NSF Workshop: Community Sedimentary Model for Carbonate Systems
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INTRODUCTION, SOCIETAL RELEVANCE, AND WORKSHOP SUMMARY

Developing predictive models of carbonate systems has important implications for monitoring and managing global climate change affecting societies around the world. Carbonate sediments and rocks form an important part of the global carbon cycle. More than 80% of Earth's carbon is locked up in carbonate rocks. Almost all of the remainder is in the form of organic carbon in sediments. About 0.05% of Earth's carbon is present in the ocean in the form of the carbonate and bicarbonate ions and dissolved organic compounds, whereas 0.0008% is tied up in living organisms, and about 0.002% is in the form of CO_2 in the atmosphere. Carbonate rock is the primary ultimate sink for CO_2 introduced into the atmosphere.

Throughout most of Earth history, precipitation of mineral carbonate has been closely linked to the metabolism and activities of living organisms. An important but often neglected part of understanding the carbon cycle requires that we understand how mineral carbonate is produced, how it accumulates into sedimentary deposits, how it is altered after burial, and how it is recycled back into mobile chemical species.

Although we have learned a lot about carbonate fixation, deposition, and dissolution in open ocean deep-sea environments, our knowledge of the rates of formation of mineral carbonate in shallow waters remains rudimentary. Knowledge of the changes of rates of deposition and dissolution with rises and falls in sea level associated with climate change is largely speculative and becomes increasingly uncertain for the more distant geologic past. A better understanding of these processes is essential to progress in understanding the effects of alterations of the carbon cycle resulting from the introduction of fossil fuel CO_2 into the atmosphere.

Reefs and carbonate platforms, in general, are sensitive climatic indicators, are "global sinks of carbon", and contain important records of past climate change. They are reservoirs of biodiversity, and provide critical fisheries habitat. Changes in global climate dramatically affect carbonate systems, and the peoples that live amongst them. Rising sea level heightens erosion of islands, reduces shoreline stability, causes marine flooding of coastal freshwater aquifers, and displaces indigenous people (e.g., South Pacific). Increased global CO_2 causes ocean acidification, which in turn affects the ability of many modern carbonate-producing organisms and processes to function optimally.

Ancient carbonate platforms and systems play a significant role in the global economy. They are the raw material for construction, both as building stone and as the parent material required for manufacture of cement. Through their high permeabilities and porosities, carbonate rocks serve as important aquifers and as petroleum reservoirs. They are major freshwater aquifers critical to the health of urban and rural areas (e.g., Edwards Aquifer, central Texas, USA), and in many island nations, the primary source of fresh water. Likewise, carbonate rock reservoirs host more than half of the world's petroleum. Finally, carbonate systems that fringe island nations across the planet form the basis of tourism and food for island peoples.

Workshop Summary

In response to the needs discussed above, an NSF-sponsored workshop on carbonate systems and numerical systems modeling was held in late February, 2008, at the Colorado School of Mines. The purposes of the workshop were to identify grand challenges for fundamental research on ancient and recent carbonate systems, and to identify promising areas for advancing the next generation of numerical process models to enhance our ability to meaningfully and accurately model carbonate systems. Thirty-one attendees from academia and industry worked to initiate a carbonate community across a broad spectrum of disciplines, including sedimentology, stratigraphy, geobiology, oceanography, paleoclimatology, numerical process modeling, and carbonate diagenesis. Although attended by a small subset of the greater potential community, this workshop served to open dialog, and began to define the necessary inputs to improved modeling of carbonate systems. The results of this first carbonate systems workshop are posted on the Community Surface Dynamics Modeling System (CSDMS) website (http://csdms.colorado.edu/meetings/carbonates_2008.html). Workshop participants, through a series of presentations, break-out groups, and open dialog, evaluated recent findings and research directions on the influences of climate, ocean systems, ecology, and diagenesis on carbonate deposits, and then began to identify the "grand challenges" (e.g., modeling large facies heterogeneities; numerical simulation of diagenetic history) to the understanding and modeling of ancient and recent carbonate systems.

