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Proceedings of the Cross Discipline Ecosystem Modeling and Analysis Workshop

August 15-17, 2000

U.S. Environmental Protection Agency
EPA Administration Building
79 T.W. Alexander Drive
Research Triangle Park, NC 27709

Cross-Discipline Ecosystem Modeling and Analysis Workshop
August 15-17, 2000

Tuesday August 15, 2000

8:00	Registration for visitor passes begins, coffee will be available	

4:35 - 5:15 **Discussion (Facilitator: Christa Peters-Lidard):** Opportunities for future collaboration

5:15 Adjourn

Wednesday August 16, 2000

Framework Developments for Coupled Multimedia Models

Break (10:10 - 10:25)

Lunch (12:15 - 1:45)

Tools and Techniques for Integrated Environmental Modeling

Break (3:05 - 3:20)

5:00 Adjourn

August 17, 2000

Landscape and Subsurface Characterization

Data Visualization and Analysis Tools

This proceedings has been reviewed in accordance with the U.S. Environmental Protection Agency's peer review and administrative review policies and approved for presentation and publication.

Cross-Discipline Ecosystem Modeling and Analysis Workshop: Introduction

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The complexity of environmental problems we face now and in the future is ever increasing. Process linkages among air, land, surface and subsurface water require interdisciplinary modeling approaches. The dynamics of land use change spurred by population and economic growth, and the impact of Best Management Practices in urban and agricultural areas must be considered in environmental exposure and risk assessments. An abundance of related research and model development is proceeding in Universities, Federal agencies and research laboratories, and related research is being sponsored by industry-based research foundations. Thus, one of the primary goals of this workshop is to bring together stakeholders from many of these diverse groups for exchange of information about their modeling needs and research activities with special emphasis on techniques, tools, and frameworks for model integration, characterization of landscape and subsurface features, and data visualization and analysis tools.

EPA is interested in fostering a "community approach" to multi-disciplinary ecosystem modeling and analysis. The emerging problems are larger than one group or one agency can expect to solve, so our goal is to work together toward open-architecture problem solving environments that facilitate the integration of state-of-the-science process models/modules, application domain specification and data preparation, and decision support. A flexible Problem Solving Environment will enable exploration of a variety of modeling approaches dealing with multiple scale and stressor interactions. Object technology, new computing algorithms and architectures, and intelligent data analysis techniques offer promise for overcoming previous computing limitations and modeling inflexibility. During the workshop, investigators from the 1996 EPA STAR grants for High Performance Computing and Communications will be presenting the results of their three year research efforts, and investigators for the 1999/2000 EPA STAR grants for Computing Technology for Ecosystem Modeling will be presenting their research directions for the next three years. Numerous other researchers and stakeholders engaged in ecosystem modeling and monitoring will also be presenting progress-to-date on their projects. The anticipated outcomes of the workshop are better understanding of 1) cross-media exchange processes and scale issues, 2) a variety of framework approaches for dealing with cross-discipline model integration and application issues, and 3) identification of inter-disciplinary opportunities for collaboration.

* On assignment from Atmospheric Sciences Modeling Division, National Oceanic Atmospheric Administration, U.S. Department of Commerce

Office of Water (OW) Water Quality Modeling Program: BASINS

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BASINS, EPA's GIS-based modeling system, makes it easier to locate potential sources of pollutants and estimate their effects on drinking water, recreational waters, aquatic life, wildlife habitat, and other critical uses of waters in a watershed. BASINS makes it easier to evaluate management strategies and perform "what if" scenarios in a particular watershed. Many factors affect water quality in a watershed, and each watershed is different. By using data compiled in BASINS, in conjunction with local data sources, users can evaluate large amounts of pollutant source, chemical discharge, and stream flow information for every watershed in the continental United States. Users may add their own data to that contained in BASINS, thus insuring use of the most current, reliable, and accurate data that exists for each watershed. They also may run models to estimate changes to water quality that may result from different land use practices. The watershed models use weather data to generate stream flow, estimate loadings to streams from non-point sources, combine these non-point source contributions with facility discharges, and calculate changes in pollutant concentrations (e.g., sediment, nutrients, bacteria, and toxic substances) as they are diluted and flow downstream. This presentation provides an overview of the features found in BASINS v 3.0 and presents a discussion of design considerations associated with working with evolving commercial software (ArcView) and Object Oriented programming languages.

Near Laboratory Ecological Research Area Studies in the Neuse River Basin

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Two years ago NERL began to establish field research sites in order to support methods development under EPA's Office of Research Development risk assessment strategy. The near lab sites will serve as this research platform. This will provide a scientific framework for risk reduction and target available resources at those environmental stressors that account for the greatest impact on human and ecological communities and will define newly emerging problem areas. To this end, four locations were chosen. 1- the Little Miami River Basin in Ohio 2- the Lower Colorado Basin in Nevada, 3- the Savannah River Basin in Georgia and South Carolina and 4- the Neuse River Basin in North Carolina.

The advantages of these NLERA sites are

1- Facilitates Ecological Research Planning
2- Reductions in Costs & Logistic Efforts
3- Enhanced Research Quality
4- Encourages Collaboration (Federal, State and Local)
5- Integrate programs and leverage resources

In the Neuse River Basin there are three base sites

1- Hill Forest on the Flat River northwest of the Triangle in the Piedmont region and is also one of the headwaters of the Neuse
2- Cunningham Farms in the coastal plain section of the state at Kinston NC. Neuse River/ Contentnea Creek
3- And a coastal site near Havelock NC ,Cherry Point Marine Air Station.

In addition to these base sites, NERL has secured access to eight swine farms in the Neuse Basin and two of these farms are the scene of an intensive study by four Federal Agencies, two State Agencies and two Universities to define the impact of CAFOs (confined animal feeding operations) on the surrounding environment

There are many environmental stressors to be found in this Basin ranging from urban and industrial pollution, agriculture pollution to natural stressors is harmful algae blooms, and coupled with rapid growth and development and changing economies. The Neuse represents a valuable ecological research resource.

Neuse River/Estuary Monitoring

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In the early to mid 1990s, the occurrence of several large fish kills together with the intense hype surrounding the pfiesteria organism helped to galvanize public opinion about the need for significant management action to resuscitate water quality in the Neuse River Estuary (NRE). In response, the NC General Assembly passed House Bill 15A NCAC 2B.0232 1997 requiring that a 30% reduction in external nitrogen (N) loading (based on a mean 1990-1995 N loading "cap") be in place by 2003. Concurrently, the State became more proactive in funding monitoring programs to provide information necessary to develop effective management strategies. This talk will provide an overview of two monitoring programs.

In 1997, the Neuse River Estuary MODeling and MONitoring (MODMON) program was initiated. The principal objectives of the MODMON program have been (i) to develop water quality models of the NRE to assist staff at the NC Department of Environment and Natural Resources in evaluating the effectiveness of proposed Total Maximum Daily Loads (TMDLs) and (ii) to develop a monitoring program that would support these modeling efforts and furthermore allow the detection of trends in water quality parameters that were presumably responding to management actions.

In 1999, the RiverNet program was funded to provide water quality monitoring data in the freshwater sections of the Neuse to (i) continuously monitor river nutrients & physical water quality parameters, (ii) transfer the data from the remote stations to NCSU and disseminate the data on the web so that the data can be accessed by policy makers, scientists, educators, scientists, government agencies, as well as university, middle and high school students, and (iii) obtain long term records of nutrient flux in various portions of the basin to determine associations with land use changes and climatic cycles. At the present time there are 3 of the 15 stations are installed.

