An Information Technology Infrastructure Plan to Advance Ocean Sciences
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Executive Summary

The field of ocean sciences is currently faced with extraordinary opportunities for progress. Three interrelated developments now permit oceanographers to study the natural system with an unprecedented degree of realism: enhanced observational capability, improved numerical models and formal methods for linking observations with models. The impact of these developments on our understanding of oceanic processes pervades all disciplines within the field, as well as cross-disciplinary linkages between physical, biological and chemical oceanography, and marine geology and geophysics. Unfortunately, many aspects of these activities are severely limited by the Information Technology Infrastructure (ITI) available to the ocean sciences community. Ongoing efforts to establish modeling/data assimilation “nodes” within the National Ocean Partnership Program (NOPP) are just one example of high-priority activities within which ITI limitations are particularly acute.

In 1999, the Office of Naval Research and the National Science Foundation’s Division of Ocean Sciences jointly formed a Steering Committee to assess the immediate ITI needs of the NOPP nodes as well as the projected needs of the broader ocean sciences community, and to provide recommendations for how these needs should be met. The Steering Committee sought input from a variety of sources. The most important of these included: a survey of the ocean sciences community to establish current and projected levels of ITI use, a survey of supercomputer centers within the United States to ascertain current and projected levels of resource allocation, and a series of invited presentations by ITI experts from the ocean and computer sciences communities.

On the basis of its surveys, the Steering Committee identified several urgent ITI issues. First, ITI-intensive ocean sciences research is expected to require ten to one thousand times the current ITI hardware capacity over the next five to ten years, with the most critical bottlenecks occurring in the availability of CPU cycles, memory and mass-storage capacity, and network bandwidth. Second, significant challenges in the area of software systems also exist. These include the need to re-engineer models, and data analysis and assimilation packages, for efficient use on massively parallel computers; the requirement for significant advances in visualization techniques to deal effectively with increasing volumes of observations and model output; and the desire for well-designed, documented and tested community models of all types. Lastly, exacerbating these looming problems is the extreme shortage of skilled ITI technical personnel accessible to the ocean sciences community.
The Steering Committee considered several approaches, of both a short-term and a longer-term nature, to meet these needs. The committee concluded that the current shortfall in hardware capacity could be partially met through more effective use of, and communication with, existing supercomputer centers, in part to better articulate ocean sciences needs and the importance of its research. Additionally, in the short term, dedicated medium-scale hardware could be procured for research activities that require lengthy periods of dedicated system use. Despite the importance of these steps to partially offset short-term needs, they are inadequate to meet longer-term needs, even if the ocean sciences were to increase its share of the available resource at the national centers far beyond the 4% currently obtained.

The Steering Committee therefore recommends substantial long-term investment in ITI for ocean sciences. This long-term investment should be deployed in flexible ways and managed by a new entity, here called Ocean.IT (pronounced Ocean I T). This organization will serve four primary functions:

1. **Improve access to high-performance computational resources across the ocean sciences.** This will be accomplished by both streamlining the current allocation procedure for shared resources, and by the acquisition of new hardware for dedicated use by the ocean sciences community. The estimated hardware need is equivalent to a single “terascale” machine, distributed among perhaps three centers each with approximately 1000 high-performance processors.

2. **Provide technical support for maintenance and upgrade of local ITI resources.** Ocean.IT will provide consulting services to facilitate efficient deployment of ITI within institutions involved in oceanographic research. Staff will be responsible for continuous technical evaluation of computing and networking hardware options, will make recommendations on computer and software acquisition, and will provide guidance on hardware and software installation.

3. **Provide model, data and software curatorship.** Community models will be distributed through a central repository, with ongoing documentation of algorithmic development and improvement. Archives of key data sets and model output will be served to facilitate their use in research by the wider community. A library of diagnostic and visualization tools (e.g., generic tracer transport codes, energy and vorticity analysis packages, Lagrangian float tracking software) will be maintained.

4. **Facilitate advanced applications programming.** Technical support and training will be provided to allow ocean scientists to take maximum advantage of ITI resources, including parallelization tools and advanced software interfaces.
Introduction

Background

Recent advances in observational, experimental and communication technologies have made ocean sciences research more integrative and interdisciplinary, and increasingly dependent on modern information technology (IT). Information technology is used to collect, transfer and analyze large volumes of data, model the ocean numerically, combine ocean models with ocean data in optimal ways (known as data assimilation), and connect scientists to each other and to the public. Broad access to the world wide web alone is revolutionizing observation, computation, collaboration and communication.

Scientific opportunities presented by the explosion in IT research are aptly described in the President’s Information Technology Advisory Committee (PITAC) report, “Information Technology Research: Investing in Our Future” (1999). PITAC found that, “the interlinked network of computers, devices and software ... will transform how we do research. High-speed computers and networks are enabling scientific discovery across a broad spectrum—from mapping the human brain to modeling climatic change. As a result researchers are finding innovative ways to collaborate with their colleagues across the globe. Key research technologies include high-end computing to allow high-fidelity models of complex physical phenomena, advances in collaborative environments, visualization of complex data sets, data mining techniques, and management of very large data sets and data bases.”

*In the context of this report, ocean is defined to include both its liquid content and the margins surrounding it.

Despite these opportunities, the ocean sciences community’s technology needs have outstripped available resources. A number of recent community assessment efforts, including Nowlin (1997a, b) and Powell (1998), have called for action. They persuasively argue for the need to implement sophisticated database, modeling and assimilation systems, and have described the scientific and socioeconomic benefits of increased efforts in these areas. These reports also stress that developing such sophisticated modeling and data assimilation capabilities requires considerable resources, including increased access to information technology, enhanced data collection efforts and a significant investment of human skills and effort.

At the same time, policy makers agreed that concerted action in the ocean could lead to large socioeconomic benefits for the United States. In 1997, Congress passed the National Oceanographic Partnership Act (P.L. 104-201), which led to the establishment of the National Ocean Partnership Program (NOPP). NOPP has the stated goals of assuring national security, advancing economic development, protecting quality of life, and strengthening science education and communication through improved knowledge of the ocean. Prototypes for regional and global observatories, integrative ocean modeling, data assimilation efforts and data management systems have been initiated with NOPP stimulus and support. These projects are demonstrating that the ocean sciences community is ready and able to develop the observing, data-handling, modeling and assimilation systems.
Terms of Reference for an Ocean Information Technology Infrastructure Steering Committee

9/21/1999

The Steering Committee (SC) for the Ocean Information Technology Infrastructure is charged with developing a flexible and comprehensive implementation plan for a distributed information technology infrastructure (ITI) that can:

1. Meet the immediate ITI needs of the NOPP Modeling/Data Assimilation nodes as well as the projected needs of other modeling teams and the broader ocean modeling community over the next decade.

2. Be readily integrated with future observational, data management and educational components of the “Hub/Node” enterprise.

3. Be easily upgraded, as information technology advances, with minimal disruption to users.

The implementation plan should:

1. Assess existing ITI activities and concepts in the U.S. science community (e.g., PACI, ASCI, MSRC) and their adequacy in addressing current and future ITI needs of the ocean science community.

2. Anticipate future ITI needs of the ocean community (current and projected NOPP nodes; other teams and individual PI’s).

3. Include a strategy for providing efficient allocation of resources and easy access to all ocean science users conducting highly meritorious research programs with large IT requirements.

Three fundamental operating principles of the SC must be:

1. That it will seek broad community input and, to the extent practicable, develop a plan that has broad community support.

2. That it involves in the planning process all of the main disciplines that make up ocean sciences as well as experts drawn from existing ITI activities like the PACI program.

3. That it takes into account the variety of data streams from remote sensing, in situ water column, and seafloor observatories that can be reasonably expected over the next decade.
it has envisioned. As these systems come on line to meet research and operational objectives, a considerably enhanced ocean information technology infrastructure (OITI) will be needed. The sections that follow present an outline of potential scientific and societal payoffs with illustrative examples, an assessment of the current state of OITI resources and of the ocean sciences community's future needs, and a set of detailed recommendations describing the steps that are necessary if ocean sciences' IT needs are to be met. These findings are the product of an 18-month, sustained study by the Ocean Information Technology Infrastructure Steering Committee.

**OITI Steering Committee**

In the fall of 1999, the Office of Naval Research and the National Science Foundation’s Division of Ocean Sciences formed a community-based Steering Committee to consider future needs in the area of ocean information technology infrastructure. The Steering Committee was charged with developing a flexible and comprehensive implementation plan for a distributed information technology infrastructure for the ocean sciences community. Terms of reference for the Steering Committee are listed on the opposite page. Committee membership included 11 members from a range of academic and governmental institutions, and with a range of information technology expertise. The chronology of Committee activities is shown in Appendix 1.

Given the immediate OITI resource needs of the NOPP Modeling and Data Assimilation nodes, and the growing use of forward and inverse modeling in most subdisciplines of the marine sciences, the Committee focussed its attention, as a starting point, on IT requirements for these activities. In compiling its community profile of IT use and future need, however, the Committee made a serious attempt to poll a representative cross-section of the ocean sciences community (Appendix 2). Though IT needs were identified in all areas of ocean sciences, the types of needs, and the quantitative demand for future resources, varied considerably by subfield. The implementation plan developed by the Steering Committee attempts to come to grips with this disparity by broadly assessing the future of OITI in the United States. Elements of this vision necessarily encompass both computational (hardware) enhancements for those subdisciplines with immediate and advanced needs, as well as new software tools and user services for those in other of the marine sciences whose activities, though less modeling intensive at present, are nonetheless IT limited.

Lastly, several issues intrinsically related to the Committee’s discussions—for example, observation systems and ocean monitoring, networking and communications, and manpower availability and recruitment—were identified as important, but outside the range of expertise represented within the Committee membership. Several recent reports have addressed some of these issues (Nowlin, 1997a and b; Frosch et al., 2000; National Research Council, 2001), while others merit further study.
Scientific Needs and Payoffs

The scientific case for enhanced OITI resources is founded on the experience derived from a decade of global ocean programs (e.g., TOGA, WOCE, JGOFS, RIDGE, GLOBEC, CoOP, CLIVAR) and the scientific challenges and opportunities identified by two recent reports, “NSF Geosciences Beyond 2000” and “Ocean Sciences at the New Millennium” (herein referred to as GEO2000 and OS2001, respectively). These reports concluded that currently available IT resources are inadequate to carry out the scientific vision of the ocean sciences community.

In this section we highlight some of the scientific opportunities, specific to ocean sciences research, that can only be realized with enhanced IT resources. Woven into this overview are several representative examples of scientific problems currently being tackled and significant advances that would result from greatly increased IT resources. The reader is referred to the two reports cited above, and other ocean sciences planning documents, for a detailed description of the “grand challenges” in oceanography.

Scientific Opportunities in Ocean Sciences*

- Ocean Turbulence
- The Complex Coastal Ocean
- Non-Equilibrium Ecosystem Dynamics
- Long-Term Ocean Observations and Prediction
- The Ocean’s Role in Global Climate
- The Ocean Below the Seafloor
- Dynamics of Oceanic Lithosphere and Margins

* from “Ocean Sciences at the New Millennium”
Why Now?

One of the fundamental lessons learned by geoscientists in the late twentieth century was “the recognition that the Earth’s environment cannot be explained by studying any element in isolation. The combined effects of many processes interact in complex ways to influence the behavior of other components within the Earth system” (GEO2000). Within the Earth system, the oceans are an excellent example of a complex system where biology, chemistry, geology and physics interact on spatial scales ranging from millimeters to the size of ocean basins, and at temporal scales ranging from milliseconds to millennia.

The present knowledge of the basic state of the ocean and the seafloor below has come about mainly through geographically broad exploration of the ocean, but during only brief time windows. Prompted by the difficulty of studying the ocean’s behavior in both spatial and temporal domains, an often-invoked assumption has been that the ocean acts in a quasi-steady or stationary manner. As more observations become available, oceanographers have come to quantitatively appreciate that the ocean system is complex, and many of the processes acting within it are nonlinear in character.

Evidence is also accumulating that even at large scales and far below the ocean surface, the ocean is unsteady—sometimes on surprisingly short time scales. The few time-series observations collected have shown that the ocean is far more variable than previously believed and can undergo rapid change from one persistent state to another. For example, “…long periods of little change can be punctuated by short periods of rapid change in species composition. These departures from “equilibrium” conditions are not necessarily transients from which ecosystems will quickly rebound, but may represent the more typical states experienced by most organisms in the sea” (OS2001). Similarly, the paleoceanographic record and idealized modeling studies suggest that the meridional overturning circulation can reorganize itself on time scales of a few decades. Irregular fluctuations between slow and rapid rates of change characterize the physical, chemical and biological structure of the ocean.

Complex temporal behavior is one consequence of the fundamental nonlinearity of the ocean in which intrinsically nonlinear processes at different spatial scales are coupled through nonlinear interactions. Mixing processes on centimeter scales effectively control the global ocean circulation. Small increases in concentration of trace nutrients such as iron can lead to large increases in phytoplankton biomass. The deep ocean and subseafloor are proving to be the most diverse ecosystems on Earth in spite of their harsh environmental conditions. However, their spatial and temporal structure is highly irregular as a consequence of the variability of sources of energy and nutrients, and of the genetic and ecological dynamics of the biomes.
These discoveries are paving the way for extending the exploration of the ocean as a collaborative, integrated, interdisciplinary pursuit of the nonlinear interactions among components of the ocean system.

In the last decade of the twentieth century, unprecedented efforts were made to observe the ocean with both in situ instruments and satellite-borne systems. These greatly increased the number of ocean observations (Figure 1). The development of additional satellite-based instruments as well as other novel observing systems has created significant new demands on IT resources. Some of these demands have to do with storing, managing and accessing the data. Others are associated with the task of analyzing and interpreting these often very large data sets.

No matter how comprehensive the observing system, many aspects of the ocean’s behavior will be very difficult to understand solely from observations. Fortunately, oceanographers, in collaboration with applied mathematicians and statisticians, are developing the ideas and tools needed to define and describe complex systems, while developments in computational science have provided powerful means for studying and investigating such systems. Ocean numerical models, as representations of the accumulated knowledge of ocean processes, are playing an increasingly important role in testing ideas of how the ocean and seafloor below work. Ocean state estimation and inverse models of the ocean and of Earth’s crust, and formal ways to combine models and observations through data assimilation, will permit synthesis of the diverse, but still sparse, observations into a dynamically consistent and quantitative picture of the time-evolving marine system.

Figure 1: Comparison of amounts of in situ data collected during the WOCE (1990-2000) and pre-1990 periods (courtesy of the WOCE International Project Office).
Data Challenges

A global, multi-scale observing system enabled by rapidly evolving technology is being deployed to gather the data necessary to put together a full picture, in space and time, of the complex ocean (Nowlin and Malone, 1999; Frosch et al., 2000). Information technology is fundamental to exploiting this comprehensive observing system. Fast and reliable data links are needed to assure near-real time delivery of these ocean observations to desktop computers of individual scientists as well as operational centers. Significant new IT resources are needed to process the exponentially increasing volume of data once they are delivered. Figure 1 shows how a climate program like WOCE has in ten years more than doubled the amount of physical in situ data collected over the previous 100+ years. While the in situ data streams are becoming computationally significant, they are dwarfed by the data streams that will be obtained from satellite-borne sensors and seafloor mapping instrumentation (see Ocean Fronts box on page 10, and Data Sets of the Seafloor on page 34).

The challenge, however, extends well beyond a need for more computational resources. It requires a fundamental change in the culture of the research community regarding the way they document, share and save the data they collect and the products they produce. It also requires an infrastructure that supports these changes. As data volumes and their use in interdisciplinary studies grow it will become increasingly difficult for researchers to obtain all of the required data sets from colleagues on a one-on-one basis as they have in the past and to reformat each of these data sets for use in their applications. The IT infrastructure of the future must permit machine-to-machine data exchanges that are semantically consistent (exchanges in which the variable names, units, data flags, etc. are well known) whether the data reside in a national archive or on a colleague’s computer. There also must be a clear data migration path from the data collector to the national archives, and there must be polices in place that address issues such as what data are to be saved, the level of documentation that is required for these data and the consistency of this documentation for the semantic content of the data sets and for the organizational structure in which they are held.
Ocean fronts are relatively narrow zones of enhanced horizontal gradients of physical, chemical and biological properties. Although encompassing only a small fraction of the ocean, frontal regions are particularly important because they are thought to play a disproportionately large role in critical oceanographic processes such as mixing and primary production. It is, in fact, their relatively small lateral size that makes them so interesting, but also makes them very difficult to study.

Ships, moored buoys and drifters, although useful in providing a measure of their vertical structure, are of little value in studies of the horizontal distribution and/or evolution of fronts. Satellites, on the other hand, possess the spatial and temporal resolution needed to quantify the location and evolution of fronts. Unfortunately, insufficient computational resources are available to process the full satellite data stream from some of the more data-intense sensors (e.g., MODIS and GOES) that capture the geophysical fields used to detect ocean fronts, such as sea surface temperature (SST). Even data from the lower data rate AVHRR sensor have only been processed to SST at quarter resolution (9 km) globally because of the lack of computational resources at the time the processing was initiated, although the resources for this task are now available. Reliable cloud-screening algorithms that do not eliminate regions of large SST gradient are also computationally intensive, often requiring significantly more time to screen for clouds than that required to develop the base SST field. Finally, edge-detection algorithms are generally even more computationally intensive than either the basic retrieval algorithms or the cloud-screening algorithms.

Cloud-screening and edge-detection algorithms applied to the quarter resolution AVHRR global SST data set for the period 1985-1996 required eight DEC Alpha months in 1999. The figure shows all the fronts for the boreal spring of 1988 resulting from this effort. To perform the same analysis with the more frequent temporal coverage of GOES for the North and South Atlantic would require at least one order of magnitude more computational resources than this. To develop SST and/or ocean color frontal fields for one year of the MODIS data stream at full resolution would require computational resources similar to those used for the entire Pathfinder period. To apply these algorithms to the full resolution (approximately 1 km), local AVHRR data streams collected at any of the existing receiving stations would require similar computational resources per year to those used for the Pathfinder data processing.

References:
Computational Tools

The numerical simulation activities pursued by ocean and computational scientists fall into one of five general categories: Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), Regional, Basin-scale and Global. Each model can be combined with data assimilation methods to test its validity, conduct observing system design experiments or estimate the state of the ocean. The further development of these models has been highlighted in the OS2001 report as crucial to making progress in the first five thematic areas listed in the box on page 6. Examples of their application are discussed below in the context of their IT requirements.

Table 1 shows how these five numerical tools can be used within current IT capabilities (numbers in green) in terms of the range of scales they can encompass and the periods that are typically simulated. It also summarizes the types of scale ranges and temporal durations that are required by some of the problems of fundamental interest to ocean scientists (numbers in purple). The table illustrates the need for tenfold or better increases in both the range of spatial scales and in the duration of the simulation covered by these classes of numerical models. Note that because these are four-dimensional models (x,y,z,t), a tenfold increase in the range of scales encompassed by a model will usually require an increase in computational cycles of order 10^4, with commensurate increases in computer memory and storage. In addition, most scientific problems require sensitivity studies that vary key parameters or ensembles of simulations involving 10 to 100 runs.

The breadth of the energy and biological variance spectra of the ocean makes it likely that for any application, key processes will have to be parameterized. The lack of spectral gaps and the inhomogeneity of energy at most scales makes the task of identifying sensible cutoff scales and parameterizing unresolved processes problematic.

<table>
<thead>
<tr>
<th>Type of Simulation</th>
<th>Resolved Scale</th>
<th>Domain Size</th>
<th>Duration of Simulation</th>
<th>Applications (Understand and Forecast)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNS</td>
<td>0.01 m 0.01 m</td>
<td>0.02 km 0.1 km</td>
<td>1 hour 1 day</td>
<td>Ocean Turbulence</td>
</tr>
<tr>
<td>LES</td>
<td>0.1 m 0.1-5 m</td>
<td>1 km 5-50 km</td>
<td>1 month 1 year</td>
<td>Ocean Turbulence and Boundary Layers</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Coastal and Estuarine Systems</td>
</tr>
<tr>
<td>Regional</td>
<td>1,000 m 10-100 m</td>
<td>500 km 1,000 km</td>
<td>1 year 1-10 years</td>
<td>Coastal Systems</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Marginal and Semi-Enclosed Seas Systems</td>
</tr>
<tr>
<td>Basin-Scale</td>
<td>10,000 m 1,000 m</td>
<td>10,000 km 10,000 km</td>
<td>10 year 500 years</td>
<td>Ocean Variability</td>
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<td></td>
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<td>Ecosystems</td>
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<td>Biogeochemical Cycles</td>
</tr>
<tr>
<td>Global</td>
<td>40,000 m 4,000 m</td>
<td>40,000 km 40,000 km</td>
<td>100 year 1,000-10,000 years</td>
<td>Climate Change and Prediction</td>
</tr>
</tbody>
</table>

Comparison among the various types of numerical simulations used to tackle oceanographic problems. The numbers in green show what is routinely possible with the IT resources available to the ocean sciences community. The numbers in purple show what needs to be done to resolve the phenomena of interest for problems ranging from ocean turbulence to global climate change.
very challenging (Figure 2). Thus, in addition to expanding the range of scales resolved by each class of models, it is equally important to increase the scale of overlap among them to help decide what processes can be expected to be parameterized in increasingly larger models.

The Gulf Stream system illustrates the difficulty of deciding the smallest scale that should be explicitly resolved in a climate model (see Eddy-Resolving Ocean Modeling box on page 14). In this example, both the position and the transverse structure of the Gulf Stream are not correctly represented when the spatial resolution is too low. There is a strong, bidirectional, nonlinear interaction between the "mean" flow (Gulf Stream front and adjacent inertial recirculations) and the "eddy" field (associated mesoscale eddies). Much of the mesoscale eddy activity near the Gulf Stream is driven by instabilities of the Gulf Stream front, and the eddies perform a climatologically significant function: they transport mass, nutrients, heat and potential vorticity across the Gulf Stream front and between the Gulf Stream and the adjacent recirculations. The envelope of eddy energy is strongly peaked near the Gulf Stream front. In a coarse-resolution climate model one would like to parameterize the mesoscale eddy-driven fluxes as a function of the flow field that is resolved. But, the feature that drives the mesoscale eddies is in the wrong place in this model. Its potential vorticity structure is resolution dependent, making any reasonable attempt at parameterization highly resolution dependent. Additionally, frontal features such as the Gulf Stream become diffuse and almost steady. The dynamical role that the ocean plays in climate is therefore suppressed in such models. The deep limbs of the meridional overturning circulation are similarly misrepresented. While one might be able to produce approximations to idealized steady-state climates with models that contain coarsely resolved oceans, such models may not accurately simulate rapid climate change and are therefore unlikely to capture the dynamics of decadal variability and carbon dioxide uptake.

The intricacy and inhomogeneity of mesoscale ocean structure is well illustrated by the calculation shown in the High-Resolution Ocean Circulation box on page 15. This calculation, which only begins to capture the mesoscale structure of the ocean, is extremely expensive computationally. This prototype calculation was performed at a state-of-the-art DoD computer facility. Given its resource demands, it is difficult to see how it could be carried out at one of the general purpose NSF supercomputer facilities under their current access and allocation policies. Ensembles of runs at durations adequate for addressing climate problems are not viable with the present infrastructure.
Community Models

Community models are emerging in all aspects of ocean sciences research, from ocean circulation and climate to ecosystem, sedimentation and tectonics. Within the field of ocean general circulation modeling, there are four classes of numerical models that have achieved a significant level of community management and involvement, including shared community development, regular user interaction, and ready availability of software and documentation via the world wide web. These four classes are loosely characterized by their respective approaches to spatial discretization (finite difference, finite element, finite volume) and vertical coordinate treatment (geopotential, isopycnic, sigma, hybrid). These codes are typically maintained within government labs or by university user groups. Although the user communities for these codes have been increasing in size and interdisciplinary character—and though they have therefore achieved, de facto, the status of a community resource—very few of these modeling systems has received sustained funding for development, testing, and outreach and training activities.

Similarly, four decades of modeling sedimentary processes has recently led to a coordinated effort to construct a Community Sedimentary Model. One of the anticipated roles of such a model is to help synthesize and interpret observational results acquired during programs such as ONR’s STRATAFORM project and the NSF-funded MARGINS program. One possible component of such a community model is one describing the filling of marine sedimentary basins such as the SedFlux model. At shorter time scales, sediment transport models are being developed, such as the community sediment transport model under development with NOPP funding. Coupled to models of the turbulent ocean bottom boundary layer, they are being used to investigate the evolution of the morphology of the water-sediment interface. Another class of marine geophysical model that requires significant computational resources is that of models of magmatic and tectonic processes.
Virtually all atmospheric and oceanic motion systems owe their existence to uneven solar heating of our planet, and the resulting large-scale circulations are nearly always directed so as to reduce this heat imbalance.

Heat-carrying currents on Earth typically organize themselves either into vertical “overturning” loops or into horizontal, thermally asymmetric eddies such as those seen on weather maps. Due to angular momentum constraints imposed by Earth’s rotation, the overturning mode is nearly absent in the atmospheric extratropics but can be sustained in the ocean with the help of frictional torques exerted by continental margins on north-southward flowing currents. In other words, the ocean is less dependent on eddies for heat transport than the atmosphere. Nevertheless, eddies do play an important role in the oceanic redistribution of heat and other properties.

Attempts to resolve in an ocean circulation model the special type of flow instability that gives rise to eddies face one major hurdle: the relatively small size—typically a few tens of kilometers—of the eddies. While a hint of the instability mechanism can be seen in models using a mesh size of 50 km, experience gained in the past decade tells us that a mesh size of 5 km or less is required before one can begin to describe a model as “eddy-resolving.” Resolving the eddy field in a basin model, let alone a model of the world ocean, therefore is a major computational challenge.

The accompanying figures (taken from Bleck et al., 1995) show the effect of grid resolution on the depiction of the Gulf Stream in two North Atlantic basin simulations that are identical in all respects except horizontal mesh size. The eddy-resolving simulation [mesh size 0.08 deg cos(lat.)] shows a Gulf Stream that begins to spawn vigorous meanders and eddies almost immediately after separating from the coast. This behavior agrees well with satellite observations.

Sea surface height maps from two North Atlantic Basin simulations at differing horizontal resolutions: ~1 degree (left panel) and ~1/12 degree (right).

References:
Global High-Resolution Ocean Circulation Experiments

Contributed by Julie McClean, Naval Post-Graduate School and Mathew Maltrud, Los Alamos National Laboratory

A long-standing debate in the climate modeling community is the grid resolution necessary to properly represent the ocean’s role in climate. To address this issue, recent comparisons of circulation models with 0.1° and 0.28° grids were completed using the extensive North Atlantic surface drifter data set for the years 1993-1997. The spatial and temporal coverage of these drifters is extensive, providing an excellent database from which to calculate statistics of the surface circulation. Eulerian statistics showed that flow features in the coarser run were unrealistic or misplaced and the variability was under-represented relative to the observations and the 0.1° simulation. The intrinsic Lagrangian (trajectory-based) scales from the 0.1° Parallel Ocean Program (POP) were not statistically different from the observed quantities, while those from the 0.28° model differed significantly (McClean et al, 2001).

Based on these and other results (Bryan et al., 1998), it was concluded that a global simulation with horizontal and vertical resolutions of at least 0.1° and 40 vertical levels respectively, (3600x2400x40 grid points) needed to be used. This simulation is underway using 500 processors on the IBM SP3 at the Naval Oceanographic Office and requires about ten days of wall-clock time and about 1 TB of storage per model year. The model uses a displaced pole grid whereby the North Pole is rotated into Hudson Bay, avoiding the issue of the polar singularity, and is initialized using the Navy’s 1/8° January climatology outside of the Arctic, and the University of Washington’s Polar Hydrography winter climatology in the Arctic. Surface momentum, heat, and salinity fluxes were calculated using bulk formulae based on the model surface temperature and an atmospheric state comprised of daily and monthly data from a variety of sources. To date, five years of the spin-up have been completed.

Preliminary comparisons of sea surface height variability from TOPEX/POSEIDON and the global 0.1° spin-up show improvements in the model variability compared to lower resolution global models, particularly in the magnitude and location of the variability in eddy-active regions.

References


DNS and LES modeling are two critical aspects of ocean sciences that are entirely dependent upon IT. DNS calculations allow oceanographers to look at fundamental processes at small scales with a minimum number of assumptions about the unresolved processes. Examples include the way in which localized patches of turbulence develop and decay in sheared and stratified flows, prey-predator interactions, the structure of oceanic boundary layers (see Turbulence Modeling box on opposite page), and the links between microscale and fine-scale physics (which helps the interpretation of data from specialized instrumentation used to study intermittent mixing in the ocean).

A major OITI requirement is to have sufficient computer resources to use the same simulation codes to understand a variety of physical, biological and geological problems, such as the interaction between larval behavior and turbulence, the small-scale dynamics of sediments, the role of breaking waves and bubbles in air-sea gas exchange, and the way in which doubly diffusive salt fingers drive the formation of thermohaline staircases. Both the smallest scale (e.g., individual organisms, particles, micro-breaking of capillary waves) and the largest relevant scale (e.g., energy-containing eddies, mean shear, boundary layer thickness, internal waves) of flow must be resolved at sufficiently high Reynolds numbers for the simulations to be representative of oceanic conditions.

Understanding the details of mixing processes will also help develop better physically based parameterizations of sub-grid scale physics in Large Eddy Simulations. At the same time, LES calculations are exploring the relationship between ocean turbulence and larger-scale processes such as convection, dense overflows and coherent vortices in the ocean mixed layer, as well as the dynamics of processes such as nonlinear internal wave fields, the interaction of tides and topography, and the transport of larvae, sediments, pollutants and mass. With a greater range of resolved scales, from turbulent scales to mesoscale features, LES “can help explain observations and point the way to parameterizations that allow upper-layer physics to be represented in circulation models” (OS2001). Another promising avenue for high-resolution LES models is the study of the circulation and ecosystem of constricted regions such as submarine canyons, bays and estuaries, coastal inlets and sounds, either as stand-alone models or embedded in more traditional ocean circulation models.

Ocean Turbulence and Mixing at Small Scales
**Turbulence Modeling**
Contributed by Eric Skyllingstad and William Smyth, Oregon State University

Large Eddy Simulation (LES) directly models scales of motion that contain the most turbulent kinetic energy. Scales of motion that are smaller than the model grid resolution are simulated via a sub-grid parameterization. Direct numerical simulation (DNS) models are similar to LES models, but use a constant kinematic viscosity, assuming either a small-scale domain or a low Reynolds number fluid. A critical need for simulating turbulence with LES and DNS is adequate spatial resolution and domain size. This need is most pronounced for complex flow problems involving stratification or shear, where the scales of turbulent eddies decrease. In LES models, this restriction limits our ability to simulate stratified or highly sheared boundary layers, whereas in DNS flow problems, it is difficult to model flows at realistic Reynolds numbers.

For example, two simulations of a wind-forced mid-latitude mixed layer with identical forcing but different grid spacing and domain size, show significant differences in the downward vertical transport of horizontal momentum (Figure). With coarse resolution (\(\Delta x = 2.0 \text{ m} \)), turbulent velocities are oriented mostly in a downwind direction with relatively weak vertical velocities. In contrast, increased model resolution (\(\Delta x = .75 \text{ m} \), lower panel) produces strong vertical motions and a deeper mixed layer, as shown by the plots of the horizontally averaged momentum and temperature. Normally, simulations using LES depend on resolving a portion of the turbulence kinetic energy spectrum that is in the inertial subrange (\(-5/3\) slope). However, resolving a \(-5/3\) slope may not be sufficient in sheared, stratified boundary layers because eddies smaller than the model resolution are critical to maintaining the overall boundary layer turbulence. If results are to be trusted, then the role of these small eddies must be addressed by increasing resolution and domain size. Increasing the resolution of this problem by the needed factor of 4 in each direction requires a 256-fold increase in computational power and more powerful visualization tools, which are beyond presently available resources.

References:


Vertical cross sections from a mid-latitude mixed layer simulation showing turbulence current vectors (every fourth grid point) and temperature perturbations.
(a) Coarse resolution: \(\Delta x = 2.0 \text{ m} \)
(b) Fine resolution: \(\Delta x = 0.75 \text{ m} \)
The Complex Coastal Ocean

The coastal ocean is of fundamental importance to many activities—including fisheries, defense, recreation and human health. It is also a region of the ocean in which human activity has perhaps the strongest impact through the modification of freshwater runoff, the introduction of large inputs of nitrogen and other nutrients, the episodic release of pollutants, the physical modification of the seafloor by dredging, and the manipulation of ecosystems by fishing. In the coastal ocean, the physical circulation is extremely complicated, the seafloor morphology itself evolves as a result of sediment transport, and the structure of biological communities varies rapidly on relatively short space and time scales. The coastal ocean is also a region of intense observational activity with coastal observatories such as LEO-15 (see Coastal Prediction box on opposite page), a spreading network of coastal radars that map surface currents, video recorders that monitor the nearshore wave field and other instruments that provide routine fisheries observations. The coastal ocean is a place where many of the pressures on IT resources that were described earlier in this section are acutely felt. The potential payoff from making more IT resources available is large. “Recent advances in computational capabilities, combined with increasingly sophisticated observational technologies (e.g., remote sensing, telemetry, networking, autonomous underwater vehicles, long-term monitoring systems) present unprecedented opportunity to advance understanding of shelf and estuarine systems and their management” (OS2001). The challenges presented by the analysis of coastal data (see Visual Super Computing box on page 40), the assimilation of coastal biogeochemical and physical data, and the development of whole-system models that integrate physics and biology and combine small scales (e.g., river estuaries and coastal inlets) with large scales (e.g., continental shelves of the United States) are profound.
Coastal Ocean Prediction
Contributed by Dale Haidvogel, Rutgers University

Permanent, continuously operating, real-time coastal ocean prediction systems are required to support a variety of critical activities in the coastal environment, including navigation and marine operations, response to oil and hazardous material spills, search and rescue, and prediction of harmful algal blooms and other ecosystem or water-quality phenomena. The implementation of such systems in turn requires advanced technologies in sensors and observing systems, and numerical models and data assimilation, as well as the infrastructures necessary to jointly use them.

Coastal ocean observation networks are now operating or are being constructed at numerous locations around the United States. Enabling technologies that make this possible include the rapid advances in sensor and platform technologies, multiple real-time communication systems for transmitting the data, and the emergence of a universal method for the distribution of results via the world wide web. Future sensors and platforms that will expand observation capabilities include new ocean color satellites, altimeters, HF Radars and autonomous vehicles. For example, the figure shows a schematic of the coastal observatory at LEO-15, which occupies a 30 by 30 km region in the New York Bight.

Concurrently, physical and ecological models for the coastal zone have been developed, and are beginning to show considerable skill. Such models by themselves are quite costly in terms of IT requirements (computing power, network speed, etc.). However, when they are linked via data assimilation to observation networks for the purpose of real-time forecasts, their IT requirements increase dramatically. For example, a single four-day forecast cycle of currents, temperature and salinity at LEO-15, using an ensemble-based assimilation technique, requires roughly 100 cpu hours on an Origin 3000 and the transfer of 10 GB of data. Parallel computing and rapid network connectivity are therefore essential for real-time operation. Scaleup of this system to cover the entire Northeast U.S. continental shelves and the inclusion of biological tracers, both envisioned for the near future, will increase these IT costs by several orders of magnitude.

The Rutgers Longterm Ecosystem Observatory (LEO-15)

References:
Recent studies have gone a long way to dispelling the old assumption that most marine ecosystems are in a state close to equilibrium. In part, this may be a result of changes in physical conditions or changes in the supply of nutrients. However, the strongly nonlinear nature of predator-prey interactions provides internal mechanisms for sustaining intrinsic ecosystem variability and for increasing the sensitivity of marine ecosystems to external perturbations. Changes in the composition of marine communities can play a role in regulating the degree of variability within an ecosystem. Another aspect of non-equilibrium ecosystem dynamics that is attracting considerable attention is the deliberate manipulation of ecosystems, for example, research into the effects on productivity, community structure and carbon sequestration that results when iron or other trace nutrients are added to pelagic ecosystems.

Efforts to understand marine ecosystems are driving a rapid growth in biogeochemical data assimilation and modeling (see, for example, Biogeochemical Simulations box on opposite page). Some of these efforts, particularly those focusing on large domains, rely on multi-compartment modeling techniques such as the various offspring of NPZ (Nutrient-Phytoplankton-Zooplankton) models. These simplified models only track bulk properties (such as nutrients, phytoplankton, zooplankton, detritus), but require that the underlying physical circulation be well-resolved in a high-resolution model to give reasonable estimates of primary production. Adding these four scalar variables to a circulation model doubles the computing requirements.

The more realistic biogeochemical models under development will require about five times more variables to represent the main functional groups for phytoplankton and zooplankton and the most critical nutrients. Other efforts, currently restricted to relatively small domains, and sometimes only in two dimensions, track individuals, following their growth, reproduction, death and feeding in the appropriate physical environment (see Biophysical Interactions box on page 22). Learning more about the strengths and weaknesses of these approaches and how they might be most fruitfully combined in three-dimensional models that simulate both biological and physical components is a task that is entraining a rapidly growing number of researchers. The pressure on IT resources comes both from the increasing complexity of modeling efforts and from the increasing number of investigations.

“New classes of models that incorporate nonlinear interactions, explicit spatial structure and non-equilibrium climate conditions need to be developed.”
(OS2001)
During the first half of the 1980s, it became clear that geochemical estimates of new production in large regions of the open ocean far surpassed that which could be sustained by nutrients supplied by vertical mixing (Jenkins and Goldman, 1985). Where might this “missing nutrient” come from? The notion that mesoscale processes could be an important vehicle for nutrient transport in the world’s oceans has been debated for some time. Several different lines of evidence now suggest that eddy-induced upwelling causes intermittent fluxes of nitrate into the euphotic zone of a magnitude sufficient to balance the nutrient demand (McGillicuddy et al., 1998). However, it was not until very recently that mesoscale phenomenology has become accessible in large-scale ocean models. Increased computational capability, together with progress in ocean modeling, have facilitated some of the first truly eddy-resolving, basin-scale simulations (Smith et al., 2000). Such calculations provide a framework in which the impact of mesoscale processes on biogeochemical cycling can be studied (Figure). Diagnosis of the model solutions suggests that, except for the wintertime period of deep convection, the dominant mechanism of nutrient input to the euphotic zone is vertical advection by eddies. This simple one-tracer biogeochemical simulation run together with the physical model was a very large undertaking by today’s computational standards (2 months of a dedicated 128-processor SGI Origin 2000). If the ocean sciences community is to address such problems with more biogeochemical realism (using on the order of ten tracer fields), then a significantly enhanced computational infrastructure will be required.

References:
**Coupled Three-Dimensional Biophysical Interactions**

Contributed by Christopher A. Edwards, University of Connecticut and Harold P. Batchelder, Oregon State University

Coastal upwelling zones have long been known to be regions of intense biological production (Ryther, 1969). Large, standing stocks of phytoplankton translate into high zooplankton biomass, which supports many productive commercial fisheries. Seasonal, equatorward wind stress drives offshore Ekman transport and upwells cold, nutrient-rich water near the coast. This forcing also results in a complex physical environment often characterized by an equatorward mean flow but contorted by a substantial mesoscale structure.

The predominantly equatorward and offshore, near-surface transport pose a challenge for planktonic organisms to remain nearshore and in preferred latitudinal zones. While mesozooplankton are unable to counteract strong horizontal flows directly, those that migrate vertically over the diel cycle may substantially reduce their net horizontal transport as a result of the large vertical shears in horizontal flow. Such biophysical interactions in coastal upwelling regions are now being explored numerically through combinations of nested physical and biological models that track individual zooplankton (Batchelder et al., 2001). In two dimensions, such Lagrangian calculations reveal the benefit of diel vertical migration (DVM) for nearshore retention (Figure) and can be explored using standard desktop workstations.

Of course, the physical environment is three-dimensional, and even passive particle trajectories in the vicinity of variable bathymetry reveal interesting fluid pathways. Understanding the complexity of the biophysical interactions, particularly when combined with variations in physical forcing on event, seasonal, interannual and interdecadal time-scales leads to nested problems requiring vast computational resources. Tracking ten million individual plankters having dynamic behavior and vital rates in stored three-dimensional physical fields representing a coastal upwelling zone for only three months requires 45 days of computation using 25 UltraSparc II processors on a Sun Enterprise server. Future problems requiring increased numbers of individuals tracked on longer time scales will require orders of magnitude increases in computational resources.

**References:**


Data Assimilation in the Context of Long-Term Ocean Observations and Prediction

“To understand and predict the changing ocean, there is a great need to capture in detail its baseline physical, biological, chemical and geological properties. The strict oceanic analog of weather forecasting would be to predict the amplification and decay of oceanic mesoscale eddies, tides and wind-waves. While these events are relevant because of their impact on marine resource management and ship movement, ocean prediction spans a much wider range, from climate change involving the global ocean circulation to the adjustment of a marine ecosystem following the introduction of an exotic species” (OS2001). Intensive use of IT is required for meeting these challenges through the combination of advanced numerical models and observations once the shortcomings and error covariances of these models are better understood.

A first class of applications for data assimilation is the testing of models and the assessment of the efficacy of observing systems. When a phenomenon of interest is well observed, the procedure can be used to quantify a model’s ability in representing the dynamics of the phenomenon (See Data Assimilation Tests Models box on page 24) or, alternatively, to check the adequacy of a data set for testing a particular dynamical hypothesis. Conversely, when only sparse observations are available, data assimilation with a comprehensive numerical model can be used to guide the design of an observing system. Models are conventionally tested by solving the equations of motion exactly, with given inputs (interior forcings, initial conditions and boundary conditions), and then comparing the solutions with observations. The agreement is rarely if ever within the experimental error of the data, even after the data have been low-pass filtered to suppress signals inconsistent with the scales of the model dynamics. The challenge is to find small enough perturbations to the model inputs, which lead to solutions agreeing well enough with the data. ‘Small enough’ and ‘well enough’ mean: consistent with prior assumptions about the variances and correlation scales of the errors in the inputs. If suitably small perturbations can be found, then the model has survived a rigorous test. Accordingly, the state estimates so produced would have credibility, and analyses of the conditioning of the fitting process could be trusted to reveal the efficiency of the instrumental array for observing the hypothesized flow regime. Such hypothesis tests are no more than conventional regression, but the calculations have not been feasible in the past owing to the nonlinearity of ocean models, and especially to the very large number of computational degrees of freedom in any realistic model. Limited tests of models with simplified dynamics have shown the power of the approach. Modern computers and emerging algorithms are just beginning to prove adequate to the task for more realistic ocean models.
Data Assimilation Tests Models
Contributed by Andrew F. Bennett, Oregon State University and ONR Science Unit, Monterey

A nonlinear, intermediate coupled model of seasonal to interannual variability in the tropical Pacific has been tested against monthly mean TAO mooring data (Bennett et al, 1998, 2000) to determine the adequacy of simplified dynamics at capturing and predicting El Niño events. The time series in Figure A shows that the solution of a perturbed model (solid line) fits the data to within standard errors of measurement. Figure B shows the SST field estimate (corresponds to solid line in Figure A) at the height of the 1997 El Niño event. The estimate has little choice but to agree with the TAO data to within experimental errors. However, the significance test for the total regression ($C^2$, not shown) is failed by many tens of standard deviations, owing to large standardized residuals in the equations of motion. Thus the SST estimates lack dynamical credibility. There is no prospect for salvaging this model by hypothesizing even greater standard errors in the dynamics. The term balance for the heat equation, expressed as time series at any one location, indicate that the residual or imbalance not only exceeds the levels of error as originally hypothesized, but is also the dominant term in the balance. There were $4 \times 10^7$ computational degrees of freedom and 2,500 data in this nonlinear, least-squares fitting exercise or ‘generalized inversion.’

Calculations of this kind with high-resolution, primitive equation models having as many as $10^9$ computational degrees of freedom, and as many as $10^5$ data, can now be performed on current computers. Future computers will permit even bigger calculations, once parallel programming and 4D display techniques (8D for covariances) have been mastered. Algorithmic refinements will permit the detailed testing of parameterizations of flux tensors, component by component. Modular software now in development will facilitate the application of this information technology to new ocean models.

References:

A. Time series of inverse estimates of the anomalous state at three TAO moorings (SS, 0, 5N) along 94W. The centered symbols are the 30-day average TAO data. All data of the same type are assigned the same standard error so only one bar is shown per panel, but note that the amplitude scale and bar length vary from panel to panel. Results here are for December 1996 to May 1998. (a) SST, +/- 0.3K, (b) Z20, +/- 3m, (c) u-ats, +/- 0.5m/s, and (d) v-ats, +/- 0.5m/s.

B. Anomalous SST and winds for mid-December 1997, contour interval 0.5K.
Another application of data assimilation, ocean state estimation, can be a powerful synthesizing force for many observing and modeling activities (see Global Ocean State Estimation Box on page 26). It permits the combining of diverse observations into a dynamically consistent and quantitative picture of the time-evolving ocean circulation and its constituents. The only way we can advance our understanding of the connections between the lower and higher levels of the marine food web, for example, and thus bring new insight into fisheries issues that affect U.S. industry and coastal communities, is to approach it as a problem in complexity. Modern IT will permit further coupled-model data studies of the intricacies of the marine carbonate system, and the ocean’s role in absorbing anthropogenically produced carbon. Assimilation of physical, biological, chemical and geological components in the ocean system is a cornerstone activity for understanding how the world ocean regulates climate. Modernizing ocean information technology will increase our chance of understanding and projecting seasonal-to-decadal variability of the coupled ocean-atmosphere system. These improvements will have a direct impact on our ability to forecast major, short-term weather events such as hurricanes and coastal storms and may permit better seasonal to decadal climate predictions for use in agriculture, infrastructure and water-resource management.
Global Ocean State Estimation
Contributed by Detlef Stammer, Scripps Institution of Oceanography

The ocean changes on a wide range of time and space scales. This variability greatly complicates observing and modeling the rapidly changing flow field, the ocean’s temperature distribution and, more generally, the consequences of those changes for climate. The extent of ocean observations is growing at a rapid rate. Quantities currently sampled on global scales include temperature, salinity, velocity, nutrients and halocarbons. Satellites provide, with nearly global coverage, data on sea-surface height, sea-surface temperature, wind stress and the near-surface distribution of chlorophyll. Despite these efforts, the ocean’s interior is under-sampled and will remain so for the foreseeable future. Information extracted from these observational data can be maximized, however, by supplementing them with the dynamical information inherent in high-quality numerical models of the ocean. One such technique for combining information from data and models to obtain the best possible description of the changing ocean is ocean state estimation.

Ocean state estimation offers the greatest promise for developing a complete, dynamical description of ocean circulation. It will provide insights into the nature of climate-related ocean variability, major ocean transport pathways, heat and freshwater flux divergences (similar for tracer and oxygen, silica, nitrate), the location and rate of ventilation, and the ocean’s response to atmospheric variability. Future oceanographic and climate research requires the ability to do ocean state estimation on a routine basis. The aim of the current “Global Ocean Data Assimilation Experiment” (GODAE) is to develop a prototype system to demonstrate the practicability of continuous ocean state estimation in the physical domain.

A pilot global ocean state estimation (Stammer et al., 2001) was conducted as part of a collaborative effort among Scripps, JPL and MIT, with a coarse resolution (2 degree) ocean circulation model over a short time period (1992-97). The model uses the MIT ocean model, which is part of ECCO. The lower part of the figure shows the estimated mean velocity field at 27 m depth. All major current systems are present, but with the low model resolution, they are too smooth. The upper part of the figure shows that the inclusion of ocean observations and ocean dynamics in the state estimation suggest that substantial corrections need to be made to the NCEP surface heat flux used to force the ocean model.

State estimation places very heavy demands on IT resources, from computational cycles to memory, storage and data transfer. A 1000-fold increase in available computational cycles is needed to address the community’s present, limited objective of depicting the time-evolving ocean state with spatial resolution up to 1/4° globally and with substantially higher resolution in nested regions, over a 50-year period. Future efforts will extend state estimation to include biogeochemical fields, adding even more to the IT requirements.

References:
The estimated mean sea-surface height and velocity field at 27 m depth are shown in the lower part of the figure. The figure shows all major current systems, but with low model resolution they appear too smooth. The upper part shows an instantaneous field of wind stress and net heat flux that is being used to force the model. The time-varying forcing is a control variable that is being estimated to bring the model into consistency with the data. Substantial corrections to the NCEP surface heat flux fields used as first guess are required. Changes relative to NCEP estimates are within error bounds and are for the heat flux field in the range of +/- 20 W/m² over large parts of the ocean. Over boundary currents changes can reach +/- 80 W/m² but are still consistent with our understanding of NCEP heat flux errors.
The Ocean’s Role in Global Climate

Ocean processes hold the key to understanding large-scale shifts in climate. The ocean is an important reservoir of carbon dioxide and heat, and “oceanic circulation, either through large-scale currents, mesoscale motions or diffusive processes, is responsible for the distribution of heat, freshwater and carbon dioxide that are gained from atmospheric exchange” (OS2001). Small shifts in ocean circulation can cause significant changes in regional climates. Regional variations in ocean climate can lead to regional changes in marine ecosystem productivity (see Coupled Climate Models box on page 30). Small fluctuations in oceanic carbon dioxide content may have a significant impact on atmospheric carbon content.

The ocean delays the impact of global warming induced by elevated atmospheric carbon dioxide concentrations by acting as a large-capacity heat sink. An analysis of historical oceanic data shows that for at least the past 50 years there has been a warming trend in the upper kilometer of all of the major ocean basins, with deeper penetration of warming in the North Atlantic. Ice-core records demonstrate that in the geologic past there have been periods in which atmospheric temperatures have changed with great rapidity (on time scales of a few decades). Sediment records suggest that in some regions ocean-surface temperatures and planktonic community structure changed at roughly the same time as the atmospheric temperature fluctuations.

Rapid or abrupt climate change is a complicated phenomenon involving many intricately linked processes. Theoretical considerations point to a possible major role for the ocean’s meridional overturning circulation (MOC). Some preliminary model results provide support for these ideas. Recent observations have demonstrated that the MOC can transmit information about changes in surface conditions in high northern latitudes to the tropics, via the deep ocean, in one decade. To get a clear understanding of how rapid changes in ocean heat transport might occur will require basin-scale ocean models integrated for several centuries with enough resolution to resolve deep boundary currents and better represent deep mixing.

Numerical models play an important role in the study of the mechanisms that govern climate dynamics. Depending on the nature of the problem addressed, these may be ocean-only models, fully coupled climate system models or intermediate hybrids. Fully coupled climate models are also used for assessments and estimates of current and future climate change. The needs of the coupled climate modeling community are comparable to those of the ocean sciences community and are addressed in the NRC report, “Improving the Effectiveness of U.S. Climate Modeling” (NRC, 2001). Here, guided by the charge to the Committee (page 4), we focus on the IT needs of those sectors of the ocean and climate science communities that are concerned with unraveling the ocean’s role in climate dynamics and with improving coupled climate models by improving the representation of ocean dynamics.

One goal of climate modeling is to get a better understanding of how the ocean takes up carbon dioxide, stores it, transports it, sequesters it in sediments and releases it back to the atmosphere. This builds on all the modeling efforts described earlier and will involve data assimilation (see previous section). At the smallest scales, DNS modeling is required to better understand carbon dioxide transport across the ocean surface and within the ocean mixed layer (see Turbulence Modeling box on page 17). At the largest scales, basin and global biogeochemical modeling is needed to study the
transport of carbon vertically, between the euphotic zone and the deeper ocean, and laterally, through ocean basins (see Biogeochemical Simulations box on page 21). The nonlinearity of the system leads to the conclusion that “locally observed variability of physical and biogeochemical cycles is... best addressed by considering processes at basin scales” (OS2001).

It has often been stressed that climate is one of the grand challenges in oceanography. One reason for this is the dependence of climate on the integrated effects of many oceanic processes covering a broad range of scales. The processes of heat transport in the ocean are fundamentally different from those in the atmosphere. They involve a much greater degree of three-dimensional anisotropy. They are more difficult to observe and model because both large-scale (global scale) and small-scale (boundary currents, deep overflows, highly inhomogeneous coherent eddy fluxes) components of flow are involved. At basin scales, parts of the ocean's thermal structure adjust within a few years while other parts possess thermal inertia of centuries or longer. The challenge of describing and testing ideas about a mechanism of which small and large space and time scales are integral parts makes computational science an indispensable tool.

Success in understanding Earth’s climate depends on progress across many topics in ocean sciences and on concurrent advances in the science of atmospheric and terrestrial systems. Climate-related needs in ocean sciences include:

1) obtaining far denser observations of the ocean than are currently made, particularly in the poorly sampled deep ocean;
2) expanding the collection and study of paleoceanographic data;
3) advances in methods to objectively design observing systems based on currently available data and dynamical knowledge (page 23),
4) rigorous testing of deductions about the climate system, from data and dynamical constraints, that data assimilation can provide (page 24),
5) synthesizing oceanographic and paleoceanographic observations permitted by state estimation (page 26),
6) an understanding of the different processes that determine horizontal and vertical transports within the ocean among the organically rich ocean margins, the ocean surface, the ocean interior and the chemically and biologically active ocean floor (pages 14, 15, 17 and 19),
7) an understanding of how the dynamically, chemically and biologically important processes interact to produce the constantly changing patterns that are climate (page 30).

Progress requires a close synthesis among observations, data analysis and modeling. The effectiveness of synthesizing observations and climate models has been demonstrated in the tropical Pacific where the synthesis of experiments like TOGA, the TAO observing system and simple, but illuminating, ENSO models has greatly enriched our understanding of the ENSO phenomenon. Large community research programs such as CLIVAR and GLOBEC, as well as the planned initiative to examine the oceanic component of the global carbon cycle, are designed to develop more ambitious syntheses. Data analysis, data assimilation and modeling are critical parts of these programs. A substantial, if still inadequate, observing infrastructure, costing many tens of millions of dollars annually, is already in place. This observing infrastructure is continually expanding. The available ocean IT infrastructure is much less well developed, despite the heavy dependence that programs such as CLIVAR, as well as the efforts of individual and small groups of ocean climate scientists, put on the use of major IT resources. So that climate research does not stall, comparable attention must be paid to establishing an ocean IT infrastructure.
Coupled climate modeling is computationally intensive, and the availability of computer cycles is a significant limiting factor to model development and application. A 100-year simulation with the current version of the CCSM takes approximately 1 month of dedicated time on 100 processors of an IBM SP-2 cluster (Winterhawk nodes). An ensemble of 3 to 6 multi-century simulations desirable for any particular emission scenario therefore takes 6 to 12 months; the long control integrations (thousands of years) needed to characterize natural climate variability or explore paleoclimate conditions (e.g. glacial/interglacial transitions) require comparable lengths of time. The problem is only compounded by current trends to improve model resolution and physics and incorporate active chemistry and biology (e.g., the carbon cycle) into climate models (Figure C, from Boyd and Doney, 2001), which can each add factors of 2-10 to the computational expense.

