Simulating Large-scale Complex Geophysical Flows on Massively Parallel High-performance Computing Platforms

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Many of the challenges that society faces at present, including global climate change, environmental degradation, and natural and human-induced disasters, require powerful simulation tools that utilize very high spatial resolution. To achieve this lofty goal, a three-pronged approach is needed to advance computational algorithms, software engineering, and high-performance computing architecture.

Over the last decade, we have been developing sophisticated models that build upon advancements in all of these areas. The result is a next-generation geophysical fluid dynamics model called SELFE (Semi-implicit Eulerian-Lagrangian Finite Elements) [1]. SELFE is an open-source community-supported modelling system, based on unstructured grids in the horizontal dimension and hybrid terrain-following S-Z coordinates in the vertical, designed for effective simulation of 3D baroclinic circulation across river-to-ocean scales. It employs a semi-implicit finite-element method together with an Eulerian-Lagrangian method (ELM) to solve the Navier-Stokes equations (in either hydrostatic or non-hydrostatic form). As a result, numerical stability is greatly enhanced and errors from the "mode splitting" method are avoided. The model also incorporates wetting and drying in a natural way, and has been rigorously benchmarked for inundation problems [2][3].

With a world-wide user base, SELFE has been demonstrated to be accurate, efficient, robust, and flexible. It has been certified by the U.S. National Tsunami Hazard Mitigation Program (NTHMP) and officially endorsed by three state agencies in the U.S. and four government agencies in Europe.
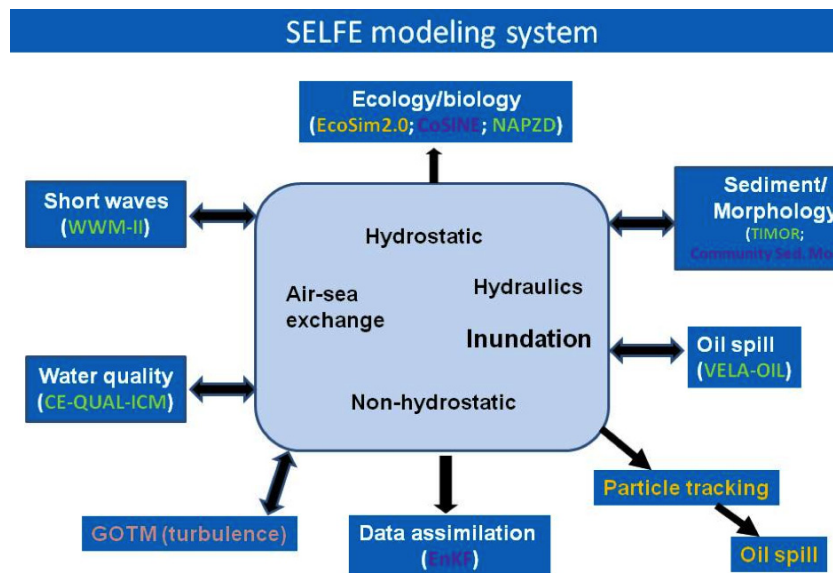
Figure 1: *SELFE modelling system as of Nov. 19, 2012.*

In collaboration with external users, we have also built a comprehensive modelling system around SELFE (Fig. 1), which now incorporates a wide range of physical processes. Key components include:

- A community-developed wind-wave model (WWM-II) which couples waves to currents [4].
- A water quality module (CE-QUAL-ICM) originally developed by Harry Wang's group at VIMS.
- Two ecological modeling packages (EcoSim 2.0 and CoSINE [5][6]) for simulating biological materials and processes in the water column.
- A sediment module which is adapted from earlier work by Courtney Harris and her colleagues [7].
- A comprehensive oil spill module which incorporates surface slicks, mixing in the water column, coastal deposition, and weathering [8].
- A flexible particle tracking module which can be used for simulating the movements of anything from oil droplets to fish.

The whole SELFE modeling system has been fully parallelized using domain decomposition and the MPI message-passing protocol, which greatly boosts its efficiency. The scalability is as good as an implicit model allows. The largest application of SELFE to date was implemented on a horizontal grid of 10 million nodes (20 million triangles) and 31 vertical levels, with finest resolution down to 5m. With 2048 CPUs of NASA's Pleiades cluster, the baroclinic simulation on this grid runs ~70 times faster than real-time.

