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 (Data Assimilation Framework based on C-Coupler2.0, 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 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

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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 the ensemble run of members from the same model.
- 40 With the rapid development of science and technology, numerical forecasting systems are evolving 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 earthEarth 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; Penny
- 45 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 such as the Data Assimilation Research Testbed (DART; Anderson et al., 2009) and the Grid point
- 55 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 achieve flexibility and convenience in software integration; however, the extra I/O accesses of disk files as well as the extra
- 60 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 Passing Interfaces)-based data exchanges between the model ensemble members and DA procedures can produce better
- 65 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). Considering that existing observation processing systems can introduce different observation frequencies corresponding to

- 70 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 crossdomain error covariance matrix to account for the impact of the same observational information on different component models cooperatively (Tardif et al., 2014, 2015; Lu et al., 2015a, b; Sluka et al., 2016).
- 75 The remainder of this paper is organized as follows. Section 2 introduces the overall design of the new DA framework named DAFCC1 (Data Assimilation Framework based on C-Coupler2.0, version 1). The implementation of DAFCC1 areis 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.

2 Overall design of the new framework

- 80 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<u>that handles the data</u> exchanges via MPI functionalities 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, and global communications of with MPI_gatherv and MPI_scatterv
- 85 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 thebut is inefficient because of inefficient global communications are generally inefficient and there are idle processes almost at any time because due to sequential running of the model ensemble and the DA method generally work sequentially but not simultaneouslymodules in the sequential DA systems. In PDAF, a DA method is transformed into a native procedure that is called by the corresponding models via the PDAF
- 90 application programing interfaces (APIs). Thus, a Thus, a model and a DA method can be compiled into the same executable, and the DA method can share the processes of the model ensemble. The code releases of PDAF (<u>http://pdaf.awi.de/trac/wiki</u>) provide template implementations of data exchanges for a default case where a DA method shares all is running on the processes of the first ensemble member of the corresponding model(for example, given that there are 10 ensemble members and keepseach member uses 100 processes, the DA method is running on 100 processes) and uses the same parallel
- 95 decomposition (grid domain decomposition for parallelization) with the corresponding model. When users want a case different from the default (e.g., a DA method does not use the same processes with the first ensemble member or uses a parallel decomposition different from the corresponding model), users should develop new code implementations for 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, and using the formats of PDAF APIs) will be developed.

- 100 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 <u>for</u> the <u>resultresults</u> 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 <u>target an improved-improve the</u> implementation of the data exchange
- 105 functionality, which in at least three aspects: 1) the new implementation does not use global communications of with MPI_gatherv and MPI_scatterv; 2) the new implementation enables a DA method to share almost all run on the processes of the model ensemble and all ensemble members (for example, given that there are 10 ensemble members and each member uses 100 processes, the DA method can run on 1000 processes); 3) the new implementation does not require users to develop extra codes in any case. When a DA algorithm uses processes no matter whether a DA method and the corresponding model use the same of different from aparallel decompositions. A DA method requires to exchange data with each model ensemble
- member, the <u>When a</u> DA algorithm will use uses a parallel decomposition that differs from the model ensemble members. Thus, the data exchange between the DA algorithm and a component model <u>an</u> 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). Each of whichthese couplers 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
- registered as a component model of C-Coupler2.0. As shown in Fig. 1a, based on the coupling configurations registered to C-Coupler2.01a, most 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.
- 125 A-most significant challenge here is that C-Coupler2.0 can only handle coupling exchanges between two component models or intrawithin one component model, while coupled ensemble DA requiresbut cannot handle coupling exchanges between a DA algorithm and acach model ensemble that includes a set of ensemble members each of which has been registered as a component model of C-Coupler2.0.member. To address this challenge, DAFCC1 automatically generates a special C-Coupler2.0 component model (called ensemble-set component model hereafter) that covers all ensemble members for running
- 130 <u>a DA algorithm. Thus, coupling exchanges between a DA algorithm and each model ensemble member can be transformed</u> into the coupling exchanges between the ensemble-set component and each ensemble member. Specifically, DAFCC1

<u>introduces</u> three new steps, i.e., initialization, running and finalization of DA instances (instances of DA algorithms), are <u>inserted intoto</u> the model flowchart with C-Coupler2.0 (Fig. 1b). These <u>three</u>-steps enable <u>a DA instance to run on the processes</u> of all ensemble members-in a, and achieve automatic coupling exchanges between a DA algorithm and each model ensemble

- 135 to use a DA algorithm cooperativelymember. The software architecture of DAFCC1 based on C-Coupler2.0 is shown in Fig. 2. It includes a set of new managers (i.e., DA algorithm integration manager, ensemble component 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<u>declare</u> its input and output fields and to obtain various information from the model. <u>AWhen a</u> DA algorithm <u>can include a set of procedures includes multiple independent modules (</u>such as observation operators and analysis modules;), each <u>of whichmodule</u> can be called <u>separately</u> by the model <u>separately</u>. The framework uses the dynamic link library (DLL) technique for the <u>connection of is used to connect</u> a DA algorithm program to a model, where <u>a program. The</u> DA algorithm program is compiled into a DLL that is dynamically linked to a model when an instance of the DA algorithm is initialized. WithUsing the DLL technique; allows us to couple a <u>new-DA</u> algorithm <u>can be used by</u> and a
- 145 model without modifying and recompiling the model codes, and <u>it provides greater independence and convenience because</u> the original configuration and compilation systems of <u>athe</u> 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 communicatorgoverns the communicators of ensemble members of each component model. The online DA procedure manager provides several APIs that enable the ensemble members of a component
- 150 model to initialize, run and finalize a DA <u>algorithm</u> instance cooperatively, <u>automatically handles the</u>. <u>The</u> data exchanges between the ensemble members and the DA algorithm with a set of operations.are also handled automatically in this manager. The ensemble DA configuration manager enables the user to flexibly <u>specify thechoose</u> DA <u>algorithm</u>, <u>DA frequencyalgorithms</u> and <u>the operationsset parameters</u> for <u>the data exchange in</u> a DA simulation <u>throughvia</u> a configuration file.
- 155 Guided by With the software architecture in Fig.-2, we implemented and the new framework (seedetailed implementations in Section 3 for detailed implementation), which, DAFCC1 enables a coupled ensemble DA system to achieve the following features:
 - 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,
- 160 components 1, 2, and 4 in Fig. 3 <u>useperform</u> DA <u>algorithms at with</u> different <u>frequencies,time periods (e.g., component 4</u> <u>performs DA more frequently than component 1 and 2)</u>, while component 3 does not use DA <u>algorithms</u>.
 - 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. 3 for example, components 2 and 4 use different instances of the same DA algorithm 2 independently.

