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A study on coupling technique and implementation of the wave-circulation coupled model①

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Abstract

The coupler is fundamental for a coupled model to realize complex interactions among component models. This paper focuses on the coupling process of Wave-Circulation (W-C) coupled model which consists of MASNUM (key laboratory of marine science and numerical modeling wave model) and POM (Princeton Ocean Model). The current coupling module of this coupled model is based on the inefficient I/O file, which has already become a performance bottleneck especially when the coupled model utilizes a large number of processes. To improve the performance of the W-C model, a flexible coupling module based on the model coupling toolkit (MCT) is designed and implemented to replace the current I/O file coupling module in the coupled model. Empirical studies that we have carried out demonstrate that our online coupling module can dramatically improve the parallel performance of the coupled model. The online coupling module outperforms the I/O file coupling module. When processes increase to 96, the whole process of EXP-C takes only 695.8 seconds, which is only 58.8% of the execution time of EXP-F. Based on our experiments under 2D Parallel Decomposition (2DPD), we suggest setting parallel decomposition strategies automatically to component models in order to achieve high parallel efficiency.

Key words: coupling technique, model coupling toolkit (MCT), W-C coupled, online coupling module, 2D Parallel Decomposition (2DPD), parallel performance

0 Introduction

The accurate forecast of ocean conditions at the time of atrocious weather is of great importance to marine operations. An accurate and timely tracking of the distribution characteristics of thermocline is the key to a successful submarine voyage. The main method of marine forecast is the ocean numerical simulation through coupling wave models and circulation models. Wave height, direction, wave-induced momentum, circulation velocity, temperature and current-induced momentum, these data are all acquired from coupled models. The interactions among these physical quantities are the leading factor of the ocean movement, especially of the upper layer. The upper ocean mixing processes are important for ocean models, especially for small-scale coastal simulations. Experts have spent numerous time and energy to study, develop and apply W-C coupled models. Mellor, et al.[1,2] derived the equations for W-C interactions. Xie, et al.[3] extended their W-C coupled modeling system to incorporate depth dependent radiation stress and bottom shear stresses. This paper focuses on the coupled model consisting of POM and MASNUM[4] which has been deployed as a numerical forecast system in China National Marine Environmental Forecasting Center.

The coupling module is crucial for the coupled model to realize the complex interactions among component models. Some couplers have been developed for coupling models[5], including Ocean Atmosphere Sea Ice Soil (OASIS)[6], Coupler of Community Earth System Model (CPL)[7], Earth System Modeling Framework (ESMF) project[8] and MCT[9], etc. All these couplers utilize message passing interface (MPI) to transfer data between component models to improve

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parallel performance. However, the coupled model of MASNUM and POM still utilize the inefficient I/O file as a coupling module which lacks of flexibility and leads to poor parallel performance, especially when the coupled model utilizes a large number of processes.

To improve the parallel performance of the coupled model with MASNUM and POM, we have made the following contributions:

(1) A flexible coupling module based on MCT has been designed and implemented to replace the current I/O file coupling module in the coupled model. It is believed this flexible coupling module can be also used in other coupled models;

(2) Lots of studies carried out by us demonstrate that our online coupling module can dramatically improve the parallel performance of the coupled model, because it avoids the overhead of writing I/O file and makes MASNUM and POM integrate at the same time.

The remainder of this paper is organized as follows. The W-C coupled model and coupling module are illustrated in Section 1 and a flexible online coupling module is designed in Section 2. The simulation results and performance are reported to validate the online coupling module in Section 3. Conclusion and remarks are given in the last section.

1 Background and related work

1.1 W-C coupled model

This part describes the basic theories of the W-C coupled model containing MASNUM and POM.

(1) MASNUM

The wave direction spectrum in wave number space is simulated by working out the wave number spectrum balance equations and combining the wind input and W-C interactions source functions into consideration. Thus wave height, wave period, wave direction and wave-induced mixing coefficient are obtained as well. The mixed characteristics numerical computational scheme has been applied in the spherical coordinate system in the model integral calculation. [10, 11]

(2) POM

POM is developed by Blumberg and Mellor of Princeton University. The time splitting method is used in its algorithms to reduce computation time. The external mode is two-dimensional and requires a small time step due to fast gravity waves, while the internal mode is three-dimensional and uses a larger step. The calculation of the three-dimensional variables is divided into a vertical diffusion time step and an advection plus horizontal diffusion time step. The external mode is implicit whereas the internal mode is explicit. [12] The output parameters include water level, sea temperature, salinity, ocean current velocity and direction which change with time. The higher resolution is used in the upper ocean layer and the lower resolution is used in the deep ocean layer.

