Narrative Summary
NOAA Atmospheric Chemical Modeling Workshop
October 10-11, 2007
Earth System Research Laboratory
Boulder, Colorado

Background

The NOAA Atmospheric Chemical Modeling Workshop included 48 NOAA participants from various laboratories and divisions of OAR, NWS, and NESDIS. The aim of the meeting was to review the current state of atmospheric chemical modeling across NOAA and, from this basis, describe a route to develop NOAA's global chemical modeling capability.

The first day of the meeting was composed of presentations that summarized the current state of atmospheric chemical modeling within NOAA. These presentations closely followed the structure and format of the NOAA Atmospheric Chemical Modeling Inventory (attached). The requirements, needs and applications for an integrated global chemical model were presented from weather forecasting, air quality forecasting, air quality regulatory, and climate perspectives. NOAA global chemistry models that already exist or are under development were then discussed, including the existing AM3/MOZART and RAQMS models and developments such as the GFS/NUOPC effort and the ESRL Chemical Model. The afternoon wrapped up with a discussion of the Earth System Modeling Framework (ESMF) by Cecelia DeLuca, ESMF project lead from UCAR. The second day of the workshop involved two working group breakout sessions. Leaders for Group I were Drs. Ramaswamy and Paula Davidson, and those for Group II were Drs. Steve Fine and Fred Toepfer. The participants were randomly assigned to working groups, with roughly equal participation from all line offices and laboratories in each group. The detailed discussion from each group was recorded by rapporteurs (Janet Intrieri, Rohit Mathur, and Gregory Frost). The following two questions were addressed:

> *1) What are the aims and anticipated applications of an integrated NOAA global chemical model?*
> *2) What steps are needed to construct and evaluate an integrated NOAA global chemical model?*

The issues brought up during the working groups were wide-ranging and comprehensive. These issues were presented to all workshop participants after each breakout session. After the workshop, the discussion points were collated and then circulated to the workshop's organizing committee for comments. The discussion points were rewritten in a narrative format in order to be more accessible to workshop participants and other interested parties. The rest of this document presents this narrative summary and a summary of the organizing committee's recommendations for next steps. It is hoped that this document might serve as the basis for a white paper that could help guide the design of NOAA's global chemical modeling capabilities.

Summary of NOAA Global Chemical Modeling Working Group Discussions

QUESTION: What are the aims and anticipated applications of an integrated NOAA global chemical model?

The workshop participants began with the question of whether we are seeking an integrated *model* or an integrated *framework* and decided that an integrated *framework* would most effectively meet NOAA's mission goals for Science Serving Society. It was recognized that the vision for NOAA's global chemical modeling capability cannot be realized with any single existing model. Rather, our goal should be the development of an integrated, seamless modeling 'system' that is scalable across space and time scales and physical process representation. This system would consist of a framework building on the scientific chemical modeling strengths across the NOAA community. The modeling system's development would rely on collaboration throughout NOAA in order to bring the best approaches to a continuous spectrum of capabilities, including:

- atmospheric chemistry over a range of temporal and spatial scales
- monitoring, understanding and tools for environmental stewardship
- simulating chemistry of climate processes and climate change
- global weather forecasting with chemistry/aerosol/cloud radiative feedbacks
- national air quality forecasts
- air quality predictions and evaluations for regulatory scenarios and approaches

An integrated chemical modeling approach would benefit NOAA by providing efficiency through the use of a common modeling framework to manage these capabilities. The use of a common modeling framework increases the effectiveness of transitioning capabilities from Research to Operations (and from Operations to Research). A unified modeling system would create controlled conditions for experiments that evaluate model components, leading to more effective use of resources.

