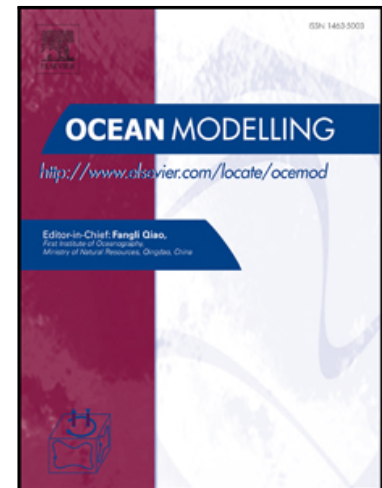


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Highlights

- Parallel DA framework is fused with ESMF to bring DA ability for coupled models.
- Obvious improvement of model skill is achieved for idealized and realistic cases.
- This DA tool incurs minimal overhead even using large core counts.

Journal Pre-proof

Development of a flexible data assimilation system for a 3D unstructured-grid ocean model under Earth System Modeling Framework

Hao-Cheng Yu^{1*}, Y. Joseph Zhang¹, Lars Nerger², Carsten Lemmen³, Jason C.S. Yu⁴, Tzu-Yin Chou⁴, Chi-Hao Chu⁵, Chuen-Teyr Terng⁵

¹Center for Coastal Resource Management, Virginia Institute of Marine Science, College of William & Mary, Gloucester Point, 23062, USA

²Alfred-Wegener-Institut Helmholtz-Zentrum für Polar und Meeresforschung, Bremerhaven, 27570, Germany

³Institute of Coastal Systems Analysis and Modeling, Helmholtz-Zentrum Hereon, Geesthacht, 21502, Germany

⁴Baytech Environment and Engineering Inc., Kaohsiung, 80143, Taiwan

⁵Marine Meteorology and Climate Division, Central Weather Administration, Taipei, 100006, Taiwan

*Correspondence to: Hao-Cheng Yu (hcyu@vims.edu)

Abstract. We develop a new data assimilative (DA) system by combining two parallel frameworks: the Parallel DA Framework (PDAF) and the Earth System Modeling Framework (ESMF). The new DA system is built on ESMF at the top level driving PDAF and any combination of Earth system model (ESM) components, thereby allowing maximum flexibility and ease of implementation of DA in fully coupled ESM applications, with minimal intrusive code changes to the original model components. We demonstrate the new DA system using the 3D unstructured-grid ocean model SCHISM as the ESM component. The new system is validated using both simple benchmarks and a realistic simulation of the Kuroshio current system around Taiwan. The new system improves the model skill for temperature and surface elevation before, during and after typhoon events. The flexibility and ease of implementation make the new system widely applicable for other coupled ESMs, thus paving the way for a new generation of data assimilative cross-scale ESMs.

Keywords: data assimilation; coupled cross-scale models

1. Introduction

Ensemble based data assimilation (DA) approaches are popular choices for DA and are less intrusive to the original model code than adjoint based approaches; numerous successful applications using either ensemble or adjoint approaches have been presented before (Kalnay et al., 2007, Carrassi et al., 2018, Vetra-Carvalho et al., 2018). However, so far, the utility of DA for cross-scale problems has not been well demonstrated, despite the obvious fact that the distribution of the observation points is highly uneven (e.g., sparse observation offshore vs dense observation nearshore). Therefore, it is highly desirable to develop DA capability for fully coupled, next generation cross-scale Earth System Models (ESMs).

A prominent example of a community-supported DA package is the Parallel Data Assimilation Framework (PDAF; Nerger et al. 2005, Nerger and Hiller 2013), which has been successfully used with several domain models such as FESOM, NEMO, or MITgcm. It is model agnostic and can handle different types of ESM component models written in modern parallel computing languages, including those represented by structured or unstructured grids, or solved explicitly or implicitly. PDAF allows to choose offline and online coupling between the DA component and the ESM components. While the offline coupling mode interfaces between the model and data assimilation codes using disk files and is hence less intrusive to the model code, the online mode (model system code with augmented DA functionality) is more efficient and allows the direct feedback from DA results to the ‘forward’ model. We focus on the online mode in this paper.

A large and growing selection of ensemble filters of both ensemble Kalman and particle filters is available inside PDAF (Table 1). Furthermore, 3D variational (3DVar) methods (see Bannister, 2017) are supported by PDAF; parameterized covariances can be used to represent the uncertainty in the model state or ensembles, which are propagated using the same ensemble infrastructure as the ensemble filters for maximum efficiency. For operations, PDAF supports two modes: (1) a fully parallel mode where all ensemble members are executed simultaneously during time stepping, and (2) a flexible mode where subsets of members (‘cohorts’; cf. Fig. 2) are executed in batches. The fully parallel mode allows maximum efficiency as measured by ‘time-to-solution’, but the flexible mode is more practical because computational resources may not always be sufficient to support the fully parallel mode (Valcke 2022).

So far, PDAF enabled DA applications have mostly focused on a single ESM component at a time, like the ocean (e.g. Nerger et al. 2007, Brune et al. 2015), sea-ice (e.g., Yang et al., 2014, Mu et al., 2019), ocean-biogeochemistry (e.g., Pradhan et al., 2019, 2020; Goodliff et al., 2019), atmospheric transport (Pardini, 2020), or the solid Earth (Fournier et al., 2013; Schachtschneider et al. 2022). *While extension to cover multiple coupled components has been demonstrated with PDAF (Nerger et al., 2020, Kurtz et al. 2016; Tang et al. 2021), this often involves non-trivial amount of developmental work.* The ensemble based DA systems such as PDAF require time-stepping of multiple ensemble members of the forward model, often written in domain decomposition based MPI parallelism (Gropp et al., 1994). While PDAF allows partitioning of global (‘world’) communication space into sub-communicators for each ‘instance’ of the model (ensemble member), it is challenging to generalize it to account for complex nonlinear coupling between ESMs without intrusive changes to the original model code. Therefore, here we implement the new DA system under the umbrella of a parallel coupling framework, the Earth System Modeling Framework (ESMF, <https://earthsystemmodeling.org/>, last access: 28 Feb 2024). This allows DA to be performed on fully coupled ESMs running on different grids/meshes, as ESMF can perform efficient regridding and interpolation between various ESM components.

In this paper, we develop a DA system based on ESMF-PDAF that can be easily extended to assimilate observations into multiple coupled ESM components simultaneously, with minimal changes to the original component codes (even under the most flexible mode). To clearly demonstrate the methodology, however, in this paper we will focus on the unstructured-grid ocean model (SCHISM), while extension to coupled ESMs (e.g., ocean-atmosphere-biology etc.) is

demonstrated using a simple coupled atmosphere-ocean model. This new capability represents a major step toward improving the skill of cross-scale coupled ESMs (such as SCHISM) via data assimilation.

The paper is organized as follows. We first describe the building blocks and overall structure of the new DA system in Section 2. We then validate the new system using a simple twin experiment in Section 3.1 and a simple coupled atmosphere-ocean model. In Section 3.2 we apply the DA system to a challenging realistic case of northwestern Pacific. Efficiency and overhead of the new DA system are examined in Section 3.3 using the realistic case. Finally, we summarize the major findings in this paper and future work in Section 4.

2. SCHISM-PDAF implementation under ESMF

ESMF is a suite of software tools for developing high-performance, multi-component Earth science modeling applications. Such applications may include many components representing atmospheric, oceanic, terrestrial, or other physical domains, and their constituent processes (physical, chemical, biological, etc.). Often these components are developed by different groups independently and must be “coupled” together using software that transfers and transforms data among the components in order to form functional simulations. ESMF introduces a set of simple and consistent component interfaces that apply to all types of components, including couplers themselves. These interfaces explicitly expose in the inputs and outputs of each component. ESMF offers a variety of data structures for transferring data between components, and libraries for regridding, time advancement, and other common modeling functions. ESMF coupling has been used to construct modular ESMs at low, high, and flexible granularity. In general, using ESMF as mediator to link all components leads to less intrusion to the model code and to maintain independence of each library.

Once the parallel world is partitioned into smaller worlds using ESMF for each ensemble member used in the DA, which is executed by a persistent execution thread (PET), the ESM and PDAF interface codes are inserted into the main ESMF driver (Fig. 1). The PDAF interface consists of initialization (at the start of simulation) and a few subroutine calls to PDAF during time stepping. The latter include `PDAF_get_state()` for updating member state and `assimilate_pdaf()` at the specified times of assimilation. Code intrusiveness is minimized with only these two calls to be added to the original ESMF component code; all other changes required are outside the original component code: inside the driving application and in the ‘binding’ codes for each ESM component. The types of filters available in the latest PDAF version are described in Table 1. Currently we have implemented 7 types of filters, in this work we focus on 2 filters ETKF (Hunt et al. (2007) and ESTKF (Nerger et al. (2012a, 2012b) together with their localized variants (LETKF, LESTKF). The choice of these filters is motivated from the fact that both are widely used, computationally efficient and highly effective in their DA skills.

We first supply PDAF with the required ‘binding’ (interface) codes to link PDAF and the ocean model, SCHISM (Semi-implicit Cross-scale Hydroscience Integrated System Model; <http://ccrm.vims.edu/schismweb/>, last access: 28 Feb 2024; Zhang et al. 2016). PDAF is designed to link with any ESM with a more generalized interface through a set of functions

(Fortran subroutines in our case), whose linking into any model is described in the PDAF tutorial (<http://pdaf.awi.de/trac/wiki/PdafTutorial>, last access: 28 Feb 2024). Here we list the major interface codes:

- 1) collect_state_pdaf/distribute_state_pdaf: create functions to fill model the state vector array with specified SCHISM variables or update SCHISM variables with values from state vector;
- 2) init_dim_obs_all: provide interface to read in observation data including error estimates for each observation type;
- 3) PDAFomi_obs_op_schism: choose an observation operator to project model state onto observed state;
- 4) init_dim_l_pdaf: specify local analysis domain, e.g., a vertical grid column, and localization radius within which observations are utilized by the local filter;
- 5) l2g_state_pdaf/g2l_state_pdaf: add ‘local to global’ / ‘global to local’ model state conversion routine for local filter;
- 6) output_netcdf_pdaf: add interface to output DA (ensemble mean and its spread) result.