Through these efforts, participants recommended forming working groups to synthesize the current knowledge and research needs within each of five broad areas of carbonate research – physical processes, biological processes, diagenesis, analytical tools for studying carbonate systems, and modeling. Modeling in this context, includes all types of numerical models, such as dynamic process-based models, stochastic, and fuzzy-logic models. Although the emphasis was on addressing the needs for enhanced models, participants emphasized the need for robust data to be applied to modeling inputs (e.g., carbonate biological and physio-chemical production rates). These working group syntheses could entail collaboration between the carbonate sedimentary and modeling communities to identify gaps in documentation of parameters and/or development of algorithms.

Participants agreed that a more coordinated research effort in carbonates would be beneficial to advancing understanding, with the ultimate goal of advancing a set of quantitative predictive models for carbonate deposition and diagenesis. As a start to achieving some of the broad research objectives, workshop participants recommended interdisciplinary efforts focus on identifying a limited number of sites to conduct integrated research in selected key subsets of: (1) the modern and Pleistocene systems, to examine in quantitative and predictive detail, the effects of ocean conditions and climate change on carbonate accumulations, and the evolution of sediments into beds and strata; and (2) important analog field areas that combine outcrop, behind outcrop, and the subsurface, to build a new generation of 3-D carbonate analogs to test the validity of numerical models. A companion effort will be needed to build an archive system to capture and share data. From this standpoint, the CSDMS Integration Facility is in an ideal position to facilitate the development, and hosting of such an archive system.

Importantly, the workshop also attempted to identify promising areas for advancing the next generation of numerical models, to enhance our ability to meaningfully and accurately model carbonate systems, including both depositional processes and diagenesis (Figure 1). An important result of the workshop was the recognition of the need to integrate carbonate modeling efforts into other Earth-surface modeling efforts such as the Community Surface Dynamics Modeling System. The workshop resulted in the development of a plan for creation of a work-bench platform for carbonate knowledge generation via a suite of integrative modules that is available to the carbonate community. As a result of the participants' efforts, this workshop has served to open the dialog, and to begin to define the necessary inputs to the modeling of carbonate systems from sedimentation through burial.

This workshop also aimed to establish a framework for future workshops to engage an expanded community interested in carbonate systems, and that can better define research goals and objectives. As part of this goal, a carbonate working group has been initiated within CSDMS, providing a hub and framework to facilitate future workshops. Subgroups, covering the five areas of physical processes, biological processes, diagenesis, tools, and modeling could be established within this broader working group.