Workshop participants recognized that a unified atmospheric chemical modeling system is a useful but somewhat idealistic concept. A major obstacle to a unified chemical modeling system is the level of complexity required to address the wide range of problems that are currently being addressed by specialized models. The level of detail required to simulate specific process interactions dictates how models should be built, which explains the wide variety of chemical models currently used by NOAA researchers. Architecture development and science code advancement should proceed independently, and we must acknowledge that today's ideal framework might not be so ideal in treating every future scientific problem.

Having acknowledged the inherent developmental challenges, the participants discussed the specific attributes of the ideal global chemical modeling system. In order to be workable, the system should be built on a framework of consistent coding and data standards, interchangeable computational modules, interfaces, and architectures. The Earth System Modeling Framework (ESMF) was discussed as one possible candidate. The ideal modeling system would be scaleable, spanning spatial domains ranging from urban to regional to global and time scales spanning days to decades. It should be based on a flexible framework that includes nesting capability (both 1- and 2-way), hydrostatic and non-hydrostatic treatments, the ability to adjust the number and types of chemical species, and incorporate a range of physical process representations. The system would have scalable chemistry, including a variety of mechanisms for both aerosol and gas phase chemistry in both the troposphere and stratosphere. The model would allow for consistent and appropriate communications between regions of the earth system, i.e., ocean, land, atmosphere, and cryosphere. It would be capable of online and offline execution, i.e., employing either concurrent or sequential calculations of dynamics, emissions, and chemical reactions. The model system would also include diagnostic tools for evaluation. It would be capable of ensemble forecasting, in that multiple simulations resulting from combinations of model components, settings, and input data could be used to improve forecast skill.

The participants discussed specific objectives and applications for which an integrated atmospheric chemical modeling system would be well-suited. These are listed here in no particular order, along with considerations discussed for each objective.

1. Meteorological and chemical re-analyses and real-time analysis:
   The current NCEP/ERA-40/20 re-analyses are not appropriate for transport/tracer applications. There is a need for higher resolutions in order to resolve processes not currently captured in these re-analyses. The re-analysis system could be extended to real-time monitoring purposes.

2. Boundary conditions and coupling between scales:
   A multiple-scale system would benefit existing regional air quality models by providing improved lateral boundary conditions and other external constraints, on time scales from days to decades. It could also lead to better two-way coupling between different spatial scales (e.g. between the regional and global scales).

3. Improved use of observational data:
   A unified modeling system would be useful for building and improving chemical data assimilation capabilities and observing network design (satellite, surface, aircraft, profiling networks). Observing System Simulation Experiments (OSSEs) could be used for future network design. The system should be validated with measurements to improve both its meteorological, air quality, and climate predictions.

4. Climate modeling and analysis:
   There is a need for both prognostic and retrospective climate analyses on multiple time scales. To properly handle this problem, the modeling system would have to treat not only the atmosphere (both troposphere and stratosphere) but also the cryosphere (including sea ice and permafrost) and the biosphere, in which land-use, vegetation, and CO_2 uptake schemes are crucial. Because multiple earth systems would be treated, the integrated model system could help improve connections to related advances for internally consistent use, such as land-use schemes. The system could provide boundary conditions of GHGs for regional analyses. An integrated modeling approach would be particularly useful in evaluating mitigation and adaptation strategies and regulatory scenarios for climate forcing agents. Such a comprehensive system would stretch existing computing resources.

5. Seasonal forecasting and longer term climate projections:

Projections of seasonal and longer-term changes in stratospheric ozone, aerosol forcing, vegetation feedback and carbon cycling, tropospheric ozone and aerosols, and air quality-climate coupling would benefit from an exploration of sensitivities to many environmental variables and process treatments. An integrated modeling system that incorporates multiple approaches would facilitate these studies.

6. Detailed AQ-climate process studies:
   An integrated chemical modeling system could lead to improved process-level understanding of air quality-climate interactions, since feedbacks would be coupled on multiple spatial and temporal scales. Inclusion of both criteria pollutants (e.g. NO_x, CO, and VOCs) and GHGs would be crucial in evaluating the direct and indirect forcing of aerosols and forcing by clouds. An integrated modeling system would allow evaluation of emission inventories that account for both GHGs and criteria pollutants.

