Developing a common, flexible and efficient framework for weakly coupled ensemble data assimilation based on C-Coupler2.0

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Abstract. Data assimilation (DA) provides initial states of model runs by combining observational information and models. Ensemble-based DA methods that depend on the ensemble run of a model have been widely used. In response to the
15 development of seamless prediction based on coupled models or even Earth system models, coupled DA is now in the mainstream of DA development. In this paper, we focus on the technical challenges in developing a coupled ensemble DA system, especially how to conveniently achieve efficient interaction between the ensemble of the coupled model and the DA methods. We first propose a new DA framework DAFCC1 (**D**ata **A**ssimilation **F**ramework based on **C**-**C**oupler2.0, version 1) for weakly coupled ensemble DA, which enables users to conveniently integrate a DA method into a model as a procedure
20 that can be directly called by the model ensemble. DAFCC1 automatically and efficiently handles data exchanges between the model ensemble members and the DA method without global communications, and does not require users to develop extra codes for implementing the data exchange functionality. Based on DAFCC1, we then develop an example weakly coupled ensemble DA system by combining an ensemble DA system and a regional atmosphere-ocean-wave coupled model. This example DA system and our evaluations demonstrate the correctness of DAFCC1 in developing a weakly coupled ensemble
25 DA system and the effectiveness in accelerating an offline DA system that uses disk files as the interfaces for the data exchange functionality.

1 Introduction

Data assimilation (DA) methods, which provide initial states of model runs by combining observational information and models, have been widely used in weather forecasting and climate prediction. The **en**semble **K**alman **f**ilter (EnKF; Houtekamer
30 and Mitchell, 1998; Evensen, 2003; Lorenc, 2003a; Anderson and Collins, 2007; Whitaker, 2012) is a widely used DA method that depends on an ensemble run of members. Other DA methods that can be performed a single model run, such as the

Nudging method (Hoke and Anthes, 1976; Vidard et al., 2003), Optimal Interpolation (OI; Gandin, 1965), Ensemble OI (EnOI; Oke et al., 2002; Evensen, 2003), three-dimensional variational analysis (3D-Var; Anderson et al., 1998; Courtier et al.1998; Gauthier et al., 1999; Lorenc, 2000) and four-dimensional variational analysis (4D-Var; Courtier et al., 1994; Kalnay, 2003;

35 Lorenc, 2003b; Rabier et al., 2007), can be technically viewed as a special case of ensemble-based methods with only one member in the ensemble when we attempt to design and develop a software framework for data assimilation. Moreover, hybrid DA methods, such as hybrid Ensemble/3D-Var (Hamill, 2000; Etherton and Bishop, 2004; Wang et al., 2008, 2013; Ma et al., 2014) and ensemble-based 4D-Var schemes (Fisher, 2003; Bishop and Hodyss, 2011; Bonavita et al., 2012, 2016; Buehner et al., 2015), also depend on an the ensemble run of members from the same model.

40 With the rapid development of science and technology, numerical forecasting systems are evolvinginvolving from only an individual component model (such as an atmospheric model) to coupled models that can achieve better predictability (Brown et al., 2012; Mulholland et al., 2015), and earth system models are being used to develop seamless prediction that spans timescales from minutes to months or even decades (Palmer et al., 2008; Hoskins, 2013). Along with the use of coupled models in numerical forecasting, common and flexible DA methods for coupled models are urgently needed (Brunet et al., 2015;

45 Penny et al., 2017). Coupled DA technologies have already been investigated widely and DA systems have been constructed (Sugiura et al., 2008; Fujii et al., 2009, 2011; Saha et al., 2010, 2014; Sakov et al., 2012; Yang et al., 2013; Tardif et al., 2014, 2015; Lea et al., 2015; Lu et al., 2015a, b; Mochizuki et al., 2016; Laloyaux et al., 2016, 2018; Browne et al., 2019; Goodliff et al., 2019; Skachko et al. 2019), in which ensemble based DA methods have already been applied (e.g., Zhang et al., 2005, 2007; Sluka et al., 2016).

50 To develop a coupled ensemble DA system, besides the scientific challenges regarding DA methods, there are also technical challenges to be addressed, such as how to achieve an ensemble run of a coupled model, how to conveniently integrate the software of a coupled model and the software of ensemble DA methods into a robust system, and how to conveniently achieve efficient interaction between the ensemble of the coupled model and the DA methods. The existing ensemble DA frameworks supporting coupled DA coupled ensemble DA systems such as the Data Assimilation Research Testbed (DART; Anderson et

55 al., 2009) , the ensemble coupled data assimilation system (ECDA; Zhang et al., 2005, 2007), and the Grid point Statistical Interpolation (GSI; Shao et al., 2016) combined with EnKF (Liu et al., 2018a), employ disk files as the interfaces of data exchange between the model ensemble members and the DA methods, and iteratively switch between the run of the model ensemble and DA using software-based restart functionality that also relies on disk files. Such an implementation (called offline implementation hereafter) can guarantee software independence between the models and the DA methods, so as to

60 achieve flexibility and convenience in software integration; however, the extra I/O accesses of disk files as well as the extra initialization of software modules introduced by the data exchange and the restarts are time-consuming and can be a severe performance bottleneck under finer model resolution (Heinzeller et al., 2016; Craig et al., 2017). The Parallel Data Assimilation Framework (PDAF; Nerger et al., 2005; Nerger and Hiller, 2013; Nerger et al., 2020) and the Employing Message Passing Interface for Researching Ensembles (EMPIRE; Browne and Wilson, 2015) framework have shown that MPI (Message

65 Passing Interfaces)-based data exchanges between the model ensemble members and DA procedures can produce better performance for DA systems, because they do not require disk files or the restart operations.

Noting that most existing couplers for Earth system modeling have already achieved flexible MPI-based data exchanges between component models in a coupled system, we design and develop a common, flexible and efficient framework for coupled ensemble data assimilation, based on the latest version of the Community Coupler (C-Coupler2.0; Liu et al., 2018b).

70 Considering that existing observation processing systems can introduce different observation frequencies corresponding to different component models, we take consideration of weakly coupled ensemble DA where the data from different component models are assimilated independently by separate DA methods (Zhang et al., 2005, 2007; Fujii et al., 2009, 2011; Saha et al., 2010, 2014) in this work, and in further work will then target strongly coupled ensemble DA, which generally uses a cross-domain error covariance matrix to account for the impact of the same observational information on different component models

75 cooperatively (Tardif et al., 2014, 2015; Lu et al., 2015a, b; Sluka et al., 2016).

The remainder of this paper is organized as follows. Section 2 introduces the overall design of the new DA framework named DAFCC1 (**D**ata **A**ssimilation **F**ramework based on **C**-**C**oupler2.0, version 1). The implementation of DAFCC1 are described in Section 3. Section 4 introduces the development of an example weakly coupled ensemble DA system based on DAFCC1. Section 5 evaluates DAFCC1. Finally, Section 6 contains a discussion and conclusions.

80 **2 Overall design of the new framework**

The experiences gained from PDAF and EMPIRE show that, a framework with an online implementation where all ensemble members of the model and all procedures of DA methods are combined into a single MPI program is essential for improving the interaction between the model and the DA software. There can be different strategies for the online implementation. In EMPIRE, a DA method is compiled into a standalone executable running on the processes distinct from the model ensemble,

85 and global communications of *MPI_gatherv* and *MPI_scatterv* are used for exchanging data between the model ensemble and the DA method. Such an implementation can maintain the independence between the DA software and the model, while the global communications are generally inefficient and there are idle processes almost at any time because the model ensemble and the DA method generally work sequentially but not simultaneously. In PDAF, a DA method is transformed into a native procedure that is called by the corresponding models via the PDAF application programing interfaces (APIs). Thus, a DA

90 method can share the processes of the model ensemble. The code releases of PDAF (http://pdaf.awi.de/trac/wiki) provide template implementations of data exchanges for a default case where a DA method shares all processes of the first ensemble member of the corresponding model and keeps the same parallel decomposition (grid domain decomposition for parallelization) with the corresponding model. When users want For a case different from the default (e.g., a DA method does not use the same processes set with the first ensemble member or uses a parallel decomposition different from the corresponding model), code

95 implementations users will be required to develop extra codes for implementing the corresponding data exchange functionality following the rules of PDAF ((e.g., using the PDAF communicators for the model, the filter and the coupling exchanges

between them, of COMM_COUPLE, COMM_FILTER, COMM_CPLMOD and COMM_MODEL, and using the formats of PDAF APIs)) will be developed.

Most DA software consists of parallel programs that generally can be accelerated by using more processor cores. When running an ensemble DA algorithm for a component model in an ensemble run, all ensemble members of the component model are synchronously waiting the result of the DA algorithm. Therefore, all the processor cores corresponding to all ensemble members of the component model can be used to accelerate the DA algorithm. To develop a new framework for weakly coupled ensemble data assimilation, we should target an improved implementation of the data exchange functionality, which does not use global communications of *MPI_gatherv* and *MPI_scatterv*, enables a DA method to share almost all the processes of the model ensemble and does not require users to develop extra codes in any case. When a DA algorithm uses a processes set different from a model ensemble member, the DA algorithm will use a parallel decomposition that differs from the model ensemble members. Thus, the data exchange between the DA algorithm and a component model ensemble member will introduce a challenge of transferring fields between different process sets with different parallel decompositions.

Fortunately, such a challenge has already been overcome by most existing couplers (Craig et al., 2012; Valcke, 2012; Liu et al., 2014; Craig et al., 2017; Liu et al., 2018b), each of which can transfer data between different process sets with different parallel decompositions without the global communications. We therefore use the C-Coupler2.0 (Liu et al., 2018b), the latest version of the Community Coupler (C-Coupler), as the foundation for developing DAFCC1. Moreover, C-Coupler2.0 has more functionalities that DAFCC1 can benefit from. For example, C-Coupler2.0 can handle data exchange of 3-D or even 4-D fields where the source and destination fields can have different dimension orders (e.g., vertical+horizontal at the source field, and horizontal+vertical at the destination field). It will be convenient to combine ensemble members of a coupled model into a single MPI program based on C-Coupler2.0 because each ensemble member can be registered as a component model of C-Coupler2.0. As shown in Fig. 1a, based on the coupling configurations registered to C-Coupler2.0, mMost operations for achieving data exchanges can be generated automatically because C-Coupler2.0 can generate coupling procedures between two process sets even when the two sets are overlapping.