Furthermore, to accommodate the flexible mode of PDAF, i.e., using fewer number of PETs than the number of ensemble members, the time stepping part of SCHISM code needed to be generalized. The flexible mode requires ‘rewinding’ of time clock after an ensemble member reaches the next assimilation time. This is because another ensemble member shares the same memory space, and the external forcing (wind, etc) needs to go back to the starting time to redo the time stepping (Fig. 2). To this end, we have modified the reading of forcing inside SCHISM to allow arbitrary rewinding.

The lowest level of the DA system is the ESM component. In this paper we will focus on a single component, the ocean model. SCHISM is an open-source 3D baroclinic model for cross-scale hydrodynamic and hydrologic applications. It uses unstructured quadrangular-triangular elements in the horizontal dimension and a very flexible vertical gridding system (Localized Sigma Coordinates with Shaved Cell, LSC²; Zhang et al. 2015). The model has been successfully applied to many nearshore and offshore systems around the world (see <http://ccrm.vims.edu/schismweb/> for a complete publication list). Related to this study, the model has been used as the engine for the operational forecasting system for Taiwan since 2011 (Yu et al. 2017; https://npd.cwa.gov.tw/NPD/resident_product/marine_model?version=public, last access: 28 Feb 2024).

Extension to coupled ESMs with the current DA system involves preparation of the binding codes (1-6) for each ESM component, and addition of ESM interfaces inside the main ESMF driver similar to the SCHISM part in Fig. 1. The complex model coupling is handled by ESMF in a modular way using high-level function calls. To demonstrate the DA capability for coupled ESMs, in this paper we use a simple atmosphere model whose wind is a function of Sea-Surface Temperature (SST):

$$U_x^{n+1} = \alpha \frac{U_x^n}{T_w} - \beta (T_w - 16) \quad (1)$$

$$U_y^{n+1} = 0.1 * U_x^{n+1} \quad (2)$$

$$\alpha = 1 \text{ (}^\circ\text{C)}, \beta = 0.5 \left(\frac{m}{s^\circ\text{C}}\right) \quad (3)$$

where n and $n+1$ are time step index, and T_w is SST. This simple coupling is used here only to demonstrate the mechanics of nonlinear coupling and is not meant to represent any real physics. The time stepping for the atmospheric model is inserted

before SCHISM stepping routine in ESMF (Fig. 3); the wind vector is updated in each time step and its effects fed back to ocean surface. For the code of assimilation, following steps described above, we only need to include wind vector in model state vector, and insert corresponding operator to derive atmosphere model state in the code, as well as its output interface and other small changes in the original binding code (Fig. 3). Real application with coupled ESMs follows a similar procedure.

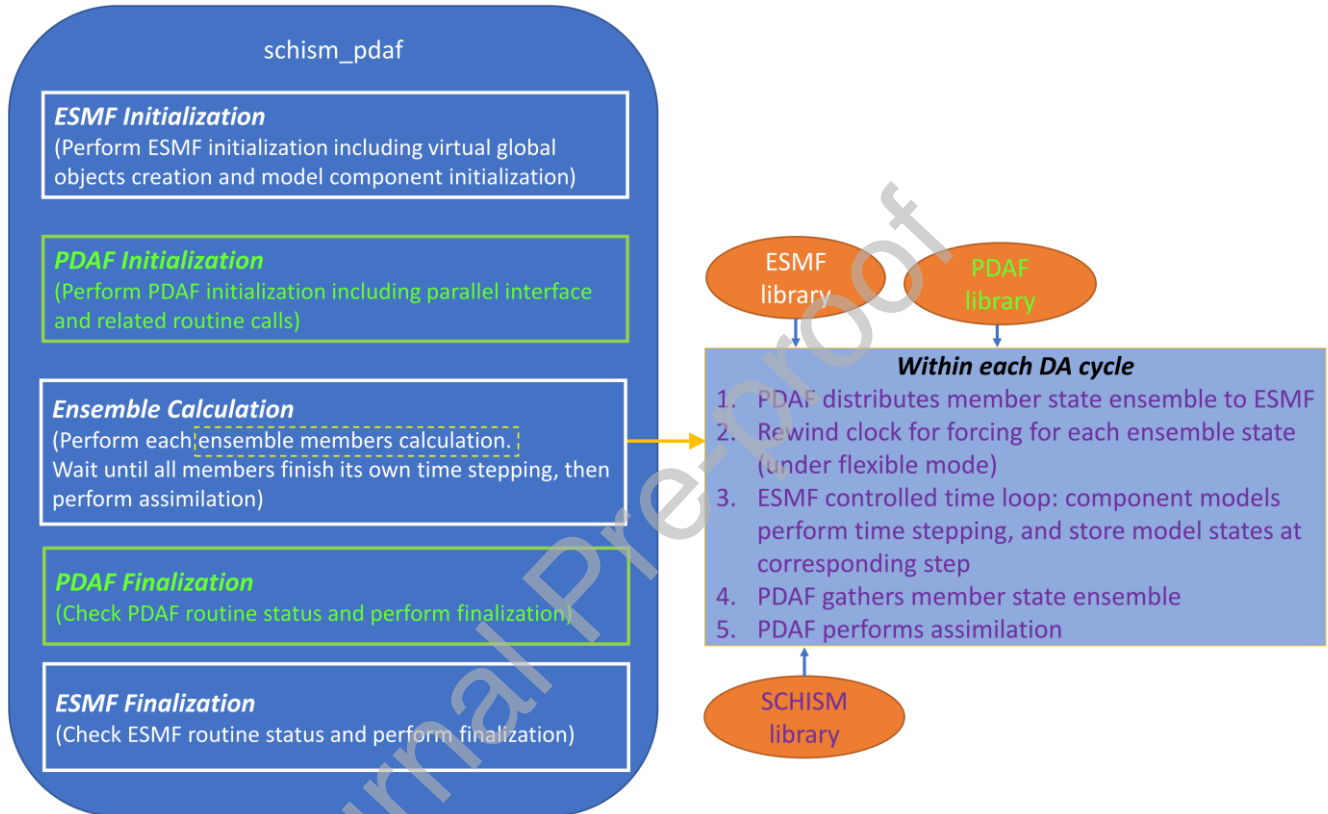


Fig. 1: Schematic code structure for the new DA system. At the top level, ESMF is used to orchestrate the parallel environment and model coupling. It initiates the environment for PDAF (for each ensemble member) and for ESMs. The code requires multiple libraries: ESMF, PDAF and one for each ESM (SCHISM in this case).

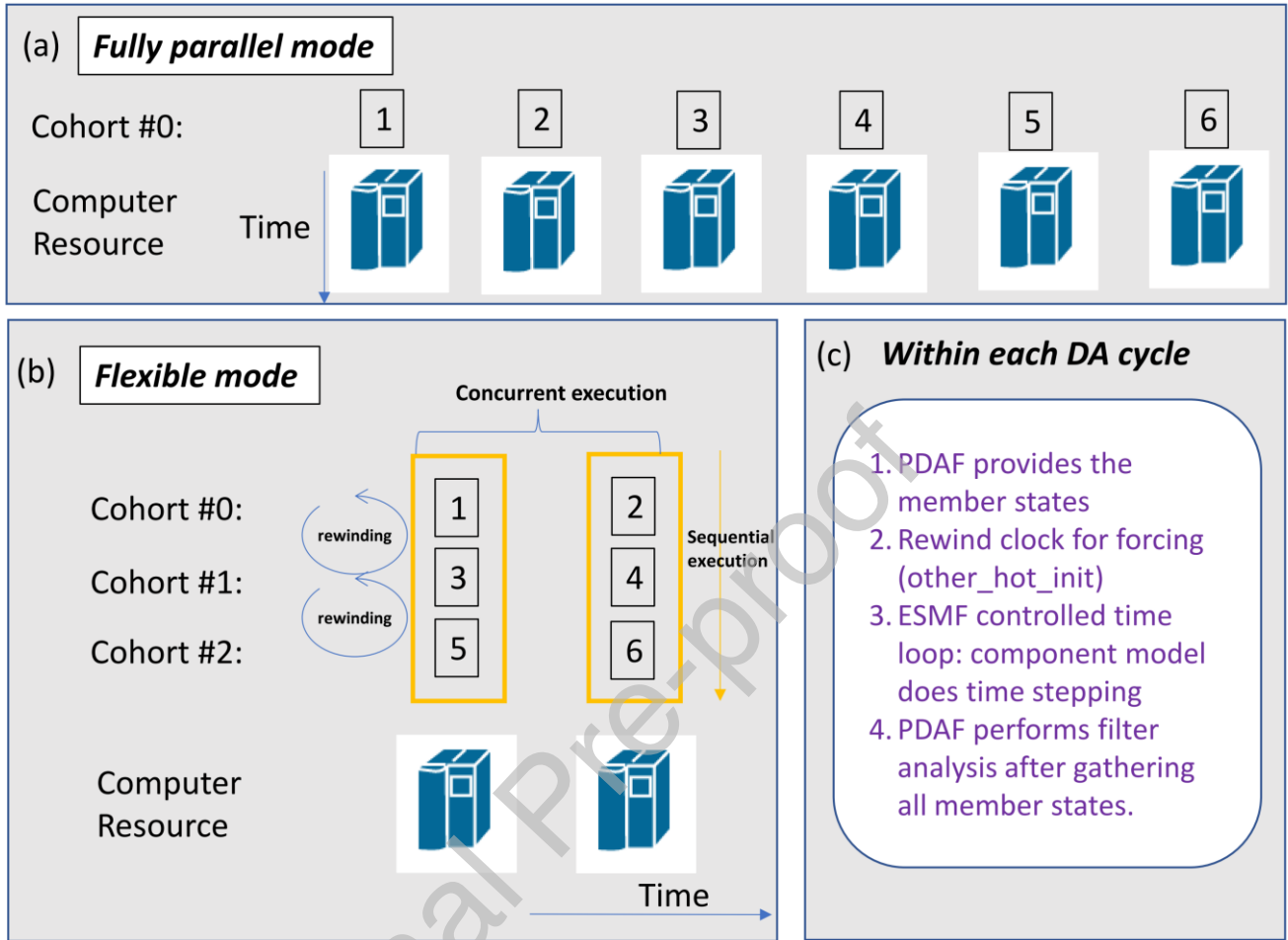


Fig. 2: Time stepping part of the new DA system (i.e., the dashed yellow box in Fig. 1) under (a) fully parallel mode and (b) flexible mode. Task IDs (1,2,...6) are distributed into 3 'cohorts' for concurrent execution in ESMF under the flexible mode of PDAF. The task IDs in each orange box in (b) are executed on the same PET sequentially, and the clock needs to be rewound during the hand-over between '1' and '3' etc via the subroutine 'other_hot_init'. Under either mode, model state will be updated from previous analysis and use the 'right' clock time forcing to restart the model stepping in each DA cycle as shown in (c).

