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14. ABSTRACT

This award funded a planning year for a project of larger scope. The objectives of the planning year were to: 1) participate in the planning process for the HRES field campaign; and 2) construct an LES code applicable to the HRES high wind regime. In order to accomplish the latter goal we improved the parallelization of our base LES code and developed an algorithm to allow simulations of turbulent winds over nearly arbitrary 3-D wave fields.

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Turbulent Flow and Large Surface Wave Events in the Marine Boundary Layers

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LONG-TERM GOALS

The long term objective of our research for the "High Resolution Air-Sea Interaction" (HRES) Departmental Research Initiative (DRI) is to identify the couplings between large wave events, winds, and currents in the surface layer of the marine boundary layers. Turbulence resolving large eddy simulations (LESs) and direct numerical simulations (DNSs) of the marine atmospheric boundary layer (MABL) in the presence of time and space varying wave fields will be the main tools used to elucidate wind-wave-current interactions. A suite of turbulence simulations over realistic seas using idealized and observed pressure gradients will be carried out to compliment the field observations collected in moderate to high winds. The database of simulations will be used to generate statistical moments, interrogated for coherent structures, and ultimately used to compare with HRES observations.

OBJECTIVES

Our near term goals are: 1) participate in the planning process for the HRES field campaign; and 2) construct an LES code applicable to the HRES high wind regime. In order to accomplish the latter goal we are improving the parallelization of our base LES code and developing an algorithm to allow simulations of turbulent winds over nearly arbitrary 3-D wave fields.

APPROACH

We plan on investigating interactions between the MABL and the connecting air-sea interface using both LES and DNS. The waves will be externally imposed: (1) based on well established empirical wave spectra; or (2) ultimately provided by direct observations of the sea surface from field campaigns. The main technical advance is the development of a computational tool that allows for nearly arbitrary 3-D wave fields, *i.e.*, the sea surface elevation $\eta = \eta(x, y, t)$ as a surface boundary condition. The computational method will allow time and space varying surface conditions over a range of wave scales $\mathcal{O}(10)$m or larger.

WORK COMPLETED

During the past year we attended a PI meeting in Irvine, CA to outline the HRES field campaign. The discussion focused on the atmospheric measurements to be collected from aircraft and from R/V FLIP with particular attention paid to the surface layer pressure measurements. The field campaign strategy will be further refined at a meeting in Monterey, CA in early December. A summary of the discussion is available from C. Friehe (U.C. Irvine).

In an effort to link modeling and observations, high-resolution turbulence calculations will be carried out as part of the HRES program. In anticipation of these computationally-intensive simulations and the need for a more general surface boundary capability we undertook several code enhancements. First, we built and tested a new highly parallel algorithm for our "flat" LES code, *i.e.*, the baseline LES code with a flat lower boundary. This allows us to design and implement the code parallelization without the additional complexities of a moving lower boundary. The resulting code will be further modified for HRES applications.

A detailed description of the parallel algorithm and an evaluation of the code performance for varying problem sizes and machine architectures is provided in Sullivan & Patton (2008). The design criteria for the new parallel algorithm are: 1) accomplish 2-D domain decomposition using solely MPI (Message Passing Interface) parallelization; and 2) preserve our well established numerical algorithm based on pseudospectral (FFT) spatial differencing and Runge-Kutta time stepping (Sullivan *et al.*, 1996). The ability to use 2-D domain decomposition, *i.e.*, splitting the computational work across two computational directions, has significant advantages in pseudospectral simulation codes as it allows direct numerical simulations of isotropic turbulence on large meshes, 2048^3 or more (*e.g.*, Pekurovsky *et al.*, 2006). In our 2-D decomposition each processor operates on three-dimensional "bricks" sub-sampled in x, y, or z directions. Brick-to-brick communication is a combination of transposes and ghost point exchange. To preserve pseudospectral differencing in the horizontal directions a custom MPI matrix transpose was designed and implemented. Finally, a new pressure Poisson solver was coded to match the domain decomposition (further details are given in Sullivan & Patton, (2008)).

With these enhancements our new algorithm allows very large number of processors $\mathcal{O}(10^4)$ to be utilized. In our previous code the total number of MPI tasks is limited by the number of vertical gridpoints typically $\mathcal{O}(10^2)$. This increased flexibility allows simulations in anisotropic computational domains, for example boxes with large horizontal and small vertical extents. The transpose and ghost-point exchange routines are general and allow arbitrary numbers of mesh points, although the best performance is realized when the load is balanced across processors. Single files, similar to FORTRAN direct access files, are written and read using MPI I/O. We find MPI I/O makes the code robust across different machine architectures and simplifies the logic required for restarts, especially if the number of processors changes during the course of a simulation. Finally, the code is compliant with the FORTRAN-90 programming standard.