(3) Wave-induced mixing coupling

The velocity, temperature and salinity are expressed as average and fluctuating components in the wave-induced mixing coupling theory developed by Yuan et al. and Qiao et al. The velocity fluctuation is decomposed into wave-induced part and current-induced part. $\overline{U_i}$ and $\boldsymbol{u}_i$ represent the means and fluctuations of velocity, and subscripts $i, j = 1, 2, 3$ represent axes of the Cartesian coordinates (x, y, z). The velocity fluctuation can further be decomposed into a turbulence portion $\boldsymbol{u}_{ic}$ and a wave-induced fluctuation $\boldsymbol{u}_{iw}$. $-(\overline{\boldsymbol{u}_{iw}\boldsymbol{u}_{jc}} + \overline{\boldsymbol{u}_{ic}\boldsymbol{u}_{jw}})$ is the momentum mixing induced by surface wave motion. How the wave-induced current momentum is stirred as[10,11]

$$-(\overline{\boldsymbol{u}_{iw}\boldsymbol{u}_{jc}} + \overline{\boldsymbol{u}_{ic}\boldsymbol{u}_{jw}}) = \begin{pmatrix} 0 & 0 & \boldsymbol{B}_V \frac{\partial \overline{\boldsymbol{U}_1}}{\partial z} \\ 0 & 0 & \boldsymbol{B}_V \frac{\partial \overline{\boldsymbol{U}_2}}{\partial z} \\ \boldsymbol{B}_V \frac{\partial \overline{\boldsymbol{U}_1}}{\partial z} & \boldsymbol{B}_V \frac{\partial \overline{\boldsymbol{U}_2}}{\partial z} & 2\boldsymbol{B}_V \frac{\partial \overline{\boldsymbol{U}_3}}{\partial z} \end{pmatrix} \quad (1)$$

The wave-induced mixing coefficient is shown as

$$\boldsymbol{B}_V = \boldsymbol{a}\iint_{\vec{k}} \boldsymbol{E}(\vec{k}) e^{2kz} d\vec{k} \frac{\partial}{\partial z}\left(\iint_{\vec{k}} \boldsymbol{w}^2 \boldsymbol{E}(\vec{k}) e^{2kz} d\vec{k}\right)^{\frac{1}{2}} \quad (2)$$

The distribution of wave spectrum is simulated by MASNUM. $\boldsymbol{B}_V$ is figured out with the wave spectrum in Eq. (2), $\boldsymbol{a} = \boldsymbol{O}(1)$ is a parameter which should be determined by observations or numerical experiments, wave number spectrum $\boldsymbol{E}(\vec{k})$ can be computed by integrating a wave number spectrum numerical model, $\boldsymbol{w}$ is the wave angular frequency, k is the wave number, and z is the vertical coordinate axis downward positive with $z = 0$ at the surface. It is superimposed on the eddy-viscosity coefficient and diffusion coefficient in POM. Accordingly, the total vertical mixing coefficient is obtained. So, the effect of wave stirring is included in the circulation model.

(4) Integration based on I/O file

The coupling method of the current W-C model is based on I/O file. The topographic data is obtained by interpolation based on the earth topography five minute gridded elevation data set (ETOPO5). And the initial temperature and salinity of the model are obtained from Levitus monthly climatology datasets. The heat fluxes are from the 1° × 1° mean monthly comprehensive ocean-atmosphere data set (COADS). The coupled model gets the wind field using reanalysis data from the National Centers for Environmental Prediction (NCEP).

The original integration scheme is a sequential execution mode. Firstly, MASNUM runs 3-day integration and the output elements especially including the wave-induced mixing coefficient $\boldsymbol{B}_V$ are exported to a file by I/O. Then the POM integrates 72-hours by reading the file that includes coupling data. The coupling process structure is shown in Fig. 1.