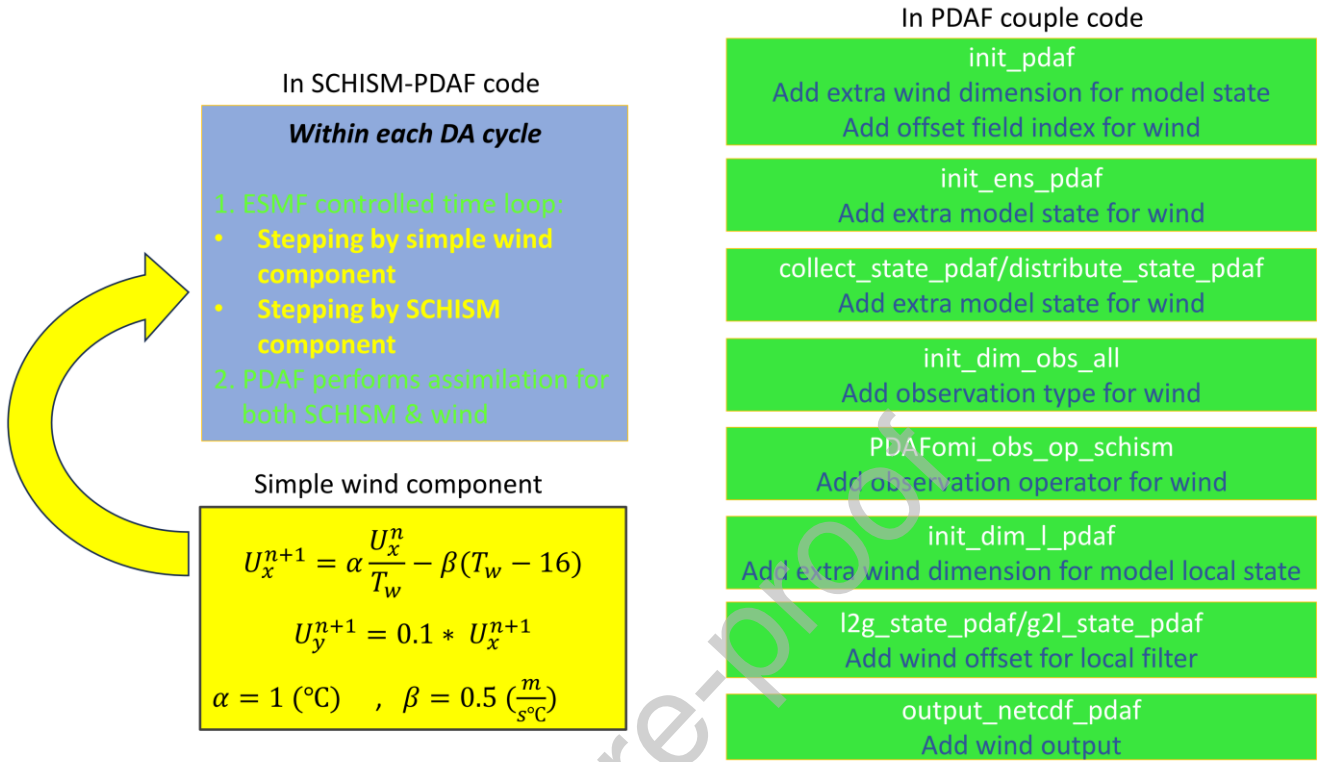


Fig. 3. Extra SCHISM-PDAF code added in coupling the simple atmosphere model.

Table 1: Types of filters supported in SCHISM-PDAF

Filter	Localized version	Implementation status	Reference
Error-Subspace Transform Kalman Filter (ESTKF)	LESTKF	Ready	Nerger et al. (2012a, 2012b)
Ensemble Transform Kalman Filter (ETKF)	LETKF	Ready	Bishop et al. (2001) Hunt et al. (2007)
Ensemble Kalman Filter (EnKF)	LenKF	Ready	Evensen (1994)
Singular Evolutive Extended Kalman (SEEK)		Ready	Pham et al. (1998b)
Singular Evolutive Interpolated extended Kalman (SEIK)	LSEIK	Ready	Pham et al. (1998a, 2001)
Non-linear Ensemble Transform Kalman Filter (NETF)	LNETF	Ready	Tödter & Ahrens (2015)

Particle Filter with resampling (PF)		Ready	Vetra-Carvalho Sanita et al. (2018)
3Dvar with parameterized covariance matrix (3Dvar)		In development	Bannister (2017)
3Dvar using ensemble covariance matrix (3DenVar)	Ensemble perturbations are updated with the LESTKF filter	In development	Bannister (2017)
Hybrid 3Dvar using a combination of parameterized and ensemble covariance matrix (Hyb3Dvar)	Ensemble perturbations are updated with the LESTKF filter	In development	Bannister (2017)

3. Validation and application of the new DA system

In this section, we will first validate the new DA system using a simple idealized test with simulated ‘observations’. We then apply the system to a realistic and challenging case of simulating typhoons in the northwestern Pacific with a focus on the regions near Taiwan using satellite and in-situ profiler observations. We will also demonstrate the efficiency and overhead of the DA system in the realistic case.

3.1 Lock-exchange test

3.1.1 Test description

To verify that this DA framework works as intended, we start from a simple test case provided by a lock-exchange experiment. This test case is initialized with a horizontally varying (but vertically uniform) temperature distribution (10°C at $x=0$ km and linearly increases to 16°C at $x=20$ km) in a narrow, closed tank with sloped bathymetry (Fig. 4). The tank dimension is 20 km in length with 1km width, with depth varying from 50m to 10m with a linear slope between $x=6$ km and 13 km (Fig. 4). The only external forcing is the surface wind that mixes the water.

3.1.2 Generation of ensemble and observation

The generation of an initial ensemble of model state realizations is a key step in PDAF and a good ensemble spread is desirable to cover potential model state trajectory to ensure success of assimilation (Vetra-Carvalho et al., 2018). Here we follow Pham’s method (Pham, 2001) to generate member states as suggested by PDAF. We first conduct a 5-day free model run and extract hourly snapshots of the model state during the entire simulation period. With EOF-decomposition analysis, singular vectors and values are extracted from these snapshots. The ensemble member states are then initialized from these values. For this a

particular matrix that represents the model mean and covariance is generated by multiplying each singular vector with the corresponding singular value. This matrix is then multiplied by a random matrix with properties that ensure conservation of the mean state and covariances to yield the ensemble perturbations. The random matrix is created from independent random vectors with unit norm, which are projected to be orthonormal to each other and orthogonal to the vector whose elements are one (for details see the Appendix of Nerger et al., 2012b). This method basically utilizes the inherent variability of model dynamics to represent uncertainty.

We follow the common twin-experiment setup here. The free run snapshots are used as “truth”. Observation data is then extracted from the “truth” by adding Gaussian-distributed random values within a standard deviation of 0.15°C that represents the observation error. To assess how well the assimilation can rectify the ‘erroneous’ model states, the ensemble model mean is initialized by intentionally adding -1°C to the first 24-hour mean state. Note, that this biased model state represents a sub-optimal case for the data assimilation, because the ensemble filters assume unbiased errors. The error statistics shown below are calculated with respect to the “truth”.

Major DA parameters include filter type, frequency of DA cycle, forgetting factor, localization radius and observation error (Carrassi et al. 2018). The observation error, whose estimates usually come with observation data, is found to be an important control. For practical applications, we have implemented 3 types of observation error input options. The first option sets the errors uniformly for all observation types. The second option allows different errors to be used for different variables, such as elevation, temperature etc. The third option is the most flexible, allowing the errors to be specified at each observation point, and is most useful for operational forecasts.

3.1.3 DA experiments

To examine the code performance, we conduct 4 experiments (Table 2) based on vertical profile observations. Exp.1 uses only 1 observation profile. Exp.2 is same as Exp.1 but examines how different observation errors affect the results (note that even though we know the exact value for this error in this simple case, we do not know this information in realistic cases). These two experiments will be discussed in Section 3.1.4. Exp. 3 (Section 3.1.5) uses multiple observation profiles with different filters. Exp. 4 (Section 3.1.6) is same as Exp. 3 but uses a coupled atmosphere model to demonstrate how to perform coupled DA. The wind forcing is not perturbed except in Exp. 4.

Table 2. Lock-exchange experiments and settings

	OBSERVATION	OBSERVATION ERRORS ($^{\circ}\text{C}$)	WIND SPEED (MS^{-1})
EXP 1	Single profile	0.15	0.5 (West)
EXP 2	Single profile	0.5, 0.15, 0.01	0.5 (West)
EXP 3	Multiple profiles	0.15	0.5 (West)
EXP 4	Multiple profiles	0.15	Coupled with atmospheric model

3.1.4 Results from assimilating a single profile

To clearly see how DA rectifies the model state, we start with only assimilating one temperature profile (down to 40m). LESTKF filter is used here with 8 ensemble members and 1000m as the localization radius to perform the analysis. The possibility to use small ensemble size (8 here) came from the use of Pham's 2nd-order exact sampling to initialize the ensemble because this ensures that the major covariance structure is represented already in a small ensemble. The local filter gives better results than the corresponding global filter in this test (Nerger et al. 2006). Figure 4(a) shows the difference between background and analysis ensemble mean (i.e., analysis increments). The analysis results indicate that the local filter (LESTKF) alters the model state mostly in the specified localization radius (1000 m).

The sensitivity to the observation error can be clearly seen in Fig. 4(b). Smaller observation errors lead to results closer to the 'observation', as expected. However, we remark that in general smaller observation errors do not always guarantee the analysis result is closer to the "truth" because 'observation' inevitably contains errors. In practice, observation errors must be set appropriately to achieve desired results. In summary, Fig. 4 indicates that the DA system works as intended.