A most significant challenge here is that C-Coupler2.0 can only handle coupling exchanges between two component models or intra one component model, while coupled ensemble DA requires coupling exchanges between a DA algorithm and a model ensemble that includes a set of ensemble members each of which has been registered as a component model of C-Coupler2.0. To address this challenge, three new steps, i.e., initialization, running and finalization of DA instances (instances of DA algorithms), are inserted into the model flowchart with C-Coupler2.0 (Fig. 1b). These three steps enable all members in a model ensemble to use a DA algorithm cooperatively.

The software architecture of DAFCC1 based on C-Coupler2.0 is shown in Fig. 21. It includes a set of new managers (i.e., DA algorithm integration manager, ensemble component manager, ensemble data exchange operation manager, online DA procedure manager, and ensemble DA configuration manager) and the new APIs corresponding to these managers. The DA algorithm integration manager enables the user to conveniently develop driving interfaces for a DA algorithm based on a set of new APIs that enables the DA algorithm to register its input and output fields and to obtain various information from the

model. A DA algorithm can include a set of procedures such as observation operators and analysis modules, each of which can be called by the model separately. The framework uses the dynamic link library (DLL) technique for the connection of a DA algorithm program to a model, where a DA algorithm program is compiled into a DLL that is dynamically linked to a model when an instance of the DA algorithm is initialized. With the DLL technique, a new DA algorithm can be used by a model without modifying and recompiling the model codes, , so thatand the original configuration and compilation systems of a DA algorithm can generally be preserved for greater independence of the DA algorithms from the models, and for less work in integrating a DA algorithm. The ensemble component manager is responsible for generating and managing the communicator of ensemble members of each component model. The online DA procedure manager provides several APIs that enable the ensemble members of a component model to initialize, run and finalize a DA instancea DA algorithm cooperatively, and automatically handles the data exchanges between the ensemble members and the DA algorithm with a set of operations. The ensemble DA configuration manager enables the user to flexibly specify the DA algorithm, DA frequency and the operations for the data exchange in a DA simulation through a configuration file.

Guided by the architecture in Fig. 21, we implemented the new framework (see Section 3 for detailed implementation), which enables a coupled ensemble DA system to achieve the following features:

1) Each component model can use different instances of DA algorithms online independently, and the execution of a DA algorithm in the MPI processes of a component model does not force other MPI processes to be idled. For example, components 1, 2, and 4 in Fig. 2Fig. 3 use DA algorithms at different frequencies, while component 3 does not use DA.

2) Given a common DA algorithm, it can be used by different component models under different instances with different configurations; e.g., the fields assimilated, the observational information used, and the frequency. In Fig. 2Fig. 3 for example, components 2 and 4 use different instances of the same DA algorithm 2 independently.

3) An instance of a DA algorithm can either use the processes of all ensemble members of the same component model cooperatively or use the processes of each ensemble member separately. For example, each DA algorithm instance in Fig. 2Fig. 3 uses the processes of all ensemble members of the corresponding component model cooperatively, except procedure 1 of DA algorithm 1 that uses the processes of each ensemble member of component 1 separately.

4) Besides employing the DLL technique for integrating DA algorithm programs, a configuration file is designed for increasing the flexibility and convenience in using a DA algorithm (see Section 3.4 for detailed implementation).

4)

3 Implementation of DAFCC1

In this section, we will detail the implementation of DAFCC1 in terms of the ensemble component manager, DA algorithm integration manager, online DA procedure manager, and ensemble DA configuration manager. Moreover, we will provide an example of how to use DAFCC1 to develop a DA system.

3.1 Implementation of the ensemble component manager

In C-Coupler2.0, the model coupling resources, including MPI communicators, time steps, timers, model grids, parallel decompositions, coupling field instances, and coupling interfaces, are associated with each component model that is registered to C-Coupler2.0 via the API *CCPL_register_component*. When running an ensemble of a model in a single MPI run, each ensemble member should be used as a separate component model. In C-Coupler2.0, model names are the keywords to distinguish different component models. To distinguish different ensemble members of a model that generally share the same code or executable, we update the API *CCPL_register_component* to implicitly generate different names of ensemble members by appending the ID of each ensemble member to the model name (the parameter list of the API *CCPL_register_component* is unchanged). The ID of an ensemble member is given as the last argument (formatted as "CCPL_ensemble_{ensemble numbers}_{member ID}") of the corresponding executable when submitting an MPI run (see ~~Fig. 3~~Fig. 4 as an example), where "*ensemble numbers*" marks the number of ensemble members and "*member ID*" marks the ensemble member ID of the current component.

Given an ensemble run of a coupled model, all ensemble members of the component models of the coupled model can be organized as one level of models (see ~~Fig. 4~~Fig. 5a), although we recommend constructing two hierarchical levels of models with the first level corresponding to all ensemble members of the coupled model and each ensemble member including the component models at the second level (~~Fig. 4~~Fig. 5b), because the hierarchical organization retains the original architecture of the coupled model through a simple additional registration of the coupled model to C-Coupler2.0.

As a DA algorithm that handles ensemble fields can run on the MPI processes of all ensemble members of a component model (~~Fig. 2~~Fig. 3), a special C-Coupler2.0~~an ensemble-set~~ component model that covers all ensemble members of the component model (this special component model is called ensemble-set component model hereafter) is required ~~for~~to us~~e~~ing the DA algorithm (~~Fig. 4~~Fig. 5b). The ensemble component manager provides the capability to generate an ensemble-set component model, which does not introduce global synchronization and only involves the ensemble members of the corresponding component model.

3.2 Implementation of the DA algorithm integration manager

A pair of a model and a DA algorithm have essentially the relationship between a caller and a callee in a program, where the callee generally declares a list of arguments that includes a set of input and output variables, while a caller should match the argument list of the callee when calling the callee (herein, the model is referred to as the host model of the DA algorithm). For a caller and a callee that are in the same native code, a corresponding compiler can guarantee the consistency of the argument list between them, regardless of the data structure of each argument. However, compilers cannot guarantee such consistency between a host model and a DA algorithm that is enclosed in a DLL but not in the native code of the host model.

To address the above challenge, we designed and developed a new solution for passing arguments between a host model and a DA algorithm, and tried to make such a solution as flexible as possible to improve the flexibility of DAFCC1 in serving

various DA algorithms. There are three driving subroutines for initializing, running, and finalizing a DA algorithm; their subroutine names share the name of the DA algorithm as the prefix and are distinguished by different suffixes. We tried to make the explicit argument list of each driving subroutine as simple as possible (e.g., only a few integer arrays), and developed a set of C-Coupler APIs for flexibly passing implicit arguments between the host model and the DA algorithm. Based on these APIs, the DA algorithm can obtain the required information from the host model and the grids via C-Coupler2.0 and can also declare any field instances that the DA algorithm has registered to C-Coupler2.0 as implicit input or output arguments, at the initialization stage of the DA algorithm. Figure 65 shows an example of the driving subroutines where the running and finalization driving subroutines are very simple. In the initialization driving subroutine, besides the original functionalities of the DA algorithm such as determining parallel decompositions, allocating memory space for variables and other operations for initialization, there are additional operations for obtaining information from the host model and grids using C-Coupler2.0, registering the parallel decompositions, required grids, and field instances to C-Coupler2.0, and declaring the field instances as implicit input or output arguments. In the running driving subroutine *DA_CCPL_RUN*, there are no explicit calls for data exchange, because the data from the model ensemble to the DA algorithm is transferred automatically and implicitly by DAFCC1 before running *DA_CCPL_RUN*, while the data from the DA algorithm to the model ensemble is transferred automatically and implicitly after running *DA_CCPL_RUN*.

The use of DAFCC1 requires some native code of a DA algorithm to be further updated accordingly. For example, the original communicator of the DA algorithm needs to be replaced with the communicator of the host model that can be obtained through the corresponding C-Coupler API, and the original I/O accesses for the model data in the DA algorithm can be turned off.

3.3 Implementation of the online DA procedure manager

To enable different component models to use the same DA algorithm but with different configurations, a component model can use a distinct instance of a DA algorithm with the corresponding configuration information. Corresponding to the three driving subroutines of a DA algorithm, there are three APIs (*CCPL_ensemble_procedures_inst_init*, *CCPL_ensemble_procedures_inst_run*, and *CCPL_ensemble_procedures_inst_finalize*) that enable a host model to initialize, run, and finalize the DA algorithm instance, and handle the data exchanges between the host model and the DA algorithm instance automatically. In a general case in Fig. 1b, the API *CCPL_ensemble_procedures_inst_init* is called when initializing the ensemble DA system before starting the time loop, the API *CCPL_ensemble_procedures_inst_finalize* is called after finishing the time loop, and the API *CCPL_ensemble_procedures_inst_run* is called in the time loop, which enables different assimilation cycles to share the same DA instance without restarting the model and DA algorithm. When a component model initializes, runs, or finalizes a DA algorithm instance, all ensemble members of this component model should call the corresponding API at the same time.

3.3.1 API for initializing a DA algorithm instance

The API *CCPL_ensemble_procedures_inst_init* for initializing a DA algorithm instance is designed and implemented with the following steps.

1) Determine the host model of the DA algorithm instance according to the corresponding information in the configuration file. If the DA algorithm instance is an individual algorithm that operates on the data of each ensemble member separately (e.g., Procedure 1 of DA algorithm 1 in ~~Fig. 2~~Fig. 3), each ensemble member will be a host model. Otherwise (i.e., the DA algorithm instance is an ensemble DA algorithm that operates on the data of the ensemble set; e.g., Procedure 2 of DA algorithm 1 in ~~Fig. 2~~Fig. 3), the host model will be the ensemble-set component model that will be generated automatically by the ensemble component manager.

2) Prepare information from the host model, such as model grids, parallel decompositions, and field instances, which the initialization driving subroutine of the DA algorithm can obtain via the corresponding APIs.

3) Initialize the corresponding DA algorithm instance according to the corresponding algorithm name and DLL name specified in the corresponding configuration file, where the corresponding DLL will be linked to the host model and the corresponding initialization driving subroutine in the DLL will be called. This implementation enables the user to conveniently change the DA algorithms used in simulations via the configuration file without modifying the code of the model.