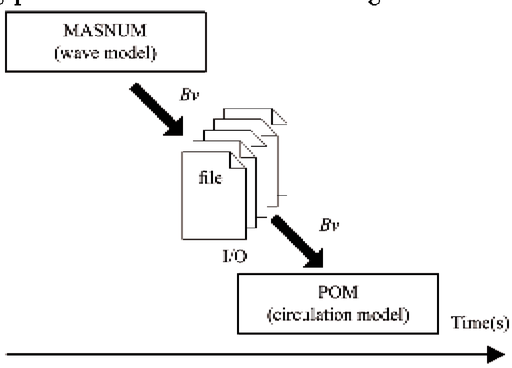

Fig. 1 Integration based on I/O file

1.2 Coupling module

With the increasing studies of numerical simulation, how to integrate independent models expediently and efficiently has become a focus with wide attention. The two-way coupling that is needed in data exchange cannot be realized based on I/O file. The spatial resolution and the time step of models are different and the location of grid points is not consistent. Individual components can be created, modified, or replaced without necessitating code changes in other components. The interpolation and smooth are required when the physical data of a model are transferred to another model. The framework assures that all heat, mass and energy fluxes in the system are conserved. All of these are the core of model coupling that is a complicated system. Its contents relate to not only mathematics and meteorology but also computer science, such as parallel computation and I/O technique, on which the models depend.

There are three kinds of coupling methods according to the compact degree among models. They are tight coupling, moderate coupling and loose coupling[13]. The tight coupling has a strong dependence on the components that data are passed by parameters. Powers, et al.[14] designed an air-sea model in tight coupling. Ren, et al.[15] set up a model that the message was transferred by pipe technique in moderate coupling. Each component maintains its independence by MPI in loose form. The common coupling modules include:

OASIS is a new fully parallel coupler for Earth System Models (ESMs). The configuration of one particular coupled ESM simulation, i. e. the coupling and I/O exchanges performed at run-time between the components or between the components and disk files, is done externally by the user also through XML files.[6]

CPL is based on a framework which divides the complete climate system into component models that are connected by CPL. The coupler controls the execution and time evolution of the system by synchronizing and controlling the flow of data in the various components.[7]

ESMF is a software infrastructure that enables different weather, climate, and data-assimilation components. It also includes toolkits for building components and applications, such as regridding software and parallel communications.[8]

MCT is a set of tools for supporting coupled models and can be used to couple message-passing parallel models to create a parallel coupled model. It is the basis of ESMF and CPL[7,8]. It is not only used in global climate models but also used in meso-scale models or weather models. MCT is used to couple the Weather Research & Forecasting Model (WRF) and the Regional Ocean Modeling System (ROMS) to study hurricane. It is also used to couple the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS) and ROMS to simulate the coastal atmosphere.[16]

2 The online coupling module

Modularization and flexibility are the major requirements of the coupling modules. Although the effort is being spent on improving W-C interactions, an efficient and effective method has yet to be developed. Obviously, it is not appropriate to use the wave model as a sub-module of ocean model and coupling offline. Therefore the online coupling technique is inevitably the only choice. The OASIS, CPL and ESMF are very complex because their emphases are on the global climate models. MCT is a coupling library for creating coupled model and is mainly oriented to the basic developing parallel environment, therefore, it is not suitable for the model experts who do not master parallel technology. For this reason, a flexible coupling module is designed for the W-C coupled model based on MCT. And then a generalization of this coupling module is given to other mesoscale or weather coupled models.

The designed coupling module includes three parts: coupling application layer, coupling driver layer and coupling parallel environment layer.

The structure is shown in Fig. 2. In the configuration system, the coupling parameters and computing resources are set. The coupling driver layer is the core of the coupling module. Its main functions are parallel communication, solving sparse matrix interpolation, etc. The coupling parallel environment layer mainly provides MPI library and other high performance computing libraries.

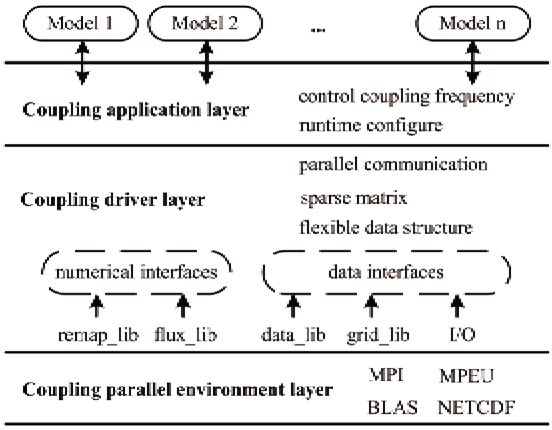

Fig. 2 Structure of the online coupling module

2.1 Coupling application layer

The functions of this layer are realized through the configuration information system. Coupling component model, coupling physical quantities, coupling frequency, integrate time, simulation areas and boundary conditions are set by configuration files. In addition, the computing resources are distributed and allocated in this layer. The function is achieved by using Multi Program-Components Handshaking[17].

