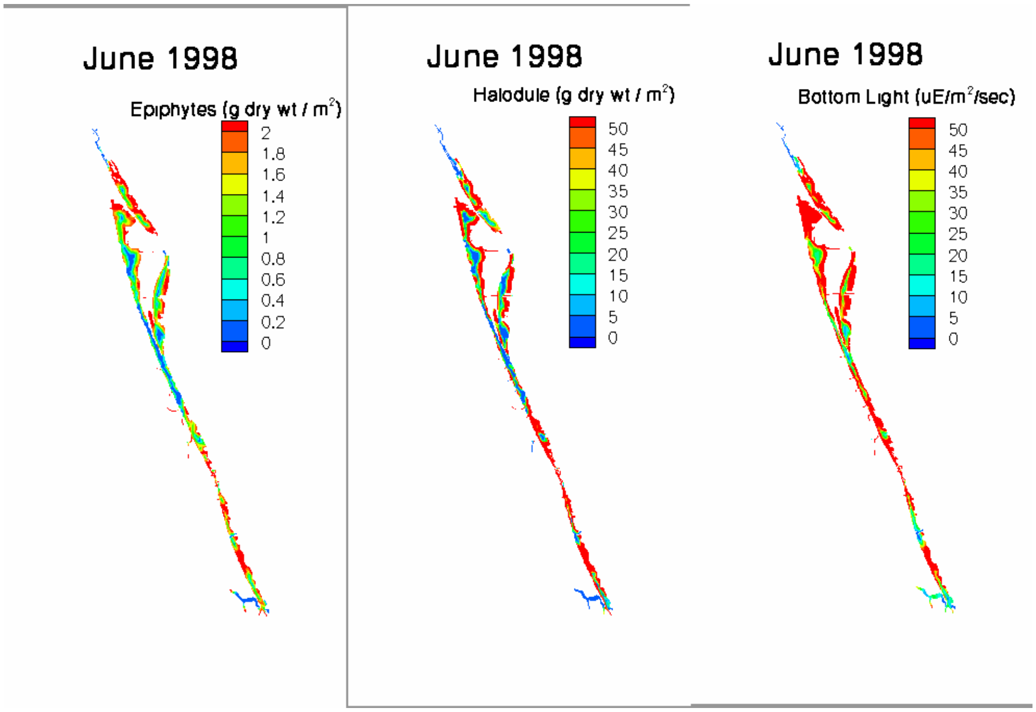


Figure 4. Simulated bottom PAR (photosynthetically available radiance) (right panel), epiphyte biomass (left panel), and Halodule boimass (middle panel) in the Indian River Lagoon on June 30, 1998.