- 165 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. 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
- 170 increasing the flexibility and convenience in using a DA algorithm (see Section 3.4 for detailed implementation).

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.

175 **3.1 Implementation of the ensemble component manager**

In C Coupler2.0, the model<u>To achieve</u> coupling resources, including MPI communicators, time steps, timers, model grids, parallel decompositions, coupling field instances, exchanges between a DA algorithm 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 runeach ensemble member, each ensemble member should be used as a separate component model, registered to C-Coupler2.0 via the API *CCPL_register_component* (Please refer to Liu et al. 2018b for more details). In C-Coupler2.0, model names are used as 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_fensemble numbers]_(member ID)") of the corresponding executable when submitting an MPI run (see Fig. 4 as an example) where "ensemble numbers" marks the

corresponding executable when submitting an MPI run (see 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.

<u>C-Coupler2.0 can manage hierarchical relationship among models, where a model can have a set of children models.</u> Given an ensemble run of a coupled model, <u>although all ensemble members of the all</u> component models of the coupled model can
 be organized as oneinto a single level of models (see Fig. 5a), <u>although we recommend constructing two hierarchical levels of models with the first level corresponding to all ensemble members of the coupled model and(see Fig. 5b), where each ensemble member <u>includingof the coupled model is at the first level while</u> the component models <u>of each ensemble member are</u> at the second level (Fig. 5b), because the. This hierarchical organization retains the original architecture of the coupled model through a simple additional registration of, and only requires users to simply register the coupled model to C-Coupler2.0.
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- 195 As-In order to enable a DA algorithm that handles ensemble fields canto run on the MPI processes of all ensemble members of a component model (Fig. 3), a special C Coupler2.0an 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 usingcalling the DA algorithm (for example, the green box in Fig. 5b)- corresponds to an ensemble-set component model). As the ensemble-set component model does not exist in the original hierarchical levels in Fig. 5b, it should be generated with
- 200 <u>extra efforts.</u> The ensemble component manager provides the capability to generate an ensemble set component model, which does not introduce global synchronization and only involves of automatically generating the corresponding ensemble-set component model when initializing a DA instance. The MPI communicator of the ensemble-set component model is generated through unifying the communicators of the ensemble members of the corresponding component model that runs the DA instance.

205 3.2 Implementation of the DA algorithm integration manager

A pair of a model and When a DA algorithm have essentiallyruns on the relationship between-processes of a component model, the model and the DA algorithm can be viewed as a caller and a callee respectively in a program, where the <u>A</u> callee generally declares a list of arguments that includes a set of input and output variables, while and a caller should match the argument list of the callee when calling the callee (herein, the model that calls a DA algorithm is referred to ascalled the host model of the

210 DA algorithm). For hereafter). When a caller and a callee that are in the same native code, a corresponding statically linked together, a compiler generally can guarantee the consistency of the argument list between them, regardless of the data structure of each argument. However, it is a challenge that 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 and dynamically linked to the host model.

To address the above challenge, we designed and developed a new solution in DAFCC1 for passing arguments between a

- 215 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. These subroutines are enclosed in the same DLL with the DA algorithm. Specifically, names of these subroutines 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., the explicit argument list only includes a few
- 220 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 of 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 a set of implicit input or output arguments, at the initialization stage of the DA algorithm of fields. Figure 6 shows an example of the driving subroutines where the running and finalization driving subroutines are veryquite simple. In the The initialization
- 225 driving subroutine, <u>besides includes</u> the original functionalities of the DA algorithm such as determining parallel decompositions, allocating memory space for variables and other operations for initialization, there are. Moreover, it includes additional operations for obtaining <u>the information fromof</u> the host model and grids using via C-Coupler2.0, registering the

parallel decompositions, required grids, and field instances to C-Coupler2.0, and declaring the a set of field instances as implicit input or output arguments. InData exchanges between the host model and the DA algorithm are conducted automatically and

- 230 <u>implicitly by DAFCC1 (Section 3.3.2), so</u> the running driving subroutine DA_CCPL_RUN, there are no_does not include 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, while the data from the DA algorithm to the model ensemble is transferred automatically and implicitly after running DA_CCPL_RUN exchanges.
- The use of DAFCC1 requires some <u>native codefurther changes to the codes</u> 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 <u>throughvia</u> 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 enablemake the same DA algorithm used by different component models to use the same DA algorithm but with different configurations, DAFCC1 enables a component model canto use a distinct separate instance of athe same DA algorithm with 240the 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 are directly called by the code of a host model-to. These APIs initialize, run, and finalize thea DA algorithm instance, and handle the data exchanges between the host model and the DA algorithm 245 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 evcles without restarting the model and the DA algorithm. When a component model initializes, runs, or finalizes a DA algorithm instance, all ensemble members of this component model should 250 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* includes the following steps for initializing a DA algorithm instance-is designed and implemented with the following steps.:

DetermineDetermining 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. 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. 3), the host model will be the ensemble-set component model that will be generated automatically by the ensemble component manager.