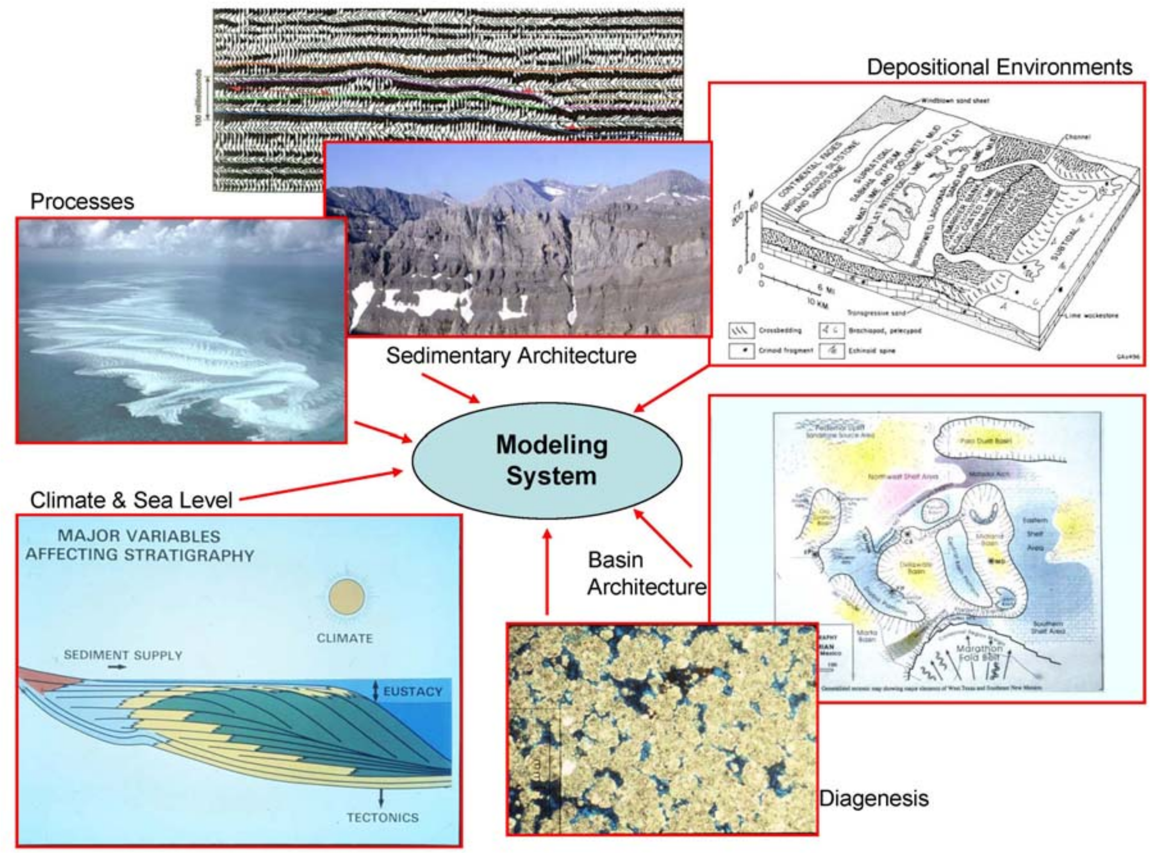

Figure 1. Components of Carbonate Community Model System.

RESULTS AND RECOMMENDATIONS

The following sections summarize workshop discussion and conclusions, and are divided into five topical areas: physical controls, biologic controls, diagenesis, numerical modeling, and tool development. They include some identified short- medium- and long-term goals for each of the topical workshop areas.

1) Physical Controls on Carbonate Deposition -

All carbonate community members face the grand challenge of quantitatively understanding and modeling facies heterogeneities, developed over various geologic timescales, as influenced by changing biotic, paleoceanographic, paleoclimatic, and sea level conditions. The first step is understanding the nature and origin of the patterns of sediment accumulation. Whereas we have a good qualitative understanding of patterns on carbonate platform tops, a rigorous quantitative understanding is lacking. Similarly, patterns and processes on platform slopes and deepwater reefs await better qualitative and quantitative exploration. Major knowledge gaps include a lack of a rigorous understanding of:

1) the effects of sea level fluctuations on sediments,

2) how to predict sedimentation patterns in a non-linear and complex system, as opposed to assessing sediments in a 1:1 linear relationship vs. depth;
3) the processes that lead to development and evolution of geomorphic and facies patterns, and the time scales of development;
4) the respective roles of quotidian and storm processes in sedimentologic and geomorphic evolution;
5) how to most accurately develop separate sector models for different environments (reefs, shoals, platform interior and tidal flats). This requires a clearer understanding of the different controls in these areas, and how sector models should be employed;
6) the interplay between physical processes and the occurrence of cemented areas (hardgrounds) and benthic mats that can influence accumulation; and
7) the effects of changes in sea water chemistry through the Phanerozoic on long-term facies development in carbonate systems.

Short-Term Goals: Participants noted a number of short term goals that entail assembling existing data, including:

1) Assemble an inventory of modern platforms types and depositional systems and an associated inventory (database) of physical measurements and models from these systems. This could lead to a new classification of different platform types and depositional environments and would show where there are gaps in physical measurement data that are necessary for modeling;
2) Take existing carbonate numerical modeling packages and run sensitivity analyses on ranges of parameters in those models, to put bounds on certain physical parameters that need to be measured or better understood. For example, the "friction factor" in CARB3D$^+$ seems to be quite important although its physical meaning is vague.
3) Assemble a catalog of existing numerical siliciclastic models to assess parameters these models use as input, and explore for possible overlap.