7. Ecosystem and other impact assessments:
   Interactions of the atmosphere with the larger ecosystem, including ocean acidification, ocean water quality, and biogeochemistry, would benefit from a comprehensive global chemical modeling effort.

8. Improving weather forecasting skill:
   A principal goal of an integrated chemical modeling system would be improving the accuracy of operational weather forecasts. By using a consistent set of physical and process treatments in both weather forecasting tools and a unified chemical model, the transfer of knowledge from research to operations would be streamlined. NWS has already noted that some chemical processes should be included in future weather forecasting models, including aerosol direct and indirect effects, improved cloud-radiation interactions, 5-10 day predictions of stratospheric ozone, the use of improved initial conditions (e.g. using satellite data assimilations), and short and long range dispersion forecasts.

9. Improving weather forecast products:
   Another application of an integrated modeling system would be in improving weather forecast products. These include aviation weather forecasts (particularly visibility / optical properties), emergency response, space weather forecasts, military applications, hydrological applications, and providing support to field measurement campaigns.

A number of issues for further consideration were mentioned, but there was not time to address them during the workshop. It will be important to decide how the success of an integrated modeling effort will be measured. A diversity of modeling approaches is important for addressing systematic error and noise. Integration of different models should move in a stepwise fashion. We should learn from existing models/science approaches, e.g. the WRF framework and ECMWF’s current effort. For example, the ECMWF effort has resulted in improved end-to-end capability in building a collaborative system, but their approach hasn’t yet been systematically compared to recognized climate models.

QUESTION: What steps are needed to construct and evaluate an integrated NOAA global chemical model?

Workshop discussions on this question included general considerations on how to approach this problem and specific steps that NOAA might follow to build an integrated global chemical modeling system. Some general considerations and discussion surrounding each were as follows:

- Existing models must fit within the new global chemical modeling framework:
  Any new modeling framework should be built to include existing models since the system must be constructed of reliable components. Evaluation criteria for these components are application dependent, however, each component must exhibit fidelity in simulating test cases. Whatever model components are chosen must also be suitable for operations.

- Coupling global scales with other spatial scales:
  Scalability is critical, particularly when comparing hydrostatic vs. non-hydrostatic treatments. There must be consideration of the timescales for exchanging information between spatial scales. An effective model framework can facilitate development of methods to simulate two-way chemical exchange, which is crucial for handling the complexity of non-linear chemistry. A standard set of tests using key observations must be designed to examine the theoretical and numerical aspects of this coupling.

- NOAA Earth system modeling:
  We should take advantage of a common framework to facilitate investigations in coupled earth systems, such as biosphere-atmosphere, ocean-atmosphere, and cryosphere-atmosphere interactions.

- Interfacing global chemical model with numerical weather prediction:
  Science advancements and operational needs are connected. An ideal unified modeling system accommodates internally consistent transfer of mass and energy across interfaces and includes flexible options for the degree of coupling. There are numerous technological considerations for portability and interoperability of ESMF (or other frameworks) in regard to existing systems.

- Evaluating accuracy of simulated chemical concentrations:
  The required time interval for observation-model comparison depends on the reactive lifetime of each chemical species. The accuracy needed for a given time interval is defined by the application.

- Databases for test cases and model evaluation:
  A crucial component to this effort is the compilation of observation datasets for model evaluation purposes. These datasets should be accessible through system libraries for stand-alone validation. Tracers and long-lived greenhouse gases (GHGs) are ideal for testing transport schemes. Analysis and re-analysis data are also useful in this regard. The databases for a unified model validation would require diverse community access that is broader than just the originating model development group. For a global chemical model system, a general set of observations for a comprehensive list of species is required, including reactive gases,

long-lived GHGs, and particulates. Some important aspects of model testing include vertical transport, tracer monotonicity, conservation of mass, and the diurnal development of the planetary boundary layer.