PreparePreparing information from the host model, such as model grids, parallel decompositions, and field instances, which <u>can be obtained by</u> the initialization driving subroutine of the DA algorithm <u>can obtain</u> via the corresponding APIs.

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- 3) InitializeInitializing the corresponding DA algorithm instance according to the corresponding algorithm name and DLL name specified in the corresponding configuration file, (Section 3.4), 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 <u>different</u> simulations via the configuration file without modifying the code of the model.
- 4) SetSetting 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 within each 270 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 275 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 280 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 thethis 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 namesname of the coupled model and the component model 1 in Fig. 5 are "*coupled*" and is "*comp1*", respectively, in the one-level model hierarchy in Fig. 5a, the full names of ensemble members of the component model 1 are "*comp1_1*" to "*comp1_N*", and the common full name of the ensemble members of the component model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given the two-level model hierarchy in Fig. 5b, the full name is "*coupled_*@comp1*"; (given the two-level model hierarchy in Fig. 5b, the full name is "*coupled_*@comp1*"; (given the two-level model hierarchy in Fig. 5b, the full name is "*coupled_*@comp1*"; (given the two-level model hierarchy in Fig. 5b, the full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"; (given model 1 are "*coupled_1@comp1*" to "*coupled_N@comp1*" and the common full name is "*coupled_*@comp1*"

that the name of the coupled model is "*coupled*"). Such a common full name can be used for generating the ensemble-set component model when the DA algorithm instance is an ensemble algorithm.

- 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. 3.
- 300 A<u>An optional</u> list of model grids and parallel decompositions, which are optional arguments that enable the DA algorithm instance to obtain the 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 assimilationDA. 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
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APIs.

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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 includes the following steps for running a DA algorithm instance 310 with the following steps:

- 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. The statistical processing regarding the time window or the ensemble is done at the same time.
- 315 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.

Each DA algorithm instance has a timer specified via the configuration information, which determines when the DA algorithm instance is run. The <u>API_CCPL_ensemble_procedures_inst_run</u> can be called for thea DA algorithm instance can <u>be called</u> at each time step, while the above three steps will be executed only when the correspondingspecified 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 and then recover the current directory for calling the running driving

325 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

- The configuration information of all DA algorithm instances used in a coupled DA simulation is contained enclosed in an XML 330 configuration file (e.g., Fig. 7), and each). Each DA algorithm instance has a distinct XML node (e.g., the XML node "da instance" in 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 inassociated with the API "CCPL ensemble procedures inst init"), which enables the user to specify the following configurations-:
- 335 1) The DA algorithm specified in the XML node "external procedures" in Fig. 7, where the the attribute "dll name" in the XML node specifies the dynamic link library, and the attribute "procedures name" specifies the name of the DA algorithm. which will be used to choose the's name associated with the corresponding 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.
- The periodic timer specified in the XML node "periodic_timer" in Fig. 7, which enables users the user to flexibly set the 340 2) frequency as well as the periodic 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 345 "local lag count" of 3.
- 3) Statistical processing of input fields specified in the XML node "field instances" in Fig. 7, where the the attribute "time processing" specifies the statistical processing in each time window determined by the periodic timer-and the. 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". BesidesAll fields can share the default specification of statistical processing shared by all fields, while a field can have its own statistical processing specified in a sub node of the XML node "field instances".
- The working directory and the scripts for pre- and post-assimilation analysis (e.g., for processing the data files of 4) observational information) optionally specified in the XML node "processing control" in 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.

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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

- 360 weakly coupled ensemble DA system by combining the ensemble DA system GSI/EnKF (Shao et al., 2016; Liu et al., 2018b) and a regional First Institute of Oceanography Atmosphere-Ocean-Wave (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
- 365 (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

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- 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

375 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.,

380 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 8a 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.

 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.

- 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
 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
- 395 CRTM coefficient files) as input, and produces an observation prior (observation innovation) file for the ensemble mean 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.
- 400 5) EnKF for calculating analysis increments. EnKF is initiated for calculating analysis increments of the whole ensemble. It 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

- 405 When adapting GSI/EnKF to DAFCC1, an ensemble-set component model derived from the ensemble forecast of WRF (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. 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
- 410 step in Section 4.1.1. This is because the online DA procedure manager of DAFCC1 enables a DA algorithm instance to 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
- 415 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. 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.

420 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. 8b and Fig. 8a).

430 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. 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

- 435 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.
 - Using the ensemble component manager, set up the two hierarchical levels of models shown in 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.
- 440 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. 8b, the example ensemble DA system of FIO-AOW follows the process layout in Fig. 12, which is essentially a real case of the process layout in Fig. 3.

445 5 Validation and evaluation of DAFCC1

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).

450 5.1 Experimental setup

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

- 455 correlation function with horizontal localization radius of 400 km and vertical localization scale coefficient of 0.4. The example 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
 460 for manipula ensemble DA system.
- 460 for running the example ensemble DA system.

The WRF-GSI/EnKF integrates over an approximate geographical area generated from a Lambertian projection of the area $0^{\circ}-50^{\circ}$ N, $99^{\circ}-160^{\circ}$ 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

- 465 WRF, an existing physics suite 'CONUS' (<u>https://www2.mmm.ucar.edu/wrf/users/ncar_convection_suite.php</u>) and 32 vertical 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; <u>https://www.emc.ncep.noaa.gov/mmb/data_processing/NCEP_BUFR_File_Structure.htm</u>) and Prepared BUFR (<u>https://www.emc.ncep.noaa.gov/mmb/data_processing/prepbufr.doc/document.htm</u>), including_conventional_observation
- 470 data and satellite radiation data, are assimilated every 6 hours (i.e., at 0000, 0600, 1200, and 1800 UTC). The air temperature (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 ($0^{\circ}-50^{\circ}N$, $99^{\circ}-150^{\circ}E$) with the same horizontal resolution of $0.5^{\circ} \times 0.5^{\circ}$ 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),
- 480 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-

- 485 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 490 integration are used for the comparison.

