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BIOGEOCHEMISTRY AND PARTICULATE DYNAMICS

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# **INTEGRATED MODELING OF THE SOUTHERN CALIFORNIA COASTAL OCEAN: BIOGEOCHEMISTRY AND PARTICULATE DYNAMICS**

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## **INTRODUCTION**

The Southern California Coastal Ocean (SCCO), defined as the region inclusive of the Southern California Bight and the Santa Barbara Channel, from the shoreline to beyond the continental shelf, has significant anthropogenic injections of many materials through the air, rivers, runoff, outfalls, sediments, and marine spills. These inputs are superposed on a dynamic system of internal processes including water motions, biological production in the surface layers, particle sinking, dissolution, and scavenging. In spite of lengthy and continuing sequences of SCCO measurements at various scales, a synthehtical understanding and an ability to make skillful predictions and comprehensive assessments of the fate and transport of these materials in the SCCO remains illusive. In many cases the interpretation of localized measurements lacks a regional context. Conversely, there is little information on the regional impacts of localized sources. It is clear that an integrated computational model of the most relevant processes is needed before these goals can be achieved. An integrated model will be of great value to environmental managers responsible for sewage discharges, storm water discharges, and coastal fisheries. The overall project objective is to develop, test, and use for practical purposes an integrated computational model of the physical, chemical, and biological processes relevant to the distributions of natural and anthropogenically injected materials in the Southern California.

## **MODEL DEVELOPMENT**

During the past four years we have developed a new model, called the Regional Ocean Modeling System (ROMS). ROMS represents an evolution from the family of terrain-following, vertical-coordinate models---specifically from SCRUM (Song & Haidvogel, 1994)---developed by scientists at Rutgers University, with whom we are also coordinating the ROMS development. ROMS, like SCRUM, is a conservative, finite-volume discretization of the hydrostatic primitive equations in 3D curvilinear, boundary-following coordinates with a variable free surface and a realistic equation of state. Several developments have been required to efficiently, accurately, and robustly calculate the equilibrium west-coast circulation at high spatial resolution and to include various biogeochemical processes.

### **Computer Engineering**

The original SCRUM code was designed to run on workstations (hence restricted to small domains, coarse resolution, and/or short intervals) and on vector supercomputers. However, many current and most future supercomputing power will be on clustered or massively parallel multiprocessor machines with from 4 to 128 or more processors, and we have made ROMS

capable of utilizing these computers efficiently. The currently most useful target supercomputers have a shared-memory architecture (e.g., SGI/Cray, Sun, HP). The primary engineering challenges here are (1) optimization of the code for the caches (local fast memory) and (2) scalable parallelization multiple processors. We use 2D partitioning of the grid into subdomains assigned to different processors. We assign multiple subdomains to each processor so the data blocks fit into the secondary cache; e.g. in going to a larger problem, it can be advantageous to increase the number of subdomains (hence subdomains per processor) rather than increase the size of the same subdomains. In addition to subdomain blocking, we introduce a zig-zag cycling sequence for the subdomains assigned to a processor: the processor goes from its first subdomain to its last, until reaching a synchronization point, then the direction of cycling is reversed. After synchronization the processor always proceeds with data already loaded into its cache, thus eliminating some cache misses; this measure reduces the probability of mutual cache-line invalidation events. Originally the new code was designed for SGI Power Challenge and SGI/Cray Origin2000 computers, and recently it was ported to Sun Enterprise. It is presently being used efficiently on from 4 to 64 processors by several groups. To allow even larger computations on future clusters of shared-memory, multi-processor computers (e.g., IBM), a two-level parallelization is now being developed that uses multi-threaded and message-passing paradigms together.