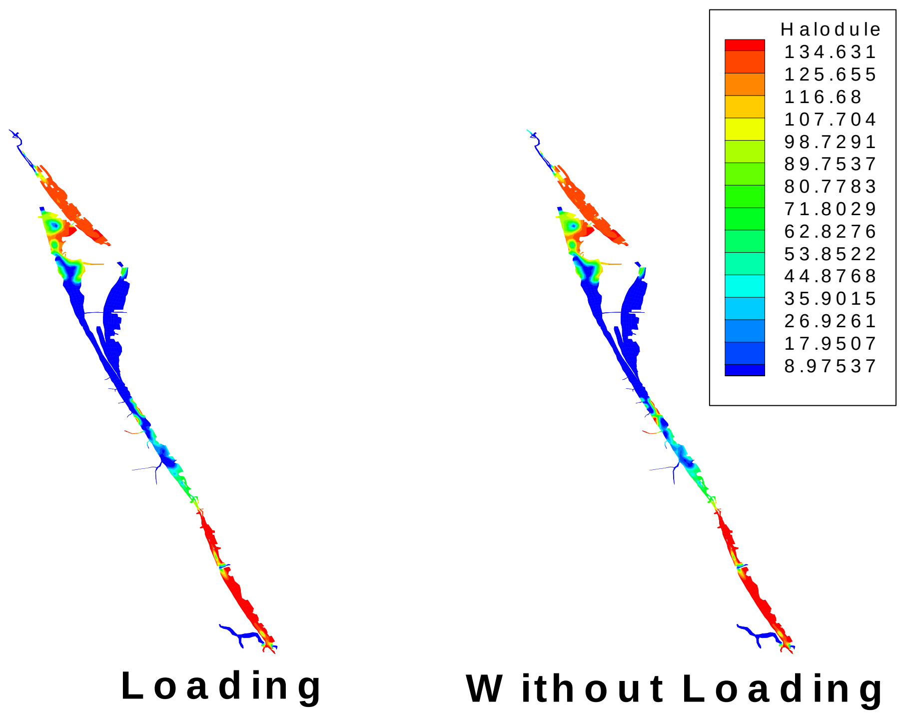


Figure 5. Simulated Halodule biomass with (left panel) and without loading (right panel) of nutrients and TSS in the Indian River Lagoon on December 31, 1998.

Simulation of Trajectory of Columbia Shuttle Debris in Atlantic Ocean

The particle trajectory model of the CH3D-IMS was recently used to simulate the trajectory of debris from space shuttle *Columbia* during its launch in January 2003. The flow field during the model simulation period is based on the output of the NOAA NCEP's Regional Ocean Forecast System (ROFS), which uses the horizontal numerical grid shown in Figure 6. Near the coast, the grid size is about 8 km. Shortly after the launch of shuttle *Columbia*, debris fell off the shuttle and impacted the Atlantic Ocean. Since the precise time of impact is unknown to us, the particle trajectory model of the CH3D-IMS was run for five particles which impacted the ocean at various time instants, ranging from 49 to 300 sec. after the launch. The results show the trajectories of the five particles for one week after their entries into water. The locations of the five particles are significantly different after one week. The results, however, could not be verified due to the classified nature of data.

Extension of the IRL Grid to Include St. Johns River and Continental Shelf

The IRL grid shown in Figure 3 only includes the estuary but not the coastal water. To enable investigation of estuary-shelf exchanges, a coastal grid must be added to the IRL grid. The coastal grid used by the debris trajectory calculation, however, is relatively coarse - 8 km. To allow investigation of estuarine and shelf processes with adequate resolution, we created a new high resolution estuary-shelf grid shown in Figure 8. The new grid has a total of 50,961 (866 x 138) horizontal grid points, vs. the 4,921 (477 x 43) grid points in the IRL grid shown in Figure 3. The new grid takes 0.92-2.2 sec per time step (60 sec), while the IRL grid takes 0.1-0.3 sec per time step, using 1-4 CPU's on our SGI Origin-300 system. This grid is sufficiently fine to resolve estuary-shelf exchange processes, by further coupling it to the ROFS grid, shown in Figure 6.

To demonstrate the feasibility of the extended grid, we simulated the tidal circulation in the entire domain during 1998. While there were water level data at the major tidal inlets and at 8-10km offshore of the inlets, there were no direct water level data at the open boundaries of the model grid shown in Figure 8. We conducted harmonic analysis of the water level data at the tidal inlets and the offshore stations, and extrapolated the water level data to the open boundaries by adjusting the amplitudes and phases of major tidal constituents such that the simulated water level at the tidal inlets agree with the measured data. Figure 9 shows the comparison between the simulated and measured water level at the Ponce, Sebastian, and Ft. Pierce inlets during Julian days 180-215.