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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. 13a). This is because DAFCC1 significantly accelerates the DA for both GSI and EnKF (Fig. 13b-d). Similarly, DAFCC1 significantly accelerates the DA as well as WRF-GSI/EnKF under different process numbers (Fig. 14, corresponding to Set 2 in Table 2)
- 500 and resolution (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. 16).
- 505 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. 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.
- 510 We note that, the execution time of the offline GSI in Fig. 13c increases when using more ensemble members. This 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. 13d and 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.

515 5.4 Correctness in developing a weakly coupled ensemble DA system

We have successfully run the full-example-DA-system with ten ensemble members, which enables us to investigate the model fields before and after DA. We find that changes to the atmospheric 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. 17. Changes to the atmospheric fields predicted based on the initial fields updated with the atmospheric analyses can also be 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

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In this paper, we propose a new common, flexible and efficient framework for weakly coupled ensemble data assimilation

- 525 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 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 that only
- 530 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 535 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

540 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. 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.

- 545 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. 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 in simulation
- 550 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.
- 555 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
- 560 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

565 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 <u>https://doi.org/10.5281/zenodo.3739729</u> (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 <u>https://www2.mmm.ucar.edu/wrf/users/downloads.html</u> and <u>https://dtcenter.org/com-GSI/users/downloads/index.php</u> respectively. For the source code of FIO-AOW, please contact the authors of (Zhao et al.,

570 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

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research, was responsible for the motivation and design of DAFCC1, co-supervised CS, and co-led paper writing. RL, XY and

575 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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References

Andersson, E., Haseler, J., Unden, P., Courtier, P., Kelly, G., Vasiljevic, D., and Thepaut, J.: The ECMWF implementation of three-dimensional variational assimilation (3D-Var). III: Experimental results, Q. J. Roy. Meteor. Soc., 124, 1831-1860,

585 1998.

- Anderson, J., Hoar, T., Raeder, K., Liu, H., Collins, N., Torn, R., and Arellano, A.: The Data Assimilation Research Testbed: A Community Facility, Bull. Am. Meteorol. Soc., 90, 1283–1296, 2009.
 - Anderson, J. and Collins, N.: Scalable implementations of ensemble filter algorithms for data assimilation, J. Atmos. Ocean Technol., 24, 1452-1463, 2007.
- 590 Bishop, C. and Hodyss, D.: Adaptive ensemble covariance localization in ensemble 4D-VAR state estimation, Mon. Weather Rev., 139, 1241–1255, 2011.
 - Blumberg, A. and Mellor, G.: A description of a three-dimensional coastal ocean circulation model, in Three-Dimensional Coastal Ocean Models, edited by N. S. Heaps, pp. 1–16, AGU, Washington, D. C, 1987.
 - Bonavita, M., Isaksen, L., and Holm, E.: On the use of EDA background-error variances in the ECMWF 4D-Var, Q. J. R.
- 595 Meteorol. Soc., 138, 1540-1559, 2012.
 - Bonavita, M., Holm, E., Isaksen, L., and Fisher, M. A.: The evolution of the ECMWF hybrid data assimilation system, Q. J. Roy. Meteor. Soc., 142, 287-303, 2016.
 - Brown, A., Milton, S., Cullen, M., Golding, B., Mitchell, J., and Shelly, A.: Unified modeling and prediction of weather and climate: a 25 year journey, B. Am. Meteorol. Soc., 93, 1865–1877, https://doi.org/10.1175/BAMS-D-12-00018.1, 2012.
- 600 Browne, P., de Rosnay, P., Zuo, H., Bennett, A., and Dawson, A.: Weakly coupled ocean-atmosphere data assimilation in the ECMWF NWP system, Remote Sens., 11, 1-24, 2005.

Browne, P., and Wilson, S.: A simple method for integrating a complex model into an ensemble data assimilation system using MPI, Environ. Modell. Softw., 68, 122-128, 2015.

Brunet, G., Jones, S., and Ruti, P.: Seamless prediction of the Earth System: from minutes to months, Tech. Rep. WWOSC-

605

- Buehner, M., McTaggart-Cowan, R., Beaulne, A., Charette, C., Garand, L., Heilliette, S., Lapalme, E., Laroche, S., Macpherson, S.R., Morneau, J. and Zadra, A.: Implementation of deterministic weather forecasting systems based on ensemble-variational data assimilation at Environment Canada. Part I: the global system, Mon. Weather Rev., 143, 2532– 2559, 2015.
- 610 Courtier, P., Andersson, E., Heckley, W., Vasiljevic, D., Hamrud, M., Hollingsworth, A., and Pailleux, J.: The ECMWF implementation of three-dimensional variational assimilation (3D-Var). I: Formulation, Q. J. Roy. Meteor. Soc., 124, 1783-1807, 1998.
 - Courtier, P., Thepaut, J., and Hollingsworth, A.: A strategy for operational implementation of 4D-Var, using an incremental approach, Q. J. Roy. Meteor. Soc., 120, 1367-1387, 1994.
- 615 Craig, A., Vertenstein, M., and Jacob, R.: A new flexible coupler for earth system modeling developed for CCSM4 and CESM1, Int. J. High Perform. Comput. Appl., 26, 31-42, 2012.
 - Craig, A., Valcke, S., and Coquart, L.: Development and performance of a new version of the OASIS coupler, OASIS3-MCT_3.0, Geosci. Model Dev., 10, 3297-3308, https://doi.org/10.5194/gmd-10-3297-2017, 2017.
 - Etherton, B. and Bishop, C.: Resilience of hybrid ensemble/3DVAR analysis schemes to model error and ensemble covariance

620 error, Mon. Weather Rev., 132, 1065-1080, 2004.