#### Physical Transport Parametrizations

Oceanic material transports by small-scale eddies remain nearly within isopycnal surfaces except in boundary layers, and small-scale parameterizations that represent this constraint yield substantial benefits (Gent & McWilliams, 1990; Danabasoglu et al., 1994). It is especially challenging to limit spurious cross-isopycnal diffusion with a terrain-following vertical coordinate, as in ROMS, since the intersection angle between coordinate and isopycnal surfaces is generally larger than with a level-coordinate model. We have improved this behavior in ROMS with a variable-stencil, isopycnal-transport scheme that dynamically aligns its stencil with the isopycnal surfaces and reduces the reach of the stencil in the cross-isopycnal direction (Shchepetkin & McWilliams, 2000a).

The atmospheric responses and biological coupling require skillfully parameterized vertical mixing in the interior and Planetary Boundary Layers (PBL). We have implemented a non-local, K-profile PBL scheme in combination with (small) interior diapycnal mixing rates due to internal waves, Kelvin-Helmholtz instability, and double diffusion (Large et al., 1994) that performs well in both data comparisons and large-domain model solutions (Large et al., 1997; Li et al., 2000), adapted to the C-grid structure of ROMS.

#### Numerical Algorithms

Once a grid resolution passes a certain threshold with viscosity decreased accordingly, the simulated flow becomes turbulent. Extensive experience of computational fluid dynamics for turbulent flows is that conventional, second-order, discretized advection schemes are not the optimal choice (weighing accuracy against computational cost) in comparison with higher-order schemes. In ROMS we have redesigned the advection operator to reduce dispersive errors and the consequently excessive dissipation rates, thereby effectively boosting the resolution on a given grid and achieving both more energetic eddy variability and reduced dependence on the grid size (Shchepetkin & McWilliams, 1998).

The vertical discretization of all physical processes in ROMS (advection, diffusion, and baroclinic pressure-gradient force) now uses local parabolic splines, limited by a density

monotonicity constraint, in a finite-volume discretization (Shchepetkin & McWilliams, 2000a,b). This approach reduces the dispersion of the vertical advection and diffusion schemes, yielding smaller numerical diffusion in the vertical (cross-isopycnal) direction. It also ameliorates the problem of loss of accuracy in the case of highly stretched, surface-concentrated grids since now all vertical profiles are treated as continuous analytical functions; this is very important for resolving rapidly changing PBL mixing and biogeochemical processes near the surface. We have implemented a hybrid vertical coordinate, which smoothly changes from terrain-following near the bottom to geopotential near the surface; this both maintains a controlled grid spacing in both PBLs, and it diminishes discretization errors in the historically problematic pressure-gradient force for terrain-following coordinates (Haney, 1991) by reducing the angle of intersection between isopycnal and coordinate surfaces in the upper ocean where the stratification is strongest.

The time-stepping scheme in ROMS allows a substantial increase in the permissible time-step size (Shchepetkin & McWilliams, 2000a). First, as is often done (e.g., Killworth et al., 1991), we time-split the rapidly evolving barotropic-velocity and free-surface fields from the slower baroclinic/tracer ones. But we do so using optimal time filter with mass and tracer fluxes that guarantee exact volume-conservation and constancy-preservation, thus removing previous restrictions of small free-surface changes, relative to the total depth, and small barotropic velocities. Second, we use a predictor-corrector time step such that once the velocity is computed for the new time step, it is immediately used for the computation of tracers, and vice versa. This scheme closely couples the fields and suppresses computational modes. The expanded regime of stability allows the larger time step.

### Open Boundary Conditions

ROMS has been improved beyond SCRUM (and most other regional models) in its treatment of open boundary conditions (Marchesiello et al., 2000a). A first requirement is that internally generated fluctuations can radiate out of the domain. We have built a radiation boundary scheme which estimates a two-component, horizontal phase velocity near the open boundaries (Raymond & Kuo, 1984; Barnier et al., 1998). However, unlike in other prototypes, we discretize both normal and tangential propagation in an upstream-biased fashion, where the normal component is treated implicitly. This scheme escapes usual time-step restrictions by large phase speeds and small-scale noise, hence it allows large time steps without loss of stability. No enhanced dissipation is needed near the boundary ("sponge layers") to maintain numerical stability. A second requirement is that external influences from remotely forced events and larger-scale flows must be conveyed through the open boundary. These influences are implemented with nudging bands along the open boundaries, where all tracer fields (including sea level) are relaxed toward specified smooth data, and a volume-conservation equation governs the mean sea level. We use an adaptive algorithm where inward and outward information fluxes (determined by the propagation algorithm) are treated separately, with much stronger nudging rates on inward fluxes. This scheme yields regional solutions, with stable statistical equilibria over many years and without evident near-boundary distortions, for both the California and Agulhas Currents (Marchesiello et al., 2000b; Penven et al., 2001).

### Ecosystem and Particle Dynamics

ROMS is intended to be a multi-purpose, multi-disciplinary ocean modeling tool. One aspect of this is biogeochemical cycling and ecosystem modeling. In a collaboration with John Moisan (NASA Wallops Island), we have incorporated a Nutrient-Phytoplankton-Zooplankton

(NPZ) model into ROMS. It is broadly similar to that of Fasham et al. (1990), adapted for the generally eutrophic California coastal region and our particular interests in particulates and comparisons with satellite ocean color measurements. It presently consists of seven biological tracers: nitrate, ammonia, phytoplankton, chlorophyll A, zooplankton, and small and large detritus. They are advected and mixed by the model transport schemes, undergo additional vertical migrations either by particle sinking or specified behavioral motions, and interact with each other biochemically. Particle dynamics are represented by an algorithm we developed for ROMS that is based on the concept that most vertical loss of mass by settling is by the sinking of large detrital particles, the rate of formation of which is a second order function of the concentration of small particles, including small detritus and phytoplankton (Jackson, 1990). ROMS is particularly suitable for such a physical-biological coupling model because of its advective fidelity, its KPP surface PBL parameterization, and its tolerance for highly stretched vertical grids (due to the vertical-spline discretization). Also, the modularity of the ROMS code allows us to configure different biogeochemical model types and investigate their behavior comparatively; for example, we are currently implementing the model of Chai et al. (1999) with multiple N, P, and Z components and a more explicit link to carbon cycling.

## **MODEL APPLICATION TO THE EQUILIBRIUM U.S. WEST COAST CIRCULATION AND PLANKTONIC ECOSYSTEM**

Our primary application of ROMS to date has been to simulate the equilibrium coastal circulation and ecosystem along the entire U. S. west coast under mean-seasonal physical forcing with nudging to mean-seasonal tracer distributions (including nitrate as the driving nutrient for the ecosystem) at the open boundaries. The domain extends in latitude from the middle of Baja California (~28N) to the Canadian Border (~48N) and about 800 km offshore, to encompass the California Current System and its regions of most energetic eddy variability well away from the open boundaries. The focus in this formulation is on the regional equilibrium dynamics intrinsic variability (mostly meso-scale) in the absence of added forced variability by synoptic and inter-annual atmospheric fluctuations. In Marchesiello et al. (2000b), we explore the latter at horizontal grid resolutions ranging from 20 km to 5 km, at the finer end of which the eddy field is approximately as vigorous in its upwelling filaments (Fig. 1) as observed. Previous circulation modeling studies (e.g., Auad et al., 1991; McCreary et al., 1991; Haidvogel et al., 1991; Batteen, 1997) are less extensive in their spatial and temporal breadth and/or less fine in their resolution, and they contain less comprehensive circulation influences and simpler transport parameterizations.

The solutions show strong seasonal variability. After a spin-up period of several years, the surface kinetic energy oscillates quasi-periodically around an equilibrium value, peaking in summer and fall, as observed with drifters and altimetry (Kelly et al., 1998). The coherent evolution of the seasonal-mean flow is conducted by the seasonal winds plus westward propagation of Rossby waves, again as observed (Lynn & Simpson, 1990; Strub & James, 1998; Hickey, 1998). A southward coastal current is generated in spring in association with upwelling fronts. This current gets stronger and moves offshore in summer. By fall, it is hundreds of kilometers offshore as the California Current. The pattern of wind forcing also moves offshore, which results in cyclonic vorticities and poleward inshore currents. South of Cape Mendocino, these currents are weak, opposite to the wind direction and spatially continuous only during fall, as long as enough vorticity is provided. North of Cape Mendocino along the coast of Oregon and Washington, a stronger, more spatially continuous poleward Davidson Current appears as the Aleutian Low moves southward. Below the surface is a continuous northward undercurrent,

as observed by Pierce et al., (2000), and its meso-scale variability is dominated by sub-surface, anti-cyclonic vortices. The intrinsic meso-scale variability in SST resembles satellite images (Strub et al., 1991), in particular with respect to cold filaments (Fig. 1). The meso-scale variability is spatially and temporally organized by the seasonal wind. In spring, frontal instabilities appear along the newly formed coastal current and roll up into vortices. Most filaments occur in summer associated with strong squirts with speeds of 1 m/s, forming hammerhead circulation at multiple scales, especially south of Cape Blanco. In fall, meanders and eddies are the dominant features, inshore and offshore of the California Current. In winter, the offshore eddy field is strongest. The eddies are most intense around capes in the zone of strong summer winds, viz., Cape Blanco, Cape Mendocino, Point Arena, Point Reyes. These are maximum variance locations in the solutions, as in drifters and altimetry (Strub & James, 1998; Kelly et al., 1998; Swenson & Niiler, 1996). The narrow temperature minima of cold filaments are generally found inshore of strong southward jets, which confirms the suggestion in Strub et al. (1991) that the cold filaments are related to in situ upwelling within the jets. They show a tight relationship with the PBL depth and the associated vertical mixing intensity, whose evident patchiness adds appreciably to biological meso-scale variability. In the Southern California Bight, the site of our proposed studies, there are a seasonally varying anticyclonic circulation and abundant island- and headland-shed eddies (Fig. 3), consistent with observations (Hickey, 1992).

As might be expected from the strong physical control of biological distributions in the California Current System (Denman & Abbot, 1994), instantaneous phytoplankton distributions show upwelling filamentary structures very much like sea surface temperature (Fig. 1), as also observed from satellite color measurements. This process is the principal determinant of the climatological phytoplankton abundance in the coastal region. With this module we have been able to simulate the average surface chlorophyll distributions in reasonable approximation to the observations (Figs. 2 and 3) (Stolzenbach et al., 2002).

We have adapted for ROMS the multi-level, fully coupled, embedded-gridding scheme of Blayo and Debreu (1999) to achieve finer horizontal resolution in local nearshore sub-domains without losing the regional or basin-scale influences simulated in the outer domain. Prototype simulations using this technique (with 1-way interaction, from the outer-domain solution to the inner ones) exist in the two configurations that will be the focus of the proposed collaborative studies: the central upwelling region between Pt. Reyes and Pt. Conception (with two grid-resolution levels *pro tem* at 15 and 5 km) and the Southern California Bight (with three levels at 18, 6, and 2 km). Fig. 4 illustrates the spatial fine-structure that arises on the inner-most grid as a result of the island wakes (Catalina) and current filaments detaching from headlands (Pt. Dume) within the Southern California Bight. The occurrence of anomalous chlorophyll concentrations trapped in the eddy centers and swept in filaments around their peripheries shows their significance for material and biological transport.

Several other simulation capabilities have been developed in ROMS but have not yet been fully configured and tested in the west coast simulations. These include 2-way interactive grid embedding, tidal forcing, sediment transport, and several biological modules including alternative NPZD ecosystems and so-called Individual-Based Models (Batchelder et al., 2002).

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Swenson, M.S., & P. P. Niiler, 1996: Statistical analysis of the surface circulation of the California Current. *J. Geophys. Res.* 101, 22631-22645.