4) Set up data exchange operations according to the input or output fields of the DA algorithm instance declared in the initialization driving subroutine via the corresponding APIs. If the DA algorithm instance is specified as an individual algorithm via the ensemble DA configuration (Section 3.4), the data exchange is intra the component model of each ensemble member. Otherwise, the ensemble-set component model is involved in the data exchange. The data exchange is divided into two levels: the data exchange between the ensemble members and DAFCC1, and the data exchange between DAFCC1 and the DA algorithm. The data exchange between DAFCC1 and the DA algorithm instance is simply achieved by the import/export interfaces of C-Coupler2.0, which flexibly rearrange the fields in the same component model between different parallel decompositions. If the DA algorithm instance is an ensemble algorithm, the data exchange between the ensemble members and DAFCC1 is also handled by the import/export interfaces of C-Coupler2.0, which flexibly transfer the same fields between different component models (each ensemble member and the ensemble set are different component models). Otherwise, the data exchange between the ensemble members and DAFCC1 is simplified to a data copy. DAFCC1 will hold a separate memory space for each model field relevant to the DA algorithm, which enables a DA algorithm instance to use instantaneous model results or statistical results (i.e., mean, maximum, cumulative, and minimum) in a time window, and enables an ensemble DA algorithm instance to use aggregated results or statistical results (ensemble-mean, ensemble-anomaly, ensemble-maximum, or ensemble-minimum) from ensemble members. The sets of data exchange operations for the input and output fields of the DA algorithm instance are generated separately.

Consistent with the functionalities in the above steps, the API *CCPL_ensemble_procedures_inst_init* includes the following arguments.

- The *ID* of the current ensemble member that calls the API, and the common full name of the ensemble members, which is used for determining the host model of the DA algorithm. When registering a component model to C-Coupler2.0, its *ID* is allocated and its unique full name formatted as "*parent_full_name@model_name*" is generated, where "*model_name*" is the name of the component model, and "*parent_full_name*" is the full name of the parent component model (if any). Given that the names of the coupled model and the component model 1 in ~~Fig. 4~~Fig. 5 are "*coupled*" and "*comp1*", respectively, in the one-level model hierarchy in ~~Fig. 4~~Fig. 5a, the full names of ensemble members of the component model 1 are "*comp1_1*" to "*comp1_N*" and the common full name is "*comp1_**" where "***" is a wildcard, while in the two-level model hierarchy in ~~Fig. 4~~Fig. 5b the full names of ensemble members of the component model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*".

- The name of the DA algorithm instance, which is the keyword of the DA algorithm instance and also specifies the corresponding configuration information. Different DA algorithm instances can correspond to different DA algorithms or the same DA algorithm. For example, the component models 2 and 4 use different instances of the same DA algorithm in ~~Fig. 2~~Fig. 3.

- A list of model grids and parallel decompositions, which are optional arguments that enable the DA algorithm instance to obtain grid data and use the same parallel decompositions as the host model.

- A list of field instances, which specify the model fields that can be used for assimilation. This list should cover all input or output fields of the DA algorithm.

- An optional integer array of control variables that can be obtained by the DA algorithm instance via the corresponding APIs.

- An annotation, which is a string giving a hint for locating the model code of the API call corresponding to an error or warning, is recommended but not mandatory, and should be provided by the user.

3.3.2 API for running a DA algorithm instance

The API *CCPL_ensemble_procedures_inst_run* is responsible for running a DA algorithm instance with the following steps.

1) Executing the data exchange operations for the input fields of the DA algorithm instance. This step automatically transfers the input fields from each ensemble member of the corresponding component model to DAFCC1 and then from DAFCC1 to the DA algorithm instance, where the statistical processing regarding the time window or the ensemble is done at the same time.

2) Executing the DA algorithm instance through calling the running driving subroutine of the DA algorithm.

3) Executing the data exchange operations for the output fields of the DA algorithm instance. This step automatically transfers the output fields from the DA algorithm instance to DAFCC1 and then from DAFCC1 to each ensemble member of the corresponding component model.

290   Each DA algorithm instance has a timer specified via the configuration information, which determines when the DA algorithm instance is run. The *CCPL_ensemble_procedures_inst_run* can be called for the DA algorithm instance at each time step, while the above three steps will be executed only when the corresponding timer is on. To store the input data such as the observational information, a DA algorithm instance can either share the working directory of its host model or use its own working directory specified via the configuration information. The API *CCPL_ensemble_procedures_inst_run* will change

295 and then recover the current directory for calling the running driving subroutine of the DA algorithm, if necessary.

3.3.3 API for finalizing a DA algorithm instance

    The API *CCPL_ensemble_procedures_inst_finalize* is responsible for finalizing a DA algorithm instance through calling the finalization driving subroutine of the DA algorithm.

3.4 Implementation of the ensemble DA configuration manager

300 The configuration information of all DA algorithm instances used in a coupled DA simulation is contained in an XML configuration file (e.g., ~~Fig. 6~~Fig. 7), and each DA algorithm instance has a distinct XML node (e.g., the XML node "da_instance" in ~~Fig. 6~~Fig. 7, where the attribute "name" is the name of the DA algorithm instance and also the keyword to match the name of the DA algorithm instance in API "*CCPL_ensemble_procedures_inst_init*"), which enables the user to specify the following configurations.

305   1)   The DA algorithm specified in the XML node "external_procedures" in ~~Fig. 6~~Fig. 7, where the attribute "dll_name" specifies the dynamic link library, and the attribute "procedures_name" specifies the name of the DA algorithm, which will be used to choose the driving subroutines. When the user seeks to change the DA algorithm used by a component model, it is only necessary to modify the XML node "external_procedures" in most cases.

  2)   The periodic timer specified in the XML node "periodic_timer" in ~~Fig. 6~~Fig. 7, which enables users to flexibly set the

310   frequency as well as the model time of running the corresponding DA algorithm. Besides the attribute "period_unit" and "period_count" for specifying the period of the timer, the user can specify a lag via the attribute "local_lag_count". For example, given a periodic timer <"period_unit"="hours", "period_count"=6, "local_lag_count"=3>, its period is 6 hours, and it will not be on at the 0th, 6th, and 12th hours, but instead on at the 3rd, 9th, and 15th hours due to the "local_lag_count" of 3.

315   3)   Statistical processing of input fields specified in the XML node "field_instances" in ~~Fig. 6~~Fig. 7, where the attribute "time_processing" specifies the statistical processing in each time window determined by the periodic timer and the attribute "ensemble_operation" specifies the statistical processing among ensemble members. For an individual DA algorithm, the attribute "ensemble_operation" should be set to "*none*". Besides the default specification of statistical processing shared by all fields, a field can have its own statistical processing specified in a sub node of the XML node

320   "field_instances".

4) The working directory and the scripts for pre- and post-assimilation analysis (e.g., for processing the data files of observational information) optionally specified in the XML node "processing_control" in ~~Fig. 6~~Fig. 7. When the working directory is not specified, the DA algorithm instance will use the working directory of its host model. The script specified in the sub XML node "pre_instance_script" will be called by the root process of the host model before the API *CCPL_ensemble_procedures_inst_run* calls the DA algorithm, and the script specified in the sub XML node "post_instance_script" will be called by the root process of the host model after the DA algorithm run finishes.

4 An example weakly coupled ensemble DA system based on DAFCC1

To provide further information on how to use DAFCC1 and for validating and evaluating DAFCC1, we developed an example weakly coupled ensemble DA system by combining the ensemble DA system GSI/EnKF (Shao et al., 2016; Liu et al., 2018b) and a regional **F**irst **I**nstitute of **O**ceanography **A**tmosphere-**O**cean-**W**ave (FIO-AOW) coupled model (Zhao et al., 2017; Wang et al., 2018). GSI/EnKF mainly focuses on regional numerical weather prediction (NWP) applications coupled with the Weather Research and Forecasting (WRF) model (Wang et al., 2014), while FIO-AOW consists of WRF, the Princeton Ocean Model (POM; Blumberg and Mellor 1987; Wang et al., 2010), the MArine Science and NUmerical Modeling wave model (MASNUM; Yang et al., 2005; Qiao et al, 2016), and all the above three model components are coupled together by using C-Coupler (Liu et al., 2014, 2018b). FIO-AOW has already been used in the research for exploring the sensitivity of typhoon simulation to physical processes and improving typhoon forecasting (Zhao et al, 2017; Wang et al., 2018). There are two main steps in developing the example system.

1) We developed an ensemble DA sub-system of WRF by adapting GSI/EnKF to DAFCC1. This sub-system helps validate DAFCC1 and evaluate the improvement in performance obtained by DAFCC1 (Section 5).

2) We merged the above sub-system and FIO-AOW to produce the example DA system that only computes atmospheric analyses corresponding to WRF currently. This system demonstrates the correctness of DAFCC1 in developing a weakly coupled ensemble DA system.

4.1 An ensemble DA sub-system of WRF

4.1.1 Brief introduction to GSI/EnKF

GSI/EnKF combines a variational DA sub-system (GSI; Shao et al., 2016) and an ensemble DA sub-system (EnKF; Liu et al., 2018a), which can be used as a variational, a pure ensemble or a hybrid DA system sharing the same observation operator in the GSI codes. It provides two options for calculating analysis increments for ensemble DA; i.e., a serial Ensemble Square Root Filter (EnSRF) algorithm (Whitaker et al., 2012) and a Local Ensemble Kalman Filter (LETKF) algorithm (Hunt et al., 2007). In this paper, we use the pure ensemble DA system without using variational DA, where GSI is used as the observation operator that calculates the difference between model variables and observations on the observation space and EnSRF is chosen for calculating atmospheric analyses and updating atmosphere model variables.

Figure 87a shows the flowchart for running the pure ensemble DA system of the WRF model in a DA window. It consists of the following main steps that are driven by scripts, while the data exchanges between these main steps are achieved via data files.

355 1) Ensemble model forecast. An ensemble run of WRF is initiated or restarted from a set of input data files, and then is stopped after producing a set of output files (called model background files hereafter) for DA and for restarting the ensemble run in the next DA window.

2) Calculating the ensemble mean of model DA variables. A separate executable is initiated for calculating the ensemble mean of each DA variable based on the model background files, and then outputs the ensemble mean to a new background

360 file.

3) Observation operator for the ensemble mean. GSI is initiated as the observation operator for the ensemble mean. It takes the ensemble mean file, files of various observational data (e.g., conventional data, satellite radiance observations, GPS radio occultations, and radar data) and multiple fixed files (e.g., statistic files, configuration files, bias correction files, and CRTM coefficient files) as input, and produces an observation prior (observation innovation) file for the ensemble mean

365 and files containing observational intermediate information (e.g., bias correction and thinning).

4) Observation operator for each ensemble member. GSI is initiated as the observation operator for each ensemble member. It takes the background file of the corresponding ensemble member, the fixed files and the observational intermediate information files as input, and produces an observation prior file for the corresponding ensemble member.