Medium-Term Goals: Participants recommended the following:

1) Collecting oceanographic measurements (waves, tides, and currents) across one or two different platforms. Longer term goals include a detailed coring program on one or more platforms to evaluate the platform depositional architecture, to provide information to test models.
2) Development of preliminary "sector models" of various specific environments to provide "modular" input to a larger community model. For example, we would envision a "reef model", one or more ooid shoal models; a tidal flat model, and a platform interior model. We do not have robust enough data to accurately model flow and sediment transport in these models.

Necessary partners for the short and medium term goals are physical oceanographers, especially to establish boundary conditions and measure the physical parameters on the platforms. This group should also partner with the biological working group for developing "sector models."

2) Biological Controls on Carbonate Deposition -

Modern tropical shallow-water coral reefs are comparatively well known, but many fundamental questions remain. Similarly, tropical meso/oligophotic reef systems, cool-water carbonate systems, and aphotic systems are poorly understood carbonate systems. Likewise, there is a broad base of paleontological knowledge of fossil biota. To better understand carbonate systems, however, a grand challenge centers on understanding how appropriate are Holocene tropical shallow-water reefs as analogues for ancient carbonate buildups, or, if they are not, how the ancient systems differ. Beyond this grand challenge, the fundamental questions of assessing how changes in biogeochemical boundary conditions (CO_2, alkalinity, salinity, and Mg/Ca ratios) have changed modes and rates of calcification remains.

Knowledge gaps identified by this group include lack of quantitative understanding of 1) the boundary conditions for hypercalcification; 2) rates of production and how they relate to rates of deposition/accumulation; 3) relative rates of bioerosion and physical erosion; and 4) the nature and origins of spatial heterogeneity. These unknowns center on aspects of rigorous understanding of the basic questions of 1) how carbonate producing communities function and how does the sediment produced accumulate; 2) the relative importance of different biota under different boundary conditions; 3) how does the seascape heterogeneity translate to stratigraphic heterogeneity; and 4) what are the origins of lime muds.

Participants suggested that experiments to understand how changes in geochemical parameters influence rates of biomineralization should be developed in collaboration with physiologists and geochemical modelers. Interaction with population ecologists will be key to interpret how changes in environment (chemical, physical, etc.) translate to population dynamics, and how that, in turn, translates to spatial heterogeneity within and between bottom types. Improved collaboration with paleontologists and carbonate sedimentologists will allow better analogue comparison between modern and ancient systems. Modern test cases should be developed as possible analogues for ancient carbonate buildups, using the full breadth of carbonate depositional systems worldwide, including tropical meso/oligophotic carbonates, cool-water carbonate systems, and aphotic communities. Studies might cross a broad range of environments (e.g., latitudinal such as E/W Australia, E/W Florida, E Africa, Hawaii to NW Hawaiian islands; current-dominated systems like the Nicaraguan Rise; across depth gradients that have changing light, trophic resources, temperature, internal waves, etc. (i.e., most modern margins); and in mixed settings that contain terrigenous sediments). Hypotheses developed in modern systems can then be tested in appropriate ancient systems. The answers to these could provide insights into understanding how seascape heterogeneity translates to stratigraphic heterogeneity, and how to characterize seascapes and the inherent dynamics of biota across turn-on-turn-off gradients in a more realistic and effective manner.

These inherently interdisciplinary efforts require diverse partners such as ocean observing system engineers, “landscape” ecologists and modelers, microbiologists, geochemists, geochemical modelers, developers of experimental mesocosms and macrocosms that test changing geochemical and atmospheric boundary conditions, physiologists to help translate implications of geochemical models to predicting how specific biota might have responded, paleontologists and paleobiologists to translate understanding of modern biotas to interpreting fossil systems, taphonomists and sedimentary geochemists to assist in constraining syndepositional loss, and paleoceanographers to understand oceanographic changes that influence fossil carbonate producing communities.

Short-Term Goals: Workshop participants suggested that in the short-term, an updated literature search of biota- and habitat- specific rates of carbonate production, accumulation, and bioerosion, including microbial contributions and interactions should provide essential information for modeling. Identification of key experimental sites and gradients provides a necessary first step for quantifying carbonate biotic heterogeneity.