Nutrient Cycling and Algal Blooms in the Neuse River Estuary

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In eutrophying coastal ecosystems like the Neuse River Estuary, nutrient-stimulated primary production and associated phytoplankton blooms have been implicated in various water quality problems. Blooms may be toxic, disrupt food webs and provide the organic matter fueling bottom water oxygen depletion or hypoxia. In the Neuse River Estuary, episodic (e.g., storm-related runoff) and chronic (low-level, long term) nutrient loading events, coupled to long residence times (30-120 days), persistent vertical stratification and elevated summer temperatures, promote blooms and hypoxia that can last for weeks and cover large areas. The timing, sources (point vs. non-point, land-based vs. atmospheric), loading characteristics (episodic vs. chronic), and levels of nutrient input are critical determinants of bloom dynamics. The ecosystem-level trophic implications are that a large component of the estuarine food web may be negatively impacted or removed, altering both the structure and function of the system. Hypoxia also alters biogeochemical (nutrient) cycling processes in affected habitats.

Nitrogen (N) is the most limiting nutrient in the Neuse. N inputs from riverine, groundwater, and atmospheric sources intensify hypoxia/anoxia potentials by stimulating phytoplankton growth and bloom formation. Changes in composition and loading rates of N sources influence both standing stock and composition of phytoplankton. If, for example, specific N inputs result in selection for rapidly-proliferating dinoflagellate, cryptomonad, and cyanobacterial nuisance blooms which are not effectively grazed, residual labile carbon will be available for fueling hypoxia/anoxia, altering benthic regeneration, nutrient cycling, and ultimately, determining the temporal and spatial patterns and magnitudes of estuarine production.

The Neuse River hydrodynamic water quality model currently lacks the information necessary to link specific nitrogen formulations (i.e., NO_x, NH_4^+, DON) with responses of phytoplankton species-specific growth and bloom events. In addition, the relative importance of acute vs. chronic loadings of these sources plays a role in determining phytoplankton competitive interactions and bloom dynamics. Because phytoplankton composition and activity play key roles in dissolved oxygen dynamics and the trophic status of the estuary, it is crucial that the water quality model account for algal group-specific responses to varying nutrient sources and concentrations. Our contribution to the Neuse River Modeling and Monitoring Program (ModMon) is designed to provide data needed to incorporate the effects of concentrations, formulations and loading characteristics of N and other nutrients on phytoplankton community structure and its contribution to O_2 depletion potentials within the model framework. The predictability of the spatial and temporal dynamics of phytoplankton blooms in dynamic estuarine environments depends on the ability of the water quality model to accurately assess the collective responses of many different ecosystem components. A mechanistic understanding of phytoplankton community dynamics and linkages to O_2 depletion potentials are critical for model validation, applications, and simulations.

Atmospheric Deposition of Inorganic Nitrogen to Watersheds/Estuarine Waters

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Atmospheric deposition of nutrients to coastal watersheds and estuaries contributes a sufficient fraction of nitrogen loading and is a contributor in nutrient stimulation. For various estuaries in the eastern U.S., the atmospheric contribution is estimated to range between 10-30% of the nitrogen load and for some estuaries the fraction is estimated to be even higher. The great majority of this deposition is in the form of inorganic nitrogen: oxidized nitrogen (ox-N = nitrate and nitric acid) and reduced nitrogen (red-N = ammonia and ammonium). This talk will provide some background on the defining characteristics of atmospheric inorganic nitrogen deposition that also relate to estuarine ecosystem modeling. This will include the two pathways of delivery of deposition (wet and dry), how gas-particle partitioning significantly affects dry deposition, and how the two inorganic forms are different and when they can be similar. The background will also include a perspective on land versus water exchange, direct versus indirect loading, and emission hot spots. The talk will then move into examination of transport lifetimes and airsheds. Because these pollutants are involved in long-range transport, the airsheds are large relative to the watersheds. Airsheds of ox-N and red-N for Chesapeake Bay and Neuse/Pamlico will be presented and compared and contrasted in terms of some of their characteristics. The characteristics of the Neuse/Pamlico reduced nitrogen deposition and airshed responsibility will also be discussed in terms of conventional wisdom (it may not be correct) and the large increase in ammonia emissions in the 1990's.

* On assignment from Atmospheric Sciences Modeling Division, National Oceanic Atmospheric Administration, U.S. Department of Commerce

Introduction: MIMS Ecosystem Modeling Integration Efforts

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The U.S. EPA Multimedia Integrated Modeling System (MIMS) is a long-term project that aims to apply advancements in software engineering to develop a problem-solving environment for multiscale ecosystem modeling and analysis. As part of the MIMS development, environmental modeling components such as atmospheric and surface hydrology models will be linked as initial prototypes to test the MIMS software architecture. This initial prototype will then be further developed to address water quality issues such as urban drainage and nitrogen flux contributions from the land surface, groundwater, and atmospheric sources, through an integrated ecosystem modeling perspective.

The focus of this afternoon session is to present environmental model development and integration efforts. For initial prototype development, terrestrial or land surface hydrology models are being linked with atmospheric and groundwater models. These linkages must address the issues of disparate scales between the individual models. Spatial scaling of these models is also being addressed to formulate strategies for modeling larger watershed and river basin domains. This is of particular concern for nutrient cycling processes where smaller vegetation zones (e.g., riparian buffers) play a significant role. In addition to ongoing projects, the new USEPA Computer Technology for Ecosystem Modeling grant program includes projects to develop new modeling approaches for surface water, swine waste land application, groundwater flow, and ecosystem exposure. It is anticipated that future MIMS prototype developments will benefit from the modeling approaches developed as part of these studies.

* On assignment from Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce

Applications of the TOPLATS Land Surface Hydrology Model, Including Strategies for Modeling Large River Basins and Coupling to Saturated Groundwater Models

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Environmental modeling has traditionally been executed separately for each major medium, e.g. air, surface water, and groundwater. Historical separation was justified on the basis that early pollution concerns were primarily confined to one medium (e.g., DNAPLs in groundwater). Ongoing work in the Chesapeake Bay, Great Lakes and the Neuse River Estuary has indicated the need for fully interactive multimedia modeling.

The TOPLATS-MM5 hydrologic-atmospheric model has been designed as part of an HPCC grant to McHenry and Peters-Lidard, and may serve as a prototype for coupling air and surface water media. TOPLATS-MM5 has been shown to improve on current state-of-science coupling of land-atmosphere media at the watershed-scale. One of the unique aspects of the coupled modeling system is that TOPLATS/MM5 incorporates an Input/Output Applications Programming Interface (I/O API) which encapsulates the complexity of coordinate systems, grid definitions, and data structures at lower software layers, and uses self-describing files and communication channels to provide this data to the coupled components.

The following three tasks are the focus of the project: 1) Apply and calibrate the TOPLATS-MM5 hydrologic-atmospheric model to the Sandy Run watershed, which is a sub-basin of the Neuse River basin in North Carolina; 2) Scope out the feasibility of applying the TOPLATS-MM5 model to the following three basins: Contentnea Creek watershed (980 mi 2), Neuse River basin (5,600 mi 2), and the Albemarle-Pamlico drainage basin (28,000 mi 2); and 3) Provide technical advice on linking TOPLATS-MM5 to grid-based (e.g., MODFLOW) or analytic element (e.g., GFLOW) groundwater models. Early results from the work, including progress developing project databases, as well as strategies for coupling environmental models will be presented.

Coupling a Mesoscale Meteorology Model to a High-Resolution Land-Surface Hydrology Model: Review of Results, Current Status, and Future Plans (EPA Grant No. CR825210)

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Current interest in the processes that govern the fluxes of heat, moisture and momentum at the land-atmosphere interest is high. It is a difficult modeling problem because the relatively small-spatial and long-temporal hydrological scales interact directly with the relatively large-spatial and rapid-temporal scales of the atmosphere. In this project, we have coupled a high-resolution land-surface hydrology model to a mesoscale meteorology model in order to represent these complex interactions. Furthermore, we have designed the coupled model to accommodate assimilation of observed rainfall and downward solar radiation in order to provide for a variety of model coupling strategies that could be useful for different types of simulation demands.