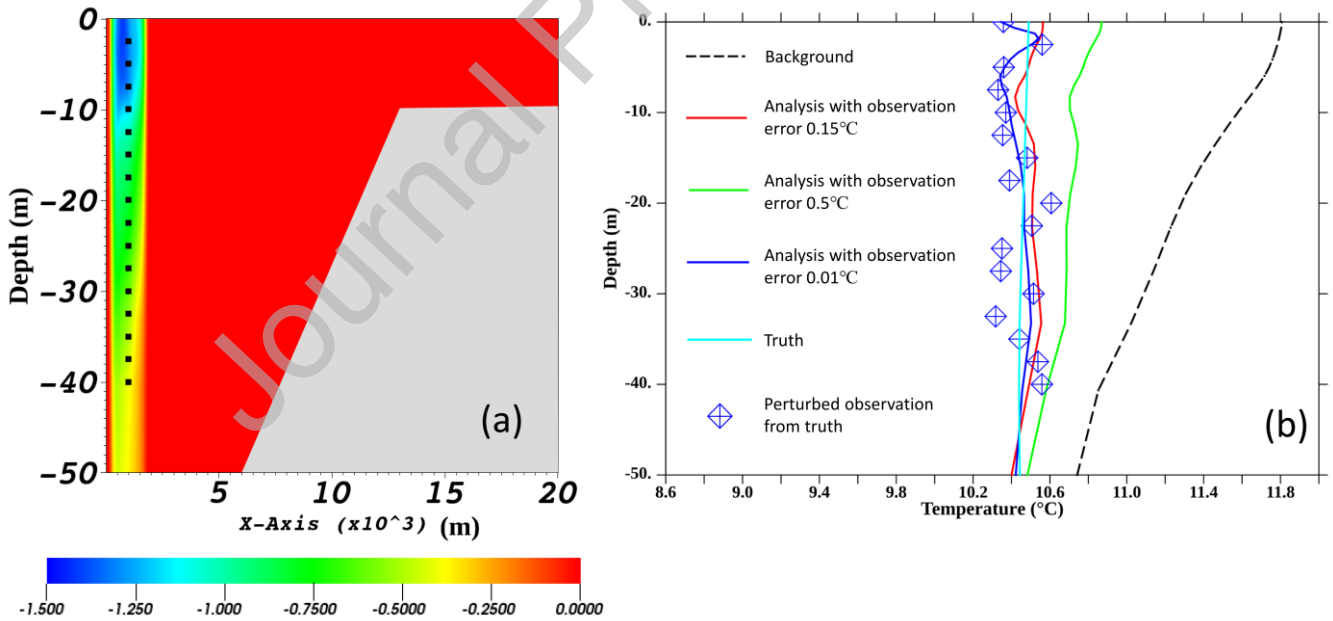


Fig 4. Lock-exchange test with 1 profile of observation. The contour plot in (a) shows transect view of the temperature *difference* before and after DA (i.e. Analysis - Background). Black dots indicate observation locations. (b) DA results with different observation errors at observation points.

3.1.5 Results from assimilating multiple profiles

In this setup, the temperature observation data points are extracted from 9 transects along the y-axis ($y=100\text{m}$, 200m , 300m ..., 900m , every 100m) direction every 250 meters in the x direction from 1 km to 19 km. In the vertical, observations are selected every 2.5 meters from surface to 40m depth as shown in the Fig. 5(a). Here we test 4 different filters including 2 global (ETKF, ESTKF) and 2 local filters (LETKF, LESTKF). Using 8 ensemble members, all those filters can immediately correct the model bias at the first DA cycle (Fig. 5). The global filters produce larger errors compared to the local filters in this case (Fig. 5). Localization suppresses spurious correlations which result from sampling errors caused by the small ensemble. In addition, the localization helps to limit the range of observation effects within the analysis domain. Due to this the local filter analysis results at both ends of the domain ($x < 6\text{km}$ and $x > 13\text{km}$) are closer to the ‘truth’. This difference can be understood from the fact that the global filter computes a global optimal ensemble combination with which the state estimate is incremented. This optimum is given by the relative errors of the model state and the observations. Since there are no observations at the ends of the domain, the assimilation results can deviate more there. In contrast the local filters decouple the computations of the optimums for distant locations from each other, so the increments on both ends of the domain are independent from each other. This effect of localization is well known for cases with abundant observations but also seems true for relatively sparse observations used here. Among the two local filters, LESTKF has certain advantages in that even if observation is locally missing for a long time, the inflation can still increase the ensemble spread for LETKF, but not the LESTKF (Nerger et al. 2012b), which may lead to over-amplified ensemble spread and thus worse analysis results with LETKF. Thus, LESTKF is generally recommended for most applications.

We have also tested with a larger number of ensemble size (40 members, Fig. 5(g-h)). The results suggest that large ensemble size can reduce errors. However, results with small ensemble size have also delivered satisfactory results as shown in this case (Fig. 5) as well as in the realistic application (Section 3.2) because of Pham’s method.

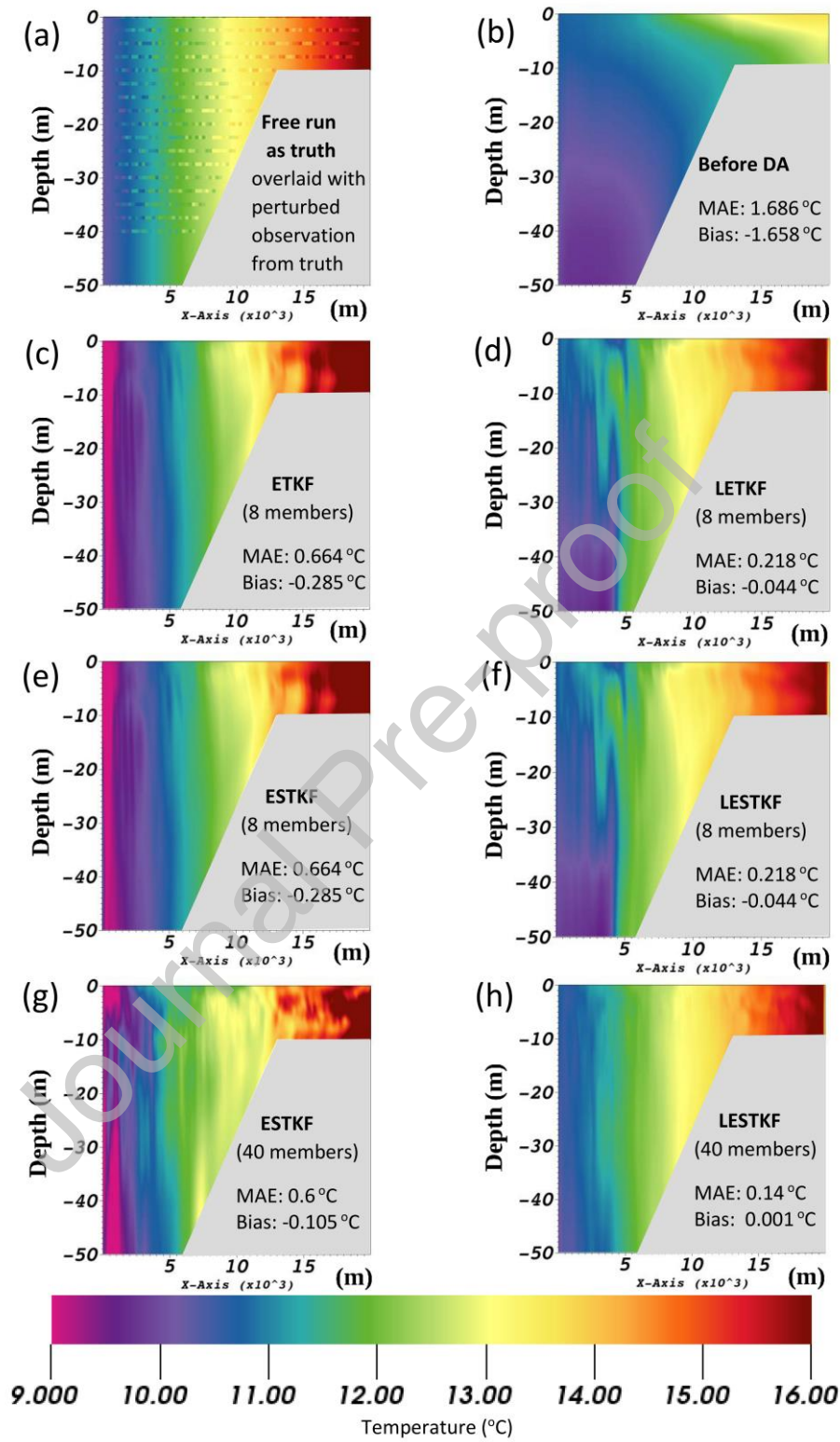


Fig 5. The vertical temperature transects after the 1st DA cycle using different filters. Initial model state is derived from 24-hour mean state with -1 °C offset. Domain-wide averaged Mean Absolute Errors (MAEs) & bias are shown for each case.

3.1.6 Coupling atmosphere model and its twin-experiment result

Lastly, the same Experiment 3 shown in the previous sub-section is used to test the simple coupled ocean-atmospheric model described in Section 2. Two filters (ESTKF & LESTKF) are tested here. The results for the water temperature and wind are shown in (Fig 6), which indicate that model states in both models can be rectified by PDAF. This simple system demonstrates that the current DA system can be easily extended to cover coupled ESMs.