**References:**


A. Projected climate-mediated changes in sea-surface temperature for the decade 2060-2070 with respect to a control run forced with 1870 conditions. The change in global mean surface temperature predicted by this model is 2°C. From the NCAR CCSM (Boville and Gent, 1998).

B. As (A) but showing changes in stratification (vertical density gradient) at 50 m depth.

C. Simulations of changes (the decade 2060-2070 minus the present) in total chlorophyll obtained by using the CCSM with an off-line, multi-species, pelagic ecosystem model. The fine black lines overlaid on the ocean are the boundaries of biogeographic provinces (Longhurst, 1998).
The Ocean Below the Seafloor and the Dynamics of Oceanic Lithosphere and Margins

The study of the oceanic crust and of the fluid flowing within it is important to a range of research. Fluids flowing through the oceanic crust contribute to the chemical balance of the ocean, but also support microbial communities at least 1000 meters below the seafloor. Fluids flowing through the oceanic crust weaken earthquake-generating faults such as those off Japan, the Aleutians and Central America. They also play a large role in the accumulation of natural resources at specific sites on and under the seafloor. Seafloor is continually being created and modified, and the topography created as a result of these processes provides critical information about Earth dynamics, influences ocean circulation patterns and contributes to the distribution of turbulence within the water column. The crust beneath the seafloor is formed at mid-ocean ridges and near-ridge faulting produces seafloor topographic roughness. Average ocean depths are controlled by the thermal structure of the oceanic lithosphere and by crustal thickness that in places is affected by hot spot activity. Island arcs, such as Japan and the Aleutians, are formed where oceanic lithosphere descends into the mantle and remelts.

There is a very wide variety of models for processes that affect seafloor formation and modification by magmatic and tectonic processes. Problems include viscous mantle flow, segregation of melt from the mantle, brittle fracture allowing melt transport and faulting. Many problems are interconnected. For example, hydrothermal circulation cools and thickens lithosphere at the ridge axis, which likely controls the size and spacing of faults. The chemical reactions of hydrothermal fluids with rocks may not only affect biologic activity, but may affect the longevity of those systems. Without continued tectonic or magmatic activity, mineral precipitation can clog up a hydrothermal system.

There are few standard model approaches to problems of the oceanic lithosphere. One reason for this is the huge range in physical parameters that may be relevant. For example, cold lithosphere may have a viscosity more than 25 orders of magnitude greater than the magma that flows through it. Moreover, we know that magma flow can affect lithospheric deformation and stress state. Likewise, faults may be places where stresses are controlled by brittle failure mechanisms while the stress in the surrounding rock is controlled by the elasticity of that rock. Typically, modelers have to approximate the behavior of one part of the system while more rigorously tracking the behavior of the rest in a numerical model. Not only are many different numerical methods used, many ways to deal with approximations are employed. As new algorithms are developed and model complexity grows, and as model resolution increases, large resources will be required to run these codes. One numerical method that is getting increasing use in a variety of these “solid-Earth” problems is a hybrid Lagrangian approach called FLAC. It can treat elastic, plastic and viscous rheologies and is robust in terms of the range of parameters it can handle. Several groups in both the United States and Europe are improving and extending codes based on this method.

The numerical modeling of mantle convection and its influence on lithospheric dynamics is increasingly relying on state-of-the-art numerical methods and employing high-performance, mas-
sively parallel computers. Modern simulations attempt to deal not only with strongly temperature-dependent viscosities but also a variety of thermodynamic and thermochemical effects that can modify or oppose the action of buoyancy forces. These numerical simulations require shared access to massively parallel HPC machines or sizable dedicated clusters.

The nature of hydrothermal circulation through the oceanic crust is important in the understanding of heat-flow processes, in the chemical modification of seawater, and for the establishment and evolution of hydrothermal vent systems. Numerical modeling is used to determine not only the influence of heterogeneity in the permeability of the seafloor but also the effects of chemical modification of seawater within the crust and the concomitant changes in buoyancy.

In addition to process-oriented models, the geophysical and geochemical research communities have in recent years developed several widely used software tools for calculating equilibrium mineral assemblages at various temperatures, pressures and bulk compositions (e.g., MELTS) and deep-Earth seismic and geochemical reference models (e.g., GERM).

As a result of the fundamental difficulty of resolving the many temporal and spatial scales over which fluid, biological, volcanic and tectonic processes occur on or below the seafloor, progress in this arena will depend significantly on technical advances for making detailed observations. From an IT perspective, there is a need for an investment in data archiving and analysis (see Data Sets of the Seafloor box on page 34 and the Three-Dimensional Imaging box on page 35). A major concern for the marine geophysics community is the archiving of rapidly growing data sets and access to archives. Advances in storage technology can accommodate the size of these data sets but as their number and size grows, how to find and efficiently access them, together with the development of tools to analyze and interpret them become significant issues. Some legacy data are essentially unarchived and identified repositories are not available for important data types, including seafloor topography and sub-bottom multichannel seismic data. Particular needs highlighted in a recent workshop (Smith et al, 2001) are for a centralized and searchable online metadata catalog summarizing the distributed data collections currently available and for a "deep archiving" capability for data in project-oriented collections. The workshop outlines 20 recommendations for how to build on the current geophysical data archive activities to create a system that can keep pace with the explosive growth in observations.

The data access, analysis and management needs of marine geophysics overlap with those of other parts of the solid-Earth research community. These needs, together with the grand challenge of developing a comprehensive understanding the dynamic Earth as an integrated interdisciplinary system, have led to the emergence of the field known as geoinformatics. Geoinformatics will provide some of the tools needed to achieve the substantial integration across disparate data types and scientific disciplines required for the development of such understanding.

In addition to data archiving, data processing needs must be considered. Scientists who use remotely sensed data, whether of the oceanic lithosphere, the seafloor, the water column or the sea surface, often do not have the computational resources and data analysis tools to process all of the data that are being acquired.

Thus, in the interdisciplinary areas of marine geoscience, there exist significant needs for data storage, data analysis, data mining and computation.
The creation and evolution of the oceanic crust is a consequence of mass and energy flux from deep within Earth to its surface. This complex process leaves its mark on the morphology of the seafloor. The challenge is to interpret the observed morphology and its spatial variations revealed by remote-sensing instruments to recover the nature of this process, and its effect on other systems such as hydrothermal circulation and biological communities.

A new “nested survey” mapping strategy has emerged to collect data very close to the seafloor. Data are now commonly collected at progressively higher resolution within subareas of the region previously surveyed, and with a variety of sensors (Figure). With these nested surveys come vastly increased data volumes. High-resolution side-scan sonar instruments collect ~1 GB of data per hour and digital cameras record ~300 MB of data per hour. Our standard software tools for visualizing these data and analyzing them are not designed to handle large-size data sets, and the side-scan and photo imagery data that are now being collected are not used at their full resolution except in very small pieces. This problem will only increase as seafloor observatories come on line, collecting vast amounts of information through continuous monitoring of seafloor physical, biological and chemical processes, and as autonomous underwater vehicles map the seafloor at increasing resolution.

The goal of seafloor mapping is a true three-dimensional rendering of the seafloor, incorporating all of the available information that can be quantitatively analyzed for feature identification (e.g., faults, volcanoes, landslides), and for pattern identification (e.g., topographic slopes, feature distributions, number densities, shapes). Currently, sufficient resources are not being devoted to developing algorithms that can automatically interpret data collected under water. Thus, some work that is very labor-intensive, such as constructing photo mosaics, is still done by hand. Resources must also be allocated to develop algorithms that integrate information provided by multiple sensors.

References:

A section of seafloor imaged at increasing resolution using different instruments. Lower panel shows multibeam bathymetry data. Each water depth represents a footprint on the seafloor that is ~30 m by 30 m. Middle panel shows a side-scan sonar image of the area outlined in the lower panel. The vehicle path is in the center of the image; white is a reflection and dark is a shadow. Each pixel represents a 2 m patch of seafloor. Top panel shows a mosaic of several digital photographs taken in the region outlined on the middle panel.
In 1999, US and Japanese scientists acquired three-dimensional (3-D) seismic reflection data of the Nankai Trough offshore of Japan. These data imaged a fault that has repeatedly produced some of Earth’s largest earthquakes and tsunamis, most recently the 1944 Nankaido and 1946 Tonankai magnitude 8.0 events. The primary objective of this investigation was to image the thrust surface and map physical properties of the thrust plane controlling fault rupture.

Although modest by oil industry standards, the .5 TB of data acquired in imaging an 8 x 80 km area of the subduction thrust represents a considerable computational challenge for academic computer facilities in both data processing and visualization. Tests of subsets of the data volume show significant enhancements to seismic images are possible with state-of-the-art seismic processing techniques used routinely by the oil industry. These tests also reveal that the required computation forces us to limit prestack migration, a particularly effective technique for imaging complex structural settings such as the Nankai Trough, to subsets of the data in some of the most critical areas. Rough estimates for computation of a single 3-D prestack depth migration of our entire data volume would be one week on a 128-processor Origin SGI. It is also reasonable to expect 5–10 iterations of migrations to determine ideal parameters.

Visualization of the seismic volume is also a challenge for high-powered computers. The oil industry has developed software for interpretation and analysis, yet there are few academic facilities capable of the 3-D data-volume rendering required to visualize and examine spatial relationships of structures in our images and in real time. In cooperation with the Texas Institute for Computation and Math (TICAM) at the University of Texas, we have conducted some preliminary tests on an older 3-D data volume. With their 16-processor SGI Onyx with eight graphics pipes, it is practical to render, in real time, a volume of 64 MB of data. The Nankai data volume is on the order of 4 GB with comparable decimation. This is more than a factor of 60 greater than what is currently practical with these facilities.

As the use of 3-D seismic imaging techniques to address academic problems in marine geology and geophysics continues to increase, much more powerful computer facilities are needed to handle the required computation.

References:

Assessment of Ocean Science IT Infrastructure

Trends in Computer Technology

Hardware Trends

In the United States, the vector supercomputers that once dominated high-end scientific computing have been replaced by systems based on commodity microprocessors. Vector supercomputers can sustain a large fraction of their peak speed on “vectorizable” problems, which include most oceanic applications. The latest vector systems sustain several Gflops per processor on such applications. Microprocessors only approach their peak speed on a very limited number of applications, with most problems (including oceanic applications) sustaining perhaps 5% to 15% of peak. In 1998, sustained performance was about 100 Mflops and now it is about 200 Mflops (Figure 3). Moore’s Law on transistor fabrication density implies that microprocessor performance doubles every eighteen months, and this historical trend is expected to continue for at least the next five years. Thus, microprocessors will be sustaining at least 1 Gflops in five years.

Until very recently, there was a large difference in floating point performance between high volume microprocessors targeted at PCs and low volume microprocessors targeted at workstations and servers. The latter were 5 to 10 times more expensive, but also 2 to 4 times more powerful. Today the mainstream Pentium 4 and Athlon microprocessors are among the fastest available for floating point applications. What still distinguishes workstation/server microprocessors is that they are 64-bit designs able to address much more memory than the 2 GB typically allowed by 32-bit designs. The improved floating point performance of inexpensive 32-bit microprocessors is a benefit to Beowulf clusters (see below), although they are typically limited by network, rather than floating point, performance on oceanic applications. There has also been a shake-out in the 64-bit microprocessor market, with Intel’s new Itanium scheduled to completely replace MIPS, PA-RISC and Alpha microprocessors over the next several years. This industry consolidation does not change the projected speed of microprocessors, which is still controlled by Moore’s Law. However, it may change the current price structure—which imposes a large cost premium on “server” characteristics such as large memory and multiple processors per node.

High speeds with microprocessors require scalable machines and applications, that is, parallelization across many processors. If moderate speedup—say, four to ten times a single processor—is sufficient, then Symmetric Multi-Processing (SMP) systems in which multiple processors share a single global memory system are typically used. Parallelization is at the

Figure 3. Ocean model performance as a function of the number of processors on several scalable systems.
Figure 4. Typical domain decomposition for parallelization of a North Atlantic model.

loop level and can either be automatic (via the compiler) or using OpenMP Fortran/C parallelization directives. Pure SMP machines are typically limited to about 16 processors, although Sun has a 64 processor SMP system and 32 processor systems that are expected to become more common in the near future.

If significant speedup, 30 to 300 times a single processor, is required then a system consisting of individual nodes connected by a scalable network is typically used. For oceanic applications parallelization is via domain decomposition with message passing between domains using the standard Message-Passing Interface (MPI) library. In domain decomposition, each processor “owns” a small subregion of the entire domain and does all calculations for that subregion. Figure 4 shows a typical decomposition, with 16x16 equal sized subdomains tiling the North Atlantic. Subdomains that are completely over land are discarded at compile time, so this example would actually run on 161 processors. However, in the typical oceanic application, frequent communication is necessary between domains, which is only efficient on a low latency network. Custom, “scalable” systems from vendors such as Cray, IBM and Compaq include relatively low latency vendor-specific network backplanes, and such systems now dominate the high-end for oceanic applications. Figure 3 shows the performance per processor of an ocean model on such systems. The result is expressed in nominal sustained Mflops, and a horizontal line indicates perfect scaling (doubling the number of processors halves the wall-clock time). Ocean models can scale to several hundred processors on these systems. The number of processors can now exceed 1,000 per system, and a recent trend is for each node to consist of an SMP multiprocessor. This has led to research into using mixed-mode, MPI and OpenMP parallelization for higher performance. This increases the programming complexity and so far has not demonstrated a large increase in performance over using MPI alone for oceanic applications.

In the 50-200 processor range, it is possible to maintain a single global memory system, providing nonuniform memory access (NUMA) speeds are acceptable, that is, some memory is “closer” to a given processor than other memory. The most popular machine of this type is currently the SGI Origin, but several vendors are expected to introduce such machines in the near future. These machines are very flexible because they can run both OpenMP and MPI applications. Distributed-memory machines with large SMP nodes (e.g., 16 or more processors per node) have similar flexibility, but without a single operating system image.

The lowest cost parallel systems are Beowulf clusters, which combine commodity microprocessor (often PC-based) nodes with a commodity networking fabric (often switched fast Ethernet) and Open Source software to produce a MPI-based system. Their exceptional price/performance make them the systems of choice for all applications they run efficiently. They have not been very effective for oceanic applications above about 16 processors because the commodity network latencies (that is, the amount
of time needed for communication among processors, nodes or elements in a network) are too high. However, systems with 100-200 processors following this design philosophy but with higher performance nodes and with lower latency networks show promise for oceanic applications. There is already a trend for higher performance Beowulf clusters to use dual-processor nodes, and SMP nodes with more processors will become increasingly common as the current price premium for multiprocessor systems shrinks. Commodity network performance and the lack of robust, parallel file systems are the weak links in current Beowulf systems, but both are expected to improve significantly over the next few years.

The Computational Grid

A long-established trend in information technology has been the transition from isolated computers to an increasingly connected grid. The advent of ARPANET in the late 1960s allowed computers separated by long distances to communicate with each other. However, the potential benefit of inter-computer communication is much greater than simple file transfer. Computer scientists quickly recognized the possibility of binding computers together into virtual machines. An important step towards this goal was the development of software such as the Network File System. This allowed small groups of computers to share disk storage by integrating storage on physically separate machines into a single logical file system. Users could access a file without having to know whether the file resides on their local machine or on a remote machine. Another step towards an integrated computing grid came with the advent of web-server and browser software that led to a global information grid popularized as the world wide web.

Much computer science research in the last two decades has been directed towards the more difficult task of implementing a computational grid in which computational projects can be distributed across a loosely connected network of computers. One long-term goal is to seamlessly integrate a widely dispersed network of heterogeneous computers into a single virtual machine. In this vision, users will log on to any computer, and then be presented with their own customized environment, regardless of location. When a computationally intensive task is submitted to the virtual machine, the underlying system software will find one or more local or remote processors that can execute it in an optimal time. This will be done in a way that is transparent to the user and which takes into account not just computational time, but also the need to transfer or merge distributed datasets (see Visual Super Computing box on page 40). Just as the electrical grid now supplies households and businesses with electricity, the computational grid will supply computational resources.

The technical challenges of grid computing are still large, but the concept is well established (e.g., Foster and Kesselman, 1999, and references therein, or www.gridforum.org). Some novel examples of the trend towards grid computing have existed for a while. The SETI@Home program (www.seti.org/science/setiathome.html) is a relatively primitive but very effective example. It has involved more than 3 million participants and averages a sustained computational rate of over 20 Tflops. It is a model that is now being considered for genome analysis, financial analysis and certain types of geoscience applications. A more sophisticated example is the Condor project (www.cs.wisc.edu/condor), which schedules compute jobs on a distributed set of machines (e.g., workstations in a department). It implements a strategy known as High-Throughput Computing and makes more effective use of a distributed set of workstations than would be the case if users were limited to their own or small subsets of workstations. For each job, Condor finds an idle machine on which to run it and automatically switches the job among different machines if a machine on which it is running begins to be used by a lo-
cal user. Although individual jobs can only be
moved to machines with similar architecture,
the Condor system itself can work on any het-
erogeneous collection of machines. Additional
examples include distributed computational fluid
dynamics calculations (see www.ipg.nasa.gov/
research/) and distributed cellular micro-physi-
ology calculations made using the AppLeS
Parameter Sweep Template and Network
Weather Service (see www.cs.ucsd. edu/
~casanova/homepage/papers/wccgsc00.ps) or
with NetSolve (see icl.cs.utk.edu/netsolve).