5) EnKF for calculating analysis increments. EnKF is initiated for calculating analysis increments of the whole ensemble. It

370 takes the model background files, the observation prior files and the fixed files as input, and finally updates model background files with the analysis increments. The updated model background files are used for restarting the ensemble model forecast in the next DA window.

4.1.2 Adapting GSI/EnKF to DAFCC1

When adapting GSI/EnKF to DAFCC1, an ensemble-set component model derived from the ensemble forecast of WRF

375 (corresponding to the first main step in Section 4.1.1) is generated as the host model that drives the DA algorithm instances corresponding to the remaining main steps. As shown in Fig. 8Fig. 9, three DA instances corresponding to the last three main steps in Section 4.1.1 (i.e., observation operator for the ensemble mean, observation operator for each ensemble member, and EnKF for calculating analysis increments) are enclosed in DLLs, without a DA algorithm instance corresponding to the second main step in Section 4.1.1. This is because the online DA procedure manager of DAFCC1 enables a DA algorithm instance to

380 automatically obtain the ensemble mean of model DA variables (Section 3.3). Although both the third and fourth main steps correspond to the same GSI, they are transformed into two different DA algorithm instances, because the third is an ensemble algorithm (i.e., it operates on the data of the ensemble set) and the fourth is an individual algorithm (i.e., it operates on the data of each ensemble member). Moreover, we compiled the same GSI code into two separate DLLs, each of which corresponds to one of these two instances, to enable these two instances to use different memory space.

For each DA algorithm instance, three driving subroutines and the corresponding configuration were developed (~~Fig. 8~~Fig. 9). In fact, the two instances corresponding to GSI share the same driving subroutines but use different configurations (especially regarding the specification of "ensemble_operation"). To enable the GSI code and EnKF code to be used as DLL, we made the following slight modifications to the code.

1) We turned off the MPI initialization and finalized and replaced the original MPI communicator with the MPI communicator of the host model that can be obtained via DAFCC1.

2) We obtained the required model information and the declared input/output fields via DAFCC1, and turned off the corresponding I/O accesses.

To drive the DA algorithm instances, the WRF code was updated with the new subroutines for initializing, running, and finalizing all DA algorithm instances. Moreover, the functionality of outputting model background files can be turned off, because the data exchanges between WRF and the DA algorithm instances are automatically handled by DAFCC1 and the WRF ensemble can be run continuously throughout DA windows without stopping and restarting. As a result, DAFCC1 saves sets of data files and the corresponding I/O access operations, while only the observation files, fixed files, and the files for the data exchanges among the DA algorithm instances are reserved (compare ~~Fig. 7~~Fig. 8b and ~~Fig. 7~~Fig. 8a).

4.2 Example ensemble DA system of FIO-AOW

FIO-AOW, which previously used C-Coupler1 (Liu et al., 2014) for model coupling, has already been upgraded to C-Coupler2.0 by us (Fig. 10a). As GSI/EnKF and FIO-AOW share WRF, the development of the example ensemble DA system of FIO-AOW in Fig. 10b can significantly benefit from the DA system of WRF~~.~~ ~~and i~~In this ensemble DA system, the ensemble of WRF computes atmospheric analyses based on the ensemble DA sub-system in Section 4.1, while each ensemble member of other component models is impacted by the atmospheric analyses via model coupling. It only took the following steps to construct the example ensemble DA system.

1) Using the ensemble component manager, set up the two hierarchical levels of models shown in ~~Fig. 9~~Fig. 11; i.e., the first level corresponds to all ensemble members of FIO-AOW while each member includes its three component models at the second level.

2) Merge the model code modifications, the DA algorithm instances, and configurations in the DA system of WRF into the example ensemble DA system FIO-AOW.

As well as being described by the flowchart involving the WRF and the DA algorithm instances in ~~Fig. 7~~Fig. 8b, the example ensemble DA system of FIO-AOW follows the process layout in ~~Fig. 10~~Fig. 12, which is essentially a real case of the process layout in ~~Fig. 2~~Fig. 3.

5 Validation and evaluation of DAFCC1

415 In this section, we evaluate the correctness of DAFCC1 in developing a weakly coupled ensemble DA system based on the example ensemble DA system (referred to as the full-example-DA-system hereafter) described in Section 4, and will also validate DAFCC1 and evaluate the impact of DAFCC1 in accelerating DA based on the sub-system with WRF and GSI/EnKF (WRF-GSI/EnKF hereafter).

5.1 Experimental setup

420 The example ensemble DA system used in this validation and evaluation consists of WRF Version 4.0 (Wang et al., 2014), GSI version 3.6 and EnKF version 1.2, and the corresponding versions of POM and MASNUM used in FIO-AOW (Zhao et al., 2017; Wang et al., 2018). In EnKF version 1.2 the default settings are used; i.e., the EnSRF algorithm is used to calculate analysis increments for ensemble DA, the inflation factor is 0.9 without smoothing, and the covariance is localized by distance correlation function with horizontal localization radius of 400 km and vertical localization scale coefficient of 0.4. The example
425 ensemble DA system is run on a supercomputer of the Beijing Super Cloud Computing Center (BSCC) with the lustre file system. Each computing node on the supercomputer includes two Intel Xeon E5-2678 v3 CPUs (Intel(R) Xeon(R) CPU), with 24 processor cores in total, and all computing nodes were connected with an InfiniBand network. The codes were compiled by an Intel Fortran and C++ compiler at the optimization level O2, using an Intel MPI library. A maximum 3200 cores are used for running the example ensemble DA system.

430 The WRF-GSI/EnKF integrates over an approximate geographical area generated from a Lambertian projection of the area 0°–50°N, 99°–160°E with center point at 35°N, 115°E. Initial fields and lateral boundary conditions (at 6 hour intervals) for the ensemble run of WRF are taken from the NCEP Global Ensemble Forecast System (GEFS) (at 1° × 1° resolution) (https://www.ncdc.noaa.gov/data-access/model-data/model-datasets/global-ensemble-forecast-system-gefs). To configure WRF, an existing physics suite 'CONUS' (https://www2.mmm.ucar.edu/wrf/users/ncar_convection_suite.php) and 32 vertical
435 sigma layers with the model top at 50 hPa are used. One-day integration on June 1st, 2016 is used for running the WRF-GSI/EnKF. NCEP global GDAS Binary Universal Form for the Representation of meteorological data (BUFR; https://www.emc.ncep.noaa.gov/mmb/data_processing/NCEP_BUFR_File_Structure.htm) and Prepared BUFR (https://www.emc.ncep.noaa.gov/mmb/data_processing/prepbufr.doc/document.htm), including conventional observation data and satellite radiation data, are assimilated every 6 hours (i.e., at 0000, 0600, 1200, and 1800 UTC). The air temperature
440 (T), specific humidity (QVAPOR), longitude and latitude wind (UV), and column disturbance dry air quality (MU) are the variables analyzed in the data assimilation. The WRF-GSI/EnKF experiments are classified into four sets, where variations of horizontal resolution (and the corresponding time step), number of ensemble members and process number (each process runs on a distinct processor core) are considered (Tables 1 and 2).

All component models of the full-example-DA-system integrate over the same geographical area (0°–50°N, 99°–150°E)
445 with the same horizontal resolution of 0.5° × 0.5° but different time steps (100 s for WRF and 300 s for POM and MASNUM,

coupled by C-Coupler2.0 at 300 s intervals). More details of the model configurations can be found in Zhao et al. (2017). The configuration of initial fields, lateral boundary conditions, and observations of WRF for the ensemble run of the full-example-DA-system are the same as for WRF-GSI/EnKF. The full-example-DA-system integrates over 3 days (June 1st to 3rd, 2016), while the first model day is considered as spin-up, and DA is performed every 6 hours in the last two model days with T, UV and MU as DA variables.

5.2 Validation of DAFCC1

To validate DAFCC1, we compare the outputs of the two versions of WRF-GSI/EnKF: the original WRF-GSI/EnKF (hereafter offline WRF-GSI/EnKF; https://dtcenter.org/community-code/gridpoint-statistical-interpolation-gsi/community-gsi-version-3-6-enkf-version-1-2) and the new version of WRF-GSI/EnKF with DAFCC1 (hereafter online WRF-GSI/EnKF) introduced in Section 4.1. As DAFCC1 improves only the data exchanges between a model and the DA algorithms, the simulation results of an existing DA system should not change when it is adapted to use DAFCC1. We therefore employ a validation standard that the WRF-GSI/EnKF with DAFCC1 keeps bit-identical result with the original offline WRF-GSI/EnKF. DAFCC1 passes the validation test with all experimental setups in Table 2, where the binary data files output by WRF at the end of the 1-day integration are used for the comparison.

5.3 Impact in accelerating an offline DA

WRF-GSI/EnKF is further used to evaluate the impact of DAFCC1 in accelerating an offline DA, by comparing the execution time of the offline and online WRF-GSI/EnKF under each experimental setup in Table 2. Considering that all ensemble members of the online WRF-GSI/EnKF are integrated simultaneously, we run all ensemble members of the offline WRF-GSI/EnKF concurrently through a slight modification to the corresponding script, in order to make a fair comparison.

The impact of varying the number of ensemble members is evaluated based on Set 1 in Table 2. DAFCC1 obviously accelerates WRF-GSI/EnKF, and can achieve higher performance speedup with more ensemble members (~~Fig. 11~~Fig. 13a). This is because DAFCC1 significantly accelerates the DA for both GSI and EnKF (~~Fig. 11~~Fig. 13b-d). Similarly, DAFCC1 significantly accelerates the DA as well as WRF-GSI/EnKF under different process numbers (~~Fig. 12~~Fig. 14, corresponding to Set 2 in Table 2) and resolution (~~Fig. 13~~Fig. 15, corresponding to Set 3 in Table 2). Considering that more processor cores are generally required to accelerate the model run under higher resolution, we also make an evaluation based on Set 4 in Table 2, where concurrent changes in resolution and process number are made to achieve similar numbers of grid points per process throughout the experimental setups. This evaluation also demonstrates the correctness of DAFCC1 in accelerating the DA as well as WRF-GSI/EnKF (~~Fig. 14~~Fig. 16).

The performance speedups observed from Figs. 11-–14 result mainly from the significant decrease in I/O accesses. Although the online WRF-GSI/EnKF still has to access the observation prior files (Section 4.1.1 and ~~Fig. 7~~Fig. 8b), most I/O accesses correspond to the model ensemble background files and model ensemble analysis files, and these I/O accesses have been

eliminated by DAFCC1 (Table 3). Moreover, more I/O accesses can be saved under higher resolution or more ensemble members.