Medium-Term Goals: Contributors suggested a need for research to constrain controls on rates and nature of calcification by key biotic groups (e.g., corals, coralline algae, calcareous green algae, larger benthic foraminifera, microbes, including cyanobacteria). They also suggested the need to constrain seascape dynamics and patterns at targeted locations, both on the surface and stratigraphically, and across gradients.

Long-Term Goals: Participants suggested that successful outcomes would include a rigorous understanding of the geochemical and physical constraints on carbonate production, and its spatial heterogeneity, and its translation into numerical models.

3) Diagenesis -

Diagenesis in carbonate systems is particularly important due to the high reactivity of carbonate minerals from their initial deposition to their deepest burial and uplift. Diagenesis on the seafloor is part of the physical controls on sedimentation. Alterations through time determine the ultimate chemistry and mineralogy of the rock (e.g., Mg cycling and dolomitization) features that are increasingly used as proxies for paleoclimate and paleoceanographic conditions in the past. Facies, diagenesis, and brittle deformation also control the heterogeneity in carbonate rock properties, and that, in turn, affects the movement of fluids through carbonate rocks. As such, diagenetic heterogeneity can affect a variety of processes of societal interest, including CO_2 sequestration, aquifer storage and recovery, contaminant plume migration in carbonate aquifers, and the production of hydrocarbons.

The grand challenge in carbonate diagenesis is to construct predictive numerical simulations of diagenetic history (e.g., mass transfer and petrophysical transformation) from pore to platform scales. Ideally, models should incorporate the entire diagenetic system and all its coupled interactions - sedimentation, chemical and biological alterations on or near the seafloor, mechanical overprints, and chemical alterations resulting from fluid flow through pore and platform burial history. Once built, diagenetic numerical models would have multiple potential uses, including: (1) evaluating general diagenetic concepts, (2) testing specific diagenetic models of ancient carbonate systems, (3) predicting rock properties (e.g., porosity) and proxies (e.g., geochemical climate or ocean signals) through time and space, and (4) evaluating the effects of decreased seafloor lithification in times of increased ocean acidification (i.e., with rising global CO_2).

In general terms, diagenetic products and processes are known as a function of various diagenetic environments (i.e., hydrochemical regimes, Figure 2). We presently have a few limited empirical and rule-based modeling tools, but these include limited linkages between sedimentation processes and post-depositional diagenesis. Major gaps in understanding include:

1) the lack of benchmarks for the 3D distribution of processes and products in time and space – decades of research has focused on establishing processes and products using representative samples along one-dimensional vertical transects.
2) significant uncertainty in many input parameters to diagenetic models – fluid chemistries, some thermodynamic and kinetic properties of carbonate minerals, and the nature of many mechanical processes.
3) the possible existence and influence of thresholds in diagenetic processes, and the nonlinear feedbacks of processes, products, and geochemical attributes is unexplored.
4) the role of biogeochemical reactions (i.e., catalysis, facilitators), empirical rules associated with some key processes (esp. cementation), and when to use transport- vs. reaction-controlled processes.
5) the nature of diagenetic outcomes at the full spectrum of scales, from thin section to platform-scale.

To explore these needs, participants suggested that access and information is required from the “right kinds of rocks” (closely spaced shallow drill cores and 3D quantitative data sets of well constrained outcrops). Large-scale monitoring sites are needed to examine seascape alterations (cementation, dissolution) and near surface post-deposition alteration (freshwater, mixing zones, refluxing brine settings). Potential partners include crystal surface geochemists, hydrologists/hydrodynamists, structural geologists, sedimentologists and stratigraphers.

Short-Term Goals: Identified goals included:

1) Dissemination of current numerical codes to grow the user community, and to develop community libraries of validation cases.
2) Develop consistent input parameters (e.g., depositional porosities), and improve most problematic of process rules.
3) Test existing tools at pore scale.
4) Establish examples of 3D diagenetic processes and products in select settings to have data sets to validate numerical codes.
5) Partner with larger community.

Medium-Term Goals: Couple second generation diagenetic models with improved sedimentary process models.