An example of the code scaling for varying workload as a function of the total number of processors NP is provided in figures 1 and 2 for 3 different machine architectures. $NP = NP_z \times NP_{xy}$ where NP_z and NP_{xy} are the number of processors in the vertical and horizontal directions, respectively. In each figure, the vertical axis is total computational time $t \times NP$ divided by total work. N_z is the number of vertical levels and $M_{x,y}$ is proportional to the FFT work in the x and y directions. Ideal scaling corresponds to a flat line with increasing number of processors. The timing tests illustrate the present scheme exhibits both strong scaling (problem size is held fixed and the number of processors is increased) and weak scaling (the problem size grows as the number of processors increases so the amount of work per processor is held constant) over a wide range of problem sizes and is able to use as many as 16,384 processors, *i.e.*, the maximum number available to our application on a Cray XT4[1]. Further, the results are robust for varying combinations of (NP_z, NP_{xy}). Generally, the performance only begins to degrade when the number of processors exceeds about 8 times the smallest dimension in the problem owing to increases in communication overhead.

RESULTS

Parallel codes allow one to simulate PBLs on fine meshes which permits a wider range of scale interactions and thereby lessens the impact of subgrid-scale parameterizations. In Sullivan & Patton (2008) we examine the sensitivity and convergence of LES solutions as the grid mesh is varied from 32^3 to 1024^3 for the classical problem of daytime dry PBL convection (Nieuwstadt *et al.*(1993) describes this flow regime). The grid sensitivity study shows that the LES solutions converge reasonably well only for meshes greater than 256^3, *i.e.*, when the ratio of the boundary layer height to the vertical mesh spacing $z_i/\triangle z > 130$. We find the skewness of vertical velocity S_w highlights the solution sensitivity to grid resolution. The variation of S_w with mesh resolution is a consequence of a Smagorinsky closure which neglects third-order SGS moments; subgrid-scale skewness has a pronounced local maximum in the surface layer and near the PBL inversion. Flow visualization of the fine mesh 512^3 and 1024^3 solutions also illustrates the impact of fine mesh resolution on coherent structures. In figures 3 and 4, we observe a a number of intriguing structural features, *viz.,* large scale plumes coupled to small scale vortical dust devils which only emerge with fine mesh resolution. The highly parallel code described above will become the baseline code for the time evolving wavy boundary computations in HRES. We expect that the small scale vortical structures and statistics found in the canonical convective PBL, as well as neutral flow statistics and structures, will be modulated by high winds and waves in the marine surface layer. Finally, we also note that our parallel code is immediately useful for simulations of the ocean mixed layer in the ONR initiative Impact of Typhoons in the Western Pacific Ocean.

IMPACT/APPLICATIONS

The computational tools developed and the database of numerical solutions generated will aide in the interpretation of the observations gathered during the HRES field campaigns. In addition idealized process studies performed with the simulations have the potential to improve parameterizations of surface drag under high wind conditions in large scale models.

TRANSITIONS & RELATED PROJECTS

We are currently engaged in analyzing data collected during the Ocean Horizontal Array Turbulence Study (OHATS) and the Coupled Boundary Layers Air-Sea Transfer (CBLAST) field campaigns. These are joint efforts between NCAR, and numerous university investigators. Also the present work has links to the ONR DRI on the impact of typhoons in the Western Pacific Ocean (ITOP).

[1]Computations on the Cray XT4 "Franklin" were carried out by Dr. E. Patton (NCAR) with computer time provided by the National Energy Research Scientific Computing Center which is managed by the U.S. Department of Energy.