The models involved are the PSU/NCAR MM5V2 and V3 and the Top-Model-based Land-Atmosphere Transfer Scheme (TOPLATS). The initial work focused on designing and constructing a flux-coupler that passes surface water and energy fluxes from TOPLATS to MM5 and passes downward directed atmospheric fluxes (precipitation, solar radiation) from MM5 to TOPLATS. The design of the coupler also accounts for the need to disaggregate fluxes passed from MM5 to TOPLATS, and to aggregate fluxes passed from TOPLATS to MM5, preserving conservation of mass and energy. The coupler is not a single subroutine but rather a set of subroutines that, when implemented in MM5 and TOPLATS, performs the desired functions.

The initial coupler was tested using a 1-dimensional column version of MM5 for a case-study that occurred in the Little Washita Watershed in 1994. Results from this study clearly suggested that the temporal variability of soil moisture in TOPLATS plays a crucial role in accurate estimation of sensible and latent heat fluxes, which in turn determine ABL characteristics. A summary of these results will be shown.

A significant amount of software re-engineering was also conducted on the TOPLATS model code in order to make it more computationally efficient. Code was re-organized in order to support parallelization, and parallel directives were added, tested and validated. In addition, by making use of "hydrological similarity," the code was optimized to eliminate pixel-based redundant calculations, improving the code performance by a factor of nearly 1000. Further, a restart capability was added, I/O was re-engineered by implementing EPA's Models-3 I/O API, and I/O API filters were built to support import of a variety of data types from both stations and remote-sensing platforms, including NEXRAD rainfall estimates. Together, this set of improvements has made it possible to regionalize TOPLATS' application domain.

At present, tests of the fully 3-D coupled system are underway, though no results will be presented at the conference. Currently, the project is focusing on three areas: the ARM-CART domain, the Neuse River basin, and the Houston-Galveston area. Though funding for the current grant will come to a close within the next year, follow-on projects have been funded based on the success of the grant work. The state of all of these projects and future goals will be outlined.

A High Performance Analytic Element Model: GIS Interface, Calibration Tools, and Application to the Niagara Falls Region

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The presentation will summarize the proposed activities of a recently funded EPA STAR project. The primary project tasks include:

- Development of a high performance groundwater flow model based on the Analytic Element Method (AEM), with an emphasis on MPI-based portability.
- Development and comparison of automated calibration/optimization tools based on: 1) nonlinear regression and 2) the genetic algorithm.
- Development of a GIS-based graphical user interface for the modeling system.
- Extensive testing of the modeling system on 3 high-performance parallel computing platforms: the SGI Origin, the IBM SP, and a heterogeneous Sun workstation cluster.
- Application of the modeling tools to a case study of regional groundwater flow in the Niagara Falls/Lake Ontario region, including comparisons with previous efforts based on the traditional finite difference approach.

The presentation will also include a brief overview of the AEM for simulating groundwater flow, with an emphasis on large scale regional applications.

Spatially Distributed Simulation of Hydroecological Processes at the Lizzy Site: Model Structure, Preliminary Applications and Coupling Issues

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We present the preliminary applications and design of a spatially distributed, hydroecological model of water, carbon and nutrient (WCN) cycling and transport to the Lizzy site. While not all required field data for model parameterization are available for this site, the form and operation of the model are illustrated to engender discussion of issues for coupling with groundwater, atmospheric and confined animal feed operation (CAFO) models. The process models for WCN cycling and transport are coupled with a GIS which functions to set up and parameterize the spatially distributed model, manage simulation runs and visualize results. The modeling system identifies a set of terrestrial, aquatic and atmospheric containers, which may be further broken down into spatial hierarchies of land (or water) units. In the terrestrial phase, the model contains successively embedded basins, slopes, patches and (canopy) strata. WCN cycling is modeled at the level of patches and strata, while lateral transport through hydrologic flowpaths occurs between patches at the levels of hillslopes and basins. The aquatic phase is described by the components of the stream network hierarchy, and contains all stream reaches, natural and built water bodies. We will describe preliminary operations and results from the hydrological portions of the model applied to the small monitored catchments in Lizzy.

Issues and Data Needs for Introducing Nitrogenous Pollutants from Swine Waste Land Application Into An Object-Oriented Ecosystem Model

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Simulation System model (RHESSys) that is implemented as a typical procedural-based code operating on global data structures. Conceptually, the model has many natural hierarchies including spatial nesting of landscape and layering of land cover. While this model provides an excellent conceptual framework for studying the effects of swine waste application to land, it is difficult for new users to understand and even harder for them to extend it. We will describe a substantial reengineering of this software into a fully object oriented system. The entire model has been subdivided into a series of namespaces and class scopes and no global data or global procedures remain. Substantial use has been made of C++ Standard Library components, as well as our own C++ library components that provide abstractions of whole-part aggregation and support for model utility needs that are common across several simulation codes. In addition, community-developed libraries that support the processing of eXtensible Markup Language (XML) are incorporated to provide for the external representation and easily extensible parsing of a series of supporting ecophysiological variable data sets used to initialize the model. All of these libraries are used to create and manage the spatial hierarchies via multiple inheritances from template base classes. The need for an explicit "atmosphere" object was identified and this functionality was abstracted out of the spatial hierarchy and the ecosystem process representations. At the lowest levels of the spatial hierarchy, where the ecosystem process representations reside, we have applied abstraction and encapsulation principles to produce abstract classes that provide the necessary interfaces for the model to function. Within the smallest spatial object, an aspatial vertical structure of above-, on-, and below-ground ecosystem or physical system abstract objects has been implemented. Concrete classes that implement the physical and ecosystem processes are derived from these interface classes. The existing procedural process codes (with significant changes in the arguments) have been used (mostly as private parts of the classes) to implement these concrete classes and these provide one example of how different process representations might be used in the model. This new design will significantly improve the education of new users and developers, permit ready modification of the system, and can more easily provide for coupling with other environmental models. We will also present a conceptual model detailing potential fates of nitrogen in land-applied liquid lagoonal swine effluent. We will summarize the results of field observations and laboratory, process-oriented studies regarding rates and environmental controls on nitrification, denitrification, N-mineralization and N 2 O emission on representative spray fields. Further, we will provide an overview of ongoing research directed toward assessing rates and controls of plant assimilation, microbial immobilization and offsite transport of N via NH 3 volatilization, and surface and ground waters. Collectively, these data will provide the information necessary to formulate and quantify significant parameters in the model.

Development of a Surface Water Object-Oriented Modeling System (SWOOMS) for the Neuse River Estuary, North Carolina

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The Neuse River Basin has experienced unprecedented growth in the past 50 years. Changing and diversifying land use practices that include forestry, agriculture, industry, and urbanization have placed increasing pressure on estuarine and coastal habitats to accommodate anthropogenic inputs of nutrients. It is widely believed that these pressures have resulted in the long-term degradation of water quality (e.g., increased nuisance and/or harmful algal blooms and fish kills) in the Neuse River Estuary (NRE). In an attempt to reverse this trend, the NC General Assembly passed legislation in 1997 requiring that a 30% reduction in external nitrogen (N) loading (based on a mean 1990-1995 N loading "cap") be in place by 2003. However, there is little evidence of how effective these measures will be in improving water quality in the NRE. It is also very unclear how to equitably and efficiently manage the highly diversified nutrient sources, (e.g., automobile, smokestack and waste lagoon emissions that are transported through the air, agricultural and urban runoff that are transported through the watershed, and point source discharges that are introduced directly into the streams and rivers), to achieve a desired nutrient loading to the estuary.

Our overall objective is to develop a prototype Surface Water Object-Oriented Modeling System (SWOOMS) that will allow us to (1) model and understand the ecological response of the NRE to varying nutrient (primarily N) loading and (2) integrate this estuary model within a larger suite of models that can track nutrients from their source in the airshed and watershed to their ultimate arrival and impacts within the estuary. Existing estuarine water quality models have not been designed to be part of such a modeling suite and therefore they are poorly suited for linking with dynamic models of other environmental media. SWOOMS will be developed using object-oriented design and implementation together with collaboration with researchers developing models in other media (i.e., the watershed, ground water and atmosphere) to yield an integrative environmental multi-media modeling system.