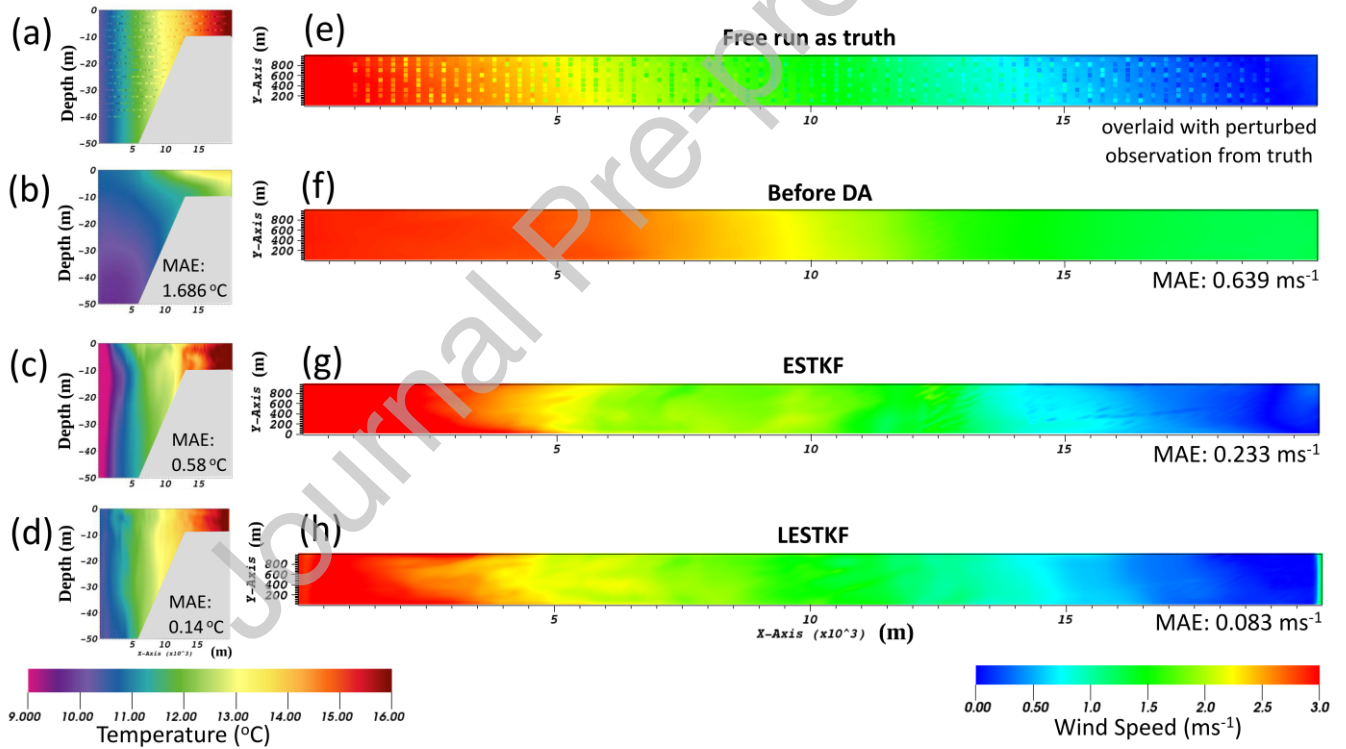


Fig 6. (a-d) Temperature results from the coupled atmosphere model, (a) Free run as truth, (b) before DA, (c) ESTKF, (d) LESTKF. (e-h) Wind speed (magnitude) after the 1st DA cycle using different filters, (e) Free run as truth, (f) before DA, (g) ESTKF, (h) LESTKF. Initial model state is derived from 24-hour mean state with a bias of -1 ms⁻¹ added. Domain-wide averaged MAEs are shown for each case.

3.2 Northwestern Pacific during typhoon events

3.2.1 DA setup

The Northwestern Pacific is a very complex system with multiple current systems interacting with each other and with complex bathymetry and geometry (Johns et al. 2001; Jan et al. 2006). A major western boundary current, Kuroshio, plays a critical role in transporting warm and salty water from equatorial Pacific to higher latitudes (Oey et al., 2013). Previously, we have successfully applied the 3D unstructured-grid model, SCHISM, to this challenging domain (Yu et al. 2017). In particular, we demonstrated that the combination of the flexible vertical gridding system with the flexible horizontal unstructured mesh is essential to capture many topographically driven processes.

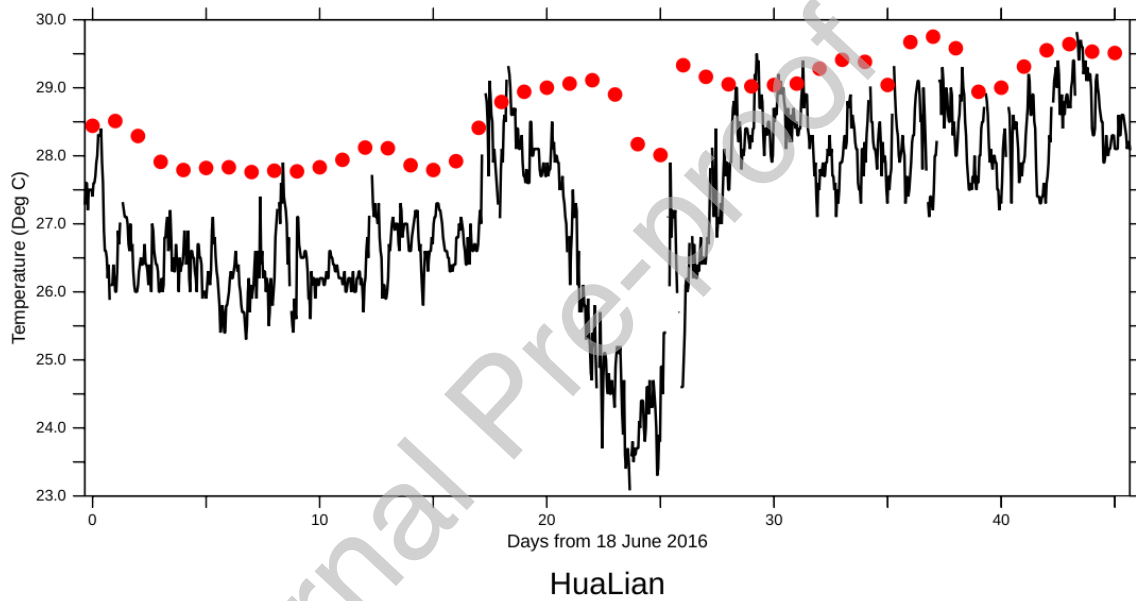
The focus here is on circulations around Taiwan, which exhibit very complex features (Jan et al. 2006). The SCHISM setup can be found in Yu et al. (2017). HYCOM GOFS 3.1 analysis (https://tds.hycom.org/thredds/catalogs/GLBv0.08/expt_57.2.html?dataset=GLBv0.08-expt_57.2, last access: 28 Feb 2024) is used for model initialization and open boundary conditions. The surface forcing is derived from ERA5 reanalysis surface field (Hersbach, H. et al., 2020). The simulation period starts from 18 June 2016 and ends on 2 August 2016 and covers the Typhoon Nepartak, which made landfall near Taiwan around 7 July 2016. We selected this period to clearly show the improvement made by DA, as the forward model (without DA) had obvious errors.

Compared to the simple case shown in Section 3.1, this realistic case is much more challenging because (1) the observation is usually much sparser than model points and often distributed unequally in space; (2) different types of observation come with different uncertainties, which may adversely affect DA results. To illustrate the 2nd point, we compare SST observations at two coastal buoys with satellite SST observations (cf. Table 3). As shown in Fig. 7, the discrepancies between the two types of observations can be as large as 2.5°C. Since the number of available buoys in the domain is too small for meaningful DA, we will not assimilate the buoy SST data. In general, conflicts between different types of observations represent a major hurdle for DA, in addition to poor data quality. In practice, users need to select best-quality observation. Table 3 summarizes the observation types used in this section. ESA CCI-SST level-4 satellite analysis products are used as the main observation (Merchant et al., 2019). In addition, there are about 20-30 ARGO floats (Argo, 2021) in our domain depending on specific periods. Figure 8 shows the ARGO distribution during our simulation period. In addition, AVISO sea level anomaly (SLA) from The Ssalto/Duacs altimeter products as produced and distributed by the Copernicus Marine and Environment Monitoring Service (CMEMS; <https://www.copernicus.eu/en/copernicus-services/marine>, last access: 28 Feb 2024) is combined with TPXO (Egbert and Erofeeva, 2002, <https://www.tpxo.net/global>, last access: 28 Feb 2024) tidal database to provide the observation for the total water elevation.

Two tests are shown here to illustrate the impact of different DA approaches (Table 4). Case A assimilates ESA CCI-SST with sparse ARGO data (about 20-30 vertical profiles each day) to correct the temperature. Case B additionally assimilates the

sea level data from AVISO and TPXO after 10 days. Validation for both cases will focus on SST and SLA around Taiwan; note that the only independent validation is against SLA for Case A (because it did not assimilate SLA directly). The observation error is provided by the data providers for the two satellite datasets. The observation errors of ARGO were set to 0.25°C for temperature and 0.25 PSU for salinity to account for the small mismatches between ARGO and ESA CCI-SST.

The approach for model ensemble member initial state generation follows that in the previous section, and we use 16 members in the test. In addition, we also tested with 40 members for Case B to examine the sensitivity. We use LESTKF with a specified localization radius of 0.5 degrees longitude and latitude. We didn't perturb lateral boundary conditions or atmospheric forcing because the influence of those perturbations is relatively minor in the interior of the domain for short duration validation cases shown in this study (see also Liang et al. 2020; Bruening et al. 2021; Koul et al. 2022). For operational applications however, we do plan to use ensemble atmospheric forcings which can be generated using the same Pham's method.



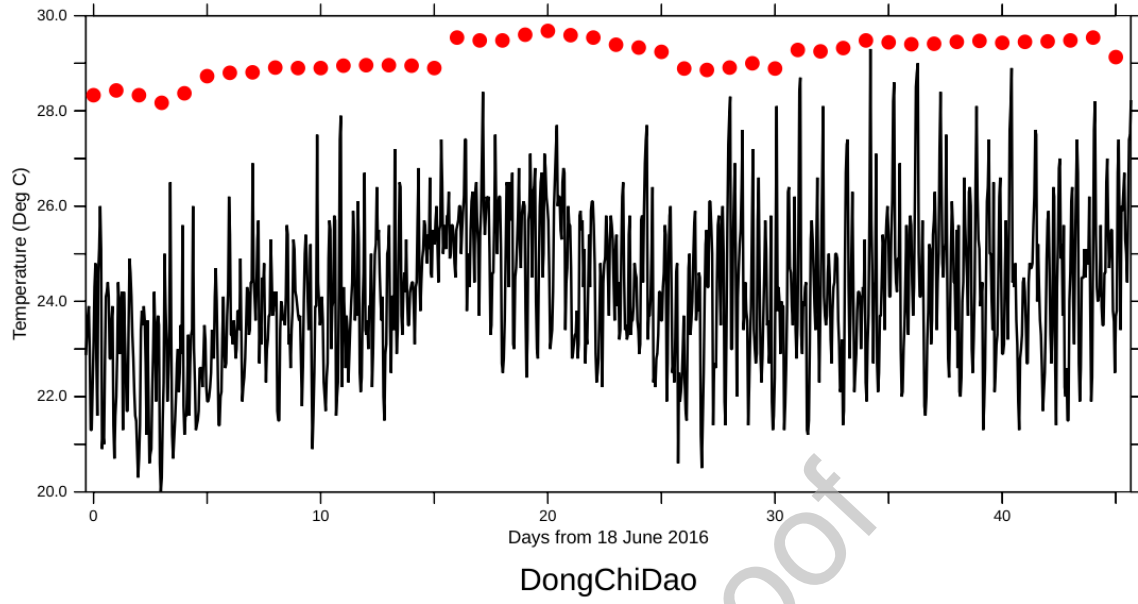


Fig. 7: Comparison of SST measured by in-situ buoys (blackline) and satellite (red dots) at two buoys near Taiwan. The buoy locations can be seen in Fig.8.