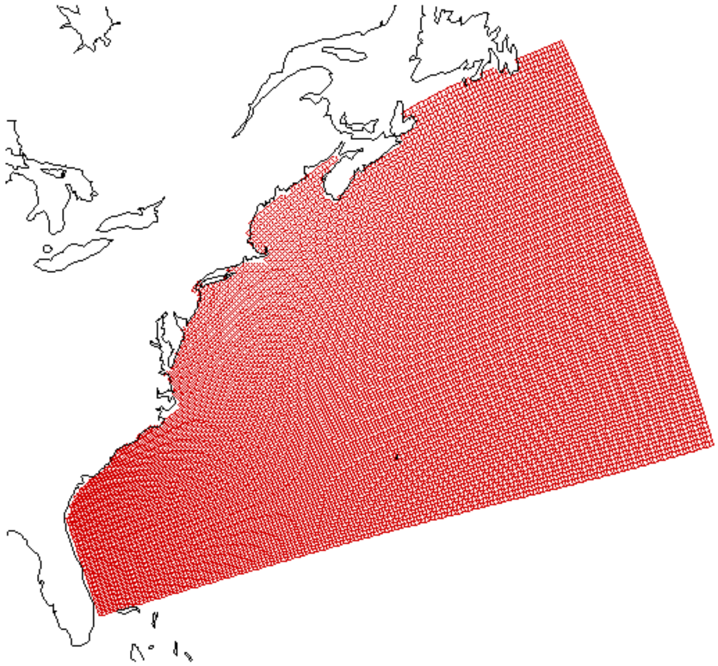


Figure 6. Numerical grid used by the NOAA Regional Ocean Forecast System (ROFS).

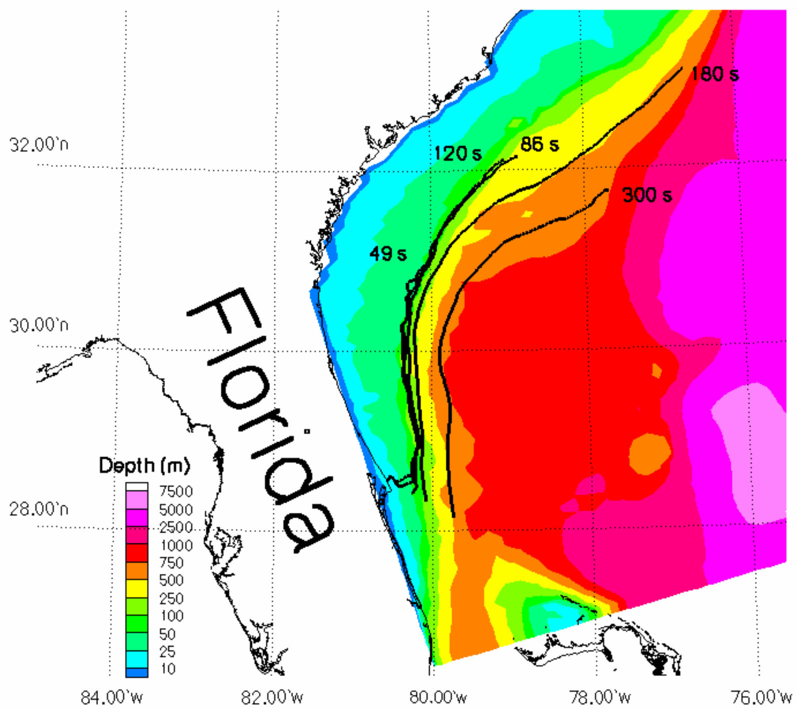


Figure 7. One-week trajectory of five hypothetical particles impacting the Atlantic ocean at various times (between 49 and 300 seconds after the shuttle launch).