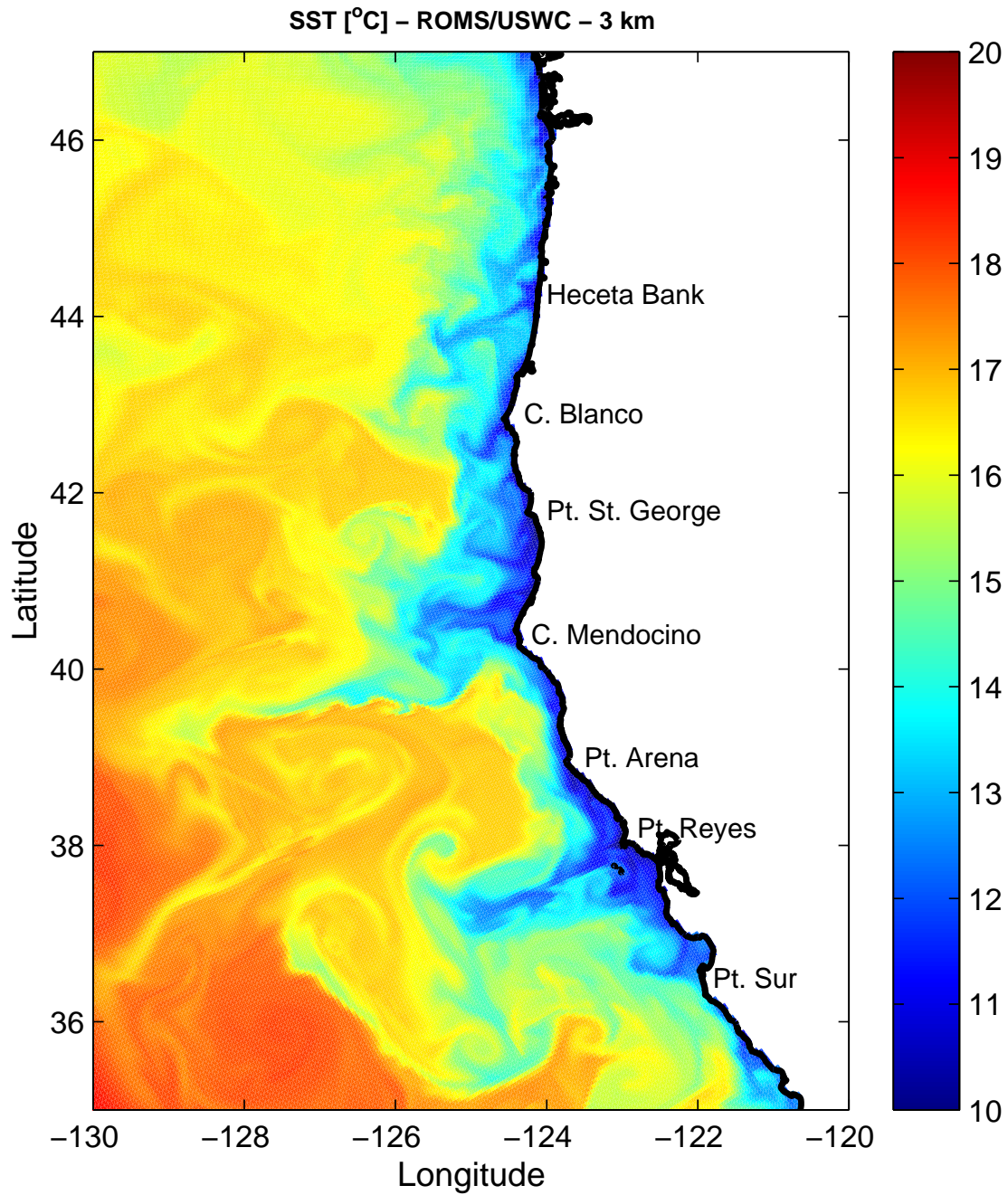


Figure 1: Instantaneous plot of ROMS simulated sea-surface temperature in summertime along the central and northern California and Oregon coasts. (Marchesiello et al., 2002.)