2.2 Coupling driver layer

The data processing and exchange functions are fulfilled in the coupling driver layer. MCT is adopted to solve the parallel coupling problem. It is built on top of a utility package called message passing environment utilities (MPEU)[18]. There are three classes that support M × N transfers: the component registry, the communications schedulers for one-way parallel data transfers and two-way data redistributions. Instead of simple arrays and MPI processes ranks, the main arguments are Router. The Router and routines are responsible for transferring data between models. Redistributing data within a single pool of processes, in principle, requires each process in the pool to send and receive data. [9]

2.3 Coupling parallel environment layer

This layer is mainly for the computing resource. The communication in component models is realized by parallel message transmission software, such as MPI, Open Multi-Processing (OpenMP). Various compilers are the basic parallel environment. The MPEU solves the parallel computing output error, resource input and so on. Moreover, more high performance computing libraries, such as BLAS, FFT, can replace general functions provided by the FORTRAN program.

2.4 Integration based on the online coupling module

In our work, the integration scheme is designed to be a concurrent mode by using the online coupling module based on MCT. The wave model and the circulation model run 3-day integration at the same time and exchange data by the coupling module which saves I/O time. Fig. 3 describes the coupling process structure.

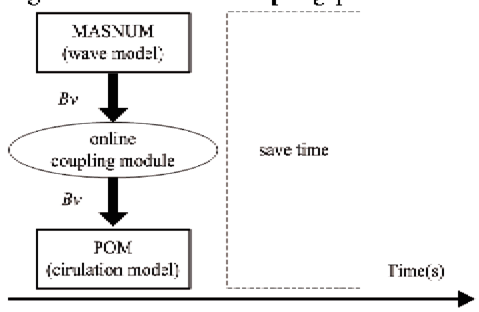

Fig. 3 Integration based on the online coupling module

3 Experimental evaluations

In this section, the parallel performance of the improved coupled model is empirically evaluated on high performance computer. First the experimental setup is introduced, second the functional correctness and calculation accuracy of our coupling moduler is proven by checking the output binary consistency and finally the detailed parallel performance is presented.

3.1 Experimental setup

To empirically evaluate the parallel performance of the coupled model, a high performance computer is used, whose name is Tansuo100 in Tsinghua University. It consists of more than 700 computing nodes, each of which consists of two Intel Xeon 5670 6-core CPUs sharing 32GB shared memory and the dominant frequency is 2.92GHz. All computing nodes are connected by the high-speed network Infiniband with a peek communication bandwidth of 5GB/sec. All tests run with one MPI process for each core and each MPI process is a single thread in the following experiments. In the W-C coupled model, The MASNUM contains 18 vertical layers and horizontal grid points of 409 × 401 (0° – 50°N, 99° – 150°E). The horizontal resolution is about (1/8)° × (1/8)° and its time step is 300s. The POM contains 30 vertical layers and horizontal grid points of 721 × 625 (15° – 41°N, 105° – 135°E). Its horizontal resolution is about (1/24)° × (1/24)°. The external and internal time steps are 4.14 seconds and 124.2s respectively.

The Argo profiling float temperature data from the Coriolis Data Centre of France is used to verify the simulation results. The results of verification show the simulations are well consistent with observation. [19] Therefore, only a 3-day integration is chosen as the control experiment (EXP CTRL) from June 8 to June 10 in 2011, and two kinds of experiments based on the same initial conditions are designed to evaluate the parallel performance. One kind is identified as the experiments coupled by I/O file (EXP-F) and the other is identified as the experiments coupling based on the online coupling module developed by us (EXP-C).

3.2 Improvement for functional correctness

In coupling module design and development, we should ensure that no change occurs in the physical meaning and complete consistency. The calculation accuracy of the coupling module based on MCT must be rigorously consistent with that of the I/O file method. In the flowing two phases check and test should be done to maintain the functional correctness and calculation accuracy.

(1) The coupling frequencies and coupling physical quantities will not be changed when we use the coupling module based on MCT to replace the current I/O file coupling module in the coupled model. The data of the output element is intercepted in every output step in order to pursue the binary consistency.

(2) The binary consistency of the circulation model output is checked and proven after the coupling process of W-C coupled model.

3.3 Performance evaluation

Table 1 lists out the detailed results of two kinds of experiments, where 2DPD of component models is the number of processes in the latitude direction multiplied by the number of processes in the longitude direction X × Y. The 2DPD of MASNUM is $X_M \times Y_M$ and 2DPD of POM is $X_P \times Y_P$ in EXP-C. The total number of processes used in EXP-C is $X_M \times Y_M + X_P \times Y_P$. The EXP CTRL is serially executed and the total execution time is 18976.7 seconds.