2014, World Meteorological Organization, 2015.

- Evensen, G.: The ensemble kalman filter: theoretical formulation and practical implementation, Ocean Dyn., 53, 343-367, 2003.
 - Fisher, M.: Background error covariance modelling, in: Proceedings of Seminar on Recent Developments in Data Assimilation for Atmosphere and Ocean, Reading, UK, 8-12 September 2003, 45–63, 2003.
- Fujii, Y., Kamachi, M., Nakaegawa, T., Yasuda, T., Yamanaka, G., Toyoda, T., Ando, K. and Matsumoto, S.: Assimilating ocean observation data for ENSO monitoring and forecasting, in: Climate Variability - Some Aspects, Challenges and Prospects, edited by: Hannachi, A., InTechOpen, Rijeka, Croatia, 75-98, 2011.
 - Fujii, Y., Nakaegawa, T., Matsumoto, S., Yasuda, T., Yamanaka, G., and Kamachi, M.: Coupled climate simulation by constraining ocean fields in a coupled model with ocean data, J. Clim., 22, 5541-5557, 2009.
- Gandin, L.: Objective analysis of meteorological fields. Jerusalem: Israel program for scientific translations, 1965
 Gauthier, P., Charette, C., Fillion, L., Koclas, P., and Laroche, S.: Implementation of a 3D variational data assimilation system at the Canadian Meteorological Center. Part I: The global analysis, Atmos. Ocean, 37, 103-156, 1999.
 - Goodliff, M., Bruening, T., Schwichtenberg, F., Li, X., Lindenthal, A., Lorkowski, I., and Nerger, L.: Temperature assimilation into a coastal ocean-biogeochemical model: assessment of weakly and strongly coupled data assimilation, Ocean Dyn., 69,
- 635 1217-1237, 2019.

Hamill, T.: A hybrid ensemble kalman filter-3D variational analysis scheme, Mon. Weather Rev., 128, 2905, 2000.

Heinzeller, D., Duda, M. G., and Kunstmann, H.: Towards convection-resolving, global atmospheric simulations with the Model for Prediction Across Scales (MPAS): an extreme scaling experiment, Geosci. Model Dev., 8, 6987-7061, 2016.

Hoke, J. and Anthes, R.: The initialization of numerical models by a dynamic initialization technique, Mon. Weather Rev.,

640 104, 1551–1556, 1976.

- Hoskins, B.: The potential for skill across the range of the seamless weather-climate prediction problem: a stimulus for our science, Q. J. Roy. Meteor. Soc., 139, 573-584, 2013.
- Houtekamer, P., and Mitchell, H.: Data assimilation using an ensemble kalman filter technique. Mon. Weather Rev., 126, 796-811, 1998.
- 645 Hunt, B., Kostelich, E., and Szunyogh, I.: Efficient data assimilation for spatiotemporal chaos: A local ensemble transform kalman filter, International Symposium on Physical Design, 230, 112-126, 2007.
 - Kalnay, E.: Atmospheric modeling, data assimilation and predictability, Cambridge University Press, Cambridge, UK, pp. 364, 2002.

Laloyaux, P., Thepaut, J., and Dee, D.: Impact of scatterometer surface wind data in the ECMWF coupled assimilation system,

650 Mon. Weather Rev., 144, 1203-1217, 2016.

- Laloyaux, P., Frolov, S., Benjamin Ménétrier, and Bonavita, M.: Implicit and explicit cross-correlations in coupled data assimilation, Q. J. R. Meteorol. Soc., 144, 2018.
- Lea, D., Mirouze, I., Martin, M., King, R., Hines, A., Walters, D., and Thurlow, M.: Assessing a new coupled data assimilation system based on the met office coupled atmosphere–land–ocean–sea ice model, Mon. Weather Rev., 143, 4678-4694, 2015.
- 655 Liu, H., Hu, M., Ge, G., Stark, D., Shao, H., Newman, K., and Whitaker, J.: Ensemble Kalman Filter (EnKF) User's Guide Version 1.3, Developmental Testbed Center, available at: https://dtcenter.org/community-code/ensemble-kalman-filtersystem-enkf/documentation, 80 pp, 2018a.
 - Liu, L., Yang, G., Wang, B., Zhang, C., Li, R., Zhang, Z., Ji, Y., and Wang, L.: C-Coupler1: a Chinese community coupler for Earth System Modeling, Geosci. Model Dev., 7, 2281-2302, doi: 10.5194/gmd-7-2281-2014, 2014.
- 660 Liu, L., Zhang, C., Li, R., Wang, B., and Yang, G.: C-Coupler2: a flexible and user-friendly community coupler for model coupling and nesting, Geosci. Model Dev., 11, 3557-3586, https://doi.org/10.5194/gmd-11-3557-2018, 2018b.
 - Lorenc, A., Ballard, S., Bell, R., Ingleby, N., Andrews, P., Barker, D., Bray, J., Clayton, A., Dalby, T., Li, D., Payne, T., and Saunders, F.: The Met. Office global three-dimensional variational data assimilation scheme, Q. J. Roy. Meteor. Soc., 126, 2991-3012, 2000.
- 665 Lorenc, A.: The potential of the ensemble Kalman filter for NWP-A comparison with 4D-VAR, Q. J. Roy. Meteor. Soc., 129: 3183-3203, 2003a.

Lorenc, A.: Modelling of error covariances by 4D-Var data assimilation, Q. J. Roy. Meteor. Soc., 129, 3167-3182, 2003b.

Lu, F., Liu, Z., Zhang S., and Liu Y.: Strongly coupled data assimilation using leading averaged coupled covariance (LACC). Part I: Simple model study, Mon. Weather Rev., 143, 3823–3837, doi: 10.1175/MWR-D-14-00322.1, 2015a.

- Lu, F., Liu, Z., Zhang, S., Liu, Y., and Jacob, R.: Strongly coupled data assimilation using leading averaged coupled covariance (LACC). Part II: GCM Experiments, Mon. Weather Rev., 143, 4645-4659, doi: 10.1175/MWR-D-14-00322.1, 2015b.
 - Ma, X., Lu, X., Yu, M., Zhu, H., and Chen, J.: Progress on hybrid ensemble-variational data assimilation in numerical weather prediction, J. Trop. Meteorol., 30, 1188-1195, 2014.
- Mochizuki, T., Masuda, S., Ishikawa, Y., and Awaji, T.: Multiyear climate prediction with initialization based on 4D-Var data assimilation, Geophys. Res. Lett., 43, 3903-3910, 2016.
 - Mulholland, D., Laloyaux, P., Haines, K., and Balmaseda, M.: Origin and impact of initialization shocks in coupled atmosphere–ocean forecasts, Mon. Weather Rev., 143, 4631–4644, doi: 10.1175/MWR-D-15-0076.1, 2015.
 - Nerger, L. and Hiller, W.: Software for Ensemble-based Data Assimilation Systems Implementation Strategies and Scalability, Comput. Geosci., 55, 110–118, 2013.
- 680 Nerger, L., Hiller, W., and Schröter, J.: PDAF The Parallel Data Assimilation Framework: Experiences with Kalman filtering., in: Use of High Performance Computing in Meteorology - Proceedings of the 11. ECMWF Workshop, edited by Zwieflhofer, W. and Mozdzynski, G., pp. 63–83, World Scientific, 2005.
 - Nerger, L., Tang, Q., and Mu, L.: Efficient ensemble data assimilation for coupled models with the Parallel Data Assimilation Framework: example of AWI-CM (AWI-CM-PDAF 1.0), Geosci. Model Dev., 13, 4305–4321, https://doi.org/10.5194/gmd-13-4305-2020, 2020.
 - Oke, P., Allen, J., Miller, R., Egbert, G., and Kosro, P.: Assimilation of surface velocity data into a primitive equation coastal ocean model. J. Geophys. Res, 107, 2002.
 - Palmer, T., Doblas-Reyes, F., Weisheimer, A. and Rodwell, M.: Toward seamless prediction: Calibration of climate change projections using seasonal forecasts, Bull. Am. Meteorol. Soc., 89, 459-470, 2008.
- 690 Penny, S., Akella, S., Alves, O., Bishop, C., Buehner, M., Chevalier, M., Counillon, F., Drper, C., Frolov, S., Fujii, Y., Kumar, A., Laloyaux, P., Mahfouf, J.-F., MArtin, M., Pena, M., de Rosnay, P., Subramanian, A., Tardif, R., Wang, Y., and Wu, X.: Coupled data assimilation for integrated Earth system analysis and prediction: Goals, Challenges and Recommendations, Tech. Rep. WWRP 2017-3, World Meteorological Organization, 2017.
- Qiao, F., Zhao, W., Yin, X., Huang, X., Liu, X., Shu, Q., Wang, G., Song, Z., Liu, H., Yang, G., and Yuan, Y.: A highly
 effective global surface wave numerical simulation with ultra-high resolution, in: Proceedings of the International
 Conference for High Performance Computing, Networking, Storage and Analysis (SC '16), IEEE Press, Piscataway, NJ,
 USA, doi: 10.1109/SC.2016.4, 2016.
 - Rabier, F., Jarvinen, H., Klinker, E., Mahfouf, J., and Simmons, A.: The ECMWF operational implementation of fourdimensional variational assimilation. I: Experimental results with simplified physics, Q. J. Roy. Meteor. Soc., 126, 1143-
- 700 1170, 2007.

685

Saha, S., Moorthi, S., Pan, H., Wu, X., Wang, J., Nadiga, S., Tripp, P., Kistler, R., Woollen, J., Behringer, D., Liu, H., Stokes,
D., Grumbine, R., Gayno, G., Wang, J., Hou, Y., Chuang, H., Juang, H. H., Sela, J., Iredell, M. T. R., Kleist, D., van Delst,
P., Keyser, D., Derber, J., Ek, M., Meng, J., Wei, H., Yang, R., Lord, St., Van Den Dool, H., Kumar, A., Wang, W., Long,

C., Chelliah, M., Xue, Y., Huang, B., Schemm, J., Ebisuzaki, W., Lin, R., Xie, P., Chen, M., Zhou, S., Higgins, W., Zou,