We note that, the execution time of the offline GSI in ~~Fig. 11~~Fig. 13c increases when using more ensemble members. This
480   is reasonable, because more ensemble members introduce more I/O accesses, as shown in Table 3. We also note that, the execution time of the offline and online EnKF in ~~Fig. 11~~Fig. 13d and ~~Fig. 12~~Fig. 14 increases when using more ensemble members. This is because the current parallel version of EnKF does not achieve good scaling performance, and thus longer execution time can be observed when EnKF uses more processor cores.

5.4 Correctness in developing a weakly coupled ensemble DA system

485   We have successfully run the full-example-DA-system with ten ensemble members, which enables us to investigate the model ~~variables~~ fields before and after DA. We find that changes to the atmospheric~~model~~ ~~variables~~ fields resulting from DA can be observed; e.g., the bias regarding T is slightly decreased and the bias regarding UV is more obviously decreased after using DA, as shown in ~~Fig. 15~~Fig. 17.

Changes to the atmospheric fields predicted based on the initial fields updated with the atmospheric analyses can also be
490   observed (e.g., the fields U and V in Fig. 18). Although only atmospheric analyses are computed currently, the model coupling in the weakly coupled DA system makes ocean and wave fields impacted by the atmospheric analyses, and therefore changes to the ocean and wave fields can be observed in a prediction (e.g., the fields SST and HS in Fig. 18).

6 Conclusions and discussion

In this paper, we propose a new common, flexible and efficient framework for weakly coupled ensemble data assimilation
495   based on C-Coupler2.0, DAFCC1. It provides simple APIs and a configuration file format to enable users to conveniently integrate a DA method into a model as a procedure that can be directly called by the model, while still guaranteeing the ~~software~~ independence of configuration and compilation systems between the model and the DA method. The example weakly coupled ensemble DA system in Section 4 and the evaluations in Section 5 demonstrate the correctness of DAFCC1 in both developing a weakly coupled ensemble DA system and accelerating an offline DA system. The development of a DA system
500   that only employs a single model run but not an ensemble run can also benefit from the advantages of DAFCC1, while the functionality of data exchanges will be automatically simplified without generating ensemble-set component models for saving extra overhead.

DAFCC1 is able to automatically handle data exchanges between a model ensemble and a DA algorithm because its design and implementation significantly benefit from C-Coupler2.0, which already has the functionalities of automatic coupling
505   generation and automatic data exchanges between different component models or within the same component model. DAFCC1 will therefore be an important functionality of the next generation of C-Coupler (C-Coupler3) that is planned to be released no later than 2022. Although the example ensemble DA system of FIO-AOW developed in this work only computes atmospheric

analyses currently, the future work similar to adapting GSI/EnKF to DAFCC1 can be conducted to further enable the computation of ocean or wave analyses. Moreover, we have considered software extendibility when designing and
510 implementing DAFCC1, which will enable us to conveniently achieve upgrades either for strongly coupled ensemble DA systems or for more types of data exchange operations in the future. As shown in ~~Fig. 7~~Fig. 8, the I/O accesses to the observation prior files for the data exchanges between DA algorithms are still retained after using DAFCC1. Although they are not currently a performance bottleneck (Table 3), we will investigate how to avoid these types of I/O accesses when further upgrading DAFCC1.

515 Regarding the evaluations in Section 5, we can only use at most 3200 processor cores, which limits the maximum number of cores per ensemble member. Consequently, we use relatively coarse resolutions of WRF and FIO-AOW. However, the results in ~~Fig. 14~~Fig. 16 from the experiment Set 4 in Table 2 indicate that DAFCC1 will also obviously accelerate the DA system when using a finer resolution and more processor cores, because it will also significantly decrease I/O accesses. DAFCC1 can tackle the technical challenges in developing or accelerating a DA system, but cannot contribute to improvements
520 in simulation results that generally depend on scientific settings which must be determined in the research environment (e.g., the DA algorithm configuration, the inflation factor, localization settings, initial states of the model ensemble run). Consequently, we did not examine the improvements in simulation results resulting from the full-example-DA-system based on various variables in Section 5.4, but only made a simple comparison of simulation results demonstrating that the full-example-DA-system can successfully run and produce simulation results.

525 The offline implementation of a DA system that relies on disk files and restart functionalities of models and DA algorithms can be a robust strategy when it comes to massively parallel computing where the risk of random task failures generally increases with more processor cores used by a task, because a failed task that corresponds to an ensemble member can be resumed from the corresponding restart files. The online implementation that unifies all ensemble members into a task enables to significantly increase the number of cores used by a task. At the same time of enlarging the risk of random task failures, the
530 online implementation can decrease such risk because it can significantly reduce disk file accesses that are generally an important source of task failures. The robustness of an online implementation can be further improved through developing the restart capability of the DA system based on the restart capabilities of the model and C-Coupler2, while users are enabled to flexibly set the restart-file-writing frequency for the online implementation that can be lower than the corresponding frequency for an online implementation generally determined by observation data frequencies. Moreover, the impact of the overhead of
535 writing restart files in an online implementation can be further decreased via asynchronous I/O support.

Code availability. The source code of DAFCC1 can be viewed via https://doi.org/10.5281/zenodo.3739729 (please contact us for authorization before using DAFCC1 for developing a system). The original source code and scripts corresponding to WRF and GSI/EnKF can be download from https://www2.mmm.ucar.edu/wrf/users/downloads.html and https://dtcenter.org/com-GSI/users/downloads/index.php respectively. For the source code of FIO-AOW, please contact the authors of (Zhao et al.,

540 2017; Wang et al., 2018). The additional codes, configurations, scripts and guidelines for developing and running the example weakly coupled ensemble DA system can also be download from https://doi.org/10.5281/zenodo.3774710.

Author contributions. CS was responsible for code development, software testing and experimental evaluation of DAFCC1 with the example DA system, contributed to the motivation and design of DAFCC1 and co-led paper writing. LL initiated this research, was responsible for the motivation and design of DAFCC1, co-supervised CS, and co-led paper writing. RL, XY and
545 HY contributed to code development and software testing. BZ, GW, JL and FQ contributed to the development of the example DA system. BW contributed to scientific requirements and the motivation, and co-supervised CS. All authors contributed to improvement of ideas and paper writing.

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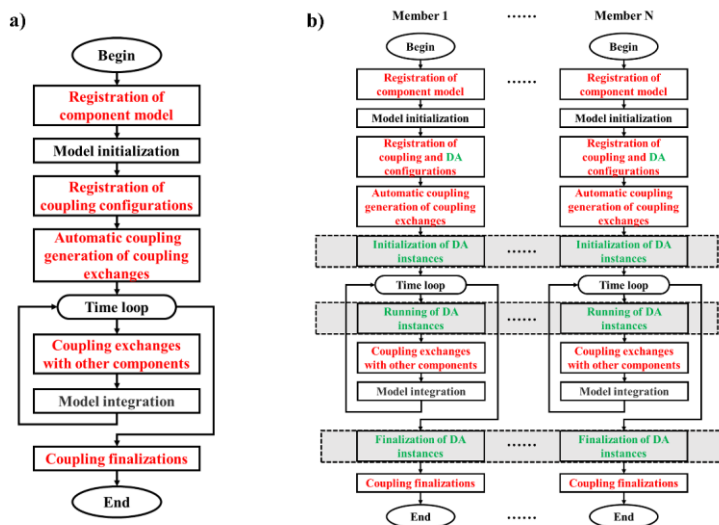

725 **Figure 1. Model flowchart with C-Coupler2.0 (a) and new model flowchart with ensemble DA based on C-Coupler2.0 (b). Black font indicates the major steps in the original flowchart of a component model without coupling, red font indicates the major steps for achieving coupling exchanges among component models with C-Coupler2.0, and green font indicates the new steps for achieving coupling exchanges between a DA algorithm and a model ensemble. The gray shadow in a dashed rectangle indicates that all members in a model ensemble cooperatively work together for the corresponding step.**

730

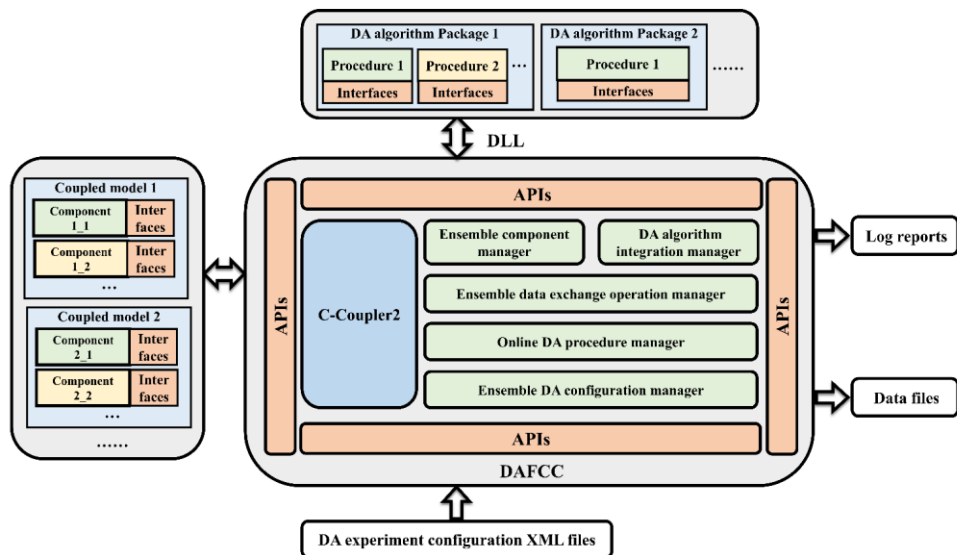
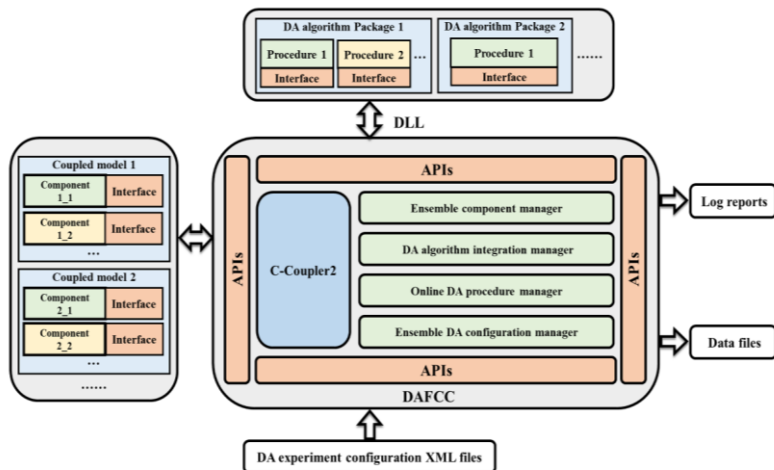



Figure 12. Architecture of DAFCC1.