While the full promise of grid computing is still
some years ahead, and its ultimate impact
uncertain, some of the developments in this
field are likely to be useful to ocean data analysis
and modeling studies for applications in which
multiple, loosely coupled tasks are supported.
Possible examples of activities that might benefit
include multi-scale nested modeling, coupled
physical-biogeochemical simulations, and some
types of data assimilation. Because many of
the traditional approaches to geophysical mod-
eling may not, at present, lend themselves well
to effective use of a distributed computational
grid, the availability of such a resource may
ultimately lead to a move towards new, non-
traditional, methodologies.

A technological trend of a different sort is to-
wards ever more powerful machines, both at
the individual-processor level and at the lead-
ing edge of parallel-computing technology. This
trend will very likely involve both an evolution
in computer architecture and the development
of new computational techniques, such as
multithreaded supercomputing, to effectively
use such machines. For example, the devel-
oment of PetaFLOPS computing, now being
actively pursued under funding from ARPA, DOE,
NASA, NSA and NSF, will involve a degree of
parallelism one to three orders of magnitude
greater than current terascale machines.

The pace of advance in software and applica-
tions is as rapid as that in hardware. The com-
mittee fully expects that by the time this re-
port is published, newer, faster commodity
hardware will have been released that could
potentially satisfy ocean sciences’ needs. This
report cannot capture these advances and cannot
address and describe all of the potential areas
of information technology that are applicable
to ocean sciences. It is the fast pace of innova-
tion and the complexity of computer sciences
advances that are part of the challenge of iden-
tifying a vision and then a workable implemen-
tation plan for using information technology for
ocean sciences.

Of the many potentially important advances
in information technology, we list some that
have begun to be explored within DoD, NSF
and the community. These application areas
include distributed supercomputing applications;
real-time, distributed, high-data-rate instrument
systems; data-intensive computing (e.g., data
assimilation, data handling); high-performance
commodity computer technologies; and
teleimmersion. To increase these areas’ use,
the ocean sciences community must find ways
to engage computer scientists to collaborate
on implementing these applications. This type
of interaction is now actively being facilitated
and funded by NOPP grants and NSF ITR grants.

Other important information technology areas
that have not yet been actively investigated
for ocean sciences applications include com-
piler optimization and applications toolkits. One
can imagine a need for toolkits for modeling
and other common ocean sciences applications
such as high-volume data processing, visual-
ization and networking in real-time observing
systems. Some groups, such as the WRF de-
velopment group at NCAR (www.wrf-model.org)
have been using more flexible programming
structures that allow modularity. Object-based
approaches for system design received some
early attention in ocean sciences (1980-90s),
but probably should be revisited. By having dedi-
cated technologists working at the informa-
tion-technology frontier in service to the ocean sci-
ences, this community’s use of information
technology will be greatly enhanced.
In recent years there has been a rapid increase in the capability of environmental observation and modeling systems to provide high-resolution spatial and temporal data from estuarine and coastal regions and, to a lesser extent, the deep ocean. The demand for these data is driven by the need for increased understanding of dynamical processes on fine scales, improved ecosystem monitoring capabilities and the management of and response to environmental crises such as pollution containment, storm preparation and biohazard remediation.

An improved understanding of aquatic systems depends upon the effective management of observed and simulated data sets and the degree to which these data sets are integrated with new visualization and analysis technologies. Because of the size and complexity of these data sets, it is no longer sufficient to visualize them as two-dimensional graphical objects on flat computer screens or only from single-user locations. To meet this visualization challenge, there has been a focus on creating persistent virtual environments, which enable multiple, globally situated participants to collaborate over high-speed and high-bandwidth networks connected to heterogeneous supercomputing resources and large data stores (De Fanti et al., 1996; Leigh et al., 1997). The use of collaborative, three-dimensional immersive environments changes the way information is viewed or manipulated and actually provides the feeling of being there, thereby aiding in the mental process of rapidly assimilating complex information (Wheless et al., 1996).

Advances in visual analysis technologies and data sharing via national high-performance networks should permit scientists to examine previously intractable environmental problems. Unfortunately, these technological improvements are not well known by the ocean sciences community, nor are they readily available for a large enough base of scientists so that large-scale, focused efforts may be easily undertaken. Clearly, the improvement of the national grid-based computing infrastructure is a requirement for conducting computationally and data-intensive activities (Foster and Kesselman, 1999). These improvements should concentrate on integrating modeling applications, database systems, archival storage systems, data display and visualization systems, and wide-area dissemination capabilities via high- and low-bandwidth network channels.

References:


Community Use of Computer Resources

Shared-resource computer centers are currently the primary source of computer cycles for both medium-sized and large oceanographic projects. These centers are being saturated with small users up to the point that large needs cannot be met adequately. As a result, it often is difficult to get access to resources, even those being allocated to a project. Moreover, the structure of many centers is not set up for long, continuous, quasi-operational simulations. Most centers assume a project will require intense computations for a few days, or maybe weeks, and then cycle out (letting a new intense project access the resources). Some ocean sciences computations fall into this category, however, oceanic applications increasingly require a daily cycle of forward modeling and/or ocean state estimation. Such applications require large computations for many months with no clear breakpoint visible for the near future. Moreover, individual runs in some cases require several days elapsed time and must run to completion to provide results (e.g., for ocean state estimation optimization problems).

In other words, many oceanographic problems have grown in computational size to the point that they require dedicated, long-term computing much the way meteorological forecast centers require a continuity of computational support. An analogy can be made to the support the ocean sciences community receives in terms of dedicated ship support by NSF and ONR. Numerical computations have been elevated to the level of importance that previously was reserved for observational programs, but the infrastructure and support required to lead the field into the future is largely missing as evidenced by the current funding process for large computing allocations (Figure 5).

The DoD High Performance Computer Modernization Program allocates 20-30% of its total resources to about 30 “DoD Challenge” projects, of which three are currently ocean modeling projects. This is the closest the community has come to adequate computer support for a project. These projects are in the 500K to 2M processor hour per year range today (the equivalent of 50-230 dedicated processors per project), with growth of at least 1.5 times per year over a project’s three-year lifetime. Even this level of support is less than desirable, and it is limited to three projects in oceanography.

The situation at NSF centers is much worse. They typically consider all projects over 100K processor hours (5% of a DoD Challenge) to be “large” and oceanography has few allocations even of this size. NSF computer centers are saturated by many users from all scientific research and applications disciplines. One of the problems here is that about 45% of available resources are allocated to four disciplines: astronomy, particle physics, biochemistry and material research, with less than 20% going to all of geosciences. One of our problems arises
from the lack of communication at all levels between supercomputer center management and ocean modelers.

Moreover, with the continuing growth of NOPP-funded activities, more and more long-term projects will be created that will require computer allocations over the projects’ duration. Typical current policy is to request computer time on an annual basis. This is rather cumbersome given that success is not guaranteed in the annual proposal submission procedure; thus funded projects can be idled as a result of the lack of required resources. The DoD Challenge projects are again an exception, with a three-year award possible.

Another obvious problem is the fact that rapid changes in computer architecture have recently put a vast burden on the scientific community to port numerical codes to modern computer platforms. The community is desperate for technical support to help optimize their programs to run on those new computers. This issue concerns groups running complex ocean models. But it likewise concerns scientists involved in computationally intense data analyses.

Figure 5. Flow chart showing the time-consuming way in which PIs currently obtain computational time on supercomputers available to the academic research community. A proposal, often in different formats, may have to be submitted to several computer centers in the hope that one of them will approve the required computer time.
Community Survey

In an effort to encourage input from all interested members of the ocean sciences community, the OITI Steering Committee conducted a survey. Topics included current OITI use, current scope of work, future OITI use, Hub functionality, Hub management and outreach (see Appendix 2). The term “Hub” used in the survey refers to a community-based resource (as described in Powell, 1998) responsible for overseeing OITI activity.

Response to the survey was requested via several avenues: advertisement in EOS, e-mail to a large (>1000 names) distribution list, and targeted contact with key individuals at 50 institutions well-known for oceanographic research. Input was solicited over a three-month period, resulting in 46 surveys returned representing 800 individuals at 35 institutions. The disciplinary makeup of the respondents spanned physical, biological and chemical oceanography, and marine geology and geophysics; a number of interdisciplinary scientists also responded. Several different types of institutions were represented, including academic, research, government laboratories and private consulting firms. Key findings are summarized next. A more detailed description of survey results can be found in Appendix 2.

- **Current Scope of Work:** The scope of respondents’ current research is tremendously diverse, including ocean circulation, climate, physical-biological-chemical interactions, seafloor geomorphology, ocean seismology, marine acoustics, sea ice and surf-zone processes. Spatial scales of interest span millimeters to global dimensions, and time scales from seconds to millennia. Computational domains range from estuaries to the global ocean. More than half of the respondents had immediate or near-term needs for real-time or near-real-time access to data. Nearly all respondents use large data sets. Advanced processing and visualization techniques are a necessity.

- **Future OITI Resource Utilization:** Respondents expect to continue to use multiple platforms in their research. Most anticipate the use of a PC/workstation for at least some fraction of their computational work. The most common response for expected monthly usage for this category was 10K cpu hours, as compared with 1K at the present time. Less than one sixth of the respondents expect to use serial architecture supercomputers in the future. Parallel supercomputers and PC/workstation clusters garnered a roughly equal proportion of responses; as in the current situation, massively parallel supercomputers are expected to be used for the most computationally intensive applications. The most common responses for anticipated needs for memory, data set archival and Internet
transfers all increased by factors of 10-1000 from current usage (1 GB to 100 GB memory; 1 GB to 1 TB per month data archival; 1 GB to 10 GB per month data transfer). Nearly all respondents foresaw the need for additional human resources to accompany expansion in computational infrastructure. Programmers, postdocs and computer specialists were the most popular choices to fill such needs. A variety of new software needs were anticipated, yet two types were by far the most frequently mentioned: parallelization tools and visualization software.

• **Hub functionality**: The most highly rated Hub functionality was that of reference archival datasets. Climatologies, topographies (the highest ranked functionality) and surface forcing all were judged to be crucial to Hub capabilities. Of the other potential archival datasets, satellite gridded data were viewed as next most useful, while both numerical model output and WOCE synthesis fields were ranked significantly lower in this capability category. As a category, the next most highly ranked resource area was that of community models. All three specific functionalities under this general heading were regarded as crucial by a significant proportion of the respondents, including codes/documentation, online tutorials and support staff. There was general support, though of varying degree, for all the specific hardware and analysis/visualization software capabilities polled. In order of average ranking in these categories, “mass storage” emerged on top, followed by analysis/visualization software, computational engines and, visualization hardware. Finally, only the items in the outreach category were rated on average to fall below the “useful” category.

• **Hub Management and Outreach**. A large majority of respondents endorsed a “mixed” distribution of facilities, with some capabilities resident at a “Hub” and the remainder distributed in some fashion over the participating “nodes.” Of its potential functions, it was suggested by many that the Hub serve as the home for only those clearly requiring a centralized facility. Examples noted by the respondents include: large-scale computing (> 1 Tflop/s) and datasets (>1 PB), rapid data transfers, and technical support staff and training activities. Many responses gave examples of what they considered to be good management “models” that might be copied by the Hub. These included: the National Supercomputing Facility, UCAR, NCAR Scientific Computing Division, NAVO, the Arctic Region Supercomputing Center and UNOLS. Several comments in favor of UNOLS-style resource management (e.g., block-funded; block awards for extended, intensive access to resources) were received. On the issue of Hub personnel, most who responded on this issue favored a minimalist approach to Hub staffing (i.e., just sufficient personnel to oversee the local facilities and to provide dedicated service functions).
Computer Center Survey

The OITI Steering Committee also conducted a survey of existing computer centers. Topics included current OITI resources, current workload, future OITI resources and centralized vs. distributed computing (see Appendix 3 for the full text of this survey). Twenty-five U.S. centers with links to ocean sciences were selected from the list of Top 500 High Performance Computer Sites (www.top500.org), and were asked to respond to the survey. Eleven survey responses were received: two from government operational environmental prediction centers, four from government laboratories, four from shared academic science resource centers, and one from a multi-campus university. Key findings are summarized below.

- **Current Resources:** The operational centers rely on machines from a single vendor, the four government laboratories each have large machines from two vendors, and the shared resource centers support two to four vendors’ machines (Appendix 3). The user base varies from 100 to 2,500, and ocean scientists are fewer than 5% of the total at all but two sites.

- **Staff:** All sites report large staffs, three sites at about 30, three at about 70 and five above 100 (Table 2). All provide 24/7/365 coverage. The government site staffs are more heavily weighted to user service roles (41% to 71% of the total, vs. 30% to 44% for academic sites), but this may in part result from the smaller number of system vendors at the government sites. Five sites indicate that at most one extra staff position would be required if a new 500-processor system were added and if it were compatible with existing machines at the site, with one site indicating that an additional one to two staff would be required if the machine was from a new vendor for the site. Nine sites indicated that adding 200 new users would require three or fewer new staff. Overall, the marginal staff costs of adding new systems and users to an existing site are very low relative to the total site staffing levels.

- **Future Resources:** Six sites estimate that capabilities would grow by 8 to 15 times in five years, with five sites estimating higher (20 to 50 times). Five sites estimate an ad-

![Figure 6. The percentage of users at U.S. supercomputer centers who are oceanographers versus all disciplines. The graph is based on surveys returned to the OITI Steering Committee by eleven computer centers.](image-url)
### Table 2

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<td>NERSC</td>
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<td>11</td>
</tr>
<tr>
<td>Discipline-Specific Specialists</td>
<td>6</td>
</tr>
<tr>
<td>Others:</td>
<td></td>
</tr>
<tr>
<td>• Database and Visualization</td>
<td></td>
</tr>
<tr>
<td>• Liaisons and Public Affairs</td>
<td></td>
</tr>
<tr>
<td>Additional Staff Requirement for</td>
<td></td>
</tr>
<tr>
<td>• 500 Processor Scalable System</td>
<td>2-4</td>
</tr>
<tr>
<td>• 200 New Users</td>
<td>0</td>
</tr>
</tbody>
</table>

Notes:

\(^{1}\) The 70 users at NERSC are all climate researchers whose simulations include an ocean component.

* Numbers include research, academic and administrative computing.
ditional growth of 8 to 12 times over the following five years, one site estimates much higher, but four sites estimate lower (2 to 3 times). SMP clusters were the favorite computational architecture for five years from now, with general agreement that the dominant architecture ten years from now is not possible to predict.

- **Central vs. Distributed Sites**: All sites agree that there would be significant cost savings from collocating a centralized oceanographic facility at an existing large computer center. Several sites also point out that a new stand-alone center might take several years to become established. The most commonly cited disadvantages of this approach were actual or perceived lack of control by the ocean sciences community and the possibility that an existing center’s mix of machines might not be a good fit to oceanographic applications. On the question of centralized versus distributed computing, many sites point out that the most demanding computational problems must be solved on a single large machine (i.e., at a central site). The most frequently mentioned advantages of distributed computer environments were flexibility and leveraging existing capabilities. The primary disadvantage was the difficulty in coordinating diverse sites to provide an acceptable overall quality of service.
Recommendations

Overview

The OITI Steering Committee recommends several solutions to short- and long-term needs identified in the surveys and previous reports. These recommendations are listed in Table 3. The recommendations labeled “Immediate” can be implemented now, but provide only temporary relief to the growing need for OITI. The “Long-Term” recommendations address current needs and growing demand for OITI.

Growing demand for OITI can be estimated by extrapolating the growth in activities shown in Figure 7. Purple represents the observatories and observing system activities. These current and future activities support an expanding observing system that dramatically increases real-time data flow and data density. The sophisticated use of real-time networks takes advantage of advances and coordination in information and communication infrastructure. Green represents the processing, serving and handling of disparate and large data sets that are being undertaken at various Data Centers (e.g., NODC, DAACs, WOCE, GLOBEC, JGOFS, GODAE). Blue areas represent the interaction of observing systems, data archiving and serving, the NOPP modeling nodes, Global Ocean Data Assimilation Experiment (GODAE), and other large-scale modeling, data assimilation and operational forecasting activities. The gray lines connecting the boxes represent the exchange of information among the various elements in the figure, the primary focus of the NOPP-funded Virtual Ocean Data System (NVODS; http://nvods.org). Thus, the blue portions of the boxes and the gray connecting lines represent the areas impacted and facilitated by the “Hub” referred to in Powell (1998) and the user survey. As each element in this diagram increases in output and sophistication, the need for OITI grows and better coordination and joint planning among the various elements will be required. The figure indicates the most obvious focus of the recommendations in this report, but these recommendations also address more subtle but equally important needs, including providing technical support, consulting expertise and technology evaluation. Not shown in the figure nor addressed in this report are additional data services such as sites for data location and additional data documentation, which are also required in an end-to-end data system.
### Issues and Road Blocks

**Allocations and access to HPC:**
- too few cpu cycles
- job duration limits
- prioritization issues
- multiple proposals to obtain resources

**Compute cycles (for users of all types of shared resources):**
- lack of long, large blocks
- lack of sufficient local processing
- lack of dedicated processors

**Power computing for medium-small resource users:**
- lack of adequate hardware, software
- lack of support for MPI code conversion
- lack of advice and consulting on networks, security, archiving

**Access to advanced software and datasets:**
- lack of access to community models/output
- lack of support for archival datasets
- lack of graphics and visualization utilities, and lack of analysis tools

**Access to applications programming:**
- difficulty with updating and converting code
- lack of expertise porting code to new machines
- lack of expertise with MPI conversions
- lack of expertise optimizing code for new compilers

### Recommendations

#### Immediate:
- add ocean community members to NSF allocations committees and other center committees; attempt to ameliorate current practices
- procure project-related, medium-scale hardware
- initiate pilot projects-Beowulf clusters
- look into excess or shared computers for ocean sciences
- provide technical support and training

#### Long-Term:
- provide hardware optimized and dedicated to ocean sciences
- act as a broker for cpu resources at HPC Centers
- secure appropriate allocations of cpu, duration
- act as a broker for cpu resources
- provide technical support
- conduct technology evaluation
- provide access to and help with community models
- provide model, data, software curatorship
- provide technical support and training
- conduct technology evaluation
- provide access to and help with community models
- provide model, data, software curatorship
- provide technical support and training
- conduct technology evaluation
Figure 7. The relationship between ocean sciences activities and information technology. Purple represents observatories and observing-system activities. Green represents data-processing serving and handling. Blue represents the interaction of observing systems, data archiving and serving, and ocean modeling.
To meet the immediate needs of the community, the committee recommends quick and easily implemented measures to access more effectively the existing computational and archival infrastructure. These are further described below.