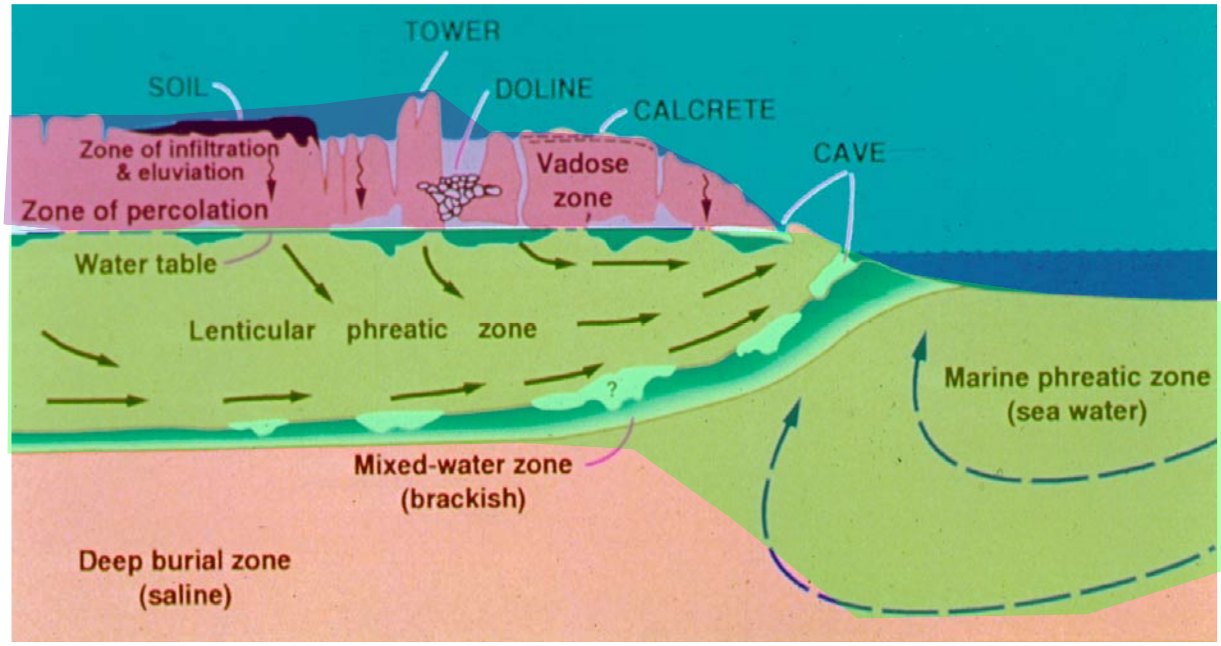

Figure 2. Diagenetic environments.

4) Numerical Modeling Strategies -

The grand challenge for numerical modeling is to make useful predictions/simulations of carbonate platform growth and diagenesis over varying time and space scales. Because it represents the numerical representation of our knowledge, this effort will require essential input and feedback from the other groups, and that the carbonate numerical community looks beyond itself, for numerical and conceptual inputs. The carbonate modeling community recognizes the need to integrate their modeling efforts into other Earth-surface modeling efforts, such as the Community Surface Dynamics Modeling System.

Knowledge gaps are wide and include 1) a lack of basic understanding of many processes, 2) uncertainties in scaling of processes temporally and spatially, 3) dearth of information on the influences of non-linearity and non-stationarity of biologic aspects of systems, 4) only qualitative insights on the feedbacks between different processes, and 5) absence of understanding of the controls on heterogeneity at different scales.

The goals for carbonate numerical process modeling are divided into four stages. The long-term goal is construction of a numerical work-bench (Figure 3) for carbonate knowledge generation that has a suite of process modules (physical, biologic, and chemical deposition, diagenesis, and structure/fractures).

Short-term goals (2 yr):

- Assign responsibilities for the cyber-infrastructure (i.e., GUI, protocols, coupling, and visualization).
- Build a module inventory and make modules available worldwide.