Specific components of the SWOOMS project are to (1) develop a finite-volume hydrodynamic/transport model, (2) integrate a water column, biogeochemical, water quality model with the hydrodynamic/transport model, (3) develop a sediment diagenesis model that is integrated with the water quality model, and (4) build the resulting surface water modeling system using an object-oriented framework that promotes seamless input/output with object-oriented models of the atmosphere, watershed, and groundwater media.

Mechanistic-based Ecosystem Exposure Modeling on a Watershed Scale

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The approaches to environmental transport and hydrological simulations on a watershed scale can be classified into three broad groups: stochastic methods, parametric methods, and physics-based mathematical methods. In the past 30 years, the watershed modeling communities have employed parametric-based models (the most famous one is the HSPF; all other parametric models are similar to HSPF, e.g., SWMM, CREAMS, STORM, ANSWERS, SWRRBWQ) for watershed management and assessment including ecological exposure assessments and TMDL calculations. Evolved from the pioneer model STANFORD WATERSHED IV, HSPF has dominated watershed simulations in the past 20 years. Physics-based, process-level chemical transport and hydrological models have been practically nonexistent until recently. It is easy to see that only the physics-based, process-level contaminant and sediment transport and fluid flow models have the potential to further the understanding of the fundamental biological, chemical and physical factors that take place in nature, and give definite and consensus predictions. It is precisely for this reason that EPA ecological research strategies (EPA, 1998) clearly stated that the first principal physical models should be used in ecological system assessment on a watershed scale. This presentation will discuss the essential elements that must be included for a model to be first-principle based. In particular, biochemical and geochemical processes must be dealt with using reaction-based approaches and rate equations must be mechanistically formulated. The presentation will address and emphasize the computational approaches that must be taken to enable the application of such a model on the field scale. This includes the development of innovative numerical algorithms to handle moving sharp fronts, the implementation of high performance computation to speed up several orders of calculations, and the inclusion of interactive graphical pre-processing and post visualizations to facilitate the application to complex watersheds and subsurface media.

Status of MIMS Architecture Design

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The Multimedia Integrated Modeling System (MIMS) is a multi-scale, cross-discipline modeling and decision support system that is intended to support ecosystem modeling and environmental health assessment. The MIMS architecture design team has collected information about MIMS requirements from stakeholders, including presentations and discussions from three prior multimedia modeling meetings, and from the team's own experience. The team has also surveyed other modeling systems and talked with a variety of model and modeling system developers. From this information the team has developed a draft MIMS architecture.

While the architecture may continue to evolve through the life of MIMS, the team intends to have a version of the architecture by the end of September that could be used to begin development. Simultaneously the architecture design team is investigating technologies, such as object databases, and collaborations that could provide the capabilities required to implement parts of the architecture.

Current MIMS Draft Conceptual Structure

One representation of the architecture is the "conceptual structure" which shows abstractions of MIMS's functional requirements and data sharing relationships among them. The conceptual structure is represented as a description of entities and a diagram (which uses an informal notation) among these entities. The lines on the diagram can be read as sentences starting with the entity at the origin of the line, followed by the text along the line, and finally the text at the destination of the line. For example, the line between the Session Manager and the System Administration Manager at the left side of the diagram could be read as "Session Manager invokes System Administration Manager."

Functional Abstractions

Files. Files on a storage device.

Databases. Databases that contain indexed information.

External Data Sources. Data services external to the organization running MIMS, such as web sites and Distributed Oceanographic Data System servers.

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* On assignment from Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce

Concurrently Executing Data Processors. In many cases, required data will be produced by other data processors.

Environmental Data Request Satisfier. Accepts requests for environmental data and determines if and how the request can be satisfied. Sources of data include files, databases, external data sources, and programs that are expected to be running. Some requests might imply aggregating, subsetting, or transforming the data. The Satisfier returns an object that provides data that satisfies the request.

Environmental Data I/O and Transformation Library. This library provides routines to read, write, subset, aggregate, and interpolate environmental data. It provides one or more APIs to support field data, tabular data, and arbitrary sets of parameters. Instances can be constructed by the Environmental Data Request Satisfier.

Persistent Object Storage. This provides storage for objects used within MIMS. It may only be accessible from object-oriented languages.

Analysis and Visualization: Performs analyses of data and prepares visualizations and reports to be used by people. A type of visualization tool that might require additional thought is one that both displays model results and allows the user to change inputs to models. For example, a control strategy development tool might display the cost and resulting air quality for a set of control strategies and allow the user to change the strategy and invoke a new simulation. It's possible that this would be a type of iteration controller.

Data Processor. One or more computational processes that perform transformations of data. Examples include what are typically called preprocessors, models, and postprocessors. Data processors can be executables, scripts, or collections of data processors. If the architecture allows data processors to be part of the framework's process space, then a data processor might simply be an object. Each data processor should be able to describe or should contain metadata that describe the resources that are required including data sets, computers, and GUIs.

Module. One or more subroutines that conform to a standard calling interface and paradigm that is designed to support interchangeable modules. An example of modules is alternative algorithms for advection that could be plugged into a model and interchanged. There could be a number of standard calling interfaces and paradigms, each supporting a different type of data processor (e.g., air quality model, meteorological model, groundwater model, emissions processor). Each module should be able to describe or should contain metadata that describe the resources that are required including data sets, computers, and GUIs.

Execution Manager. Used by Iteration Controllers (IC) and Conceptual Simulation Editors (CSE) to control execution of Data Processors.

Component Mediator. This provides configuration management functionality, where configuration items are Iteration Controllers, Data Processors, and Modules. It likely will be the Concurrent Versions System (CVS) or built on top of CVS, which will allow users to perform configuration management without using the MIMS framework.

System Administration Manager. Provides administration services, such as registering users and hosts.