To meet the growing need of ocean sciences, the committee recommends that a new entity be constituted in order to provide the leadership services described and requested by users (see previous sections). This entity encompasses some of the intended functions of the “Hub,” identified in Powell (1998). However, the OITI Steering Committee, and the majority of those who responded to the survey, felt strongly that the structure required should not be a centralized facility and that it needed to provide capabilities beyond those described in Powell (1998). For this reason, the IT resource structure recommended here will be referred to as Ocean.IT (pronounced Ocean IT). This renaming is meant to capture all aspects of the community’s IT needs and vision, including help and service in building local components of a national information technology infrastructure, and using information technology to advance ocean sciences. Starting from its initial focus on addressing modeling, data assimilation and data-processing needs, Ocean.IT’s structure and charter should be flexible enough to expand in other IT areas such as real-time communication, if needed.

Leadership, advice and service are needed within the community regardless of the level of sophistication of the project or the user. The unique role of Ocean.IT is its focus on facilitating the acquisition, allocation and use of IT infrastructure for all aspects of computer-intensive activities; this is needed not only because of the new modeling challenges undertaken through NOPP and other large research programs, but also because of the challenges posed by the analysis of the growing ocean data stream and by the rapid advance of computer science tools and IT hardware. At the highest level, Ocean.IT will serve in an advisory role to IT elements for which it is not directly responsible, such as the long-term oceanographic data archive. At the individual project-scientist and small- to medium-research group level, Ocean.IT will serve by making computational and other IT advances more available locally and remotely.

Funding for Ocean.IT will have to be sustained, with an initial level designed to substantially augment ocean sciences IT resources. Capital expenditures will, however, be continuous so that Ocean.IT can be maintained at a state-of-the-art level.

Ocean.IT will...

...provide both central and distributed human and technical resources.

...function like a scientific program office (e.g., WOCE or GLOBEC) and will provide leadership and advocacy for the infrastructure needs in ocean sciences research areas that use and need information technology.

...function as a resource center for hardware, software, archiving, data serving, and technical training and consulting.
Short-Term Recommendations

Although technical and scientific knowledge and funding have been dedicated to computationally intensive research questions, progress is hindered by inadequate access to computational resources. This situation is likely to deteriorate if no improvement can be achieved during the coming few years. Right now there is a compelling, immediate need to provide the NOPP-sponsored data assimilation, physical modeling and multidisciplinary modeling nodes with sufficient computer resources for them to meet their funded goals. During this period, new and even more computationally intensive research projects will be attempted.

The computer center survey indicates that ocean scientists who use supercomputer centers represent less than 4% of the centers’ user base and they use an even smaller percentage of the available cpu time (see pages 45 to 47). Most computer centers have a very low percentage of users that run MPI or OpenMP codes, and centers that have a higher percentage of such users appear to have no established priority system for executing this type of code. For the community that has not undergone extensive code conversions, there is a huge competition for cpu time on the few vector parallel machines that are left. The survey indicates that at all centers that have them, these vector machines are used 100% of the time and that these machines will soon be phased out.

The results of the community survey also reveal that it is not easy for the ocean sciences community to access high-performance computing resources in sufficiently large blocks of cpu allocations or for sufficient duration. The community of users of small to medium computational resources is stymied by the complexity of porting software from one machine to another, a lack of dedicated medium-size machines, which forces users to compete with large users, and a host of logistical problems within their own universities. Most users have very little access to available time, sophisticated users have very little access to dedicated time, and current allocation processes are unlikely to fill this need-provision gap.

The OITI planning activities are mostly concerned with medium- and longer-term remedies of this pressing situation, but there are a few actions that can be taken immediately to alleviate the current problems. At this time, the computer resources logjam prevents progress in the larger NOPP modeling node projects, creates frustration for the medium- to small-resource user, and hinders the progress in processing global observations. The committee recommends that funding agencies take two steps to improve the ocean sciences community’s current situation, including providing hardware and enhancing communication with computer centers and allocation panels. These steps are described in the following pages.
Supplemental Hardware

Provide hardware dedicated to serving the oceanographic community’s computational needs. The OITI Steering Committee recommends action along three lines:

**Distributed, Medium-Scale Hardware**

Funding agencies should address requests for project-related, medium-scale computer hardware support. Such funding is difficult to find with current mechanisms. For the success of individual NOPP nodes, the NOPP mechanism should consider hardware and computational time as part of the resource needs.

**Excessed or Shared Supercomputers**

A complementary action will be to provide computer cycles to the ocean sciences community and/or to NOPP projects from one or more large computer systems through the addition of computer resources to an existing, shared computer resource center. Two approaches might be taken. The DoD HPCMP centers, and perhaps others, typically budget a life cycle of three to four years for its supercomputers. At the end of that time, the hardware is offered to other organizations. These machines often still represent significant computer resources that, in principle, could be used by ocean sciences. In many cases, the cost of moving an old machine to a new institution, purchasing a new maintenance contract, and supporting the operations of a stand-alone machine will not compare favorably with purchasing new hardware to supplement an existing center. However, the committee recommends that the feasibility of maintaining such retired hardware at its original site, with in-house support and supplemental funding from ocean sciences funding agencies, be investigated to see whether it is cost-effective.

**NOPP Needs**

To meet the immediate needs of NOPP projects, a center should be identified that is willing to manage a NOPP-dedicated system and to augment one or more of its existing systems. NOPP would pay for the purchase and upkeep of the additional capability, which would be dedicated to NOPP projects, thus freeing up other resources for the rest of the ocean sciences community. Care must be taken that NOPP-specific resources do not jeopardize ocean projects running on the shared portion of the machine.

These measures resolve some of the obvious problems, but do not address the growing need for a more sophisticated, dedicated infrastructure. The medium- to long-term need will be addressed by Ocean.IT described in the following pages.
Enhancing Communications

Allocation and Advisory Committees

Increase the participation and visibility of the oceanographic community in the allocation panels and advisory committee to NSF, DoD and other supercomputer centers to articulate its computing needs.

Computer Centers

Facilitate dialog among members of the oceanographic community, computer center managers and computer center advisory committees to identify, and attempt to remedy, the most pressing problems in current computer center management practices. Examples of these issues include limited run time, a lack of queue management, a lack of job priority assignments, and lack of recognition of ocean problems as meaningful computational challenges. It is hoped that a dialog with center managers will help provide some short-term remedies to problems stemming from current practices.
Long-Term Recommendations: Establishing Ocean.IT

Ocean.IT Functional Elements

The functional elements of Ocean.IT are designed to address the issues and roadblocks identified by the community.

Issue: Allocations and Access to High Performance Computing Centers

A common thread in the computer surveys is the difficulty many ocean scientists have in obtaining access to resources at supercomputer facilities. These difficulties include getting access to sufficient quantity and duration of CPU cycles, and to mass storage allocations, and access to mass storage of model outputs. A recommended solution is for Ocean.IT to act as an agent for the ocean sciences community in obtaining a larger share of current resources, managing new resources, and simplifying the process of obtaining allocations. This brokerage and managerial service applies to both existing resources across agency-sponsored supercomputer centers and new resources that Ocean.IT would manage.

Recommendation 1: Improve Ocean Sciences Access to CPU Cycles

Allocations of CPU cycles need to be augmented, both by purchasing supercomputers and by acquiring resource allocations at national centers. The process of obtaining CPU allocations should be streamlined by combining computer resource requests as part of the original proposal review process, analogous to the way ship requests are handled. Potential users would submit a single form and Ocean.IT would broker resources either at one of the ocean sciences HPC sites or at the most suitable national supercomputing facility. Ocean.IT would argue for block allocations of computer time from these centers on behalf of the ocean sciences community. The Ocean.IT broker would also work with the HPC centers to obtain allocations in terms of numbers of processors, run duration, job priority and scheduling that are well-suited for ocean sciences.

Recommendation 2: Improve Ocean Sciences Access to Mass Storage

The surveys identified access to a common ocean sciences mass store facility as an important issue. Generally, mass storage use at a HPC goes along with the allocation of CPU time. When the allocation is used, the investigator has a limit on the residence time of the research results. This limits an investigator’s ability to use output and the community’s ability to access the output. Only investigators with an account on a machine have access to the mass storage. An additional mass storage capability is required to allow the general ocean sciences community easy access from the outside. This facility will be distributed (many mass storage facilities). Ocean.IT will facilitate access to community products. Additional challenges related to managed update, quality control, easy access and ability to serve in a rapid, online manner will also be addressed by Ocean.IT.
**Issue: Optimized Compute Cycles for All Users**

The surveys of the users and centers revealed that the nature of the computationally intensive activities featured in Figure 7 has some common requirements:

- need for large blocks of computer time;
- need for large numbers of dedicated processors;
- need for high inter-processor communication speed.

These issues motivated the committee to address the question of the likelihood that available resources at general-purpose scientific computing centers will be configured for ocean sciences needs. The conclusion of the committee is that this is not likely. The computer survey indicates that the current trend at computer centers is to purchase machines that are based on commodity microprocessors with high latency, which are effective barriers for obtaining optimum solution speed of ocean problems.

As a community with only 4% of the resources and little representation on the allocation committees, it is difficult to influence the choice of future hardware for ocean science needs at the HPC centers. This issue clearly affects the high-volume resource user, a category that is expected to grow as we tackle more complex problems. Without help, the other users will face a difficult situation as the few vector machines left are fully saturated and will soon go away entirely. The most efficient way to meet ocean sciences needs is to have dedicated resources to supplement HPC resources.

The following elements are the principal hardware needs for ocean sciences.

**Recommendation: Provide High Performance Computer Hardware Optimized for Large Ocean Sciences Projects**

This recommendation is broken down into two parts, first in terms of the capacity that is recommended, and second in terms of how that capacity should be deployed.

We recommend that the equivalent, in computing power, of the leading-edge civilian terascale computing system be acquired. (A current example is the new O(3000) processor system at the Pittsburgh Supercomputer Center.) Efforts should be made to upgrade this capability by 30% to 60% a year to keep up with improvements in technology. Initially, ~500 TB of mass storage will be required, with future capacity following an exponential growth curve.

There are two ways to accomplish this goal:

- Purchase the hardware typical of a supercomputer facility (one or more large multi-processor supercomputers, satellite clusters, mass storage, etc.) and install this in a new stand-alone ocean sciences computing center.

- Purchase the hardware typical of a supercomputer facility and disperse this among one or more existing supercomputer centers as additions to the existing facilities with this additional capacity being dedicated to ocean sciences.
The possibility of starting a new HPC center, dedicated to ocean sciences, was considered carefully by the committee, weighing comments from the ocean sciences community and from existing centers. The idea was judged to be too costly and inflexible, with the added danger that an ocean HPC center would try to drive the science.

We recommend that the hardware be located at existing centers and dedicated exclusively to ocean sciences use. This will require a budget for additional systems administration and maintenance at the selected facilities. We recommend optimizing the hardware acquisitions and configurations for ocean problems.

We recommend that the initial purchase not be a single terascale machine but that capacity equivalent to roughly one-third of a leading terascale machine be added to the facilities at existing, but separate, computer centers. Together, this capacity, dedicated to ocean science problems, will be the equivalent of creating new resources slightly greater than those of the leading terascale facility, but will be a more cost-effective and more robust approach than the purchase of a single new machine. At the present state of the art, this means the addition of O(1000) high-performance processors to the existing configuration at each host center.

We recommend that, after the initial purchase, annual increases in capability should be made. This growth should be through progressive performance upgrades of the capacity at the three “ocean sciences computing” locations. We recommend that all of the supercomputer purchases be made under performance curve contracts.
**Issue: Maintenance and Upgrade of Local IT Infrastructure**

The community survey reveals that many users struggle just to obtain the next fastest workstation, maintain connectivity to the network and implement basic security precautions. The IT departments of many universities struggle to maintain only the most basic of functions, while the research departments are functioning on the technological edge. The needs of this part of the community fall into the following straightforward categories:

- modern, high-end workstations;
- small clusters (O(10)-O(100));
- midsize clusters (O(100)-O(500));
- mass storage devices;
- consulting on purchasing options;
- advice, consulting and training for networking, security and hardware options;
- upgrade networking infrastructure at ocean sciences centers.

**Recommendation 1: Provide a Technical Evaluation Function**

Ocean.IT will provide a consultant group and advisory desk on IT related issues for the ocean sciences research community. Ocean.IT personnel will provide an ongoing service examining and testing the latest technological advances. These activities will assess improvements in hardware and software and make recommendations regarding systems for ocean sciences. An example of the technical function might be to assess the use and setup of a small Beowulf cluster. Personnel will also provide a resource center for evaluating hardware and software for users with workstation needs. Software toolboxes would be evaluated for various computer platforms. Hardware performance and archival options will also be evaluated. Recommendations would be posted on a web site as well as provided via a help desk. In the near term, special attention would be given to security issues with solutions as well as system security evaluations being provided by Ocean.IT.

**Recommendation 2: Provide Computing and Networking Hardware and Support**

Agencies will still need to support hardware purchases at the user and institutional levels. Some individuals and small groups of users will still have their needs met best by using dedicated local machines or a cluster connected to the Internet via high-speed networks. We anticipate that this need will always be present and meeting it should be an integral part of the Ocean.IT role. In addition to the need to provide robust mechanisms to fund such acquisitions at a continuous level, there will also be a need, from users, for advice on what to buy and how best to set it up. This, too, is an important role for Ocean.IT.
Issue: Access to Advanced Software and Datasets

A common need within the ocean sciences community is easy access to advanced software and data products, including numerical models, model output, analysis packages and reference datasets. The increase in complexity of handling such needs is apparent. For example, today’s models may be written in a mixture of languages, with different versions of the model meant for running on different compilers and memory systems. Typically 50% or more of the code is outside the model’s computational kernel, dealing with parallelization, forcing fields, boundary conditions, diagnostics, etc. The forcing fields, such as wind stress and heat flux, for global models require gigabytes of storage. This trend is expected to continue.

In addition, the number of hydrographic stations has increased from the 10,000 stations collected in the 100 years preceding WOCE to the 24,000 collected in the 10-year WOCE period of the 1990s (Figure 1). The increase in Lagrangian measurements is more dramatic; surface drifters have gone from less than 2000 per year (pre-WOCE) to over 5000 per year (WOCE-era) and subsurface floats from a couple of hundred to over 6000. A typical global model output for a simulation can reach many gigabytes.

The community needs simple, facilitated access to the results of observational and computational experiments. Ocean.IT will be a curator of models, data and software and a facilitator of their use and access.

Recommendation 1: Provide Model and Software Curatorship

The goal is to invest in developing advanced software while avoiding duplication of efforts among numerous PIs. The underlying software (models or tools) should conform to standard software engineering principles, including documentation. Support staff must be available to provide online help. As appropriate, formal training on these applications or software packages may be provided. The types of software and the corresponding needs are listed below.

- **Community Models:** Community models serve as software infrastructure that allows the efficient implementation, testing and dissemination of new techniques. Development of community models and their component algorithms will continue to be a distributed community-wide activity. Ocean.IT’s role will be to serve a central repository to provide easy access to community models contributed by their development groups within the ocean sciences community, facilitate access to new model algorithm developments and improvements, conduct standardized testing and performance characterizations across model classes, and archive and distribute model code and documentation. In addition to being a common access point for different types of community codes, Ocean.IT will provide a common set of user services — including workshops and online tutorials — that are logistically difficult for academic groups to provide. In the long term, frequently used components needed by several community models will be consolidated into shared tool kits, but initially, community models will be selected from existing, stand-alone state-of-the-art models. It is anticipated that an advisory board will be need to help sort out the designation of “community models.”
• **Multidisciplinary Models:** Some of the most obvious applications for archived model output are experiments that further use the physical and tracer fields for transporting other variables. One example would be the use of an archived physical model run as input to a simulation of biological or chemical processes in the ocean. For this purpose, Ocean.IT should have, in addition to core physical, biogeochemical and biogeophysical community models, generic tracer advection models and the infrastructure to run those models easily (included browsing, sub-setting, reformatting).

• **Analysis Tools:** Ocean.IT will provide a library of software tools, supplied together with software documentation, to facilitate the community’s use of oceanographic data and model output. This software toolkit would include statistics packages, time-series analysis packages, graphics packages, compression tools, translators, etc., as well as visualization tools (translators, sub-setting, etc.). Each software library and application must be documented and tested to meet quality-control standards for use as a product by a large number of scientists. See www.netlib.org as an example.

**Recommendation 2: Data Archiving and Distribution**

The design and creation of, and effective access to, data archives are persistent issues in ocean sciences. The role of Ocean.IT will be to streamline access to existing data centers, data standards, metadata, etc., and to act as a clearing house and point of connectivity to the centers of research in data access and archives in the IT, computer science, physics, health and other sciences.

• **Archives of Measurements and Model Output:** In addition to model code and documentation, Ocean.IT must be responsible for archiving model output and specific observations, and providing support for the wider community to use these data. This service needs to cover a large range of applications, from process-oriented forward runs (climatological runs, hindcasts, special processes) to ocean state estimation where models have been constrained by ocean data sets (reanalysis runs and forecast runs).

• **Data Access:** Similar to the support provided to models and model output, Ocean.IT must provide support of ocean data. This service needs to include the capability to obtain customized gridded climatologies, initial conditions for models, boundary conditions for models, data sets, surface forcing fields (such as heat fluxes) and bottom topography fields. In addition to archiving some frequently used data itself, Ocean.IT must have links to all existing archive centers, including in situ data (e.g., WOCE, JGOFS, GLOBEC, NODC, ODP and CLIVAR data centers) and satellite data (e.g., DAAC centers).

• **Permanent Archives:** Although there are thought to be policies in place for data delivery to national archives, the policies that exist are out of date, do not apply to all of the observational data being collected and are not enforced. The result is that a signifi-
cant fraction of the data are lost. Ocean.IT will work with the oceanographic community to develop a consistent set of policies for long-term retention of observational data and model output. Specifically, Ocean.IT will work on a suite of recommendations for data that should be archived at a national repository, periods of retention for these data, procedures for delivery of these data and for other issues related to the preservation of satellite and in situ observational data.