- Make available 5-9 modules that could include biogenic and inorganic production, biologic ecosystems and communities, physical and biologic syndepositional processes, dissolution-reprecipitation, cementation, hydrodynamics (e.g. Delft3D, ROMS), and sediment transport (CSDMS, e.g., SedFlux, SedFloCSTMS).
- Verify modules on appropriate time scales, and establish at least one database for testing.

Potential partners in this effort are global change community, reef health community, hydrology, industry, ecosystems, geochemistry, and ocean atmosphere communities. Start an online journal repository for modules and code documentation, possibly through the CSDMS organization, with benchmarks, and where editorial board and review involves the user community.

Medium-term goals:

- Involve students from geophysics, applied math, and computer science fields to address computational issues like grid conversion and interfaces.
- Have stage 1 modules tested and improved.
- Document results to enable informed choice of modules, and begin coupling with climate/ocean/siliciclastic models.
- Conduct initial sensitivity studies, and complete a comparative numerical scheme study, including an initial comparative verification/inverse objective cost function study.
- Conduct two international workshops in carbonate computational issues, and achieve "buy-in" with non-NSF funds for module development.
- Ensure high performance computing access, and activate partnerships.
- Have modules running efficiently on HPC, and have at least one useful prediction.
- Publish a series of peer reviewed papers using the workbench modules, and conduct a number of sedimentology courses in US using the carbonate workbench as a lab tool.

Long term goals (10 yrs):

- Numerical work-bench for carbonate knowledge generation is available to the carbonate community. The workbench will: 1) have a suite of process modules (i.e., deposition, diagenesis, deformation/fracturing); 2) accept input from other models (e.g., ocean, climate, etc.); 3) accept observations from different sources, and databases; 4) have multiple inversion/verification schemes, and multiple sensitivity/response surfaces and uncertainty quantification; 5) have multiple scales/scalability, nestedness, and up- downscaling; and 6) have multiple outputs (Eclipse, Petrel, modflo etc.).
- Workbench prediction will be able to influence observatory systems like the Global Ocean Observatory.

I/O	Light-based deposition	Parallel I/O	Fuzzy-logic
Cellular Automata	Flow	Residence time	Sediment transport
Sea-level changes	Waves	Supersaturation	Climate model integration

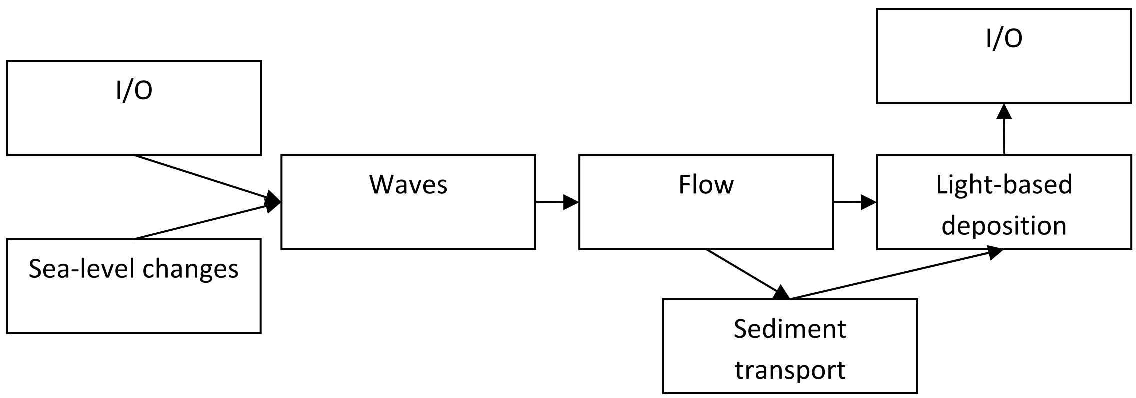

Figure 3. The carbonate "work bench" model is envisaged to contain a number of discrete modules (top), such as I/O interactions with other models, process-based factors, and stochastic process which can be linked together (bottom) to create a numerical model designed for the experiment in-hand. This frees the researcher from developing a model "from scratch" and maximizes the re-use of common functionality.