- 705 C., Liu, Q., Chen, Y., Han, Y., Cucurull, L., Reynolds, R. W., Rutledge, G., and Goldberg, M.: The NCEP Climate Forecast System Reanalysis, Bull. Am. Meteorol. Soc., 91, 1015-1057, 2010.
 - Saha, S., Moorthi, S., Wu, X., Wang, J., Nadiga, S., Tripp, P., Behringer, D., Hou, Y., Chuang, H., Iredell, M., Ek, M., Meng, J., Yang, R., Mendez, M., Van Den Dool, H., Zhang, Q., Wang, W., Chen, M., and Becker, E.: The NCEP Climate Forecast System Version 2, J. Clim., 27, 2185–2208, http://dx.doi.org/10.1175/JCLI-D-12-00823.1, 2014.
- 710 Sakov, P., Counillon, F., Bertino, L., Lisæter, K. A., Oke, P. R., and Korablev, A.: TOPAZ4: an ocean-sea ice data assimilation system for the North Atlantic and Arctic, Ocean Sci., 8, 633-656, 2012.
 - Shao, H., Derber, J., Huang, X. Y., Hu, M., Newman, K., Stark, D., Lueken, M., Zhou, C., Nance, L., Kuo, Y. H., and Brown,
 B.: Bridging Research to Operations Transitions: Status and Plans of Community GSI. Bull. Amer. Meteor. Soc., 97, 1427-1440, doi: 10.1175/BAMS-D-13-00245.1, 2016.
- 715 Skachko, S., Buehner, M., Laroche, S., Lapalme, E., Smith, G., Roy, F., Surcel-Colan, D., Bélanger, J., and Garand, L.: Weakly coupled atmosphere-ocean data assimilation in the Canadian global prediction system (v1), Geosci. Model Dev., 12, 5097-5112, 2019.
 - Sluka, T., Penny, S., Kalnay, E., and Miyoshi, T.: Assimilating atmospheric observations into the ocean using strongly coupled ensemble data assimilation, Geophys. Res. Lett., 43, 752-759, 2016.
- 720 Sugiura, N., Awaji, T., Masuda, S., Mochizuki, T., Toyoda, T., Miyama, T., Igarashi, H., and Ishikawa, Y.: Development of a 4-dimensional variational coupled data assimilation system for enhanced analysis and prediction of seasonal to interannual climate variations, J. Geophys. Res., 113, C10017, doi: 10.1029/2008JC004741, 2008.
 - Tardif, R., Hakim, G., and Snyder, C.: Coupled atmosphere–ocean data assimilation experiments with a low-order climate model, Clim. Dyn., 43, 1631-1643, doi: 10.1007/s00382-013-1989-0, 2014.
- 725 Tardif, R., Hakim, G., and Snyder, C.: Coupled atmosphere-ocean data assimilation experiments with a low-order model and CMIP5 model data, Clim. Dyn., 45, 1415-1427, doi: 10.1007/s00382-014-2390-3, 2015.
 - Valcke, S., Balaji, V., Craig, A., Deluca, C., Dunlap, R., Ford, R. W., Jacob, R., Larson, J., Okuinghttons, R., Riley, G., and Vertenstein, M: Coupling technologies for Earth System Modelling, Geosci. Model Dev., 5, 1589-1596, 2012.

Vidard, P. A., Le Dimet, F. X., and Piacentini, A.: Determination of optimal nudging coefficients, Tellus, 55A, 1–15, 2003.

- 730 Wang, G., Qiao F., and Xia C.: Parallelization of a coupled wave-circulation model and its application, Ocean Dyn., 60(2), 331–339, doi:10.1007/s10236-010-0274-6, 2010.
 - Wang, G., Zhao, B., Qiao, F., and Zhao, C.: Rapid intensification of Super Typhoon Haiyan: the important role of a warmcore ocean eddy, Ocean Dyn, 68, 1649-1661, 2018.
 - Wang, W., Barker, D., Bray J., Bruye're C., Duda M., Dudhia J., Gill D., and Michalakes J.: WRF Version 3 Modeling
- System User's Guide, available at http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V3/contents.html, 2014.
 Wang, X., Barker, D., Snyder, C., and Hamill, T.: A hybrid ETKF-3DVAR data assimilation scheme for the WRF model. Part I: Observing system simulation experiment, Mon. Weather Rev., 136, 5116–5131, 2008.

Wang, X., Parrish, D., Kleist, D., and Whitaker, J.: GSI 3DVar-based ensemble-variational hybrid data assimilation for NCEP global forecast system: Single-resolution experiments, Mon. Weather Rev., 141, 4098 – 4117, 2013.

- 740 Whitaker, J.and Hamill, T. M. Ensemble Data Assimilation without Perturbed Observations, Mon. Weather Rev., 130, 1913-1924, 2012.
 - Yang, X., Rosati, A., Zhang, S., Delworth, T., Gudgel, R., Zhang, R., Vecchi, G., Anderson, W., Chang, Y., DelSole, T., Dixon,
 K., Msadek, R., Stern, W., Wittenberg, A., and Zeng, F.: A predictable AMO-like pattern in the GFDL fully coupled ensemble initialization and decadal forecasting system, J. Clim., 26, 650-661, 2013.
- 745 Yang, Y., Qiao, F., Zhao, W., Teng, Y., and Yuan, Y.: MASNUM ocean wave numerical model in spherical coordinates and its application, Acta Oceanol. Sin., 27, 1–7, 2005.
 - Zhao, B., Qiao, F., Cavaleri, L., Wang, G., Bertotti, L., and Liu, L: Sensitivity of typhoon modeling to surface waves and rainfall, J. Geophys. Res. Oceans, 122, 1702–1723, doi:10.1002/2016JC012262, 2017.
- Zhang, S., Harrison, M., Wittenberg, A., Rosati, A., Anderson, J., and Balaji, V.: Initialization of an ENSO forecast system using a parallelized ensemble filter, Mon. Weather Rev., 133, 3176–3201, 2005.
 - Zhang, S., Harrison, M., Rosati, A., and Wittenberg, A.: System design and evaluation of coupled ensemble data assimilation for global oceanic climate studies, Mon. Weather Rev., 135, 3541–3564, doi: 10.1175/MWR3466.1, 2007.



755 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.







Figure 3. 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 765 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 770

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

775 Figure 4. 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.



780 Figure 5. 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-<u>set component model</u> that covers all ensemble members of component model 1 is generated as an example for using the DA algorithm in ensemble component

785 manager.

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 DA_CCPL_RUN
- c) 1 Subroutine *DA*_CCPL_FIN
 - 2 DA finalize
 - 3 End subroutine DA_CCPL_FIN

790 Figure 6. 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></root>
2	<pre><da_instance name="DA_algorithm1_procedure1" status="on"></da_instance></pre>
3	<external_procedures_status="on" dll_name="lib_da1_p1.so" procedures_name="algorithm1_procedure1"></external_procedures_status="on">
4	<pre><pre>cyperiodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/></pre></pre>
5	<field_instances ensemble_operation="none" status="on" time_processing="inst"></field_instances>
6	<pre><pre>cessing_control status="on" ></pre></pre>
7	<working_directory path="" status="off"></working_directory>
8	<config_scripts status="on"></config_scripts>
9	<pre_instance_script name="da1_p1_online_run.sh" status="on"></pre_instance_script>
10	<pre><post_instance_script name="" status="off"></post_instance_script></pre>
11	
12	
13	
14	<pre><da_instance name="DA_algorithm1_procedure2" status="on"></da_instance></pre>
15	<external_procedures dll_name="lib_da1_p2.so" procedures_name="algorithm1_procedure2" status="on"></external_procedures>
16	<pre><pre>cyperiodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/></pre></pre>
17	<field_instances ensemble_operation="aver" status="on" time_processing="inst"></field_instances>
18	<pre><field ensemble_operation="mem_1" name="XLAT" time_processing="inst"></field></pre>
19	<pre><field ensemble_operation="mem_1" name="XLONG" time_processing="inst"></field></pre>
20	
21	<pre><pre>cessing_control status="on" ></pre></pre>
22	<pre><working_directory path="./experiment/da1" status="on"></working_directory></pre>
23	<config_scripts status="on"></config_scripts>
24	<pre_instance_script name="" status="off"></pre_instance_script>
25	<pre><post_instance_script name="da1_p2_online_run.sh" status="on"></post_instance_script></pre>
26	
27	
28	
29	<da_instance name="DA_algorithm2" status="on"></da_instance>
30	<external_procedures dll_name="lib_da2.so" procedures_name="algorithm2" status="on"></external_procedures>
31	<pre><pre>cperiodic_timer status="on" period_unit="seconds" period_count="21600" local_lag_count="0"/></pre></pre>
32	<field_instances ensemble_operation="gather" status="on" time_processing="inst"></field_instances>
33	<pre><pre>control status="on" ></pre></pre>
34	<pre><working_directory path="./experiment/da2" status="on"></working_directory></pre>
35	<config_scripts status="on"></config_scripts>
36	<pre_instance_script name="./scripts/da2_pre_online_run.sh" status="on"></pre_instance_script>
37	<pre><post_instance_script name="./scripts/da2_post_online_run.sh" status="on"></post_instance_script></pre>
38	
39	
40	
41	

795 Figure 7. Example of the XML configuration for a DA experiment.



Figure 8. 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.



805 Figure 9. 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.



Figure 11. 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.

(a) FIO-AOW				_							(b))]	DA i	instances								
		Μ	PI P	roce	sses		$ \bot$	_	_	М	IPI_C	OMM	L_WO	RLD						GSL	obser	ver	
		1	2	3 4	1 5	6	í 🗖				F	10-A	OW							for 1	neml	ber	
		-	2	5 -		0						WR	F						r.	GSI	obser	ver	
	0	1	2	3 4	5	6						PO	М						Ior	ense	mble	: mea	n
	0	1	2	0 1	0	1					N	1ASN	UM							E	nKF		
(c)	-									N	1PI	Pro	cess	es									
	Member 1					Member 2									Me	embe	er 3						
		0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	1
		0	1	2	3	4	5	6	0	1	2	3	4	5	6	0	1	2	3	4	5	6	1
		0	1	2	0	1	0	1	0	1	0	1	2	0	1	0	1	2	0	1	0	1	I
		0	1	2							3	4	5			6	7	8					I
		0	1	2							0	1	2			0	1	2					1
		0	1	2							3	4	5			6	7	8					

Figure 12. Example of the process layout of the example ensemble DA system FIO-AOW. (a) Each ensemble member of FIO-AOW 820 (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.

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830 Figure 13. 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.



835 Figure 14. As in Fig. 13, but from experiment set 2 in Table 2.



840 Figure 15. As in Fig. 13, but from experiment set 3 in Table 2.



845 Figure 16. As in Fig. 13, but from experiment set 4 in Table 2.



850 Figure 17. 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.



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.

Table 1. Horizontal resolutions and time steps of WRF.

Horizontal	Total Horizontal	T ¹ C 4		
Resolution	Grid Points	Time Step		
45 km	160×120	180 s		
30 km	240×180	120 s		
15 km	480×360	60 s		

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

Export cot	Horizontal	Number of	Processes for each	I abel marks		
Experiment set	resolution	ensemble members	ensemble member	Laber marks		
		5		15KM_5mem_160proc		
S of 1	15 Jun	10	160	15KM_10mem_160proc		
Set I	13 KIII	15	160	15KM_15mem_160proc		
		20		15KM_20mem_160proc		
			40	15KM_10mem_40proc		
Set 2	15 Jun	10	80	15KM_10mem_80proc		
Set 2	15 KIII	10	160	15KM_10mem_160proc		
			320	15KM_10mem_320proc		
	45 km			45KM_10mem_80proc		
Set 3	30 km	10	80	30KM_10mem_80proc		
	15 km			15KM_10mem_80proc		
	45 km		40	45KM_10mem_40proc		
Set 4	30 km	10	80	30KM_10mem_80proc		
	15 km		320	15KM_10mem_320proc		

	Number of	Number of	Total I/O	Number of model	Total I/O accesses to
Horizontal	ensemble	observation prior	accesses to	ensemble	model ensemble
resolution	members	files	observation priors	background & analysis files	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

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