**Recommendation 3: Response to New Computer Technologies**

The advent of new computer technologies and platforms often necessitate modifications (sometimes massive) to existing software and procedures. As a consequence, the software to be used, the application to be undertaken, and the computational resource to be used must often be matched for effective performance.

- **Standards:** To maximize the use of observational data and model output by the community, these data objects must be freely and easily accessible (i.e., the data system must be interoperable at all levels). To achieve this requires consistent and complete descriptions (metadata) of the data sets and well-defined and widely used data access protocols. To this end, Ocean.IT will work with the community to develop standards for data documentation and transfer protocols and will help promote these standards within the community.

- **Guidance on Hardware:** Ocean.IT services must also include expert advice on new computer technology and platforms, including platform selection for a given application, help in code redesign for improved performance, and comparative information on platform speed and cost.
**Issue: Access to Applications Programming**

As computer centers struggle to maintain the cutting edge in hardware, the nature of the compilers, processors and memory use change dramatically (see the previous section on trends). To take advantage of this computational power, sophisticated programming is needed. To solve the most complex problems, ocean scientists will need to program their codes for simulation, data processing, statistics and visualization very cleverly. It is not reasonable to expect an investigator to be a master programmer when the IT industry is having trouble finding qualified staff to perform advanced applications programming. A very strong community need is to have a programmers’ resource center to train, aid and support code conversion to current hardware, optimize code for advanced projects to take maximum advantage of current hardware, support diagnostics and analysis packages, and implement connectivity to the Grid and other national infrastructure projects.

**Recommendation 1: Provide Technical Support and Training**

Ocean.IT will provide a consultancy function for higher level applications programming. We envision that they will provide a frequently asked questions file, and help with some major initiatives. A primary function will be the training of interested members of the community. To identify priorities, Ocean.IT would institute a series of workshops or courses designed to coordinate and train the ocean sciences community in various IT subjects. An annual workshop would aid in focusing the overall ocean sciences community on IT needs. Other courses would address topics ranging from setting up a new cluster to more scientific endeavors, for example, data assimilation techniques. It is anticipated that scientific issues and technical and software training requests will change as the community comes up to speed on IT concepts (e.g., parallelization support). Ocean.IT should also provide online technical help as well as through training. Staffing for this function would draw from the scientific community and from in-house technical staff.

**Recommendation 2: Sponsor Pilot Projects**

Pilot projects are needed to explore the technical feasibility of elements of the OITI plan. These projects should immediately benefit the participants and to the wider community, and at the same time motivate future OITI and Ocean.IT directions. Examples include: exploring the effectiveness of Beowulf clusters for modeling and data assimilation, for graphics and visualization, and as database servers; reducing the duplication in software development by providing standard solutions to pre-identified problems (parallel netCDF, Eulerian/Lagrangian interpolation, flux couplers for nested grids, etc.). Another possible pilot project is sponsoring a data assimilation center that creates and implements the appropriate data assimilation method for the user and model. These projects could be coordinated by Ocean.IT.
Long-Term Recommendations: Implementing Ocean.IT

The ideas on implementing Ocean.IT will continue to evolve through more community planning. This section is the OITI Steering Committee’s recommendations, with consideration of all survey input.

Staffing Requirements for Ocean.IT

Staffing estimates for initiating Ocean.IT are given below and in Table 4. These estimates were derived from knowledge of the staffing levels of a typical small computational center. As Ocean.IT takes on more activities, more staff in the different categories might be needed.

- **Management**: Ocean.IT will require a full-time Director and Technical Director. The Director will be charged with overall leadership and will be an advocate for advancing the scientific priorities of the ocean sciences community through the effective use of modern information technology. S/He will be responsible for the continuing evaluation of and planning for community needs. S/He will also provide, to the relevant federal agencies, periodic recommendations for updating the ocean IT infrastructure to ensure that Ocean.IT evolves to keep pace with advances in ocean science and computational science and technology.

  The Technical Director will provide leadership in hardware, software, computer configuration, model, data and software curatorialship, and technical expertise specifically for ocean sciences. As such s/he will be the primary interface with the IT research community, the HPC centers directors and hardware manufacturers. The Technical Director will also be responsible for providing the technical basis of recommendations to the agencies for maintaining the currency and optimization of an advanced IT infrastructure for ocean sciences.

  To ensure that Ocean.IT remains responsive to the community and the funding entities, the Director should be responsible to an oversight Board of Trustees, similar to the boards that advise UCAR, UNOLS and IRIS. The Director and staff would also draw upon the expertise of scientific advisory panels or tech-

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<tr>
<td><strong>Inaugural Ocean.IT Staffing (minimum expectation)</strong></td>
</tr>
<tr>
<td>Management (senior scientist level)</td>
</tr>
<tr>
<td>Research Scientist (specialists in various areas)</td>
</tr>
<tr>
<td>Research Scientist (virtual staff)</td>
</tr>
<tr>
<td>Computer Scientists</td>
</tr>
<tr>
<td>Applications Programmers</td>
</tr>
<tr>
<td>Systems Administration</td>
</tr>
<tr>
<td>Technical Specialists (web, data, viz specialists)</td>
</tr>
<tr>
<td>Visiting Scientists</td>
</tr>
<tr>
<td>Administrative Specialists (staff support; workshop support)</td>
</tr>
<tr>
<td>*In different disciplines of community models; in ocean observation serving or technology evaluation</td>
</tr>
<tr>
<td>**In visualization; in systems administration or technology evaluation</td>
</tr>
<tr>
<td>***In parallelization tools; help desk; model maintenance and code</td>
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technical expert panels (drawn from existing research groups and individual users) to assure responsiveness to community needs.

We also recommend that the Director have a two- to three-person technical staff for administering OITI-funded computer resources and support functions located at Ocean.IT (these are not personnel at outside centers). An administrative assistant and a financial specialist will be needed for the Director’s office.

- **Model Maintenance and Service:** Staff will be needed to support the community use of biogeochemical coupled codes, circulation models and data assimilation modules; make computational-update code improvements; and maintain version control of community models, etc. We assume a minimum of one expert per model might be needed. The staff for this category could reside at their home institution and be virtual staff of Ocean.IT; initially they could be drawn from the development teams that generated the community model/data assimilation system. As the number and complexity of these community models grow, code curatorship could occur within a central facility. We estimate that there might be four to five community models/data assimilation systems. Maintenance-code updates and code porting could be done through this central facility. The desired personnel would be highly skilled application modelers with training in oceanographic subdisciplines. This type of staffing may be difficult to obtain. Research-level scientists have the required skills but are inconsistent with the “helping” and service attitude (both for their career and the centers needs). A core staff is desirable but it might be supplemented by providing for support for visiting scientists when new model/assimilation/database systems are being developed and brought on line.

- **Data Archives and Links:** It will be necessary to have a dedicated staff member that generates, maintains and constantly updates links from the Ocean.IT to data archives around the country. As a provider of facilitated access, Ocean.IT should be comprehensive in its links and catalogues of archived data. As Ocean.IT grows in its service to the community, creating and maintaining specialized archives (such as forcing fields for models, or listings of geophysical core libraries) will be added. In addition, the difficult task of establishing compatible formats, translators and metadata would be undertaken by this staff member. It is also desirable for them to know DoD’s and other data-serving systems. Research scientists and technical research specialists that have worked in the observational ocean sciences field or related areas are the most likely candidates for this type of position.

- **Visualization:** Within the Ocean.IT there is no intention to duplicate or generate the volume of research in visualization, thus this function is best fulfilled by a staff member who can act as a liaison between the ocean sciences community and the large computer science and other geoscience research communities that are working in visualization. We anticipate that a computer scientist can provide expertise, liaison among existing systems and ocean applications of systems, technical development, and consultant services for software specific to ocean sciences. In the areas of ocean sciences dealing with very
large and dense data sets and output archives, a second specialist who is dedicated to custom visualization software development might be needed. Many of the MSRCs have this expertise in house; it may be possible to have them as virtual staff members or consultants to Ocean.IT.

- **Systems Administration:** Staff will be required to maintain the in-house systems that Ocean.IT uses to provide its services. As a link to models, data and software, we can anticipate that a considerable amount of “web serving”/routing type hardware will be resident at Ocean.IT. We expect there might be pilot projects to test new types of clusters. Staff trained in systems administration will be needed to provide technical guidance on these pilot projects; they will be needed to maintain internal systems and they will be needed to provide general technical advice to the ocean sciences community. We estimate that two to three people are needed.

- **Code Parallelization/Tools:** The center will require one to two experts to provide user support in noncommunity programming. This staffing will address the need to parallelize code (modeling and other) written by those not formally affiliated with Ocean.IT modeling and assimilation activities but who are allocated time on Ocean.IT computational resources. Ocean.IT support staff will provide assistance in determining the cost versus benefit associated with parallelizing a potential user’s code and in the actual parallelization effort if parallelization is deemed appropriate. We anticipate that a Unix application programmer and a PC-knowledgeable application programmer will be needed.

- **Web Site and Documentation:** One full-time position will be needed to maintain online documentation and an access-facilitating web site. We anticipate that a fairly advanced and experienced web designer should be part of the Ocean.IT staff to facilitate the “virtual” nature of Ocean.IT services. The web outreach and serving system also needs to have security while remaining essentially open to the public. We anticipate one web master/designer/security person and perhaps a second to generate content and documentation.

- **Technology Evaluation:** Ocean.IT could employ specialists for fixed terms of three to six years to establish new community models, a software library or instrumental protocol (following the successful example set by the ECMWF). The regular, but organized, turnover of staff will be critical to its authority and vitality.

- **Workshops:** Workshop organization will involve one to two staff members who will act as coordinators. They will be in charge of designing workshop agendas, coordinating participants and trainers and securing adequate lodging and meeting accommodations.

- **Hardware:** Although the activities managed by Ocean.IT will, in general, be distributed, the Ocean.IT technical group must also have local hardware and software resources at its disposal. These must be sufficient for evaluating and configuring new systems for ocean sciences research and should include two small clusters, several types of fast interconnect and networking hardware, routers, web servers and high-end graphics capabilities.
First Step Toward Implementing Ocean.IT

The implementation strategy for Ocean.IT should be developed by the ocean sciences community in consultation with funding agencies. As an initial step to help with this process, we recommend establishing the Ocean.IT office with a director and small administrative and technical staff (4-5 people). Within a year we expect that staffing levels will be brought up to the minimum expectation levels described in Table 4. In addition to increasing the visibility of the ocean sciences community as a major user of IT at existing HPC Centers, the office staff would start implementing solutions for the short-term needs identified on pages 52-54 and the long-term needs identified on pages 55-62. Together with the funding agencies and advisory board of ocean scientists, this five-to-six-person Ocean.IT office would develop a detailed plan for implementing the full Ocean.IT entity described in these recommendations. The immediate hardware needs might be best addressed by add-ons to HPC centers and the purchase of a few superclusters. The user support component may be best achieved initially by providing supplemental funding to research groups developing and maintaining candidate community models and software tools.
References


Acronyms

ASCI .......... Accelerated Strategic Computing Initiative
AVHRR ....... Advanced Very-High Resolution Radiometer
CCSM ........ Community Climate System Model
CLIVAR ...... Program on CLImate VARiability and predictability
CoOP ........ Coastal Ocean Processes
DAAC .......... NASA's Distributed Access Archive Centers
DoD .......... Department of Defense
DOE .......... Department of Energy
DNS .......... Direct Numerical Simulation
ECMWF ....... European Centre for Medium-Range Weather Forecasting
ENSO ........ El Niño-Southern Oscillation
GLOBEC ...... Global Ocean Ecosystems Dynamics
GODAE ...... Global Ocean Data Assimilation Experiment
GOES.......... Geosynchronous Operational Environmental Satellite(s)
HPC .......... High-Performance Computing
HPCMP ...... High Performance Computing Modernization Program
IRIS .......... The Incorporated Research Institutions for Seismology
JGOFS ...... Joint Global Ocean Flux Study
LES .......... Large Eddy Simulation
MODIS ...... MODerate resolution Imaging Spectroradiometer
MPI .......... Message-Passing Interface
MSRC .......... Major Shared Resource Center
NASA ......... National Aeronautics and Space Administration
NAVO .......... Naval Oceanographic Office
NCEP .......... National Center for Environmental Prediction
NCAR .......... National Center for Atmospheric Research
NODC .......... National Ocean Data Center
NOPP .......... National Oceanographic Partnership Program
NPACI ...... National Partnership for Advanced Computational Infrastructure
NRAC .......... National Resource Allocations Committee
NRL .......... Naval Research Laboratory
NSF .......... National Science Foundation
NUMA ....... Non-Uniform Memory Access
ODP .......... Ocean Drilling Program
OITI .......... Ocean Information Technology Infrastructure
ONR .......... Office of Naval Research
OpenMP .... Open Multi-Processing
PACI .......... Partnership for Advanced Computational Infrastructure
POP .......... Los Alamos Parallel Ocean Program
RIDGE ...... Ridge InterDisciplinary Global Experiments
SAR .......... Synthetic Aperture Radar
SMP .......... Symmetric Multi-Processing
SST .......... Sea surface temperature
TAO .......... Tropical Atmosphere Ocean project
TOGA ........ Tropical Ocean Global Atmosphere project
UCAR .......... University Corporation for Atmospheric Research
UNOLS ...... University-National Oceanographic Laboratory System
VODHub .... Virtual Ocean Data Hub
WOCE ....... World Ocean Circulation Experiment
Appendix 1

Meeting Chronology

January 5–7, 2000
National Science Foundation, Arlington, Virginia

The committee reviewed their charge and terms of reference, discussed OITI objectives, and
determined the preliminary organizational plan for OITI effort, including: 1) assessing commu-
nity needs, 2) assessing the science payoff, 3) addressing short- and long-term needs, 4) work-
ing groups, 5) surveys, 6) town meetings, 7) web pages, 8) e-mail contact point and mail groups.
This meeting also included presentations by people with experience at large computing centers
such as NCAR, PACI and the Navy.

April 20–21, 2000
University Inn, Seattle, Washington

The OITI committee (1) reviewed the community input and state of the “Ocean Information
Infrastructure,” (2) drafted an interim strategy and (3) determined and assigned necessary ac-
tions for the full report. Presentations were made from a National Academy panel and from the
data processing community.

September 11–13, 2000
Hyatt Rosemont, Rosemont, Illinois

At this meeting the committee began to review and edit pieces of the front end of the draft
report, and assessed what additional information was necessary. The committee began crafting
the recommendation section, considering the views expressed in the community survey.

January 11–12, 2001
Airlie House, Warrenton, Virginia

The committee reviewed and completed writing assignments for the draft report, and identified
all additional materials required to ready the report for community review.
Appendix 2

Community Survey

OITI Survey on Infrastructure Needs in Ocean Information and Technology (SINOIT)

A. Professional Information
1. Your highest degree (BS, MS, PhD)
2. Institution (Academic / Research lab / Industry / Government)
3. Discipline (Physical Oceanography, Biological Oceanography, Marine Chemistry, Marine Geology, Marine Meteorology, Interdisciplinary)
4. If you are responding for a group (e.g., research group or department), please identify the approximate number of group members in each of the following categories:
   - Ph.D. faculty (academic)
   - Ph.D. faculty (research)
   - Ph.D. staff
   - MS staff
   - Postdocs
   - Graduate students
   - Undergraduate students

B. Current ITI Resource Utilization
1. What ITI resources are you using for your current projects?
   a) Computational (monthly usage, hours)

<table>
<thead>
<tr>
<th>ITI Resource</th>
<th>O(100)</th>
<th>O(1K)</th>
<th>O(10K)</th>
<th>O(100K)</th>
<th>O(1M)</th>
<th>O(10M)</th>
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<tr>
<td>PCs/workstations</td>
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<td>supercomputer (serial)</td>
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<td>supercomputer (parallel)</td>
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<td>PC/workstation cluster</td>
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<td>Other (pls specify)</td>
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</table>

b) Total memory (MB):
   10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)
c) Dataset archival (monthly production, GB):
   1 / 10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)
d) Data transferred over Internet (monthly, GB):
   1 / 10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)
e) Are these ITI resources adequate to conduct your current research in an optimal manner? If not, which are not sufficient, and why not?
C. Current Scope of Work

1. Briefly describe the types of research problems on which you are working (e.g., eddy-resolving global ocean modeling, coupled physical/biological models, real-time state estimation, dataset analysis/visualization, etc.)

2. Do your projects involve real-time infrastructure needs (e.g., real-time access to and/or transfer of remote datasets, etc.)? If so, please describe these needs briefly.

3. What types of models/analyses do you utilize:
   a) dynamical models:
      diagnostic / QG / PE / reduced gravity / other (pls specify)
   b) spatial coverage:
      1D / 2D / 3D / regional / global
   c) temporal duration:
      days / months / years / decades / centuries and longer
   d) coupled components:
      biology (NPZ, etc.), geochemistry, atmosphere, sea ice, etc.
   e) advanced analysis tools:
      feature recognition, 3D visualization, statistical analysis, other (pls specify)

4. Do your activities involve the processing of large data sets? If so, please briefly describe the types of data, the processing involved, and the infrastructure required.

D. Future ITI Resource Utilization

1. What ITI resources would you require to conduct your future research in an efficient manner (5-10 years)?
   a) Computational (monthly usage, hours)

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<th>O(100)</th>
<th>O(1K)</th>
<th>O(10K)</th>
<th>O(100K)</th>
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<td>(1 cpu = 750 hrs/mo)</td>
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<td>supercomputer (serial)</td>
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<td>supercomputer (parallel)</td>
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<td>PC/workstation cluster</td>
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<td>Other (pls specify)</td>
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</table>

b) Total memory (MB):
   10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)

c) Data set archival (monthly production, GB):
   1 / 10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)

d) Data transferred over Internet (monthly, GB):
   1 / 10 / 100 / 1K / 10K / 100K / 1M / 10M / other (pls specify)
e) What human resources, in addition to those already available to you, would be required to use these resources efficiently (programmers, postdocs, computer specialists, consultants, etc.)?

f) What new software tools would be required (e.g., numerical algorithms, visualization software, parallelization tools, etc.)?

g) What ITI-intensive research issues would you tackle, that you cannot do now, if additional resources were available? Please describe the likely benefits to this research of enhanced ITI resources.

h) Which ITI-intensive research questions do you think the ocean science community as a whole ought to tackle over the next few years?