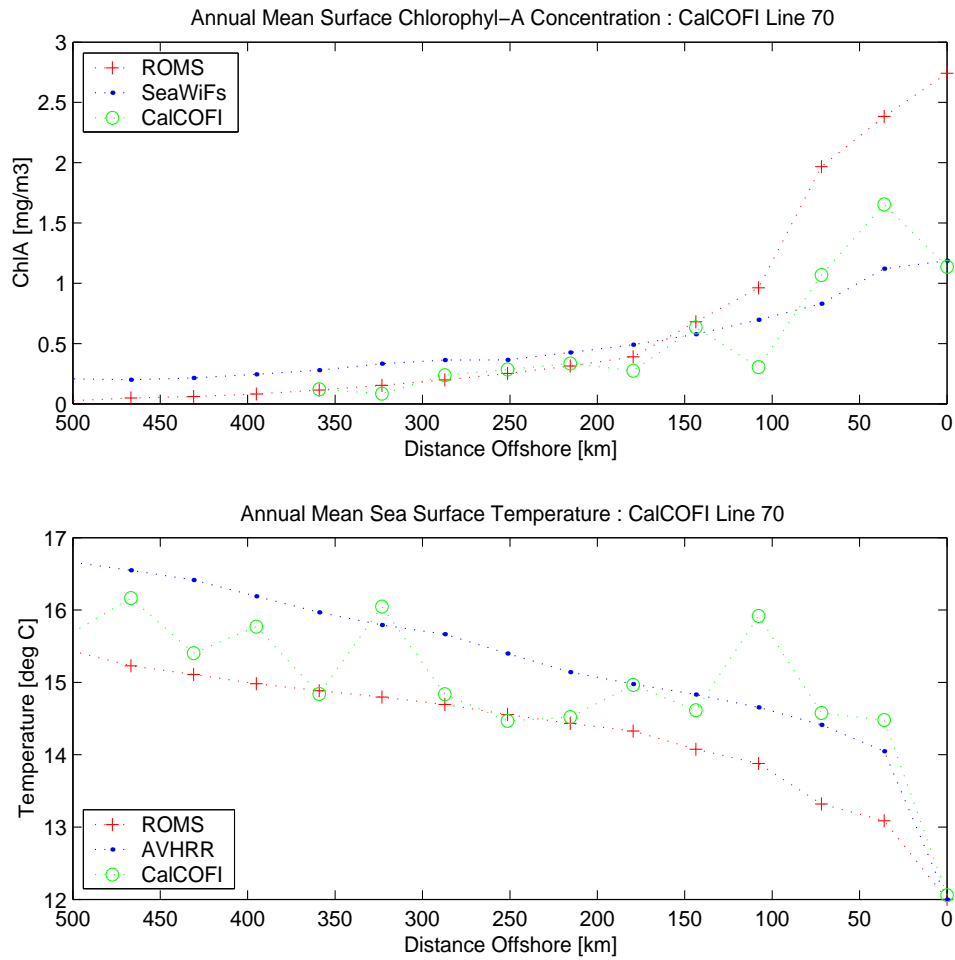