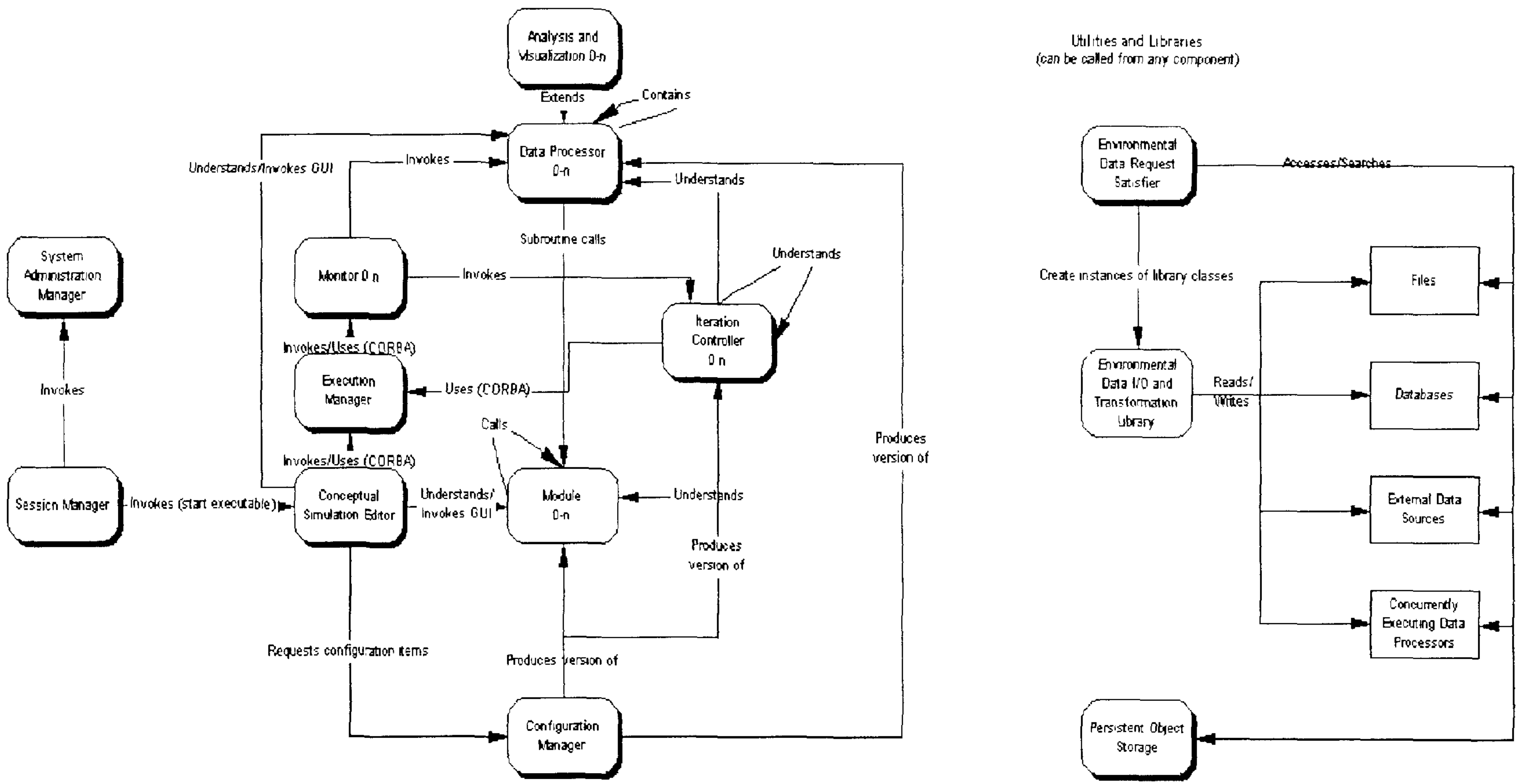
Iteration Controller. An entity that understands the characteristics of data processors, modules, and other iteration controllers; provides values for inputs that the user has specified will vary; starts the execution of the data processors and other iteration controllers; and determines if iteration is required, possibly by examining the results of previous runs. Examples of iteration controllers include a Monte Carlo simulation controller, a calibration tool, an iteration tool (e.g., repeat runs for different chemicals or time periods), an automated testing facility, and an optimization package.

Conceptual Simulation Editor. This includes functionality for building models, connecting models (planning computational studies), and specifying relevant domain, chemicals, date/time, output time steps, output parameters, scale, etc. It is undecided if this will include specification of a timeline of events (e.g., land development), or if that functionality belongs in an Iteration Controller or a model.

Session Manager. The Session Manager is what is initially started when MIMS is invoked. It performs authorization checks before starting other MIMS components. It might also keep track of which components and windows were last open and reopen those items.

Monitor. System monitors run on each platform where iteration controllers and data processors run, invoke those components at the request of the execution manager, and indicate when those components have completed. The monitor also returns information about the capabilities of the host on which it runs.

MIMS Draft Conceptual Structure
8/9/00



Notes "0-n" indicates that an arbitrary number of entities would be present
Shadows denote entities that contain one or more computational applications
Text in parentheses along the links indicates the communication mechanism used

Dynamic Information Architecture System (DIAS)

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A major challenge in modeling and simulation is the need to account for the complex, dynamic, and multi-scale nature of "real-world" systems for the purpose of experimentation, problem solving and decision support. Over the past 7 years, DIS has developed the Dynamic Information Architecture System (DIAS), an object-oriented framework with capabilities for attacking complex modeling and simulation problems. The main components of any DIAS simulation are 1) software objects (Entity objects) that represent the real-world entities that comprise the problem space; 2) simulation models and other applications that express the dynamic behaviors of the domain entities; and 3) the unique DIAS infrastructure that makes it feasible to build and manipulate complex simulation scenarios in which Entity objects can interact via numerous concurrent dynamic processes.

DIAS extends the Object paradigm of encapsulation and inheritance by abstraction of the objects' dynamic behaviors, separating the "WHAT" from the "HOW". DIAS object class definitions contain an abstract description of the various aspects of the object's behavior (the WHAT), but no implementation details (the HOW). Separate DIAS infrastructure objects carry the implementation of object behaviors (the HOW) and provide the linkage to models/applications. These models are linked to appropriate domain objects "on the fly", to meet specific needs of a given simulation context. Therefore, in a DIAS simulation, models communicate only with domain (Entity) objects, never directly with each other. From a software perspective, this makes it easy to add models, or swap alternative models in and out without major re-coding. This gives DIAS the ability to scale very well to increasingly complex problems. To adequately address the scientific domain of these new models, however, requires that intelligent domain (discipline) expertise be used in Entity object design.

Because of the wealth of existing legacy models/applications, it is important to promote model and code reuse. Application registration through DIAS provides for integration of legacy-type applications (e.g. simulation models, GIS applications, database management systems) without expensive reworking or recoding. The DIAS Java-based Application Programmers Interface (API) allows modelers to register models/applications and create DIAS simulation suites. Using the API, developers can extend existing DIAS Entity objects, create new Entities as needed, write the "wrappers" for their existing models/applications, or code new models within the DIAS framework. DIAS external applications are executed in their native languages (e.g. FORTRAN, C, etc.), and DIAS can be used to integrate disparate models, databases, or applications that can reside on multiple machines across a network, including the Internet.

Additional functionality associated with DIAS is the Framework for Addressing Cooperative Extended Transactions, or FACET. FACET is an object-based software framework that provides a mechanism for simulating complex patterns of societal interaction of multiple entities (agents) over time. FACET models are analogous to flowcharts and can be used to implement societal behavior patterns such as land management plans, business practices, government or corporate policies, clinical guidelines, etc. FACET models operate within DIAS, providing dynamic, integrated societal and natural process modeling capability.

Modular Modeling Framework for Multi-disciplinary Ecosystem Modeling

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The interdisciplinary nature and increasing complexity of ecosystem and natural-resource problems require the use of a variety of modeling approaches that can incorporate knowledge from a broad range of scientific disciplines. Optimal models for selected problems should be composed of a combination of process-simulation modules that are most appropriate for a given set of problem objectives, data constraints, and spatial and temporal scales of application. A modular modeling framework is being developed to facilitate the development, evaluation, and application of such models to a wide range of research and operational problems. The framework is an integration of modular concepts and tools from the U.S. Geological Survey's Modular Modeling System (MMS) and the Friedrich Schiller University's Object Modeling System (OMS). The framework uses the Java programming language to provide an object-oriented approach and platform independence. Model resource definition and the integration of database and GIS technologies are supported through the use of the eXtensible Markup Language (XML).

Development of Object-based Simulation Tools for Distributed Modular Ecological Modeling

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Ecological models, and supporting computing technology, have evolved to the point were it is feasible to develop truly modular approaches to model construction and implementation. A consistent, robust framework is needed to make this technology readily accessible to the ecological modeling community. The primary objective of the study is to provide this technology by extending an existing object-oriented simulation framework for ecological modeling in four focused areas: 1) underlying object-based technology for implementing and coordinating collections of simulation objects (modules) in an integrated simulation environment, 2) interobject communication technology supporting both single-machine and network-based communication between components of a modular simulation, 3) spatial and nonspatial data input, collection, analysis and visualization, and 4) development of visual programming tools for rapid definition and assembly of model modules into complete, fully functional ecological models and visual interpretation of model results.