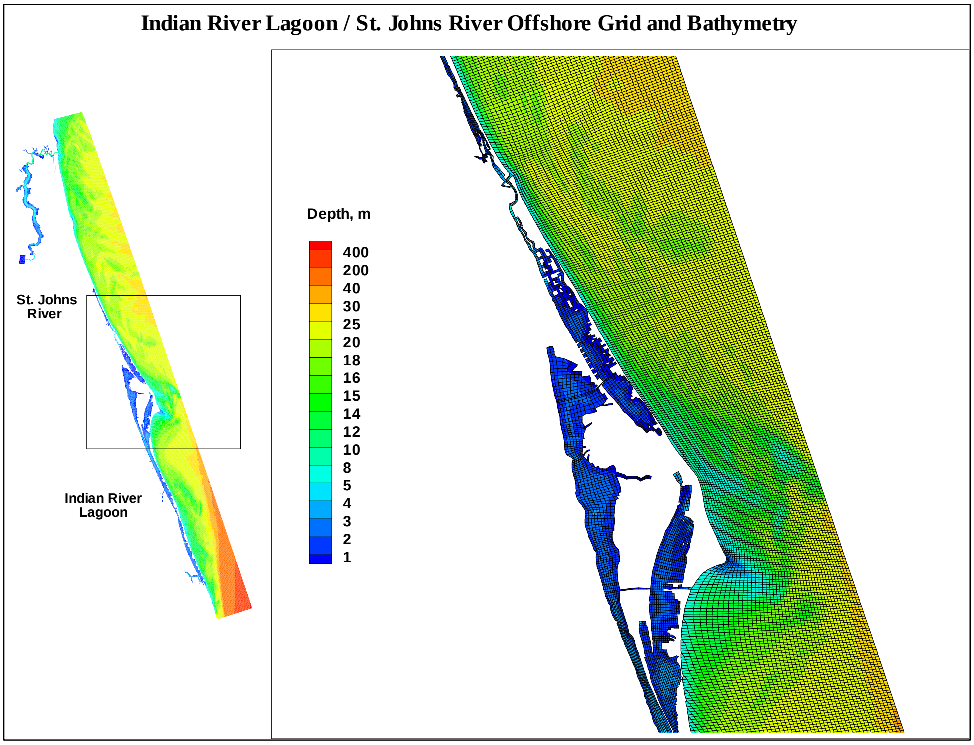
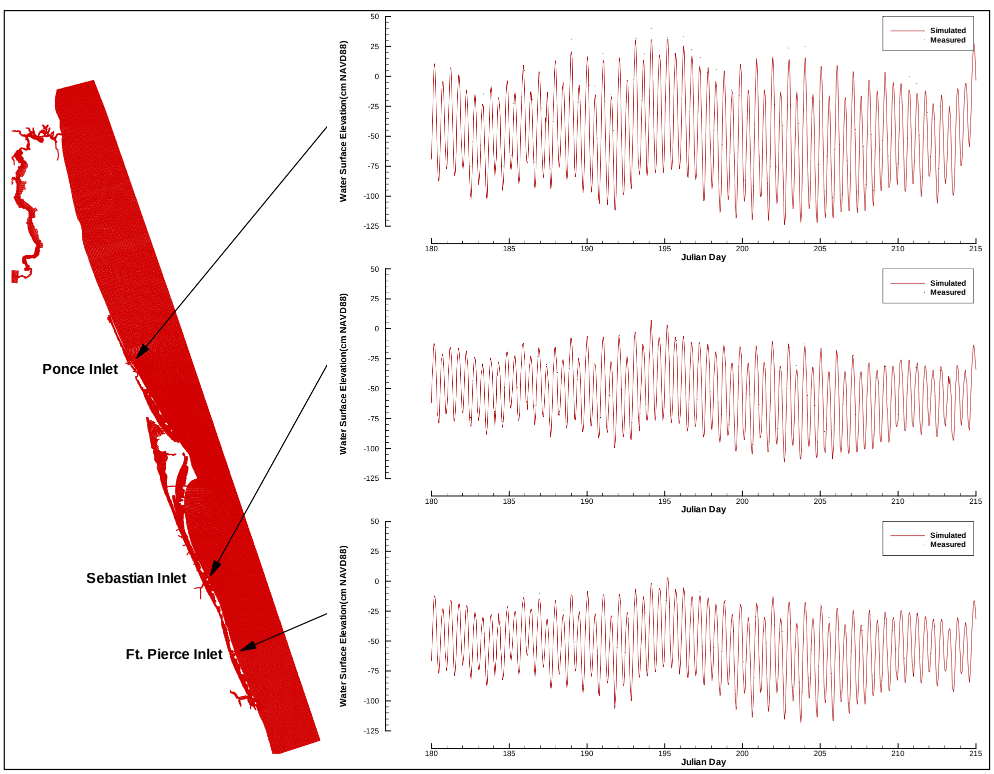


Figure 8. A horizontal numerical grid for Indian River Lagoon, St. Johns River, and a large coastal area.



T a m p a Figure 9. Simulated and measured water level at three inlets in the **B a y ,**
IRL+St.Johns+Offshore grid.

Sarasota Bay, and Gulf of Mexico

Tampa Bay is a large estuary (second largest in Florida) situated along the Southwest coast of Florida, and connected to a coastal lagoon - Sarasota Bay. Pollutant loading has resulted in hypoxia and loss of seagrass in the past 50 years. Since the mid 1990's, however, nutrient load reduction has led to improved water quality and seagrass recovery (Tomasko, 2002). The area is subjected to many storms and hurricanes.