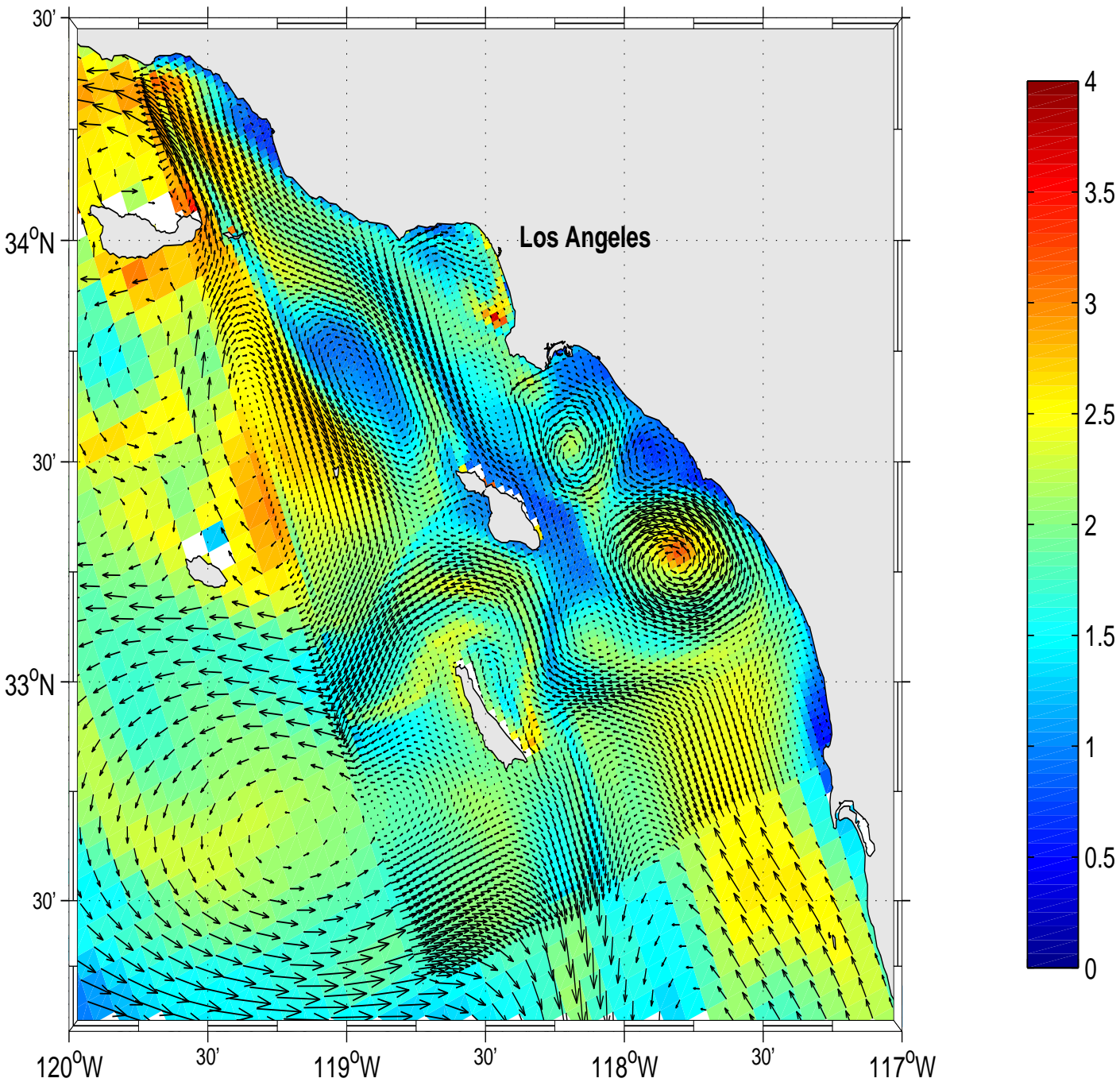