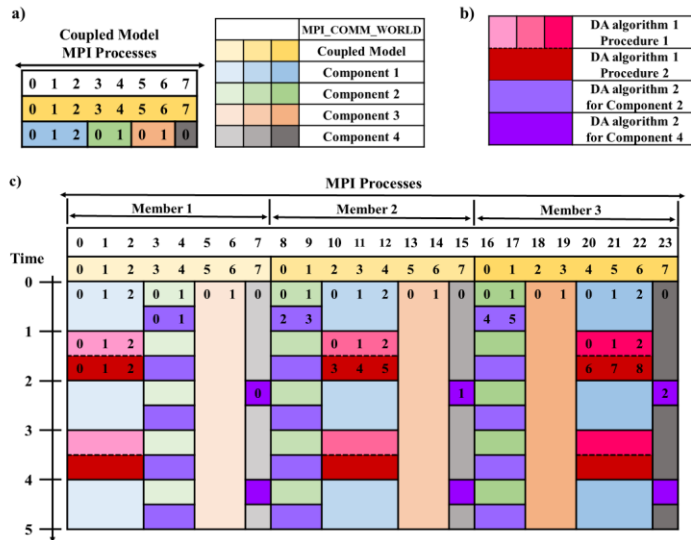



Figure 23. Example of running a DAFCC1-based weakly coupled ensemble DA system with three ensemble members. (a) Each ensemble member of the coupled model (yellow series) uses 8 MPI processes, where component 1 (blue series) uses three MPI processes, component 2 (green series) uses two MPI processes, component 3 (orange series) uses two MPI processes, and component 4 (grey series) uses one MPI process. (b) DA algorithm 1 and two instances of DA algorithm 2 (purple series) are used in this DA system, where DA algorithm 1 includes procedure 1 (pink series) and procedure 2 (red). (c) Execution of the DA system: the process layout of ensemble members of component models, the process layout of DA algorithms, and the alternative execution of a DA algorithm and the corresponding component model. Each number in the colored box in (a) and (c) indicates the process ID in the corresponding local communicator of a member of the coupled model, a member of a component model, or all members of a component model.

```
mpirun –np N1_1 Comp1 namelist CCPL_ensemble_3_1 : –np N1_2 Comp2 namelist
CCPL_ensemble_3_1 : –np N2_2 Comp2 namelist CCPL_ensemble_3_2 : –np N2_1 Comp1
namelist CCPL_ensemble_3_2 : –np N3_1 Comp1 namelist CCPL_ensemble_3_3 : –np N3_2
Comp2 namelist CCPL_ensemble_3_3
```

Figure 43. Example of the command for submitting an MPI run of three ensemble members of a coupled model that consists of Comp1 and Comp2. Comp1 can be before Comp2 at the second ensemble member, and the process numbers N1_1, N2_1, and N3_1 of Comp1 at different ensemble members can be different.

750

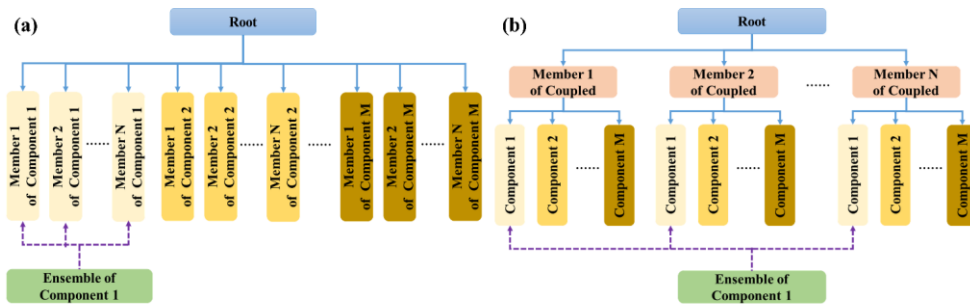



Figure 54. Two examples of the organization of N ensemble members of a coupled model consisting of M component models. (a) Single-level organizational architecture of all ensemble members of the component models in the coupled model. (b) Two-hierarchical-levels organizational architecture. All ensemble members of the coupled model are organized as the first level with all component models from each ensemble member of the coupled model at the second level. An ensemble that covers all ensemble members of component model 1 is generated as an example for using the DA algorithm in ensemble component manager.

755

a)

1	**Subroutine** *DA*_**CCPL_INIT**
2	Obtain model information and grids from C-Coupler2
3	Initialize grid and parallel decomposition
4	Allocate memory spaces of variables
5	Initialize other operations
6	Register the parallel decompositions, required grids and field instances to C-Coupler2
7	Declare field instances as implicit input or output arguments
8	**End subroutine** *DA*_**CCPL_INIT**

b)

1	**Subroutine** *DA*_**CCPL_RUN**
2	DA analysis
3	**End subroutine** D*A*_**CCPL_RUN**

c)

1	**Subroutine** *DA*_**CCPL_FIN**
2	DA finalize
3	**End subroutine** *DA*_**CCPL_FIN**

760   **Figure 65. Example of the driving subroutines in a DA algorithm. (a) Initialization driving subroutine. (b) Running driving subroutine. (c) Finalization driving subroutine. The name of the DA algorithm "DA" is used as the prefix of the three driving subroutines; different suffixes are used for distinction. Black font indicates original functionalities of the DA algorithm, while red font indicates additional operations to perform online data exchanges between the model and DA algorithm.**

```
1   <root>
2   <da_instance name="DA_algorithm1_procedure1" status="on">
3       <external_procedures status="on" procedures_name="algorithm1_procedure1" dll_name="lib_da1_p1.so"/>
4       <periodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/>
5       <field_instances status="on" time_processing="inst" ensemble_operation="none"/>
6       <processing_control status="on" >
7           <working_directory status="off" path=""/>
8           <config_scripts status="on">
9               <pre_instance_script status="on" name="da1_p1_online_run.sh"/>
10              <post_instance_script status="off" name=""/>
11          </config_scripts>
12      </processing_control>
13  </da_instance>
14  <da_instance name="DA_algorithm1_procedure2" status="on">
15      <external_procedures status="on" procedures_name="algorithm1_procedure2" dll_name="lib_da1_p2.so"/>
16      <periodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/>
17      <field_instances status="on" time_processing="inst" ensemble_operation="aver">
18          
19          
20      </field_instances>
21      <processing_control status="on" >
22          <working_directory status="on" path="./experiment/da1"/>
23          <config_scripts status="on">
24              <pre_instance_script status="off" name=""/>
25              <post_instance_script status="on" name="da1_p2_online_run.sh"/>
26          </config_scripts>
27      </processing_control>
28  </da_instance>
29  <da_instance name="DA_algorithm2" status="on">
30      <external_procedures status="on" procedures_name="algorithm2" dll_name="lib_da2.so"/>
31      <periodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/>
32      <field_instances status="on" time_processing="inst" ensemble_operation="gather"/>
33      <processing_control status="on" >
34          <working_directory status="on" path="./experiment/da2"/>
35          <config_scripts status="on">
36              <pre_instance_script status="on" name="./scripts/da2_pre_online_run.sh"/>
37              <post_instance_script status="on" name="./scripts/da2_post_online_run.sh"/>
38          </config_scripts>
39      </processing_control>
40  </da_instance>
41  </root>
```

765 **Figure 76. Example of the XML configuration for a DA experiment.**

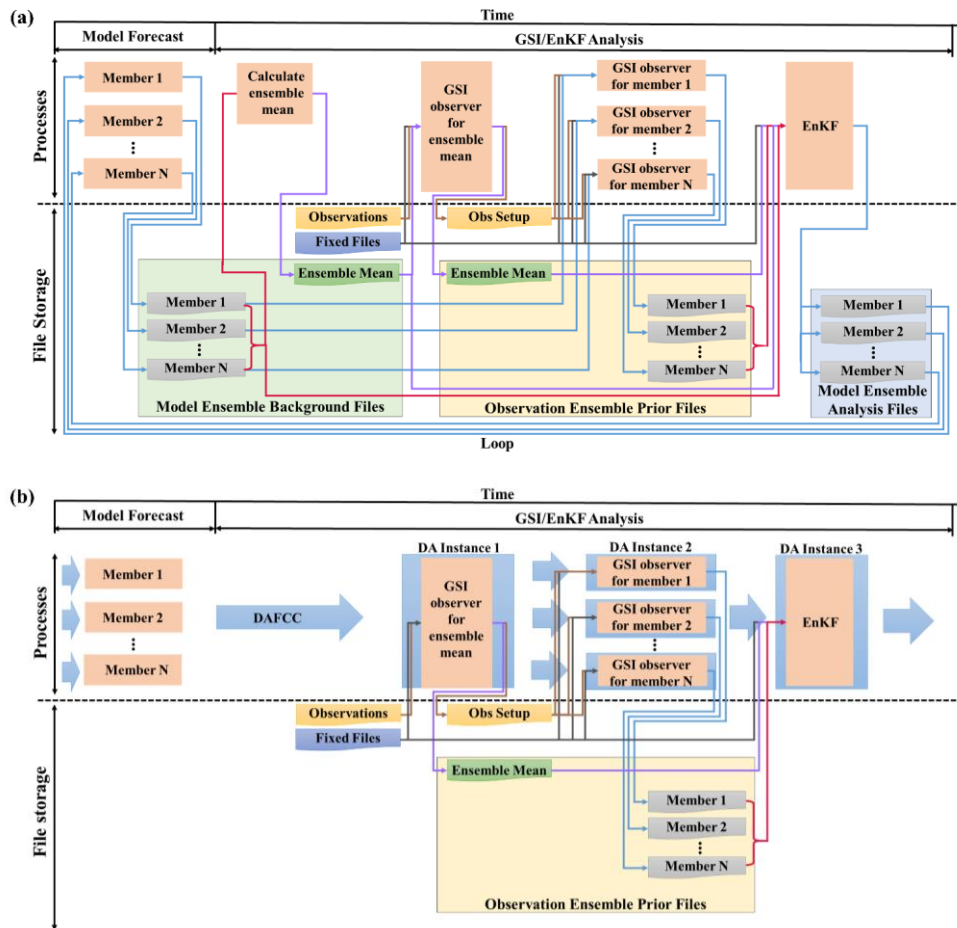
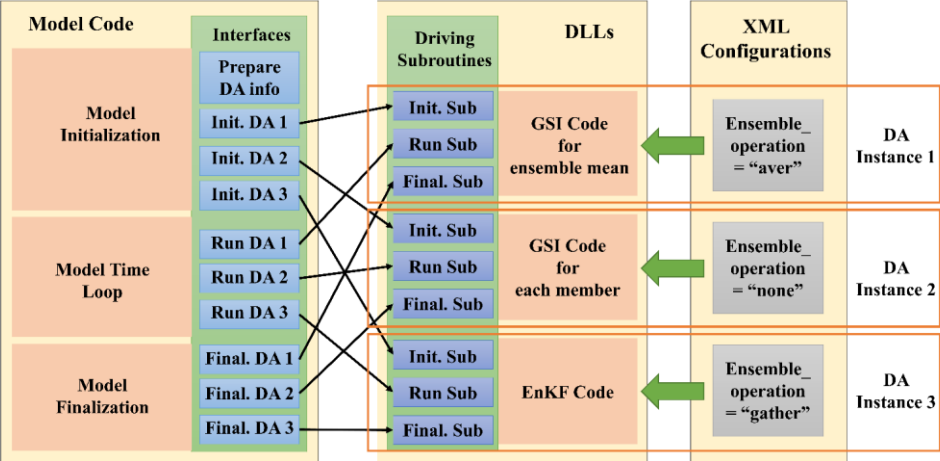