CH3D-IMS has been applied to simulate the circulation, water quality, light, and seagrass biomass in the Tampa Bay estuarine system (Sheng et al., 1996). The model successfully simulated the hypoxia event in Hillsborough Bay during 1991 (Yassuda and Sheng, 1998) and was applied to simulate the effect of nutrient load reduction on the Tampa Bay estuarine system (Sheng et al., 2001). In addition, the 2-D and 3-D versions of CH3D were coupled to the SWAN (Ris et al., 1996) and REF/DIF to simulate the storm surge and coastal flooding in the Pinellas County (Sheng et al., 2002). In the following, the results of storm surge simulation in the area, using a wetting-and-drying version of CH3D and a total of 54,476 horizontal grid cells and four vertical layers, are shown. Using one cpu, it takes 1.06 or 1.28 sec per time step (60 sec) for the model run. The results (Figure 11) show extensive flooding.

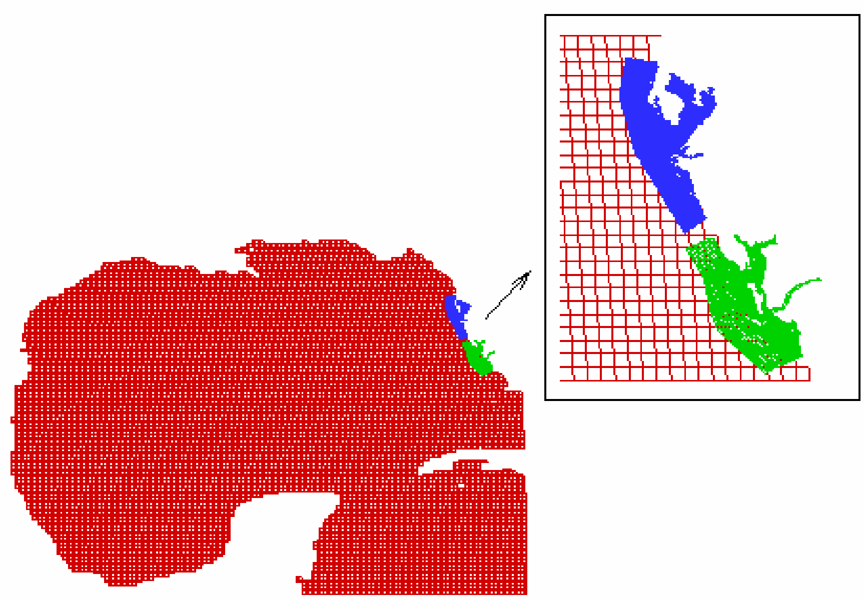


Figure 10. Numerical grids of Tampa Bay and Charlotte Harbor, which are coupled to a Gulf of Mexico grid.

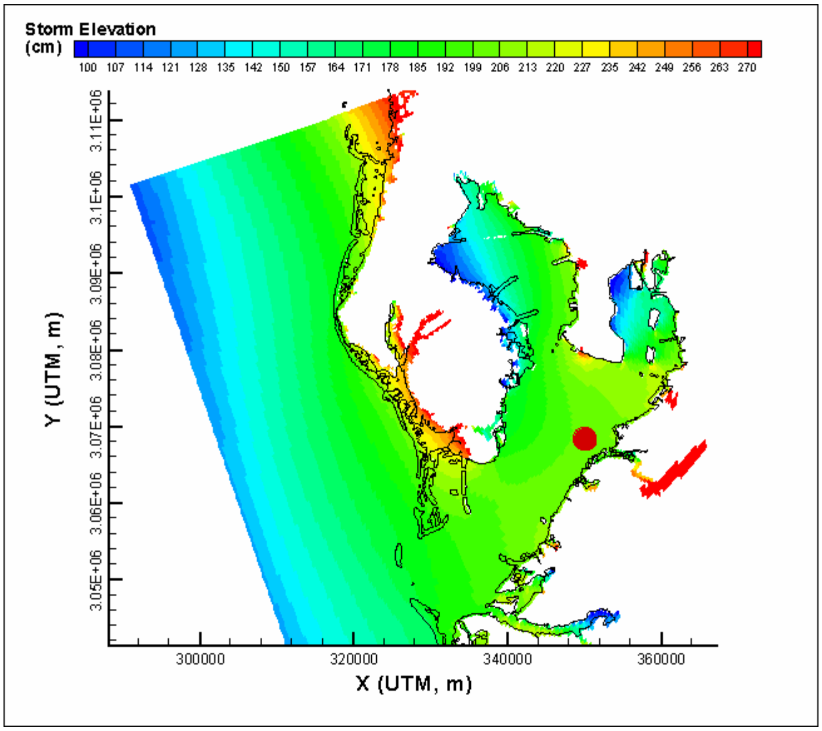


Figure 11. Simulated storm elevation in the Tampa Bay area during a hypothetical storm with uniform wind of 75 mph. The red dot indicates the center of the storm.

Charlotte Harbor and Gulf of Mexico

Charlotte Harbor is a large estuarine system along the Southwest Florida coast. One of the major issues concerning Charlotte Harbor is the determination of Minimum Flow and Level (MFL) criteria for the three major rivers (Peace, Myakka, and Caloosahatchee) due to concern of the impact of increasing demand for and withdrawal of freshwater from upstream of the estuary. The CH3D-IMS is being applied to simulate the flow and salinity distribution inside the entire estuarine system. The CH3D-IMS has been applied to simulate the circulation measured by USGS in 1986 and the water quality data measured by the State of Florida in 1996 and 2000 (Sheng and Park, 2002; 2003). Figure 12 shows the horizontal numerical grid (with 92 x 129 grid cells) used for the model simulation. Using eight vertical layers, there are a total of 94,944 grid points. The grid includes a large coastal region to allow simulation of dynamic exchanges between the estuary and the Gulf of Mexico. Using 2 CPU's on the SGI Origin-300, it takes 0.78 sec to run one time step (60 sec) of CH3D.

Recently, a real-time physical oceanographic observing system was installed near Station CH09B (Figure 13) by the University of Florida. The data include air temperature, wind velocity, relative humidity, vertical profile of horizontal currents (via ADCP), water temperature, and conductivity. The data are collected every 15 minutes and downloaded via cell phone onto a computer located at the University of Florida. Graphic forms of the data are presented on http://chharbor.coastal.ufl.edu/. The observing system has been in operation since April 2003. The following example shows the simulation of water level and horizontal currents during 6/03-8/03.

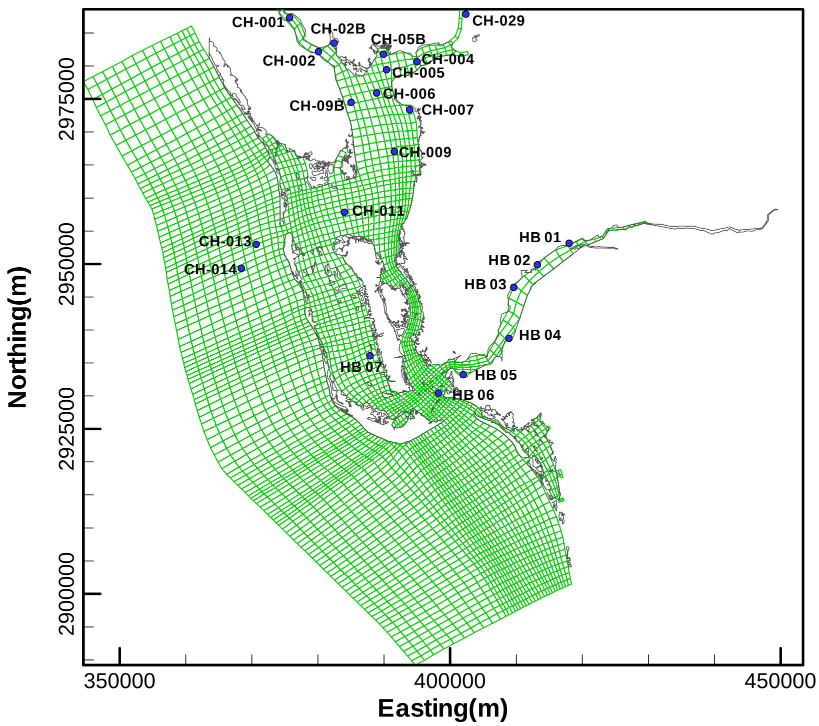


Figure 12. The horizontal numerical grid used by CH3D-IMS for Charlotte Harbor simulations, with water quality data stations labeled.