Table 1 Computation time of experiments

Execution Time (second)		Number of Processes: EXP CTRL	2		4		8		16	
		Time	2DPD	Time	2DPD	Time	2DPD	Time	2DPD	Time
EXP-F	Model Time	M: 8834.7	1 × 2	M: 5957.3	2 × 2	M: 2775.7	2 × 4	M: 1200.9	4 × 4	M: 714.2
		P: 10142		P: 7732.8		P: 4144.9		P: 2838.7		P: 2081.6
	Total Time	18976.7		13690.1		6920.6		4039.6		2795.8
EXP-C		/	M[a]: 1 × 1	10227.7	M: 1 × 2	6213.3	M: 1 × 2	3538.7	M: 2 × 3	2251.9
			P: 1 × 1		P: 1 × 2		P: 2 × 3		P: 2 × 5	
		/					M: 2 × 2	4558.7	M: 2 × 2	2603.5
							P: 2 × 2		P: 3 × 4	
Execution Time		32		48		64		80		96
		2DPD	Time	2DPD	Time	2DPD	Time	2DPD	Time	2DPD	Time
EXP-F	Model Time	4 × 8	M: 365.6	6 × 8	M: 340.3	8 × 8	M: 322.3	8 × 10	M: 343.8	8 × 12	M: 351.2
			P: 1365.9		P: 897.3		P: 838.3		P: 760.5		P: 831.8
	Total Time		1731.5		1237.6		1160.6		1104.3		1183
EXP-C		M: 4 × 4	1469.3	M: 3 × 6	924.6	M: 4 × 4	849.9	M: 5 × 8	793.4	M: 4 × 8	822.6
		P: 4 × 4		P: 5 × 6		P: 6 × 8		P: 5 × 8		P: 8 × 8	
		M: 2 × 4	1333.1	M: 3 × 4	859.9	M: 4 × 6	785.8	M: 4 × 5	729.7	M: 4 × 6	776.2
		P: 4 × 8		P: 5 × 8		P: 5 × 8		P: 6 × 10		P: 8 × 9	
		/		M: 4 × 6	1079	M: 4 × 8	899.9	M: 4 × 4	794.7	M: 4 × 4	695.8
				P: 4 × 6		P: 4 × 8		P: 8 × 8		P: 8 × 10	

a: M specifies the wave model MASNUM and P specifies the circulation model POM

Fig. 4 shows the speedup rate of these two experiments. EXP-C significantly outperforms EXP-F. When the number of processes increases, the speedup of EXP-C increases more quickly than that of EXP-F. Besides, the speedup of EXP-F even drops when the number of processes reaches to 80. When the number increases to 96, the execution time of EXP-C is 695.8 seconds, which is only 58.8% of the execution time of EXP-F.

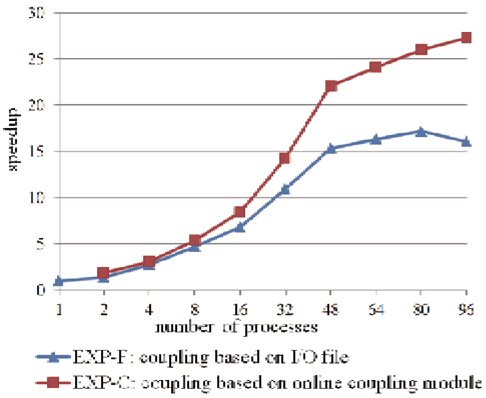

Fig. 4 Speedup of the two coupling methods

In addition, it is found that 2DPD has great influence on the computing performance of component model by experiments based on various 2DPD strategies From Table 1. Meanwhile, it is found that the load balance in coupled model needs adjusting computation resource manually.

4 Conclusions

The coupling technique based on coupler has been applied to the research field of meso-scale models. In this paper, an online coupling module based on MCT is designed and implemented to replace the current I/O file coupling module in the W-C coupled model of MASNUM and POM. Lots of studies demonstrate that our online coupling module can dramatically improve the parallel performance of the coupled model after checking the functional correctness, because it avoids the overhead of writing I/O file and makes MASNUM and POM integrate concurrently. We will popularize this flexible coupling module in other coupled models.

After comparing different 2DPD numerical results, a further suggestion is given that the component or coupled models achieves a high level of parallel efficiency by computing resource allocation. With the parallel scale increasing, automatically setting parallel decomposition strategy and task scheduling methods are demanded.

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