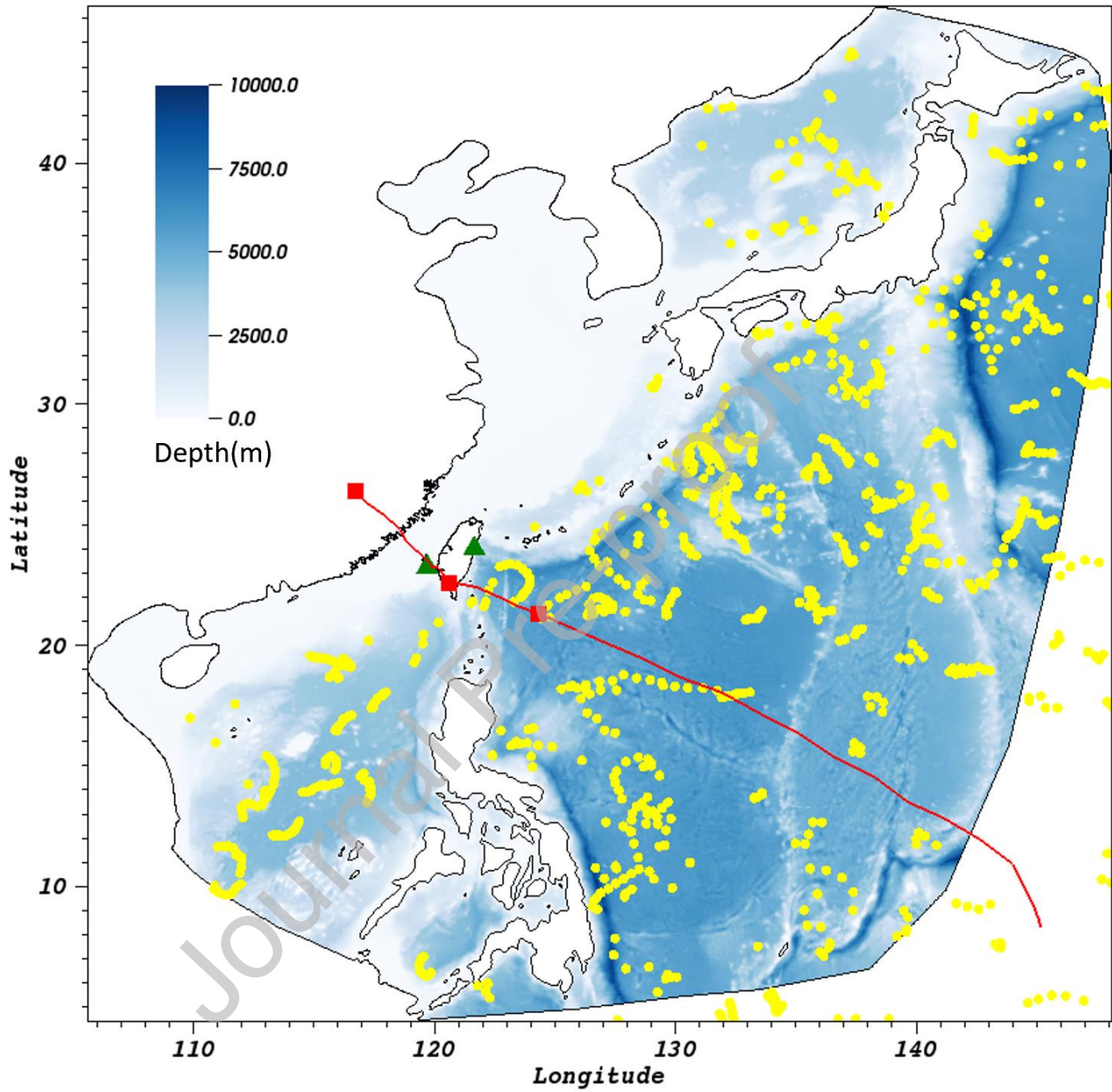


Fig. 8: Model domain for Northwestern Pacific with bathymetry, ARGO locations (yellow dots) within simulation period, Central Weather Administration buoy locations (green triangles), typhoon Nepartak track (red line), with the red squares representing the typhoon center locations corresponding to the times used in Fig. 10 & 12 (i.e., Day 19 (before), Day 20 (during), and Day 22 (after typhoon)).

Table 3 Observations data types used in DA and validation

OBSERVATION TYPE	HORIZONTAL RESOLUTION	FREQUENCY	OBSERVATION ERROR
ESA LEVEL 4 CCI-SST	0.05 degree	Daily	Directly derived from error estimation (0.16 ~ 3.66°C)
ARGO	Sparse and random	Input with daily frequency	0.25 °C & 0.25 PSU
AVISO SLA + TPXO	0.25 degree	Daily	Directly derived from SLA error estimation (range: 0.01~0.14 m)

Table 4 Real case setup

CASE	OBSERVATION ASSIMILATED
A	ESA CCI-SST, ARGO
B	EST CCI-SST, ARGO, AVISO-SLA + TPXO

3.2.2 Discussion of assimilation results

Since both cases assimilate SST data, the simulated SST is improved immediately after the first DA cycle compared to the free run without DA. This improvement is persistent throughout the entire 45-day simulation period, starting from relatively calm weather conditions to the brief severe typhoon and restoration period afterward. Figure 9 shows that after 19 DA cycles, SST from both Cases A&B have similar improvement compared to the free run and remain close to the observation in the entire domain. Closer to Taiwan, Figure 10 reveals some small differences between the two cases: assimilation of the SLA observation in Case B made a small difference in the deeper region, especially along the Kuroshio near Okinawa (in the region 124° E~128° E, 20° N~24° N; cf. the dash boxes in Fig.10). This difference persisted throughout the typhoon period (Fig. 10). Other than that, both cases perform well. Overall, the two cases have improved SST skills (Fig. 11); however, Case A shows a slightly better score in the latter half of the simulation (Fig. 11), probably due to some minor compensating effects from assimilating the AVISO. The two DA results show significant improvement from the free run (Fig. 11). Using 40 members in Case B modestly improved the overall model skill. This again confirmed that the smaller ensemble size used can already capture the model covariance because of Pham's method.

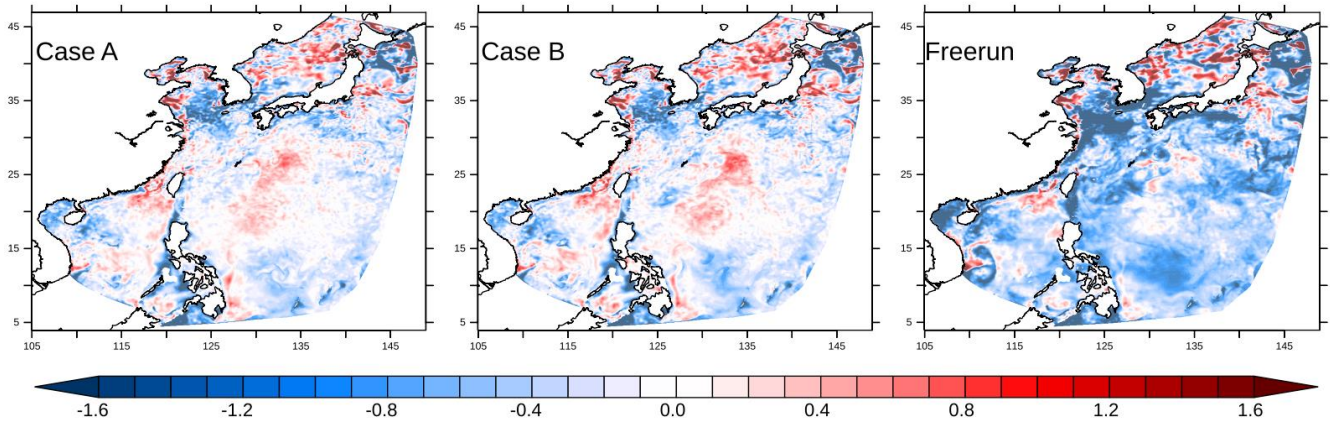


Fig. 9: SST bias ($^{\circ}\text{C}$) comparison on Day 19 (7 July 2016, before typhoon).