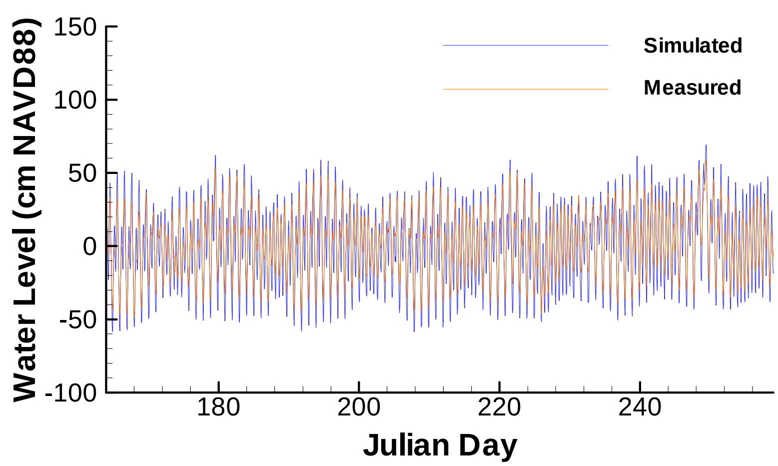


Figure 13. Simulated and measured water level at the UF station in 6/2003-8/2003.

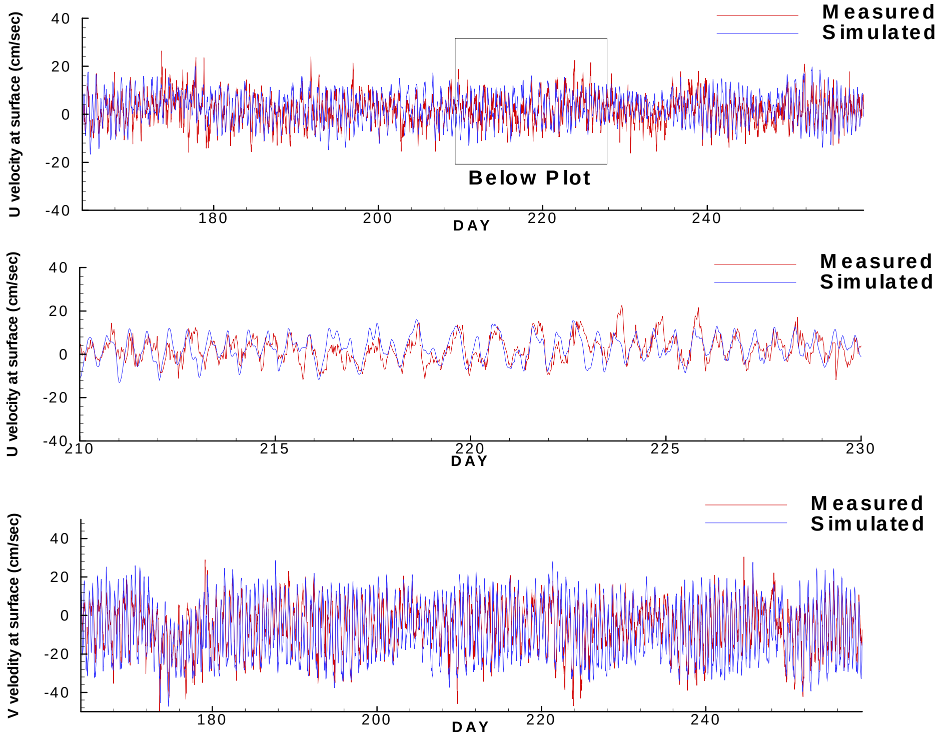


Figure 14. Simulated and measured horizontal currents at the UF station.