This research will result in a set of tools for automating and simplifying the process of developing interoperable object-oriented simulation models for spatially- and nonspatially-explicit ecological systems. The study will use current standard object-oriented languages (C++ and Java) and language-independent object technologies (CORBA/COM/DCOM) to refine and develop a collection of object classes and application programming interfaces (API's), and visual development tools geared towards ecological modelers for simplifying and automating the development of ecological models which may be both spatially distributed and networked via the World-Wide Web. We will work other modeling groups to coordinate activities and approaches to providing technology for modular model development and implementation. To test and evaluate the tools developed, the resulting simulation framework will be utilized to implement a watershed model with hydrologic, ecological and economic components currently being developed in a separate project.

Deliverables from this project will include (1) a series of interface specifications and corresponding code to allow intermodule communication and identification to facilitate modular model development and assembly, 2) a simulation environment providing coordinated execution of module collections, each potentially running as continuous or discrete object at variable timesteps, and 3) a visual assembly tool capable of query single-machine or networked model modules for identification and interface specification, able to assemble these modules into complete simulation models, execute the resulting model, and provide visual interpretation of the results. These products will be made available on the web for utilization by other modeling groups.

A Toolbox for Assembling Spatially-Explicit Multimedia Ecological Models from Reusable Components

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Simulation models have become essential tools for evaluating the effect of human perturbations on ecosystems. We have developed a system for constructing ecological models for simulating the inter-linking of processes, such as water flow and nutrient flow, and the spatially-explicit connections between adjacent ecosystems. This system is called the Ecological Component Library for Parallel Spatial Simulation (ECLPSS), and can be viewed as a toolbox for ecological simulation modeling. The goal of this framework is to permit users to design and build fully three-dimensional spatially-explicit ecological models by connecting existing reusable components and readily creating new components. In ECLPSS, models can be quickly assembled from a library of components, each representing a single function or aspect of a process. These components only communicate via state variables -- they cannot communicate directly or with any hidden variables. Because of this constraint on model looping structure, components can be readily replaced without 'breaking' the model. This functionality makes it easy to test the influence of a given representation of a process on the predictions, or to easily modify the model when understanding of a process improves. The ECLPSS framework uses component-based techniques to simulate ecosystem and ecological phenomena at multiple spatial scales. The framework is designed to take advantage of parallel processing to enable simulation of many individuals in a large spatial domain at high speeds. It is designed to operate on multiple platforms and be used across networks via a World Wide Web-based user interface.

This system allows the user to separate chemical, physical, and biological concepts from simulation support functionality. Hence biologists can readily construct new spatially-explicit models without becoming computer scientists, while computer scientists can improve the modeling support framework without being ecologists. The system assists ecologists to build robust spatially-explicit simulations of ecological processes from a growing library of reusable components representing terrestrial ecosystem processes.

With this system scientists can create models of ecological processes more reliable by using interchangeable components that can be easily replaced without interfering with other aspects of model behavior.

Software Reuse and Cluster Computing Tools for Environmental Modeling

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The Software Reengineering Laboratory (SRL) at Iowa State University has developed ParAgent, a tool for automatic parallelization of legacy codes. The SRL has assembled ParAgent and other complementary tools in a comprehensive environment to make cluster computing a reality for long-range climate and environment modeling. The software tools and their applicability will be described using the NCAR/Penn State MM5 as an example. Results of performance experiments on several Pentium clusters with different communication networks will be presented.

The Coupling-Mode Extensions of the Models-3 I/O API: Tools for Building Coupled Cross-Media Models

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The Coupling-Mode Extensions were developed in the "Practical Parallel Computing" STAR Cooperative Agreement to provide a robust and modeler-friendly set of tools for coupling multiple cooperating environmental models. Data is exchanged by means of a data access library in a selective, direct-access fashion, so that the individual models do not "need" to know whether they are running stand-alone, receiving their data from files, or whether they are running in parallel, receiving data from other processes running at the same time (on possibly different -- even remote -- computer systems). Cooperating-process models for both hydrology-meteorology and numerical air quality prediction have been constructed using the coupling-mode extensions of the Models-3 I/O API.

Model Design for High Performance on Microprocessor Based Parallel Computer Systems

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Several aspects of environmental model design and parallel decomposition have substantial effects upon the computational performance of models running on microprocessor based parallel computer systems. The "Practical Parallel Computing" STAR Cooperative Agreement studied the sensitivity of model performance to these aspects for several environmental models, across a range of several vendors' computer systems. It also studied modeler friendly means of parallelization on available systems. We discuss these results.

High Performance Computing for Large Scale Environmental Flow and Transport Processes

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The objective of this work is to develop parallel algorithms for large scale environmental flow and transport processes. We present a domain-decomposition based Least-Squares Finite Element Method (LSFEM) which can provide implicit and fully coupled transient solutions to large scale, three-dimensional Navier-Stokes equations and convection diffusion equations. The LSFEM leads to a symmetric and positive definite (SPD) system of linear equations. A parallel and matrix-free conjugate gradient method is used as an iterative solver for the SPD linear systems. Parallel computations of fluid flow problems with more than 4 million finite elements and 29 million unknowns were carried out on a HP-Convex Exemplar X-class scalable computers (SPP 2200). Efficiency of parallelization is about 65 to 86 percent.

We formulate a LSFEM for large eddy simulation (LES) of turbulent flow and transport processes. The formulation is based on a dynamic subgrid scale model, which can capture the dynamics of the wall layer and provide correct profiles of eddy viscosity and eddy diffusivity.

Other preliminary results obtained by the LSFEM include multiphase flow in porous media, pollutant dispersion in convective boundary layers, concentration fluctuations and reactive plumes.

Other activities in this project include parallel computations of open channel flows on the Roadrunner cluster.

High-Performance Modeling of Estuarine and Coastal Dynamics

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In order to develop predictive ability of long-term response of estuarine and coastal environments to natural and anthropogenic changes, high performance environmental models are needed. Multiple year simulation using existing multi-dimensional environmental models require excessive computer time on conventional single CPU computers. This work examines the application of high performance computing to models of estuarine and coastal dynamics. Both shared memory approach and message passing approach (PVM and MPI) have been tested with 1-D, 2-D and 3-D estuarine and coastal models on several different platforms (SGI Origin-2000, Sun Enterprise, Beowulf Cluster, and a cluster of various UNIX workstations).

This paper focuses on the application of high-performance modeling techniques on a curvilinear-grid multi-dimensional model CH3D which was the cornerstone of the Chesapeake Bay model. Based on our test, the shared-memory approach is very effective on the SGI Origin-2000, due to the particular solution algorithm deployed by CH3D. However, CH3D is not very amenable for parallelization on the Beowulf Cluster at UF. A new approach which uses a very fine rectangular grid and special parallel algorithms has been found to be very effective. A new parallel matrix inversion routine developed by us is being implemented into the model.

Novel Techniques for Parallel Simulations

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In this talk we discuss two novel ideas that have proven useful in coastal simulations. The first is a simple parallel algorithm for solving banded linear systems. This algorithm is optimal and practical. The second is a paradigm called LESS_TALK. LESS_TALK can be used to speedup computations in general on any parallel model of computing.

Tool-box for parallel simulation of flows in porous media

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For parallel simulation of flows in porous media we have implemented, and tested a computer system that is based on:
(a) discretization techniques utilizing finite elements and finite volumes;
(b) efficiently preconditioned iterative methods for the resulting large sparse system;
(c) error control and adaptive grid refinement; and
(d) parallel implementation on multiprocessor systems utilizing domain decomposition concepts.

The tools that we have used include:
(1) stand-alone 3-D mesh generator (NETGEN);
(2) stand-alone partitioning and load balancing software (METIS);
(3) local error control based on a posteriori error analysis and subsequent refinement procedures;
(4) parallel methods based on domain decomposition and multigrid/multilevel subdomain preconditioning;
(5) MPI and the OpenMP standards for parallel computations.

Examples of various tests on problems of flow and contaminant transport in porous media will be presented.