E. **Hub Functionality**

1. How important to your research would the following functionalities be if offered by the “Hub” (i.e., how much would you use them?):

<table>
<thead>
<tr>
<th></th>
<th>Crucial</th>
<th>Useful</th>
<th>Unnecessary</th>
<th>Don’t know</th>
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<tbody>
<tr>
<td>a) Community models</td>
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<td>i) code/documentation</td>
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<td>ii) online tutorials (how to use/apply the models)</td>
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<tr>
<td>iii) support staff</td>
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<tr>
<td>b) Archival datasets</td>
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<tr>
<td>i) numerical model outputs</td>
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<tr>
<td>ii) reference datasets</td>
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<tr>
<td>- climatologies</td>
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<td>- topographies</td>
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<td>- surface forcing</td>
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<td>- other (pls specify)</td>
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<tr>
<td>iii) other QC’ed datasets</td>
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<td>- WOCE synthesis fields</td>
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<td>- satellite gridded data</td>
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<td>- other (pls specify)</td>
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<tr>
<td>c) Hardware</td>
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<tr>
<td>i) computational engines</td>
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<tr>
<td>ii) mass storage</td>
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<tr>
<td>iii) visualization/analysis</td>
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<tr>
<td>d) Analysis/Visualization software</td>
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<tr>
<td>e) Outreach</td>
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<tr>
<td>i) onsite classes (at one of the Hub centers)</td>
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<tr>
<td>ii) classes at your institution</td>
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<tr>
<td>iii) development of ocean science curricula</td>
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</table>
F. Hub Management and Outreach

1. How would you like to see the “Hub” managed? In what type of institutional setting or settings should it be located? What type(s) of personnel and/or facilities should be associated with the “Hub”?

2. Which of these functionalities do you think are best delivered in a “centralized” facility? How should the ITI resources be distributed (centrally, distributed, mixed)?

3. What lessons can be learned from the distribution and management of current ITI resources?

4. What benefits to the public at large could be achieved with enhanced ITI resources (e.g., general awareness, education, etc.)?

5. Are there functionalities not listed above which you feel should be offered by the “Hub”? 
Community Survey: Extended Description

• Current ITI Utilization. Most respondents use a combination of computational platforms to carry out their research. Nearly all use a PC or workstation for some fraction of their computational work. Use of supercomputers is evenly split between serial and parallel architectures. Less than one sixth of the respondents indicated the use of PC/workstation clusters. Generally speaking, such platforms serve less computationally intensive needs (order 100-1K CPU hours of monthly usage), whereas the bulk of the larger applications (order 1K-100K CPU hours of monthly usage) are still the domain of supercomputers. The most common responses for memory usage was 1 GB, data set archival of 1 GB per month, and internet transfers of 1 GB per month.

Respondents who felt that current ITI is insufficient outnumbered those whose needs were being met by a margin of two to one. Of those whose work is limited by ITI resources, most indicated bottlenecks which fall into three categories:
- raw compute power (CPU plus memory capacity)
- data storage/archival
- network connectivity.

Of these three, the first two were cited more frequently than the latter by a four to one margin. Several respondents indicated frustration with the issue of raw compute power in particular, noting that their codes simply do not perform well on massively parallel architectures. Few investigators can justify the effort required to re-engineer their codes accordingly; one respondent expressed the sentiment that "life is too short to make my codes run on massively parallel machines."

• Current Scope of Work. The scope of respondents current research is tremendously diverse, including ocean circulation, climate, physical-biological-chemical interactions, seafloor geomorphology, ocean seismology, marine acoustics, sea ice, and surf zone processes. Spatial scales of interest span millimeters to global dimensions, and time scales from seconds to millennia. Computational domains range from estuaries to the global ocean. More than half of the respondents had immediate or near-term needs for real-time or near-real-time access to data. Nearly all respondents utilize large data sets. Advanced processing and visualization techniques are a necessity.

• Future ITI Resource Utilization. Respondents expect to continue to use multiple platforms in their research. Most anticipate the use of a PC/workstation for at least some fraction of their computational work. The most common response for expected monthly usage for this category was 10K CPU hours, as compared with 1K at the present time. Less than one sixth of the respondents expect to use serial architecture supercomputers in the future. Parallel supercomputers and PC/workstation clusters garnered a roughly equal proportion of responses; as in the current situation, massively parallel supercomputers are expected to be used for the most computationally intensive applications. The most common responses for anticipated needs for memory, data set archival, and Internet transfers all increased by factors of 10-1000.
from current usage (1 GB to 100 GB memory; 1 GB to 1 PB per month data archival; 1 GB to 10 GB per month data transfer).

Nearly all respondents foresee the need for additional human resources to accompany expansion in computational infrastructure. Programmers, postdocs and computer specialists were the most popular choices to fill such needs. A variety of new software needs are anticipated, yet two types were by far the most frequently mentioned: parallelization tools and visualization software.

If these additional ITI resources were to be provided, respondents anticipated wide-ranging scientific benefits.

- **Hub Functionality.** The community survey asked respondents to rate (as “Crucial,” “Useful,” “Unnecessary,” or “Don’t know”) various potential functionalities of the OITI “Hub.” Rankings were requested on sixteen specific capabilities, covering five resource areas (Community models, Archival datasets, Hardware, Analysis/visualization software, and Outreach). Table A3-1 summarizes the cumulative rankings obtained on this section of the survey.

By and large, capabilities in all resource areas except Outreach were endorsed by a majority of the respondents (average response above “Useful,” after excluding the “Don’t know” responses). By assigning arbitrary weights to the responses (two for Crucial, one for Useful, and zero for Unnecessary), we can obtain an approximate numerical ranking from which the following general statements can be made.

The only broad category of Hub functionality to receive an average endorsement nearest to “Crucial” (average > 1.50) is that of reference archival datasets. Climatologies, topographies (the highest ranked functionality), and surface forcing all were judged to be crucial to Hub capabilities. Of the other potential archival datasets: satellite gridded data was viewed as next most useful (1.45), while both numerical model output (1.18) and WOCE synthesis fields (1.07) were ranked significantly lower in this category of capability (though still as “Useful”).

As a category, the next most highly ranked resource area was that of Community models. All three specific functionalities under this general heading were regarded as Crucial by a significant proportion of the respondents, including Codes/documentation (ranked as crucial by 46%, average rating 1.41), online tutorials (36%, 1.31), and support staff (39%, 1.27).

There was general support, though of varying degree, for all the specific Hardware and Analysis/visualization software capabilities listed. In order of average ranking in these categories, “mass storage” emerged on top (1.44), followed by “analysis/visualization software” (1.33), “computational engines” (1.25) and finally “visualization hardware” (1.06). Note that the number of responses in the “Unnecessary” category is relatively high here, except for “analysis/visualization software.”

Finally, as remarked above, only the items in the Outreach category were rated on average to fall below “Useful.” This includes “onsite classes” (0.81), “classes at home institutions” (0.60) and “development of ocean science curricula” (0.87).
How important to your research would the following functionalities be if offered by the “Hub” (i.e., how much would you use them?):

<table>
<thead>
<tr>
<th>Functionalities</th>
<th>Crucial</th>
<th>Useful</th>
<th>Unnecessary</th>
<th>Don’t Know</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>a) Community models</strong></td>
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<tr>
<td>i) code/documentation</td>
<td>17</td>
<td>18</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>ii) online tutorials (how to use/apply the models)</td>
<td>13</td>
<td>21</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>iii) support staff</td>
<td>13</td>
<td>16</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td><strong>b) Archival datasets</strong></td>
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</tr>
<tr>
<td>i) numerical model outputs</td>
<td>9</td>
<td>21</td>
<td>3</td>
<td>5</td>
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<tr>
<td>ii) reference datasets</td>
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</tr>
<tr>
<td>• climatologies</td>
<td>20</td>
<td>8</td>
<td>3</td>
<td>4</td>
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<tr>
<td>• topographies</td>
<td>22</td>
<td>8</td>
<td>2</td>
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<td>• surface forcing</td>
<td>20</td>
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<td>• other (pls specify)</td>
<td>4</td>
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<tr>
<td>• WOCE synthesis fields</td>
<td>9</td>
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<tr>
<td>• satellite gridded data</td>
<td>17</td>
<td>11</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>• other (pls specify)</td>
<td>6</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>c) Hardware</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>i) computational engines</td>
<td>14</td>
<td>12</td>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>ii) mass storage</td>
<td>21</td>
<td>7</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>iii) visualization/analysis</td>
<td>9</td>
<td>15</td>
<td>7</td>
<td>3</td>
</tr>
<tr>
<td><strong>d) Analysis/Visualization software</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>12</td>
<td>2</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td><strong>e) Outreach</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>i) onsite classes (at one of the Hub centers)</td>
<td>5</td>
<td>16</td>
<td>11</td>
<td>5</td>
</tr>
<tr>
<td>ii) classes at your institution</td>
<td>4</td>
<td>18</td>
<td>12</td>
<td>3</td>
</tr>
<tr>
<td>iii) development of ocean science curricula</td>
<td>8</td>
<td>10</td>
<td>12</td>
<td>7</td>
</tr>
</tbody>
</table>

*Table A3-1*
• **Hub Management and Outreach.** The questions contained in this section of the survey addressed some of the most contentious issues, and solicited the most discursive answers. Not surprisingly, they are also the most difficult to synthesize in any complete or unified way. Nonetheless, several common themes among the responses emerge.

Taking the issue of centralization versus distributed facilities first (Question 2): a large majority of respondents endorsed a “mixed” distribution of facilities, with some capabilities resident at a “Hub” and the remainder distributed in some fashion over the participating “nodes.” Of its potential functions (see section E: Functionalities), it was suggested by many that the Hub serve as the home for only those clearly requiring a centralized facility. Examples noted by the respondents include: large-scale computing (> 1 Tflop/s) and datasets (>1PB), rapid data transfers, and technical support staff and training activities. Finally, most respondents recognized that economics and expertise issues favored an institutional setting with existing OITI capabilities and knowledge base.

The question on Hub management (Question 1) elicited a range of suggestions. Many responses gave examples of what they considered to be good “models” of management that might be copied by the Hub.

These included: the National Supercomputing Facility, UCAR (two responses), NCAR Scientific Computing Division, NAVO, the Arctic Region Supercomputing Center, and lastly UNOLS (4 responses). Several comments in favor of UNOLS-style resource management (block-funded; block awards for extended, intensive access to resources; etc.) were received. On the issue of Hub personnel, most who responded on this issue favored a minimalist approach to Hub staffing, for example, just sufficient personnel to oversee the local facilities and to provide dedicated service functions.

Question three was directed at “lessons” to be learned from current OITI practices. While not explicitly stated in this way, we hoped to get from the answers to this question some “complaints” about how these issues have been handled in the past. Among the common themes here were the issues of redundant software development, oversubscription and/or bottlenecks on currently available systems, and rapid response to changing hardware technology. Specific concerns included: redundant development of geoinformatic systems, and the inability of current OITI infrastructure to “track” innovative and evolving technologies (risk-taking). A few specific complaints about existing systems were directed at NCAR (oversubscribed, though well managed) and the DoD labs (restrictions regarding noncitizens and NAC procedures). The latter in particular led several respondents to recommend strongly that the Hub be housed in a nonclassified environment. A final issue that emerged explicitly in one response, and by implication in several others, is the issue of interoperability of datasets, services, models, etc. (the flip-side of redundant software development).

The responses to Question three (Education/Outreach) were highly diverse, with some respondents seeing a valuable opportunity for public outreach (though specific suggestions were also diverse), and others having little idea or an active disinterest. It is clear that the consensus in this area is least well developed of all issues surveyed.
Appendix 3

Survey of Computer Centers

A. Site Information
1. Institution Type: (e.g., Academic / Research lab / Industry / Government)
2. Percentage of computational workload on a fixed schedule: (fixed schedule is, for example, the same jobs every day)
3. Number of computer users?
   (a) Oceanographic disciplines:
   (b) Total (all disciplines):

B. Current Information Technology Infrastructure (ITI) Resources
1. Computer hardware: (machine type, number of processors, peak GFlops per processor, total memory in GB, total local disk in GB).
2. Data archive: (machine type, online disk capacity in GB, near-line type and storage capacity in TB, off-line type and storage capacity in TB).
3. Internal Network: (type, peak data throughput MB/s, actual average data traffic GB/day)
4. Internet access: (type, peak data throughput MB/s, actual average data traffic GB/day)
5. Staff levels: Please indicate the number of full time positions and the typical required level of knowledge/expertise in the following areas.
   (a) Management:
   (b) Systems and support:
   (c) Network administration:
   (d) User Services:
   (d) Discipline-specific specialists:
   (e) Other (please specify):
   What coverage (e.g., 24/7, normal working hours, etc.) is provided by this staffing level?
6. Approximately how many additional staff, and in what areas, would be required to support the addition of the following to your center?
   (a) A single 500-processor scalable system:
   (b) Two hundred new users:
7. What process do you use for allocating resources to projects?
8. What is the typical individual project resource allocation (e.g., processor hours), duration of allocation (e.g., per year), number of projects and percentage of your overall allocation in the following categories?
   (a) Large projects:
   (b) Medium projects:
   (c) Small projects:
9. What are the maximum individual job limits (processors, processor hours, memory, etc.), on your largest computational system, in each of the following categories? What percentage of the overall system workload is in each category?
   (a) High priority large jobs:
   (b) High priority medium jobs:
   (c) High priority small jobs:
   (d) Std. priority large jobs:
   (e) Std. priority medium jobs:
   (f) Std. priority small jobs:
   (g) Low priority large jobs:
   (h) Low priority medium jobs:
   (i) Low priority small jobs:
10. What percentage of your total computational workload uses the following approaches to scalability?
    (a) None (single processor):
    (b) Shared memory (e.g. OpenMP):
(c) Message passing (e.g. MPI):
(d) Remote memory (e.g. SHMEM):
(e) Dual-level (e.g. OpenMP+MPI):
(f) Other (please specify):

11. Percentage of overall usage from oceanography?
   (a) Computation:
   (b) Data Archive:
   (c) Internet Access:
   (d) User Services:
   (e) Discipline-specific specialists:

C. Future ITI Resources

1. How much more capability do you expect to have in 5 years (e.g., two times present, ten times present, etc.) in the following areas?
   (a) Computation:
   (b) Memory per machine:
   (c) Local disk per machine:
   (d) Data archive online capacity:
   (e) Data archive nearline capacity:
   (f) Data archive offline capacity:
   (g) Internal network throughput:
   (h) Internet throughput:

2. How much more capability do you expect to have in 10 years (e.g., two times present, ten times present, etc.) in the following areas?
   (a) Computation:
   (b) Memory per machine:
   (c) Local disk per machine:
   (d) Data archive online capacity:
   (e) Data archive nearline capacity:
   (f) Data archive offline capacity:
   (g) Internal network throughput:
   (h) Internet throughput:

3. What kind of machine architecture do you expect to provide the majority of your compute cycles in (a) 5 years and (b) 10 years?

4. What emerging hardware, software or networking trends do you expect to impact how your center works in (a) 5 years and (b) 10 years?

5. As hardware and software evolve, what are some of the major challenges that you anticipate (a) new users and (b) experienced users will encounter in trying to use your center in the future?

6. Over the next few years, do you anticipate any change in the level or type of help/consulting/training services that you supply to your users?

7. Do you anticipate dramatic growth in the computational activities of any particular segments of your user community over the next few years? If so, in which areas?

8. To what extent can the capability of a large computer center be replaced by a geographically distributed network of computer sites over the next 5-10 years?

9. What are the costs and benefits of centralized vs geographically distributed computer environments over the next 5-10 years?

10. What are the advantages and disadvantages of collocating all or part of a computational capability dedicated to oceanography at an existing computer center?
<table>
<thead>
<tr>
<th>Primary Hardware</th>
<th>Academic Centers</th>
<th>University</th>
</tr>
</thead>
<tbody>
<tr>
<td>Machine</td>
<td>NCSA</td>
<td>SDSC</td>
</tr>
<tr>
<td># processors</td>
<td>SGI Origin</td>
<td>IBM SP</td>
</tr>
<tr>
<td>Peak Speed (Gflops/processor)</td>
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<td>1.5</td>
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<tr>
<td>Memory (Gbytes)</td>
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<td>Local Disk (Gbytes)</td>
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<td>On-line Disk (Gbytes)</td>
<td>2,000</td>
<td>3,000</td>
</tr>
<tr>
<td>Near-line Disk (Tbytes)</td>
<td>60</td>
<td>500</td>
</tr>
<tr>
<td>Internal Network Speed (Mbyte/s)</td>
<td>125 peak</td>
<td>100 peak</td>
</tr>
<tr>
<td>Internet Access (Mbyte/s)</td>
<td>80 peak</td>
<td>3-80 peak</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Secondary Hardware</th>
<th>Government Labs</th>
<th>Operational Centers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Machine</td>
<td>NERSC</td>
<td>LANL</td>
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<tr>
<td># processors</td>
<td>IBM SP</td>
<td>SGI Origin</td>
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<td>Peak Speed (Gflops/processor)</td>
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<td>2,048</td>
</tr>
<tr>
<td>Memory (Gbytes)</td>
<td>1,200</td>
<td>512</td>
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<tr>
<td>Local Disk (Gbytes)</td>
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<td>On-line Disk (Gbytes)</td>
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<td>Near-line Disk (Tbytes)</td>
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</tr>
<tr>
<td>Internal Network Speed (Mbyte/s)</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Internet Access (Mbyte/s)</td>
<td>40 peak</td>
<td>N/A</td>
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<table>
<thead>
<tr>
<th>Machine</th>
<th>Cray T3E-900</th>
<th>Compaq SC</th>
<th>Compaq SC</th>
<th>C90</th>
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<tbody>
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<td>2.5 Tflops</td>
<td>256</td>
<td>8</td>
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<td>Peak Speed (Gflops/processor)</td>
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<td>Memory (Gbytes)</td>
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<td>600</td>
<td>128</td>
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<tr>
<td>Local/Near-line Disk (Gbytes)</td>
<td>1,500</td>
<td>10,000</td>
<td>4,500</td>
<td>100</td>
</tr>
</tbody>
</table>

Notes:
- Centers not in survey