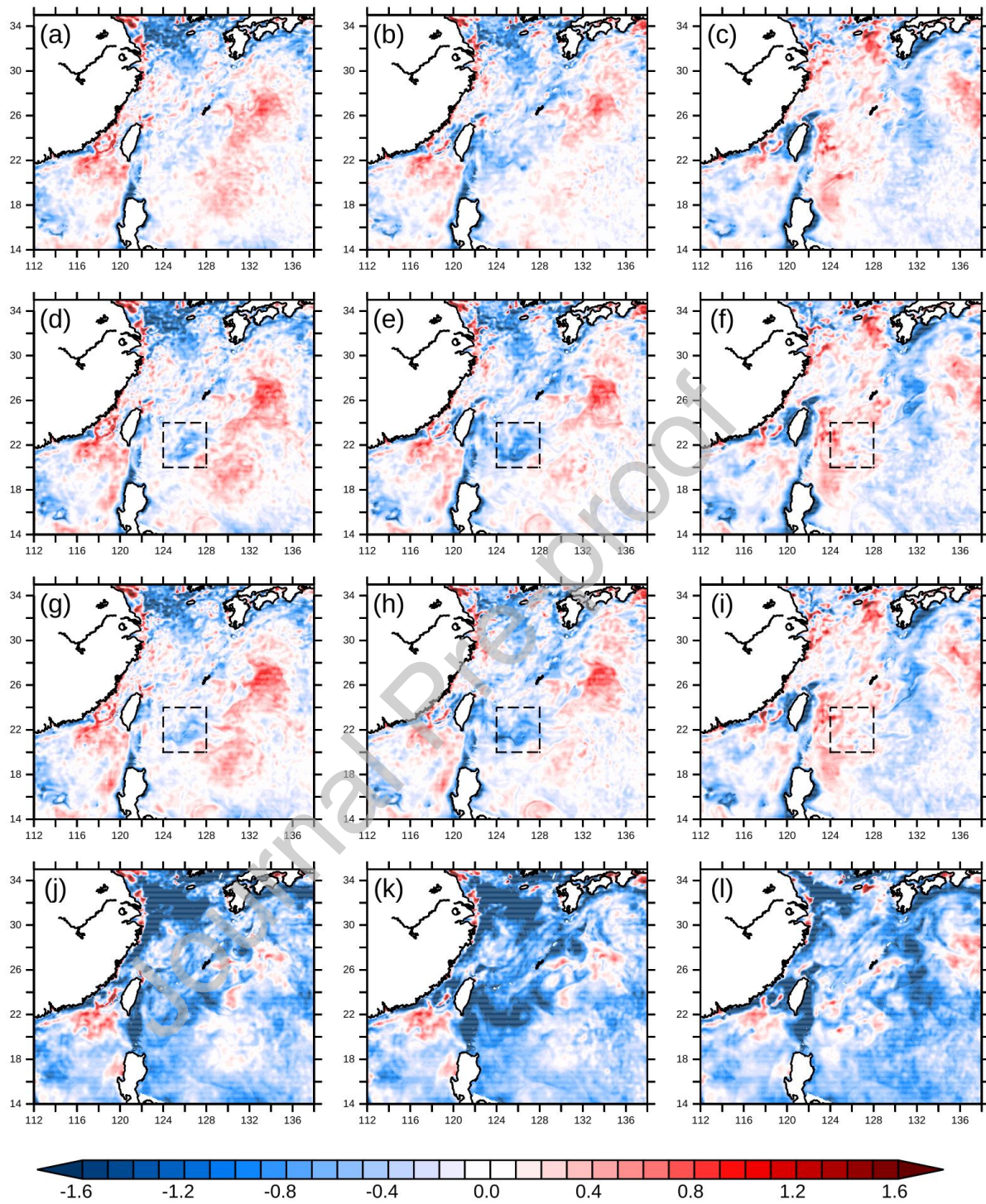


Fig. 10: SST bias (in $^{\circ}\text{C}$) comparison around Taiwan. Panels (a-c) represent Case A on Day 19 (before typhoon, 7 July 2016), 20 (during typhoon, 8 July 2016), 22 (after typhoon, 10 July 2016). The typhoon center locations are shown in Fig. 8. Panels (d-f) represent Case B; (g-i) represent Case B with 40 members; (j-l) represent the Free run.

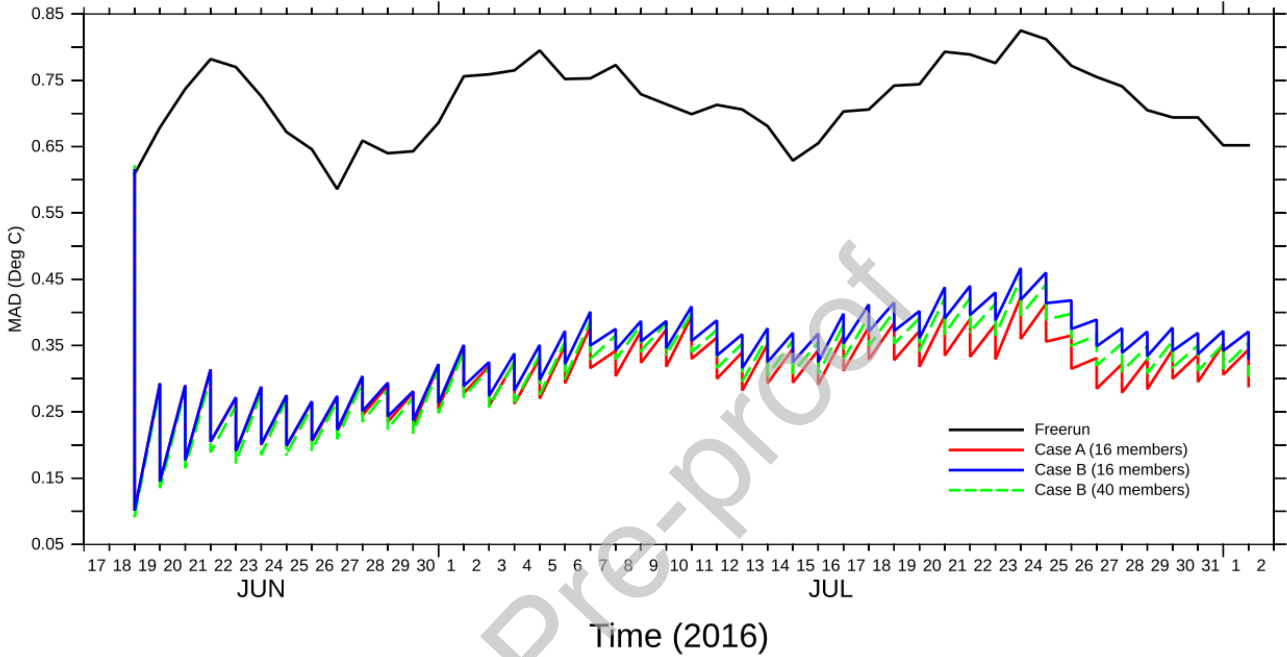


Fig 11: Comparison of averaged Mean Absolute Difference (MAD) of SST in the Taiwan region (whose extent is shown in Fig. 10a). The vertical jumps in cases A and B represent the DA effects at each analysis step.

For the SLA, both cases also deliver similar results. Case B, which explicitly assimilates AVISO, shows a slightly better performance and captures eddy location more accurately (Fig. 12). On the other hand, performance of Case A is also largely satisfactory (Fig. 12). Note that for Case A, the SLA data is considered as an independent validation dataset to evaluate how assimilating the temperature observation may improve other variables. Results from Cases A&B show improved skill from the free run in all stages of the typhoon (Fig. 12). As expected, the SLA in Case B has the best skill among all cases, especially after 10 days of DA (Fig. 13). Once again, using 40 members in Case B only marginally improved the skill (Fig. 13).

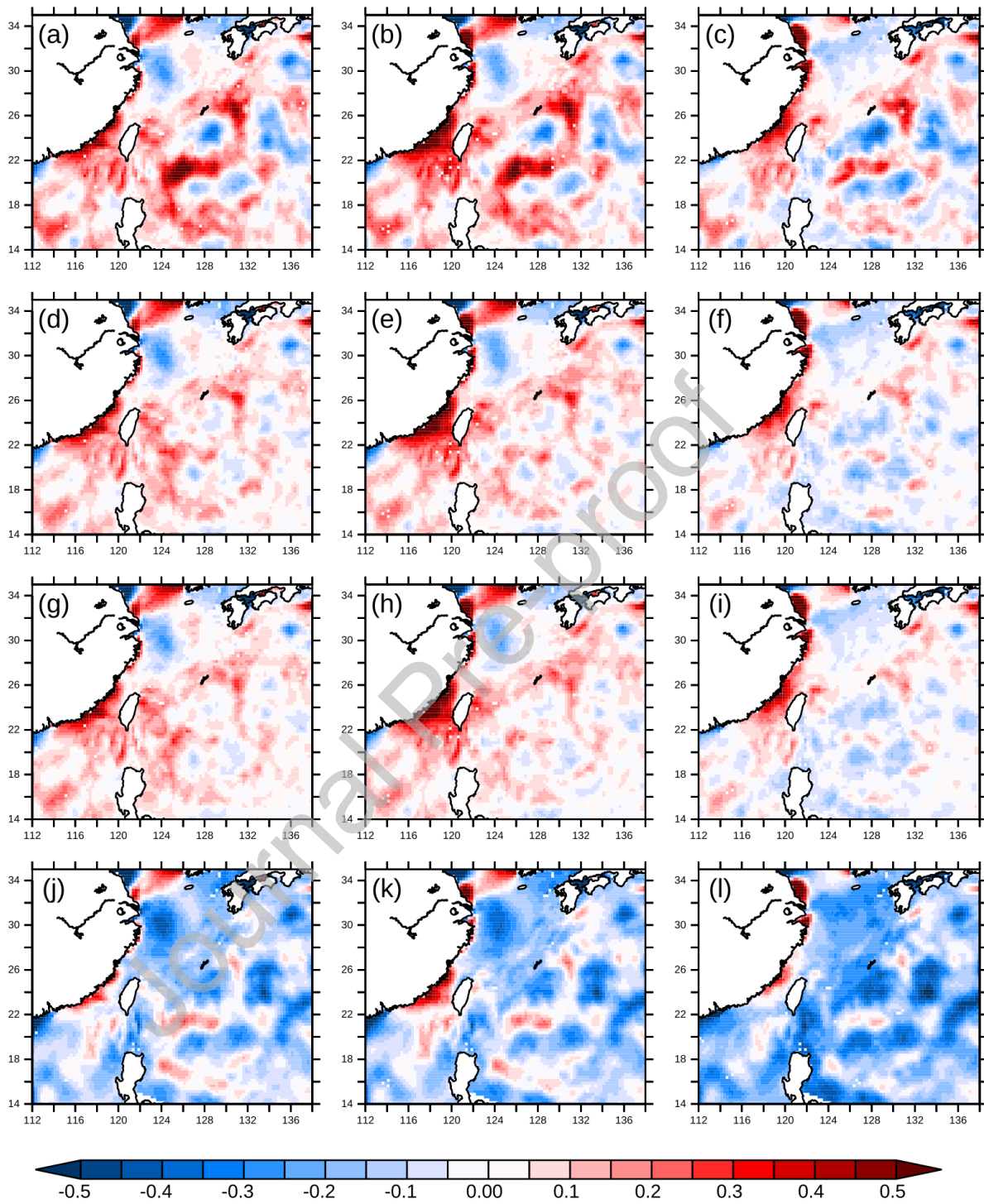


Fig 12: SLA errors (in m) comparison around Taiwan. The three columns correspond to before, during and after the typhoon. (a-c): Case A; (d-f): Case B; (g-i): Case B with 40 members; (j-l): Free run.