Development of a 1-km vegetation database for modeling biogenic fluxes of hydrocarbons and nitric oxides

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Regional air quality modeling systems are composed of an intricate network of programs that include emission processors, dry deposition algorithms, and meteorological modules. Characterizing the land surface is critical for modeling biogenic emissions, dry deposition of gases and particles, and fluxes of moisture, heat, and momentum. Existing land use inventories, such as the popular USGS 1-km satellite-derived database, lack information on the distribution of specific tree species and crop types. Emissions of isoprene, an important hydrocarbon emitted from vegetation, varies by several orders of magnitude among deciduous tree species. Similar variations occur with the emission of nitric oxide from different crop types. Less pronounced, but still significant (~factor of three), variations occur with stomatal resistance among different tree species and crop types. Stomatal resistance strongly influences dry deposition and surface energy fluxes. To support the USEPA's existing Community Multi-Scale Air Quality (CMAQ) modeling system and evolving Multi-Media Integrated Modeling System (MIMS), we have developed a 1-km vegetation database for North America. This database integrates the USGS database with forest inventories collected by the U.S. Forest Service and crop statistics complied by the U.S. Department of Agriculture. We will demonstrate the value of characterizing specific tree species and crop types in the third generation of the Biogenic Emissions Inventory System (BEIS3), which is an important emissions processor for the CMAQ modeling system.

* On assignment from Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce

Landscape Characterization and Non-Point Source Nitrogen Modeling in Support of TMDL Development in the Neuse River Basin, North Carolina

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Pfiesteria-like toxic blooms have been implicated as the causative agent responsible for numerous outbreaks of fish lesions and fish kills in the Mid-Atlantic and southeastern United States. An increase in frequency, intensity, and severity of toxic blooms in recent years is thought to be a result of surface water nutrient enrichment mediated by changing land-use practices. The goal of this research is to apply land-cover/use information to quantify the extent distribution of terrestrial sources of nitrogen contributing to harmful algal blooms and possible Pfiesteria outbreaks. This is being accomplished by coupling high resolution land-cover data sets with GIS-based nutrient models that will be calibrated and validated using a stratified subset of Neuse River basin (NRB) sub-watersheds. A high resolution land-cover/use data sets has been developed using advanced satellite based remote sensor systems including the new SPOT 4 (XS) and Landsat 7 Enhanced Thematic Mapper Plus (ETM^+) remote sensor systems to provide basin-wide land cover/use data at 0.4 ha. and 5.8 ha. minimum mapping units (MMU) or landscape patches. Also, new IKONOS sub-meter stereo imagery for the characterization riparian zone vegetation structure. NRB modeling includes the development and implementation of a nitrogen mass balance model to quantify patch specific potential nitrogen sources, coupled with a hydrologic model for routing nitrogen to water courses based on event driven precipitation.

Observations and Modeling of O_3 and SO_2 Deposition Velocity over Agricultural and Forest Ecosystems: Synthesis of a Six Year Field Program.

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Dry deposition networks, such as the CASTNET network in the United States, usually measure concentration of pollutants and infer deposition velocity from a model. In the Castnet network the multi-layer model (MLM) of Meyers is used. To evaluate the MLM and other deposition velocity models, and to provide a database that can be used to improve our understanding of dry deposition processes, we launched a field program that was designed to directly measure fluxes and deposition velocity of O_3 and SO_2 over a variety of natural and managed ecosystems that were representative of major land use types. Agricultural studies have included two studies over pasture, one over corn, and two over soybean. One of the soybean studies lasted the full growing season of the crop, from planting to harvest, and included a major drought, and a hurricane. Three studies were conducted over forests, a six week study over a pine plantation, and growing season long studies over a deciduous and a mixed coniferous-deciduous forest. Additionally, a six-week study was conducted over a salt-water estuary. This paper will summarize and synthesize these studies. It compares and contrasts the observations from each study, extracting the salient features and noting the similarities and differences in the deposition process for each pollutant between the different cover types. Besides a general "Climatology" of deposition velocity for the sites, special attention is given to issues such as the impact of water on leaf surfaces, day/night differences between plant species, the differing diurnal cycles of deposition velocity over different plants, uptake by surfaces, and other issues. The MLM was run using data from the field studies. The modeling results are shown, and its strengths and weaknesses discussed. Finally, some thoughts on a new deposition velocity model that shows promise for improved predictions will be presented.

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* On assignment from Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce

Four-dimensional (4D) acquisition, visualization and analysis of Ground Penetrating Radar data for the determination of three-dimensional hydrologic conductivity and time-dependent fluid flow

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The key problem in subsurface remediation is knowing what happens below the surface. If we knew this, we could tailor our remediation and containment activities to the processes that occur. This knowledge can partly be derived from modeling. However, modeling will always be limited by data and thus what we really need are data on subsurface processes. In all current approaches our data on the subsurface is limited to the results of single geophysical surveys and a small number of wells, most of which are not even equipped with continuous logging probes.

Sponsored by EPA Grant # GR825209-01-0, we developed and refined a methodology to use multiple three-dimensional (3D) GPR surveys (4D surveys) to image processes. Our direction of research was based on the recognition that 4D data do provide the potential to see processes but also that field 4D data were of insufficient quality to resolve many of the issues involved in understanding 4D data. We thus chose to develop our methodology in a custom-created highly-controlled environment (Columbia's subsurface imaging lab) in which we can create and control both the subsurface and the processes in the subsurface. The lab is centered around a large tank which can hold 20 tons of material which can be emplaced in a relatively simple fashion.

This lab is completely automated from data acquisition to processing and web based visualization (all of which occur in near real time). Thus, we can observe processes as they occur (which of course allows us – at least in theory - the ability to observe the effect of feed back systems on these processes). Once we collect high-density 4D data the focus shifts to how to interpret 4D geophysical data. As the temporal density of our 4D datasets is one to two orders of magnitude higher than all other 4D datasets collected anywhere else we had to develop a new approach. Our data allows us to exploit the temporal density of the data to invert for the changes in our data (which are a result of processes) to obtain information on the fluid flow. This of course requires fairly complex visualization and computational approach as we are manipulating data coming in at a rate of approximately 20 MB/hour, and we have to invert this data for processes. However, the amount of data makes the inversion feasible (if not trivial).

As the fluid flow is related to the hydrological conductivity we can – with some assumptions – derive a 3D distribution of hydrological conductivity from our data. While this methodology has been developed in a controlled setting, the only problems in expanding this approach to the field setting are engineering related and we are now close to being able to image subsurface flow (and the contamination or remediation associated with this) in field settings in real time. One caveat is the geophysical method used: while radar was appropriate for our setting it is well known not to work in all areas and we may thus have to use other geophysical methods (eg. acoustic or electrical) in other settings.

Determination of aquifer recharge, ground-water flow and basin discharge-methods and examples

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The water balance equation provides the basis for understanding movement of water and dissolved matter through a watershed. Several hydrologic and chemical techniques can be combined to understand a hydrologic system so that resulting models more accurately reflect controlling processes taking place in a watershed. Useful techniques include hydrograph separation, isotope analysis, and environmental tracers. A simple analysis using tritium data and hydrograph separation is demonstrated which can be used to separate surface runoff, deep ground water and shallow ground water contributions to streamflow. Environmental tracer data collected during the summer of 1999 (chlorofluorocarbons) are presented which can be used to verify model-predicted movement of groundwater through Coastal Plain aquifers on the Lizzie Study Site.

In order to demonstrate application of the hydrograph separation technique, a case study for mapping ground-water recharge in North Carolina is presented. The method focuses on the drainage basin, dividing the landscape into upland flats, valley slopes, and valley bottoms. The method is based on a conceptual understanding of ground-water flow within the basin, where water moves beneath the land surface from upland recharge areas to lower riverine areas of ground-water discharge. The building blocks of the recharge map are 1:24,000-scale soil-mapping-units digitized from detailed county soil surveys. These mapping units are aggregated into "hydrogeologic areas" having similar recharge characteristics. Several factors govern the rate of ground-water recharge, including: depth to the water table; slope of the land surface; and the infiltration capacity of the unsaturated soil profile. Corresponding properties of soil mapping units are: drainage class; slope gradient; and underlying geology. The Rorabaugh-Daniel streamflow recession-curve displacement technique was used to estimate ground-water recharge in selected drainage areas at representative USGS stream gauging stations. These calculated recharge values were used, in turn, to calibrate, recharge rates for the different hydrogeologic areas using a Monte Carlo simulation technique. Stream hydrograph separation techniques were used to determine the ground-water contribution to streamflow.