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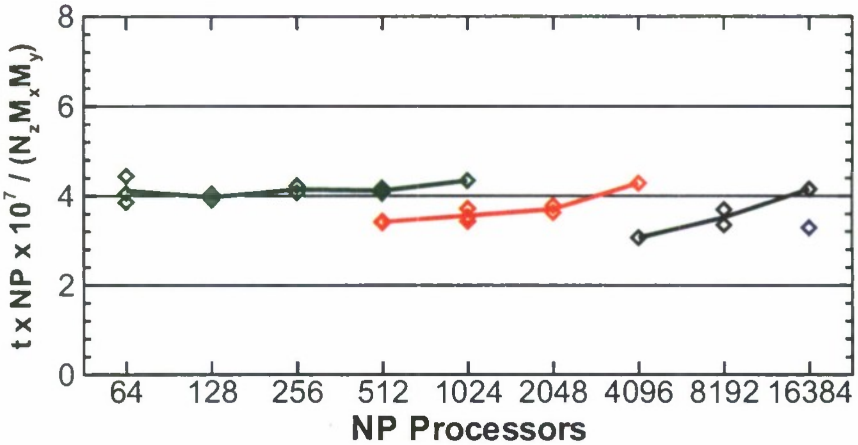


Figure 1: Computational time per gridpoint for different combinations of problem size and 2-D domain decomposition for the Cray XT4 (an example of strong scaling). a) green lines and symbols problem size 512^3; b) red lines and symbols 1024^3; c) black lines and symbols 2048^3; and d) blue symbol 3072^3. For a given number of total processors NP the symbols are varying vertical and horizontal decompositions, *i.e.*, different combinations (NP_z, NP_{xy}).

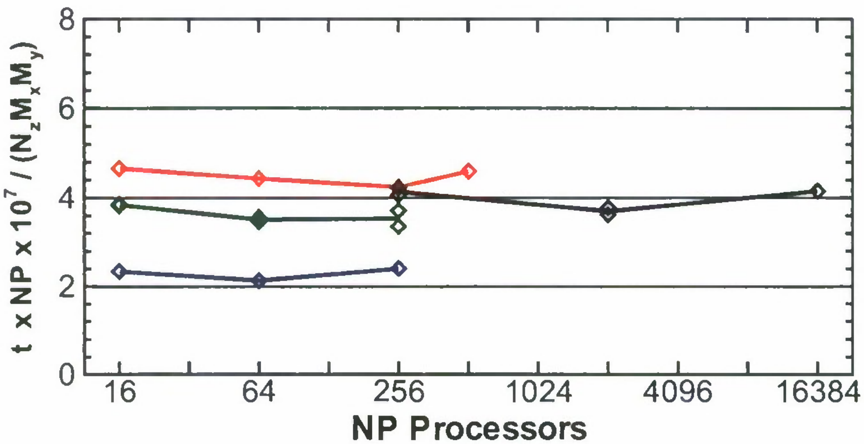
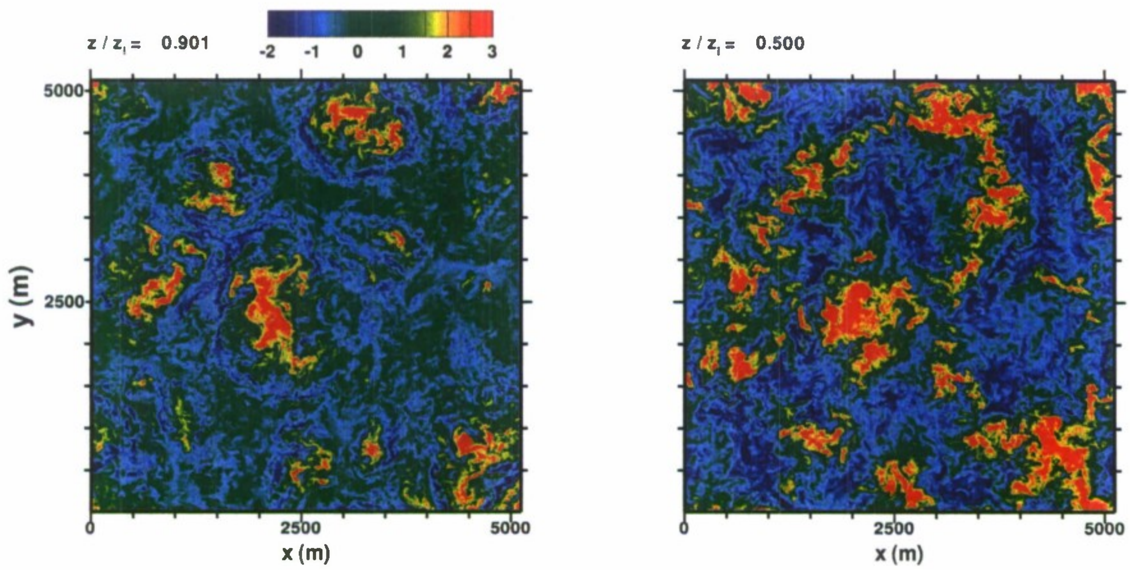


Figure 2: Computational time per gridpoint for a fixed amount of work per processor (an example of weak scaling). Red, green, and blue lines 60,000 points/processor for different machines. Cray XT4 red line; Dual core IBM SP5+ green line; Single core IBM SP5 blue line. Black lines and symbols 524,288 points/processor for Cray XT4. For a fixed number of total processors NP multiple symbols are different combinations of (NP_z, NP_{xy}).