Figure 8~~7~~. Running processes and data scheduling for (a) original GSI/EnKF used as a pure ensemble DA system, and (b) modified GSI/EnKF based on DAFCC1. Orange rectangles in the Processes panel indicate different running processes, while thick blue arrows mark data scheduling based on DAFCC1. Rectangles of various colors with a curved lower edge in the File Storage panel indicate different files, while arrows of different colors indicate the scheduling of corresponding files.

770

775   **Figure 98. Modifications of model code and the invoking of relationships to the DA algorithm in the example ensemble DA system.**

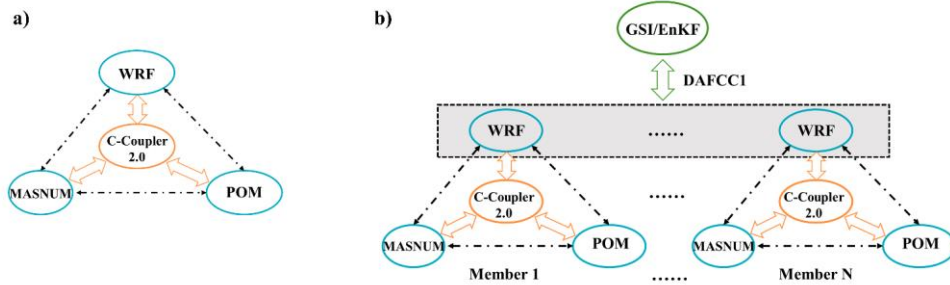



Figure 10. Architecture of FIO-AOW (a) and the corresponding example ensemble DA system (b). The gray shadow in a dashed rectangle in (b) indicates that atmospheric analyses are computed by GSI/EnKF that has been coupled with the ensemble of WRF based on DAFCC1.

780

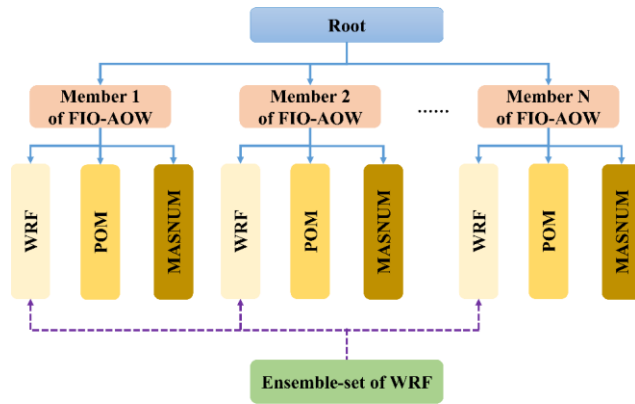



Figure 911. Two-hierarchical-level organizational architecture for N ensemble members of FIO-AOW consisting of WRF, POM, and MASNUM. All ensemble members of FIO-AOW are organized as the first level with all component models in each ensemble member at the second level. An ensemble-set that covers all ensemble members of component model WRF is generated by the ensemble component manager.

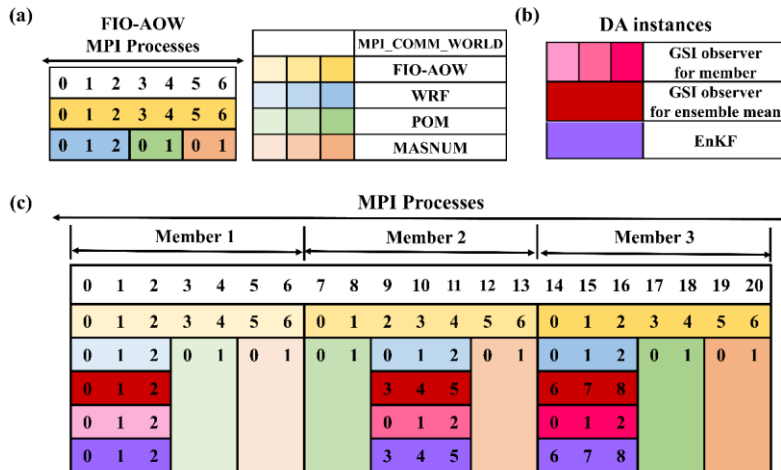
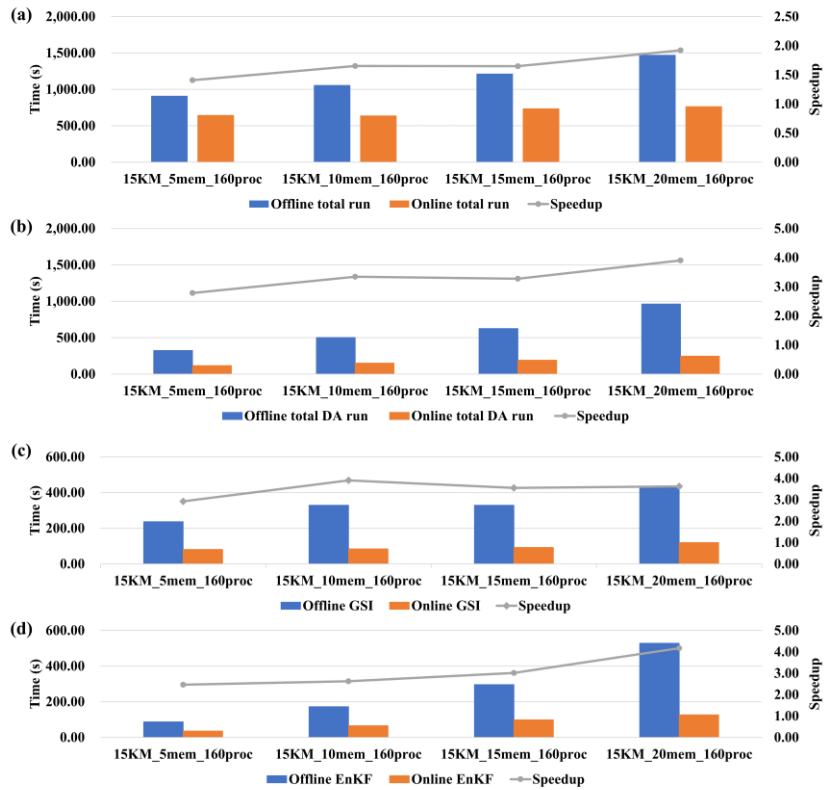
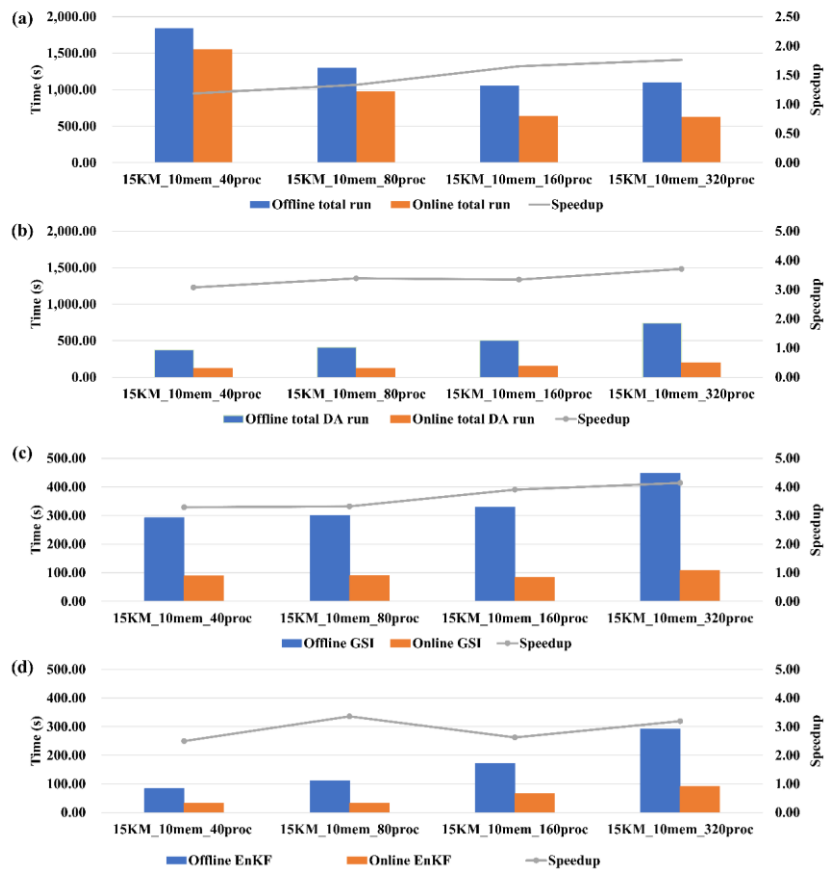
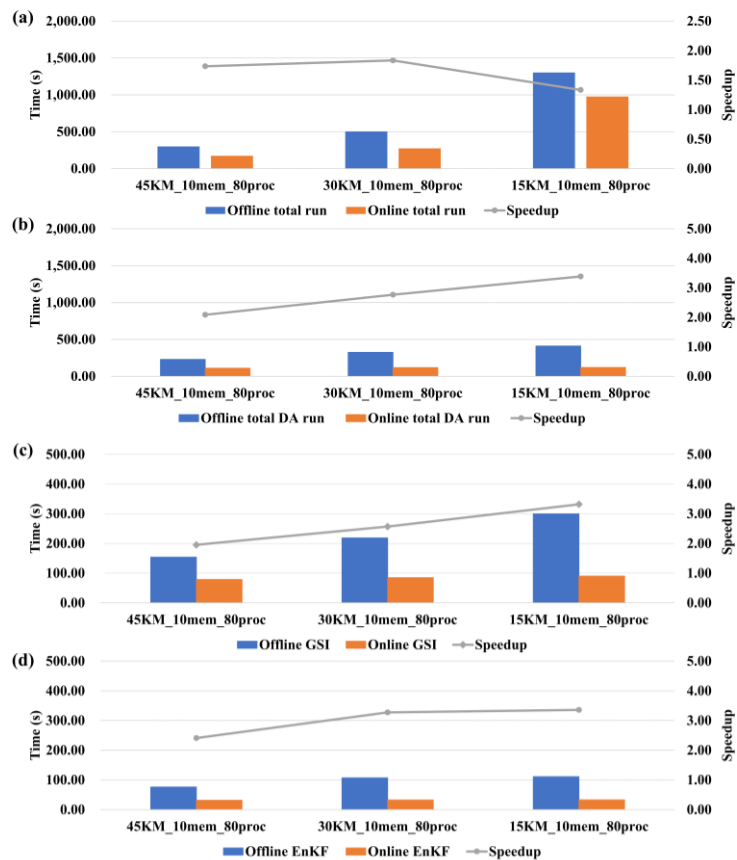
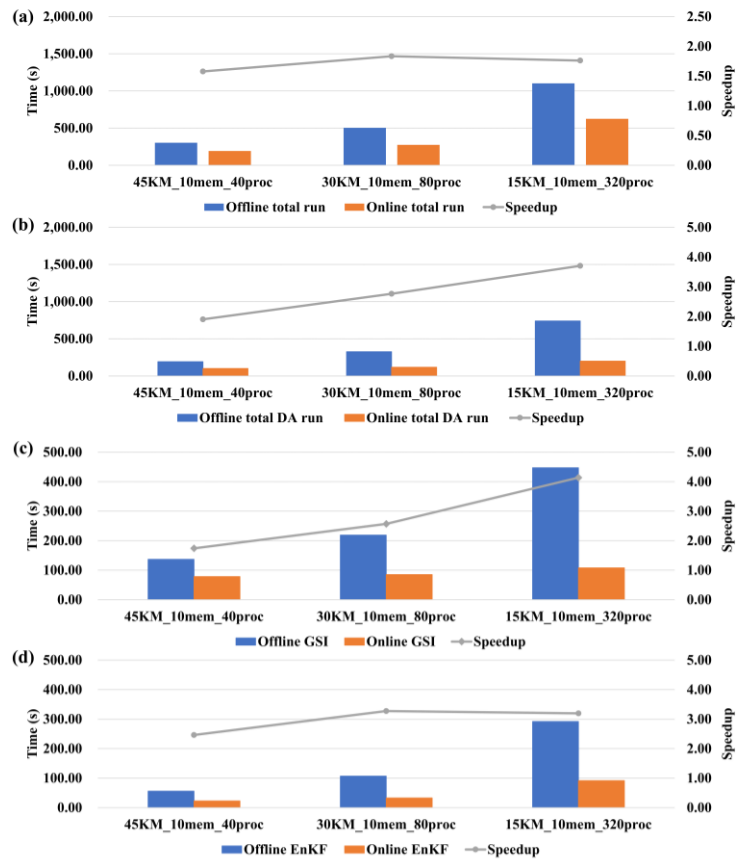
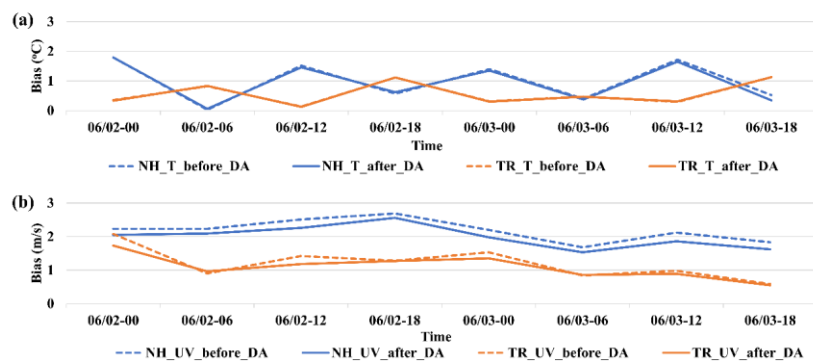