Advancement of Environmental Decision Support Through HPCC

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Decision making for single- and cross-media environmental problems is often complex and tedious. Competing design objectives and constraints, coupled with large quantities of data and sophisticated simulation models, produce problems that can seem overwhelming to a policy maker. In some cases, the time and effort spent to find feasible management strategies limits the resources available for exploring issues such as cost, equity, and uncertainty. The fields of Decision Support Systems (DSSs), Operations Research, and Decision Theory offer concepts and techniques that promise to facilitate the design process, potentially yielding more effective and efficient solutions, as well as allowing more comprehensive consideration of complex design issues. Many such techniques, however, are highly computationally intensive. While this has limited their application in the past, high performance computing is making these approaches more practical for supporting policy making in the present and future. We have performed a variety of activities to explore the use of decision support tools in regulatory decision making. Among the topics that will be discussed in our presentation are: a prototype decision support system for air quality management, optimization using distributed computing, advancements in optimization algorithms, the conjunctive use of simple and complex models, and new approaches for modeling emissions trading programs.

* Now on assignment to Atmospheric Modeling Division, National Exposure Research Laboratory, USEPA from Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce

A Framework for Creating and Managing Graphical Analyses

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Environmental data analysis often consists of a long and convoluted series of questions, with each analysis providing some answers and leading to more questions. During the exploration of the data, statistics and visualizations are a means to an end, such as a better understanding of the environment, an improved model, or a new policy. While a number of environmental data analysis tools are available, there remains a fundamental gap between the work many scientists perform and the tools that are available. Most environmental data analysis systems concentrate on only the capabilities needed to crunch numbers or create pictures. The user retains a substantial burden of repetitively explaining to an analysis package — often via low-level commands — how to process the data. At the same time, many people keep no or inadequate records of how they have analyzed their data, which can be a problem if questions arise later. Issues such as lack of awareness of tools and their capabilities further hinder scientists' data analysis efforts.

To address the gap between data analysis work and analysis tools' capabilities, we developed the Knowledge-based Environmental Data Analysis Assistant (KEDAA), a prototype software system. The KEDAA provides analysis management capabilities that provide more complete support for data analysis than is found in most analysis packages. Note that the KEDAA was intended to support people who analyze environmental data, not replace them. The KEDAA does not interpret data or draw conclusions from analyses.

The KEDAA also does not perform analyses itself. Instead, it relies on off-the-shelf data analysis packages to perform that work. In other words, the KEDAA provides an interface between the user and existing analysis packages. A user specifies an analysis to perform via the KEDAA's graphical user interface (GUI), which allows the user to select analysis techniques, variables to plot, options, panes (i.e., divide a window or page into multiple plot areas), and overlays. The KEDAA determines which of the external analysis packages that KEDAA utilizes can best satisfy the user's request and sends the appropriate instructions to that package.

The user can store the specifications of analyses in an electronic outline. Collapsing and expanding sections of the outline allows the user to review past work at the desired level of detail. Textual notes can be added to the outline to record observations, hypotheses, and conclusions, allowing a user to create an integrated record of what analyses were performed and what insight was gained. Variables read from data files and formulas for deriving variables can be assigned to topics in the outline, providing a scope for variables that are analyzed. Analyses can be copied from one topic (scope) to another, allowing complex analyses to be easily applied to different variables.

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* Now on assignment to Atmospheric Modeling Division, National Exposure Research Laboratory, USEPA from the Atmospheric Sciences Modeling Division, National Oceanic and Atmospheric Administration, U.S. Department of Commerce.

+ Currently with Sonoma Technology, Inc.

The KEDAA currently provides six types of analyses, implemented by three analysis packages, and reads files in four formats. The KEDAA has been designed in a modular manner that allows its capabilities to easily be extended with new analyses, packages, and file formats. The KEDAA is implemented in Java and has been used on several flavors of UNIX.

We believe that the KEDAA can provide several benefits for users. Users can perform repetitive analyses, for instance of multiple time periods or scenarios, by simply copying and pasting analyses. The KEDAA provides a common user interface for creating analyses with multiple packages and indicates when analysis techniques can and cannot be used, which allows users to apply new techniques to their work without learning new analysis packages or commands. Since the KEDAA provides a general graphical user interface for creating analyses, it can be used as a front-end for packages that do not have a GUI. Finally, users can produce an integrated record of analyses performed and insight gained that can be invaluable when questions arise later.

The development and evaluation of the approaches described above were terminated prematurely when the principal investigator changed organizations. The KEDAA provides significant analysis management capabilities, but users have not extensively evaluated the concepts. The KEDAA is available as open source from http://envpro.ncsc.org/keda. The distribution includes source, jar files, and on-line documentation.

Space Time Toolkit: Web-Based Integration and Visualization of Spatially and Temporally-Disparate Data from Distributed Sources

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The Space-Time Toolkit (STT) is a Java-based environment designed for interactive fusion and 3D visualization of disparate data sets. It is capable of running as either an application or an applet on virtually any workstation platform with highly interactive, dynamic 3D performance. Unlike most visualization environments, the STT does not require input data to be gridded into a common spatial domain nor stacked as common time slices in order to be integrated together. In fact, the STT acts as an on-demand transform manager that will "on-the-fly" georegister and synchronize multisource disparate data into any user-selectable display domain. A powerful capability within the STT is the presence of an Observation Dynamics Model that provides geolocation capabilities for virtually any dynamic sensor, whether hand-carried, stationary, or mounted on satellite, aircraft, ship, or automobile.

For any user-selected project, the STT determines the availability of data using web-based resource documents. All data is accessed over the web using URLs that point to Internet files, CGI scripts, or Java Servlets.

While the STT prototype was developed primarily using NASA funding, the current Java redevelopment was partially funded (10/96 - 09/99) by the EPA HPCC program under Chris Saint. The EPA Nashville SOS field experiment data has served as a testbed for merging disparate data from multiple sources. With current funding primarily coming from NASA, the STT is being extended to meet the needs of NASA's EOS and Digital Earth programs.

Field Data Model for Supporting Cross-media Modeling and Visualization of Large Diverse Time-varying Geospatial Data and Metadata

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Goal:
Research scientific data models and develop high-quality multi-language software libraries for efficient representation, integrated analysis and visualization of large diverse time-varying geospatial environmental data and metadata for supporting cross-media modeling and decision-support applications operating in a high-performance networked multi-platform computing environment.

Background:
Computer modeling of environmental processes is crucial for understanding how the environment changes due to natural and human processes and the long-term effects of these changes on ecosystems and human health. Environmental decision-making requires the support of reasonably accurate modeling of the relevant processes and summary analysis of their effects.

Environmental modeling is typically done separately in each domain - air, land surface, water, soil, groundwater, etc. - and at different scales: global, meso, regional, urban and micro. Modeling results must be compared and correlated with actual observations, samples and reported data. Also, ideally, the various kinds of models (air, terrain, soil, etc.) should be coupled to better account for the exchanges that occur at these domain interfaces, such as wet deposition of air pollutants onto the surface of a lake and biogenic emissions from surface vegetation, etc.

Decision-support analysis imposes more requirements on models such as steering (of model execution) and generation of metadata (allowing traceability during review and future analysis). Metadata necessary to support EPA's "20-year rule" is a significant challenge that must be met by such decision-support systems to help justify (e.g., in court) regulatory laws enacted based, in part, upon such computer-aided analysis.