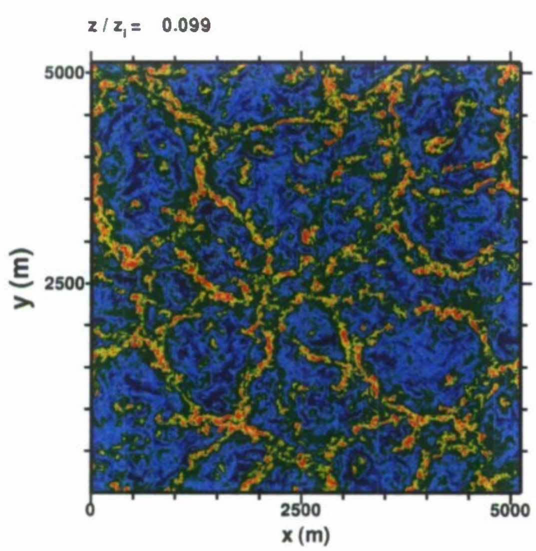


Figure 3: Visualization of the vertical velocity field in a convective PBL at different heights from a 512^3 simulation. Plumes near the inversion can trace their origin to the hexagon patterns in the surface layer. The color bar is in units of $\mathrm{m\,s^{-1}}$.

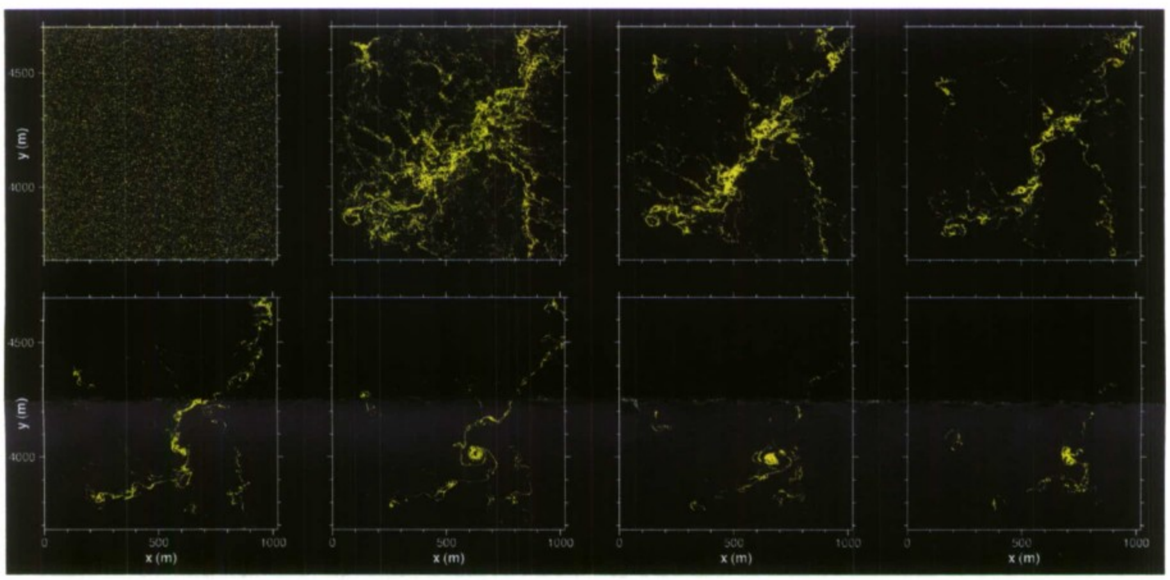


Figure 4: Visualization of particles released in a convective PBL at $z/z_i \sim 0.2$ over a limited horizontal extent from a 1024^3 simulation of convection. The viewed area is $\sim 3.8\%$ of the total horizontal domain. Notice the evolution of the larger scale line of convection into small scale vortical dust devils. Time advances from left to right beginning along the top row of images.