5) Tools Needs and Development -

Recent advances in the remote sensing of earth systems are providing numerous opportunities for detailed digital numerical data collection. Current tools in use to gather data in modern and near-modern systems include optical remote sensing, Lidar (airborne/land), bathymetry and spectral response, sonar (bottom topography and bottom sensing (backscatter)), acoustic Doppler profiling (current velocity and direction), in-situ wave profilers, synthetic aperture radar, and shore-based radar (wave/current measurements), and turbidity, temperature, alkalinity sensors. Research needs include developing higher resolution versions of the tools mentioned above, and developing the software and computing power to process ever larger quantities of data.

For ancient carbonate systems the advent and improvements of 3-D seismic data are beginning to provide the possibility of collecting extensive three dimensional data on architecture and morphology of ancient carbonate platforms. Many of these 3-D datasets come from mature hydrocarbon fields that have extensive well log, core, biostratigraphic, and production data that can be used to calibrate the seismic data. The challenge is to provide these data to academic researchers. Building academic-industry partnerships to achieve this should be a priority. Surface and near-surface tools, such as Lidar and GPR, provide opportunities to collect quantitative and 3-D data, and link with other subsurface data sets. These tools ultimately can provide quantitative high resolution data on geometry, facies, and diagenetic character (i.e., pore systems) of carbonate systems.

Enhanced understanding of ancient strata centers on the ability to gain accurate high-resolution chronostratigraphic, biostratigraphic and absolute time data, to better constrain correlations, dates, and rates. Most dating of carbonate systems involves a combination of biostratigraphic data and multiple other age determination techniques (e.g., Sr isotopes, magnetostratigraphy, high-precision radioisotope dating: U-Pb, U-Th and Ar/Ar dating recently improved to 0.1% error). Of notable concern is that in the area of biostratigraphy, many experts are of retirement age resulting in knowledge loss and very little of these data have been captured into publically available databases.

Future needs in studies of ancient carbonates require high resolution biostratigraphy resolving cyclostratigraphy to the 0.02-0.4 my level. This could involve partnering with Earthtime (NSF) and Earthtime Europe, CONOP (constrained optimization), and the high resolution event sequencing of assemblages of biostratigraphic sections that could provide resolving power better than 0.5 my time scale. Composite standards and coordination of data collection are needed to assure that all useful data are captured. Astronomically calibrated cyclostratigraphy offers resolving power at 0.02 to 0.4 my level for the Cenozoic-Mesozoic and modeling objectives should include testing for the astronomical signal in cyclic carbonate systems. Cyclostratigraphy validation tools include time series analysis tools that can potentially quantify the time-frequency evolution of carbonate accumulation. However, the method incorporates assumptions of the stratigraphic record, and further research is needed on effects of depositional (stratigraphic) breaks, and accumulation (thickness) changes. Spectral analysis does provide one means to assess variability of carbonate sedimentation as a function of frequency. An understanding of the degree of randomness of sedimentation, and identification of external forcing mechanisms is necessary to validate apparent astronomical signals.

SUMMARY & CONCLUSIONS

The grand research challenges for advancing understanding of modern and ancient carbonate systems identified in this first integrated community workshop include:

1) Quantitatively understanding and modeling facies heterogeneities developed over various timescales, as influenced by changing biotic, paleoceanographic, paleoclimatic, and sea level conditions;
2) understanding the appropriateness of using Holocene tropical shallow-water reefs as analogues for ancient carbonate buildups;
3) developing predictive numerical simulations of diagenetic history from the scale of the pore to the scale of the platform by incorporating and coupling sedimentation, chemical and biological alterations on the seafloor, mechanical overprints, and chemical alterations resulting from fluid flow;

4) resolving cyclostratigraphy to the 0.02-0.4 my level using high resolution biostratigraphy and absolute age dates;

A more coordinated research effort in carbonate systems would be beneficial to advancing these community challenges. The group recommended research that focuses on identifying a limited number of sites to conduct integrated research on selected key subsets of: (1) the modern to Pleistocene, to examine the effects of ocean conditions and climate change on carbonate sedimentation, and the evolution of sediments into beds and strata; and (2) important analog field areas that combine outcrop, behind outcrop, and the subsurface, to build a new generation of 3-D carbonate system models.

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