Selected SELFE applications include:

Columbia River estuary and plume. SELFE is at the heart of the hindcast and forecast system of CMOP's SATURN observatory for Pacific Northwest coast and estuaries. The SATURN forecast system has also been adopted by NOAA.

San Francisco Bay and Delta. We are nearing the end of the first phase of work with California's Department of Water Resources (DWR) to implement SELFE 3D for the San Francisco Bay and Sacramento-San Joaquin Delta system. Climate change is expected to exacerbate the chronic shortage of water resources in California, and this tool will be used by DWR and other agencies in their decision-making process (Fig. 2). SESAME is a closely related project sponsored by NOAA which studies Pacific salmon in the Bay-Delta system. SELFE is being used as the hydrodynamic model for this system to provide baseline information for other models.
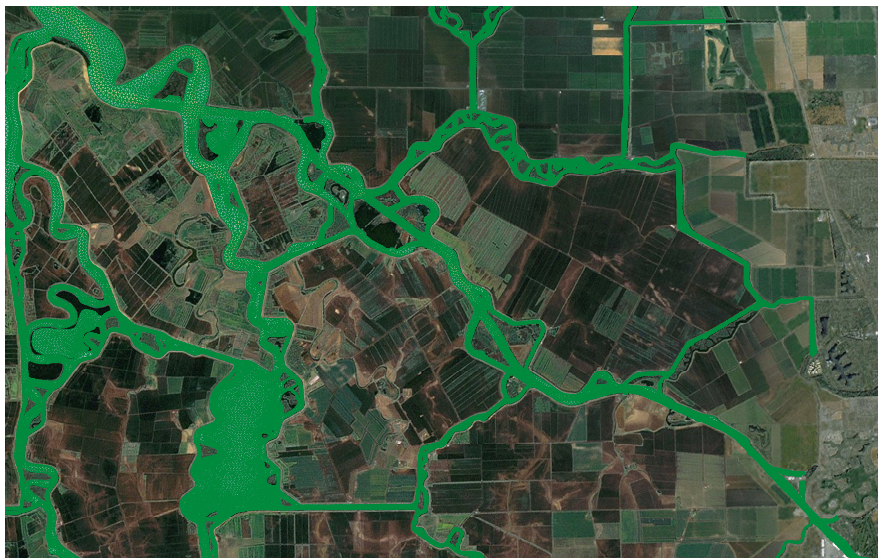

Figure 2: *Sacramento-San Joaquin Delta SELFE grid.*

Tsunami hazard mitigation. NTHMP is using SELFE for tsunami inundation modelling, after passing various benchmarks stipulated by NOAA. It has been used to generate official inundation maps for the state of Oregon, an effort spearheaded by Oregon's Department of Geology and Mineral Industries, under the auspices of NTHMP.

Storm surge inundation. SELFE is being used in a super-regional testbed for coastal inundation, sponsored by the U.S. Integrated Ocean Observing System, and led by Dr. Rick Luettich at UNC. The testbed focuses on two coastal regions that are prone to inundation hazard: Gulf of Mexico and Gulf of Maine. In addition, Harry Wang's group conducted real-time forecasting for hurricane Irene (2011) using SELFE.

Developing and maintaining a sophisticated modeling system such as SELFE is no mean feat. To use the system to its full potential, we have to leverage existing HPC platforms in this country and abroad. In collaboration with world-wide users, SELFE has been successfully ported to over 15 of the largest clusters in the USA, Europe, and Asia-Pacific region, including NASA's Pleiades, NSF's Ranger/Stampede, ECMWF's C1A/C1B, Deutsche Climate Research Center's Blizzard, Central Weather Bureau's (Taiwan) Fujitsu FX10, etc. These systems have enabled us to conduct large-scale, cutting-edge simulations.

A major bottleneck in using the national and international clusters is the slow rate for file transfers, especially for the terabytes of model output. For code testing and small-to-medium size applications, we therefore prefer to rely on smaller local clusters. In this role, SciClone serves as a critical resource for SELFE developers and users at W&M and VIMS. In fact, SELFE accounts for much of VIMS's usage on SciClone, supporting several of the projects described above with simulations using 48–160 CPUs.

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