Figure 120. Example of the process layout of the example ensemble DA system FIO-AOW. (a) Each ensemble member of FIO-AOW (yellow series) uses 7 MPI processes, where WRF (blue series) uses 3 MPI processes, POM (green series) uses 2 MPI processes, and MASNUM (orange series) uses 2 MPI processes. (b) Two DA algorithm instances of GSI are adopted for each member (pink series) and ensemble mean (red) respectively following another DA algorithm instance of EnKF in this DA system. (c) Process layout of the DA system: the process layout of ensemble members of component models and the process layout of DA algorithms. Each number in the colored boxes in (a) and (c) indicates the process ID in the corresponding local communicator of a member of the coupled model, a member of a component model, or all members of a component model.

800 **Figure 1~~3~~4. Execution time (colored bars) corresponding to the online and offline WRF-GSI/EnKF and the corresponding speedup (gray line, ratio of offline execution time to online execution time) from experiment set 1 in Table 2. (a) Total run (including model run and DA algorithms run). (b) DA algorithms (including GSI and EnKF) run. (c) GSI run. (d) EnKF run.**

805   **Figure 1~~4~~2. As in ~~Fig. 11~~Fig. 13, but from experiment set 2 in Table 2.**

810   **Figure 1~~5~~3. As in ~~Fig. 11~~Fig. 13, but from experiment set 3 in Table 2.**

815 **Figure 1~~6~~4. As in ~~Fig. 11~~Fig. 13, but from experiment set 4 in Table 2.**

820 **Figure 17̶5̲. Total bias of assimilated variables relative to corresponding observations before and after DA for (a) T and (b) UV at each DA time from the EnKF standard output file. The dotted lines indicate the bias of assimilated variables before DA and the solid lines indicate the bias of assimilated variables after DA. Blue lines are the bias in the area of 0°–25° N, and orange lines are the bias in the area of 25°–50° N.**

825

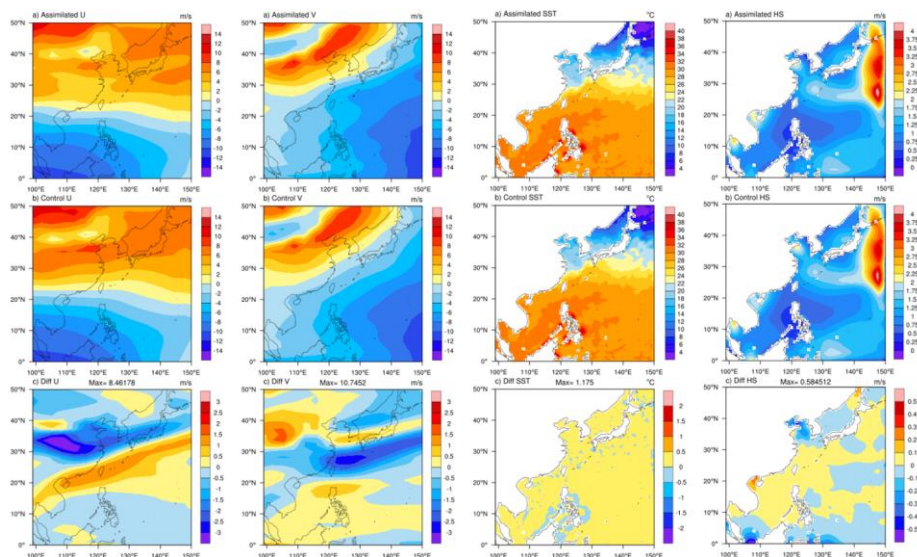



Figure 18. Simulation results of FIO-AOW (at 06:00 on June 3rd, 2016) about the fields of meridional wind (U; the first column) and zonal wind (V; the second column) produced by WRF, sea surface temperature (SST; the third column) produced by POM, and sea surface significant wave height (HS; the fourth column) produced by MASNUM. The first row shows the results of the full-example-DA-system predicted since 00:00 on June 3rd, based on the DA experimental setup in Section 5.1, the second row shows the results without DA and the third row is the corresponding differences.

830

Table 1. Horizontal resolutions and time steps of WRF.

Horizontal Resolution	Total Horizontal Grid Points	Time Step
45 km	160×120	180 s
30 km	240×180	120 s
15 km	480×360	60 s

840 **Table 2. Setup of four experiment sets in terms of horizontal resolution, number of ensemble members and number of processes**

Experiment set	Horizontal resolution	Number of ensemble members	Processes for each ensemble member	Label marks
Set 1	15 km	5	160	15KM_5mem_160proc
		10		15KM_10mem_160proc
		15		15KM_15mem_160proc
		20		15KM_20mem_160proc
Set 2	15 km	10	40	15KM_10mem_40proc
			80	15KM_10mem_80proc
			160	15KM_10mem_160proc
			320	15KM_10mem_320proc
Set 3	45 km	10	80	45KM_10mem_80proc
	30 km			30KM_10mem_80proc
	15 km			15KM_10mem_80proc
Set 4	45 km	10	40	45KM_10mem_40proc
	30 km		80	30KM_10mem_80proc
	15 km		320	15KM_10mem_320proc

Table 3. I/O access statistics corresponding to WRF-GSI/EnKF

Horizontal resolution	Number of ensemble members	Number of observation prior files	Total I/O accesses to observation priors	Number of model ensemble background & analysis files	Total I/O accesses to model ensemble background & analysis files
15 km	5	12	0.11 GB	324	129.13 GB
15 km	10	22	0.21 GB	624	251.30 GB
15 km	15	32	0.30 GB	924	373.48 GB
15 km	20	42	0.39 GB	1224	495.65 GB
30 km	10	22	0.18 GB	624	62.86 GB
45 km	10	22	0.17 GB	624	27.96 GB