Figure 2: Annual-mean surface values of chlorophyll A (top) and Sea Surface Temperature (bottom) along CalCOFI Line 70 along the U.S. West Coast. In each panel are model, in situ, and satellite results. (Stolzenbach et al., 2002.)



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Figure 3: Southern California Bight surface currents and chlorophyll in the neighborhood of the innermost embedded subdomain in a 3-level simulation (i.e., with horizontal resolutions of 18, 6, and 2 km). Note the clean transition of flow and material concentration across the between the innermost and intermediate grids. Also note the strong influences of island and coastline topography around Santa Monica Bay and the Chlorophyll anomalies associated with the mesoscale eddies.

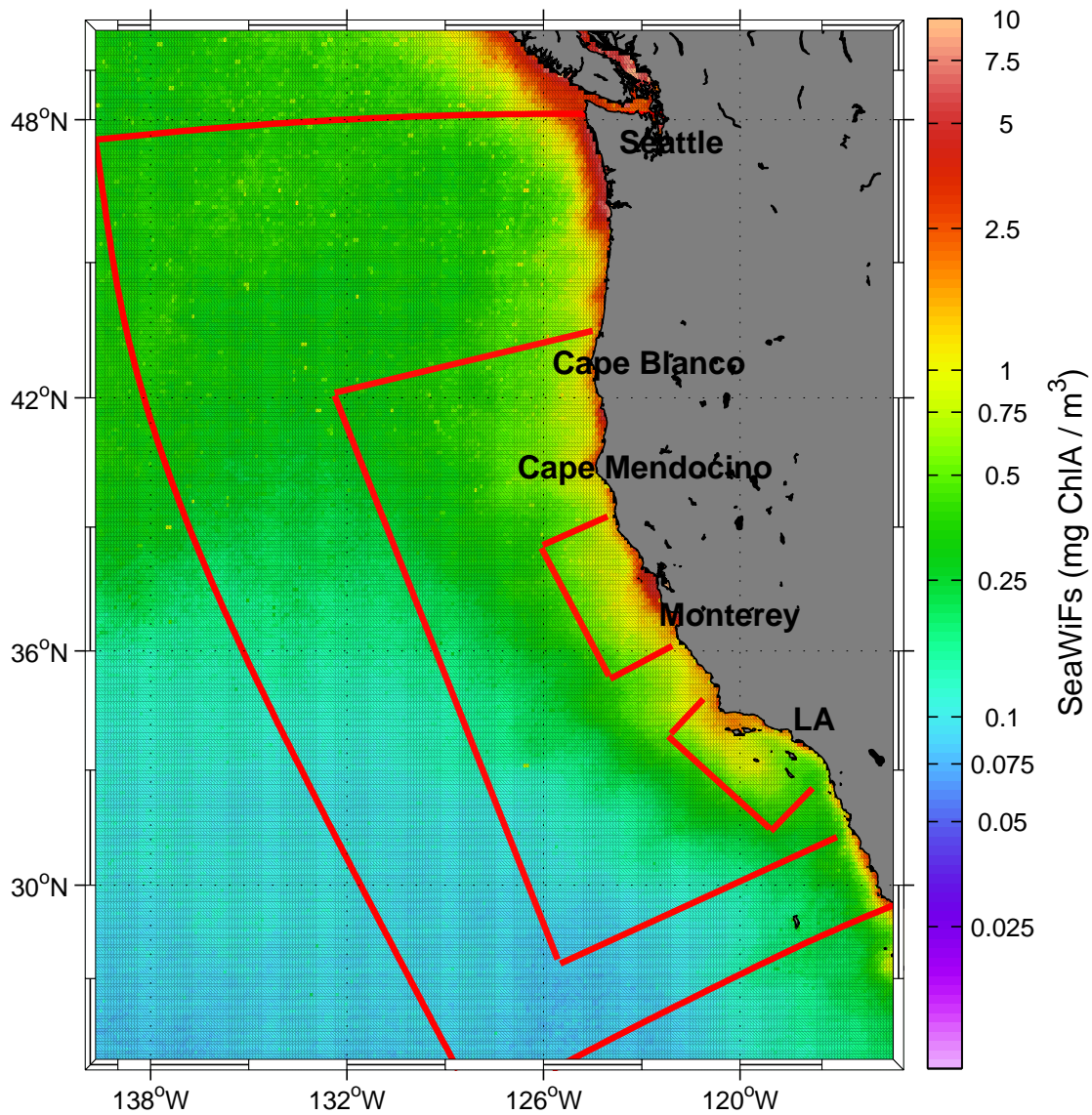


Figure 4: Approximate boundaries of the model domains for the standard configuration with 3-level embedding, superimposed on the time-mean surface chlorophyll distribution measured from SeaWiFS. The coarser grid has its horizontal resolution at 15 km, the medium grid at 5 km, and the two finer grids—Central California Coast and Southern California Bight—at 1.7 km each.