DISCUSSION

We have presented the development and recent applications of an integrated modeling system, CH3D-IMS, to several estuarine and coastal ecosystems in Florida. The integrated modeling system has been developed by the Advanced Coastal Environment Simulation (ACES) Laboratory at the University of Florida by integrating various component models and validating them with extensive field data from several estuarine and coastal ecosystems. The example applications showed the feasibility of using CH3D-IMS for predicting the response of estuarine and coastal environment to anthropogenic and natural changes. However, many aspects of the integrated modeling system need to be continually improved to make the modeling system more robust and more efficient, due to the wide range of scales and numerous processes involved in such simulations. We discuss several major issues in the following.

Computational Resource Requirement

As shown in the examples, integrated-scale and integrated-process modeling over large estuarine and coastal areas require high resolution and long-term simulations. While we are using 100-400 m grid spacing and a 60 sec time step, it is expected that resolution of 10-50 m with a smaller time step will be needed for more accurate simulations in coastal and nearshore areas. To allow efficient simulation, models should be parallelized, modular, and portable. To this end, we have created parallel versions of the CH3D-IMS for both shared memory computers and Beowulf clusters. All the example simulations of CH3D-IMS discussed required CPU time no more than 1/60 of the realtime. However, as we couple the estuarine and coastal models to the basin scale model (e.g., Gulf of Mexico model or Atlantic Ocean model) or global model, the required computational resources will be much greater and may exceed the capabilities of our computers (three SGI Origin systems and one Beowulf cluster). As the problem gets more complicated, it may become necessary to use an unstructured grid to reduce the total number of grid points for a large computational domain, and to develop fully parallel models using *MPI*. To meet the increasing demand for more computational resources, some institutions, e.g., University of Florida, are developing super Beowulf clusters with more than 1,000 CPU's. Others, which may be the majority, will continue to rely on the few supercomputing centers (with super clusters) in the nation. An attractive alternative is to link several mini-clusters into a regional "grid" (Foster et al., 2001).

Interdisciplinary Team Effort

The development of an integrated modeling system requires the integration of numerous disciplinary models, e.g., hydrodynamic, sedimentary, water quality, ecological, atmospheric, and groundwater models. This is a difficult task, since it is not only difficult to assemble an interdisciplinary modeling team, but also to achieve consensus among the team as to how to integrate the various disciplinary models. Different disciplinary models may contain very different spatial and temporal scales. Moreover, various disciplinary models are often developed with different programming languages on different computers with different operating systems. Although we have achieved the goal so far within a single research group, as the problem becomes more complicated, it will become increasingly difficult for us to integrate more disciplinary models and couple to larger scale models within the single research group.

An Infrastructure to Facilitate Collaboration Among Multiple Institutions

To deal with the two difficult issues pointed out in the last two paragraphs, it is believed that the modeling community can take advantage of the recent dramatic growth in networking and grid computing (Foster et al,. 2001). For example, within a year, the National Lambda Rails will bring 80 Gb/sec bandwidth to many universities and research laboratories in the nation. The rapid development and maturity of middleware, thanks to the NSF Middleware Initiative (NMI), will enable the development of computational grid for estuarine and coastal ocean modeling. An example coastal ocean modeling grid has been tested within the University of Florida (Davis et al., 2004). A prototype regional coastal ocean modeling grid is being developed by the University of Florida, Louisiana State University, and College of William and Mary, based on the approach proposed by Sheng and Davis (2003). Mini-clusters consisting of a combination of 1-processor, 2-processor, and 4-processor computers at each of the three institutions will be linked together into a regional "grid" via networking, middleware, and virtual machine software. This grid will allow virtual sharing of computer resources, models, data, and expertise among the three institutions.

Conclusions

Integrated-process and integrated-scale modeling of large estuarine and coastal areas is becoming increasingly important for coastal zone management and mitigation of coastal hazard. We have presented the continued development and recent applications of an integrated modeling system, CH3D-IMS. Due to increasing demand for higher resolution and longer-term simulations of complex interdisciplinary problems, the integrated modeling system needs to be continually improved to meet the challenges. To facilitate the rapid development and enhancement of integrated modeling systems , a regional coastal ocean modeling grid is proposed to provide regional virtual sharing of computer resources, models, data, and expertise. Integrated-process and integrated-scale modeling can be conducted by running different disciplinary models and different scale models at different institutions simultaneously on the modeling grid. This will revolutionize the coastal ocean modeling as we know it.

ACKNOWLEDGMENT

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