- NOAA-wide efforts toward building the model framework:
  Sharing ideas and science codes is crucial to this effort. Increasing collaboration between groups should be science-driven. These collaborations will be nurtured by management giving recognition for cross-disciplinary activity. Inter-organizational workshops and regular meetings between groups across NOAA to discuss results and coordinate activities are recommended. Regular discussion of science advances and technological/operational advances will provide opportunities for cross-fertilization.

- Research-to-Operations:
  Here we mean "Operations" to include both NOAA/NWS operations and applications as well as IPCC applications. A unified chemical modeling framework is extremely useful for research-to-operations. For this approach to be successful, a description of future operational standards and protocols and their availability is needed. Phased development and testing of a unified system is useful. NOAA should set up standard tests and thresholds for testing a global chemical modeling framework. These can also be devised for inter-comparison of existing NOAA capabilities. The workshop participants recommended that NOAA set up a model test-bed center.

The workshop concluded with set of specific steps towards developing and testing a unified chemical modeling system with the general considerations discussed above in mind. These steps target the four main applications (climate, weather forecasting, air quality, and the carbon cycle) that were identified earlier in the workshop. No explicit revising loops are listed, but these may occur based on the success or failure of each step. A number of activities should occur in parallel with the development steps outlined below, including: external collaborations; continued component evaluation; normalization/standardization of input/output data; documentation, training and outreach, transition to Operations, and development of code/data repositories..

The entire modeling framework should be open source, following ITAR (International Traffic in Arms Regulations) information exchange protocols. The development and testing process will require ongoing collaborations with data providers. Data assimilation will require a similar discussion to building a unified modeling system, but this issue was not covered at the workshop due to time constraints.

Proposed steps in developing an integrated global chemical modeling capability are as follows:

1. Component Evaluation
   a. Review of existing integrated modeling systems, what can be reused?
   b. What components are needed?
   c. What components exist already?
   d. Identify missing components.
   e. At what level of granularity should we be componentizing?
   f. What components could be combined?

g. Component characteristics (Adjoint? Parallel? Interdependencies? …)
h. Identify project management structure

2. Paper model building for each Application
   a. Do concepts make sense?
   b. Review granularity of components and evaluate lessons learned
   c. Integrate granularities across applications (climate, weather, air quality, carbon cycle)
   d. Analyze data flows and integrations, communications
   e. Evaluate data calls, revise standards, etc.
   f. Identify prototypes and complexity that could be developed now
   g. Swapping, extension, evaluate scalability and adaptability across applications
   h. Identify high priority components for testing across applications
   i. Identification of verification processes and datasets needed for model evaluation
   j. Normalization/standardization of input/output data

3. Build and test each component
   a. Build and test model components within an existing model
   b. Test components across models

4. Benchmark against existing applications, results and resource requirements. Verification against measurements, evaluation/identification of model improvements using observations

5. Demonstrate scalability and adaptability of code across spatial, temporal and process complexity

Next Steps – Proposed Next Steps discussed at the workshop:

<u>Review</u> current state of other frameworks/modeling efforts (Leads: ERSL, NCEP representatives)

- Review current state of other modeling frameworks & efforts (e.g., GEOS-5, WRF, GEMS, other European efforts, etc.)

- Present results at next workshop

<u>Plan</u> model development (Leads: ARL, GFDL, ESRL, NCEP, NESDIS representatives)

- Explore coupling issues: engineering-coupling/hardware-systems considerations, ESMF integration, at what level do we couple, etc.

- Identify a case study or two
  - Define the objective for the test case
  - Define an architecture, model application components, & coupling for the test case
  - Define time period useful for the test which span different applications

    - Provide a common set of all relevant observations for the obs period to test the model
    - Test --with a real, already existing, model

- Present results at next workshop