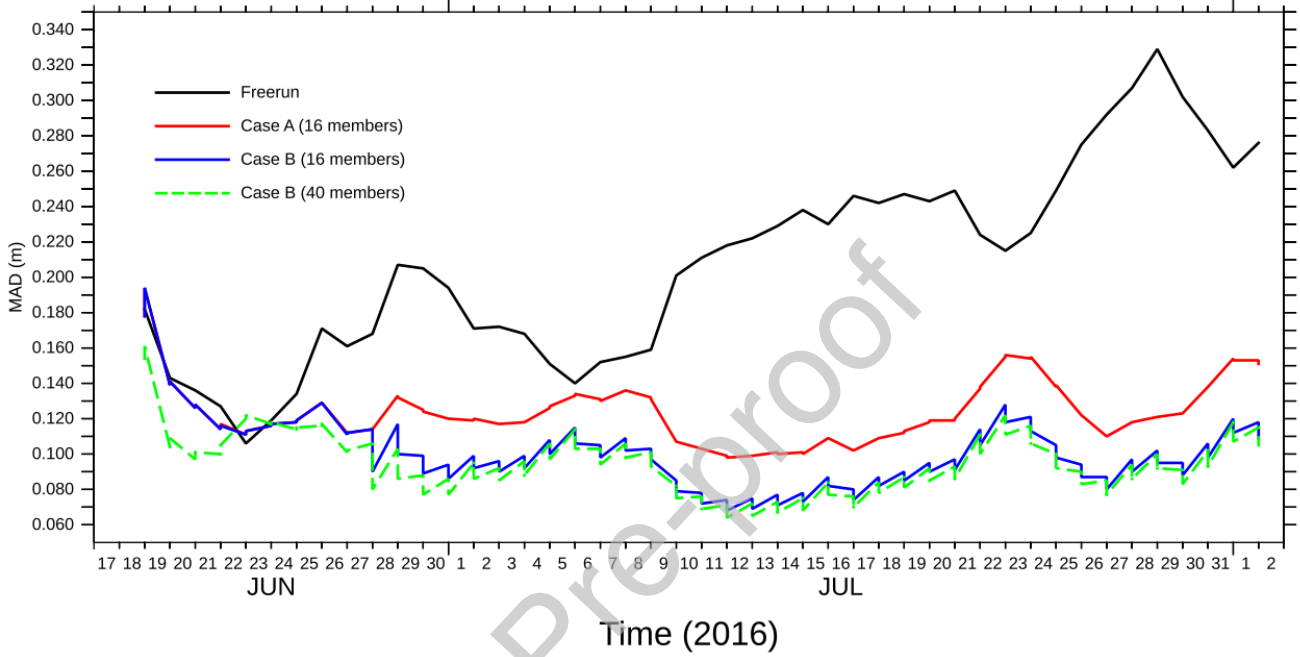


Fig. 13: Comparison of averaged MAD for SLA in the subdomain region around Taiwan; the jumps in Case B correspond to before/after DA step.

3.3 Code efficiency

PDAF allows maximum flexibility in setting up the DA experiments in either ‘flexible’ or ‘full parallel’ modes, based on availability of computational resources. If sufficient resources are available, the ‘fully parallel’ mode is the most efficient option. Under this mode, all ensemble members are executed concurrently (Fig. 2). In reality, however, computational resources are usually limited, and the flexible mode is often the only practical option especially for large applications. Under this mode, the user can specify how many members are executed concurrently in batches, and memory sharing and rewinding of clock are necessary between different cohorts (Fig. 2). Obviously, one way to maximize efficiency is to minimize the number of cohorts.

In this section we test the performance using different numbers of ensemble members under the fully parallel and flexible modes using the same test shown in Section 3.2. The simulations were conducted on Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)’s Frontera (<https://docs.tacc.utexas.edu/hpc/frontera/>, last access: 28

Feb 2024). Table 5 summarizes the simulation costs from different tests. The results indicate that there is no significant time difference between different numbers of ensemble members under the fully parallel mode, which demonstrates the excellent scaling and minimal overhead induced by PDAF and ESMF. Both ensemble forecast and assimilation analysis steps took similar amount of time. Using the flexible mode, the ensemble DA time is very close to that in the corresponding run using the fully parallel mode after factoring in the number of cohorts (4 in this case), and the time spent on the assimilation analysis step is about the same as that in the fully parallel mode. This again illustrates minimal overhead induced by PDAF and ESMF. The code can efficiently handle both modes and thus give users options to adjust the cost of ensemble simulation based on available resources. Compared to the free run, the ensemble forecast step using fully parallel mode only induces less than 4% overhead cost. Furthermore, the overhead is negligible under the flexible mode for the forecast step (after factoring in the number of cohorts). The cost for the analysis step is mainly dependent on the amount of observation data as each observation data point needs to be searched within the local analysis domain, which accounts for about 93% of the cost for the analysis step. In other words, the PDAF filter only accounts for ~7% of the cost in the analysis step, and the search algorithm is the bottleneck for DA analysis. This bottleneck will be further improved in the future using newer versions of PDAF. Overall, the DA tool adds a modest (~20%) overhead to the free run in the total time.

Table 5. Wall-clock time (for 28 days of simulation) from using different numbers of ensemble members under fully parallel and flexible mode on Frontera (with 56 cores/node).

Ensemble members	Compute Nodes	Cores	Init (mins)	Ensemble forecast (mins)	DA analysis (mins)	Total (mins)
Freerun	10	560	0.5	306	0	306.5
8 (fully parallel)	80	4480	0.5	308.3	54.4	363.2
16 (fully parallel)	160	8960	0.5	312.5	55.7	368.7
24 (fully parallel)	240	13440	0.5	312.55	55.5	368.55
8 (flexible mode, 2 members in each cohort)	20	1120	0.5	1219.98	56.4	1276.88

4. Conclusions

We have developed a new data assimilative (DA) system by combining two parallel frameworks: a parallel DA framework (PDAF) and a flexible model coupling framework (ESMF). The new DA system is built on the ESMF at the top level that drives the PDAF and any combination of earth system model (ESM) components. In addition, the new DA system supports the two operating modes of PDAF: full parallel (when sufficient resources are available) or flexible (when resources are insufficient). Therefore, the new system allows maximum flexibility and easy implementation of data assimilation for fully coupled ESM applications. The new system was successfully applied to a realistic case of Kuroshio simulation around Taiwan using remote sensed and in-situ observation, and it significantly reduced the model errors for temperature and surface elevation before, during and after typhoon events. The new DA system offers possibilities of a new generation of data assimilative, cross-scale and fully coupled ESMs, enabled by different types of ensemble filters. On-going work will extend the current system to include other types of observations (e.g., velocity measurement from Coastal Ocean Dynamics Applications Radar (CODAR), Acoustic Doppler Current Profiler (ADCP)) and realistic coupled ESM applications.

CRediT authorship contribution statement

Hao-Cheng Yu: Software, Visualization, Validation, Writing – Original draft. **Y. Joseph Zhang:** Software, Methodology, Visualization, Writing – Original Draft. **Lars Nerger:** Software, Methodology, Writing – Review & Editing. **Carsten Lemmen:** Software, Writing – Review & Editing. **Jason C.S. Yu:** Data Curation. **Tzu-Yin Chou:** Data Curation. **Chi-Hao Chu:** Funding acquisition. **Chuen-Teyr Terng:** Writing – Review & Editing, Funding acquisition.

Declaration of competing interest

The authors declare that they have no conflict of interest.

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(1) William & Mary Research Computing for providing computational resources and/or technical support (URL: <https://www.wm.edu/offices/it/services/researchcomputing/atwm/>, last access: 28 Feb 2024)

(2) the Extreme Science and Engineering Discovery Environment (XSEDE; Grant EAR21010), which is supported by National Science Foundation grant number OCI-1053575;

(3) Texas Advanced Computing Center (TACC), The University of Texas at Austin.

Code availability

The PDAF code (version 1.16 was used here) is archived at Zenodo (<https://doi.org/10.5281/zenodo.6535821>), a full code documentation and a usage tutorial, is available at <http://pdaf.awi.de> (last access: 28 Feb 2024). This package requires ESMF (version 8.1.0 was used here) which are freely available at <https://earthsystemmodeling.org/download/> (last access: 28 Feb 2024). SCHISM and its ESMF cap including the PDAF interfaces are continually developed at <https://github.com/schism-dev/schism> and <https://github.com/schism-dev/schism-esmf>. The versions used here are permanently archived at <https://zenodo.org/record/6537527> (SCHISM) and <https://doi.org/10.5281/zenodo.6535437> (SCHISM-ESMF).

Data availability

The ARGO data was downloaded from ARGO project (<http://doi.org/10.17882/42182>). Detail description can be found at <https://argo.ucsd.edu/data/acknowledging-argo/> (last access: 28 Feb 2024). ESA CCI-SST data can be downloaded from Centre for Environmental Data Analysis (CEDA) archive (Merchant et al., 2019, <http://dx.doi.org/10.5285/62c0f97b1eac4e0197a674870afe1ee6>). AVISO SLA data can be downloaded from CEMES archive (<https://doi.org/10.48670/moi-00148>). TPXO is maintained by CEOAS, Oregon State University, USA (<https://www.tpxo.net/global>, last access: 28 Feb 2024) and freely available for academic research usage.

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CRediT authorship contribution statement

Hao-Cheng Yu: Software, Visualization, Validation, Writing - Original draft. **Y. Joseph Zhang:** Software, Methodology, Visualization, Writing - Original Draft. **Lars Nerger:** Software, Methodology, Writing - Review & Editing. **Carsten Lemmen:** Software, Writing - Review & Editing. **Jason C.S. Yu:** Data Curation. **Tzu-Yin Chou:** Data Curation. **Chi-Hao Chu:** Funding acquisition. **Chuen-Teyr Terng:** Writing - Review & Editing, Funding acquisition.

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: