



# Python-Fortran Hybrid Programming for Deep Incorporation of AI and Physics Modeling and Data Assimilation (Hf2pMDA\_1.0)

Xianrui Zhu<sup>1+</sup>, Zikuan Lin<sup>2+</sup>, Shaoqing Zhang<sup>2\*</sup>, Zebin Lu<sup>2</sup>, Songhua Wu<sup>3,4</sup>, Xiangyun Hou<sup>2</sup>, Zhisheng Xiao<sup>3</sup>, Zhicheng Ren<sup>3</sup>, Jiangyu Li<sup>5</sup>, Jing Xu<sup>5</sup>, Yang Gao<sup>6</sup>, Rixu Hao<sup>7</sup>, Xiaolin Yu<sup>2</sup>, Mingkui Li<sup>2</sup>

5 <sup>1</sup>Chongben Honors College, Ocean University of China, Qingdao, 266100, China

<sup>2</sup>Key Laboratory of Physical Oceanography, Ministry of Education, and Institute for Advanced Ocean Study, and Frontiers Science Center for Deep Ocean Multispheres and Earth System (FDOMES), College of Oceanic and Atmospheric Sciences, Ocean University of China, Qingdao, 266100, China

<sup>3</sup>Qingdao Leice Transient Technology Co., Ltd., Qingdao, 266100, China

10 <sup>4</sup>College of Marine Technology, Ocean Remote Sensing Institute, Ocean University of China, Qingdao, China

<sup>5</sup>Qingdao Marine and Meteorological Institute, Qingdao, 266100, China

<sup>6</sup>Key Laboratory of Marine Environmental Science and Ecology, Ministry of Education, Frontiers Science Center for Deep Ocean Multispheres and Earth System (FDOMES), Ocean University of China, Qingdao, 266100, China

15 <sup>7</sup>College of Intelligent Systems Science and Engineering, and Engineering Research Center of Navigation Instruments, Ministry of Education, Harbin Engineering University, Harbin, 150001, China.

<sup>+</sup>Co-first authors who contributed equally to this work.

<sup>\*</sup>Correspondence to: Shaoqing Zhang (szhang@ouc.edu.cn)

**Abstract.** Artificial intelligence (AI) provides an unprecedented opportunity for advancing physics numerical modeling including data assimilation, which is a high-efficient and critically-important tool for advancing our understanding on Earth system and its applications. At the same time, deep incorporation of AI and physical modeling can make great driving to advance AI by injecting it rich physics from long time physics-based modeling development. However, since such physics models are conventionally coded in Fortran and AI algorithms usually are conveniently designed in Python, difficulties exist to directly incorporate AI algorithms into physics models, vice versa. Here, based on a f2py protocol, we have developed a procedure that implements an infrastructure which conveniently conducts Python and Fortran hybrid modeling and data assimilation (Hf2pMDA) to form a program entity so that AI algorithms and physical models can invoke mutually. As examples, within Hf2pMDA, a climate weakly coupled data assimilation (WCDA) system is naturally upgraded to a strongly CDA (SCDA) system, and a 1 km high-resolution weather DA system is conveniently implemented within a multi-layer downscaling model that has multiscale DA in different nesting layers. In the climate SCDA system, a coupled general circulation model (CGCM) and multiscale filtering algorithm is integrated by a Python main controller (PMC) that calls



30 Fortran CGCM components and WCDA modules as well as a data-trained SCDA algorithm by latent space variational autoencoder (VAE) in Python. In the high-resolution weather DA system, the downscaled model consisting of traditional Fortran DA modules in all mother domains and Python VAE DA algorithm in the central child domain is integrated by a PMC that organizes these components. With convenient realization of deep incorporation of any AI algorithm and physics model, the Hf2pMDA has a great potential to make progresses on both AI and scientific modeling.

## 35 **1 Introduction**

Since the first Electronic Numerical Integrator and Computer (ENIAC) was born in 1940s, numerical weather prediction (NWP) models have been developed progressively (Benjamin et al., 2019) and advanced rapidly in recent years (Haarsma et al., 2016). An NWP model is a set of discretized momentum (dynamics) and energy (thermodynamics) budget equations of multi-sphere fluid motions, which can be dated back to the 17th century Newtonian mechanics (Newton, 1687) and 19th century Mayer's and Joule's energy conservation law (Mayer, 1842; Joule, 1843). Nowadays, an NWP model has advanced as an Earth system model (ESM) that consists of coupled atmosphere, ocean, sea-ice, land as well as biogeochemical processes etc. multi-sphere components (e.g., Kay et al., 2015; Danabasoglu et al., 2020). Now, the ESM is pursuing precise simulation and prediction for weather-climate variations through resolving multiscale interactions in the geofluid by developing high-resolution (HR) model (Zhang et al., 2023; Mouallem et al., 2025), which is a critically-important platform for Earth science studies (Haarsma et al., 2016).

However, as the spatial resolution continuously increases, physics-based modeling encounters many challenges (Chang et al., 2020; Marotzke, 2023). For example, as a consequence of water phase changing with strong nonlinearity, the genesis and melting processes of sea-ice have scales from millimeters (freezing coagulations, for instance) to hundreds of kilometers (glaciers, for instance) and rich scale processes such as melt ponds (e.g. Feng et al., 2022), ice leads (e.g. Qu et al., 2024) and polynyas (e.g. Diao et al., 2022) between them. Each scale band plays relatively independent and important role (Kenneth et al., 2020). Such a multiscale nature makes particular difficulties on HR modeling of sea-ice, since any HR model needs a specific parameterization for its sub-grid processes (Gou et al., 2025). The other outstanding example on HR ESM challenges is parameterization of planetary boundary layer (PBL) processes (Jia and Zhang, 2020). When the model horizontal resolution comes to a level of kilometers, classic PBL parameterization that deals with low resolution sub-grid boundary processes is no longer suitable for describing turbulences induced by differently-featured underneath surface structures, such as mechanical (roughness), thermal (urban heat) and shear-induced turbulences etc. (Kadivar et al., 2021). Machine learning artificial intelligence (AI) technology provides unprecedented opportunities to resolve the challenging issues of physics-based HR modeling described above. As long as data that sufficiently represent an end-to-end process, no matter how complex the process is, it always can be resolved by a data-training procedure based on neural (deep learning) network (Hopfield, 1982; Rumelhart et al., 1986). Starting from the basic principle of least-square fitting to resolve optimal



weighting coefficients on a network, AI algorithms advance very rapidly and help greatly enhance accuracy of weather forecasts (Bi et al., 2023) and climate predictions (Ham et al., 2019). While data-driven AI technology rapidly spreads into almost every engineering and scientific discipline, the data-driven nature limits its further advancement and therefore physics-guided AI merges explosively (Faroughi et al., 2024; Yuan and Guo, 2024).

65 Deep incorporation of AI and physical models (let's call so for wording convenience) can make unbelievable opportunities to drive both even more rapidly advancing by injecting AI rich physics from long time physics-based modeling development and letting physical models being able to use any trained AI algorithm. Nevertheless, physical models are conventionally coded in Fortran (or Fortran-C hybrid) language and AI algorithms are designed and trained in Python language. Although great efforts are made for combining utilities of different languages together (Müller et al., 2024), deep incorporation of AI  
70 and physical models is still very difficult because of the lack of convenient infrastructure friendly to physical modelers between Fortran and Python. At present, on the one hand, most of the physics-guided AI employs some simplified physical expressions by Python (e.g. Häfner et al., 2018; Kochkov et al., 2024; Shu et al., 2025; Hao et al., 2025). On the other hand, physical models can only use some selected AI algorithms that can be translated into Fortran (Heuer et al., 2024) with FTorch library (Cambridge-ICCS, 2024) that does still not fully support all Torch application interfaces (Atkinson et al.,  
75 2025).

In this study, we document our developing process of Python-Fortran hybrid programming to establish a convenient infrastructure platform on which AI and physical modeling and data assimilation can deeply incorporate with respect to each other, called Hf2pMDA, based on the f2py protocol (Harris et al., 2020). Basically, through 3 steps of preparations in environment setting, recompiling of Fortran codes of physical model and plug interface, and simple programming of Python  
80 main controller, Hf2pMDA conveniently realizes the online deep incorporation of AI and physical modeling and data assimilation. Through exhibitions of two applications on climate strongly coupled data assimilation and high-precision small region weather Lidar assimilation, we show that Hf2pMDA is a readily using friendly platform to physical modelers and researchers.

This paper is organized as follows. **Section 2** describes the baseline of f2py protocol and outlines the general procedure to  
85 construct the framework of online Python-Fortran hybrid modeling and data assimilation (Hf2pMDA). **Sections 3 and 4** give examples of detailed implementation for applying Hf2pMDA to a climate model CDA system and a downscaling NWP system. Finally, summary and discussions are given in **Sect. 5**.

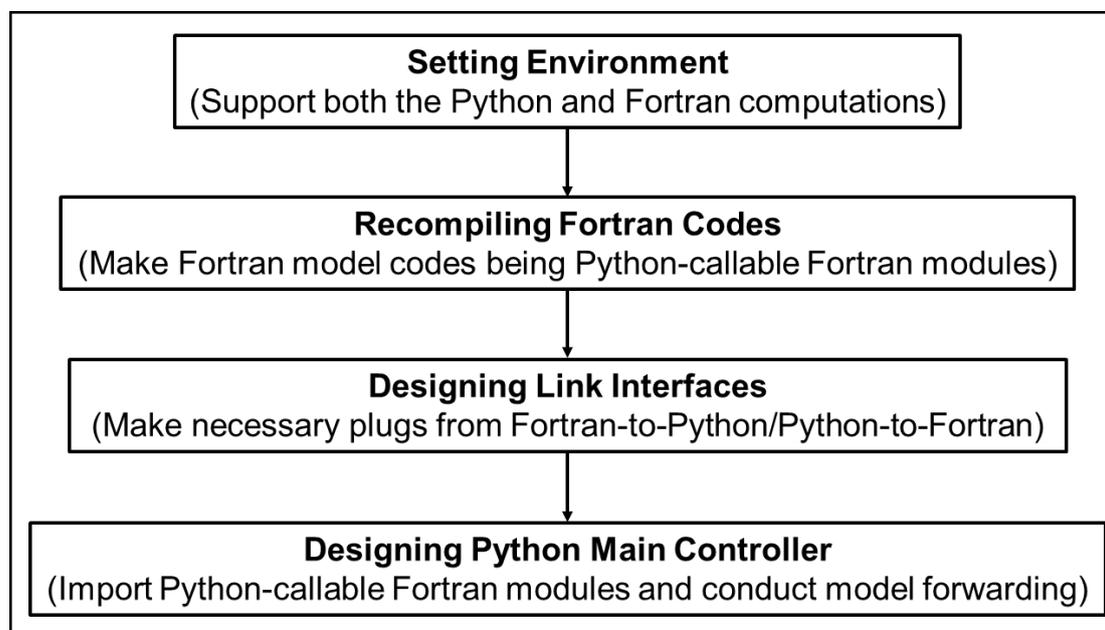
## 2 An infrastructure of Python-Fortran hybrid modeling and data assimilation (Hf2pMDA)

### 2.1 General f2py protocol and the outline of Hf2pMDA

90 The f2py protocol provides a basic idea for designing online Python-Fortran hybrid computation. A Python coded program with a kind of interpreted fashion is directly executed without pre-compiling requirement as compiled languages such as



Fortran etc. A natural way to realize hybrid computation of Python and Fortran is that Python-callable Fortran (PCF) modules can be imported into a Python main controller (PMC) as callable objects and scientific Fortran computation can call Python-coded AI algorithms as subroutine or function. To that end, there are three aspects of concerns that need to be addressed in an infrastructure of Python-Fortran hybrid modeling and data assimilation (Hf2pMDA) designed in this study: (1) computational environment needs to be set to support both the Python and Fortran computations; (2) Fortran model codes need to be recompiled so that they become PCF modules; (3) application-oriented interfaces need to be designed to link PCF modules to PMC, and let scientific Fortran computation being able to call Python-coded AI algorithms. The logistics of Hf2pMDA can be illustrated a flow-chart in **Fig. 1**.



**Figure 1:** A logic flow-chart of the design idea for the infrastructure of Python-Fortran hybrid modeling and data assimilation (Hf2pMDA).

## 2.2 General procedure of Python-Fortran hybrid computation based on f2py

### 2.2.1 Environment setting

In theory, there is no specific environment variable for f2py. However, to minimize the interruption of other computation tasks to the Python-Fortran modeling development, we strongly recommend to use an environment setting tool such as *conda* etc. to set an isolated environment for the Python-Fortran hybrid application. We may start from a Python environment by typing the command “*conda create -n f2py python=3.11*” and continue to complete the setting by typing “*conda activate f2py*” and “*conda install numpy=1.26*” for follow-ups until necessary, where 3.11 and 1.26 are environment parameters of corresponding software. For some non-standardized environment variables only necessary for specific applications, the



“source” command is a convenient complementary. Detailed description will be given in specific applications by **Sects. 3 and 4**.

### 2.2.2 Creating of Python-callable Fortran (PCF) modules

115 In order to become Python-callable, the existed Fortran codes need to be recompiled with an additional new tag “-fPIC” that makes the Fortran codes being compiled become Dynamic Link Library (DLL) candidates with a “position independent” nature. Once relatively-independent Fortran codes are all recompiled as DLL candidates, they are ready to link with the Python main controller (PMC).

To minimize complexity of the infrastructure between PMC and PCF modules, a plug-featured Fortran subroutine that well organizes the PCF modules and makes a few plug-ins for PMC needs to be encapsulated with all PCF modules to form a signature file that shows a clear structure of such plugs. We use the following command line to initially create a signature file called *appname.pyf*:

```
$ f2py app_plugs.F90 -m appname -h --overwrite-signature appname.pyf
```

where *app\_plugs.F90* consists of subroutines or functions that organize the PCF modules and serve as the plug-ins of PMC. Supposing that there are a few DLL candidates created in the compiling procedure described above called *libapp1.a*, *libapp2.a*,...etc., then, the encapsulating command looks like a continuous line of the above initial creation line of *appname.pyf* as:

```
130 $ FC="mpif90" CC="mpicc" CXX="mpicxx" LD-shared="mpif90" LD-flags="-no-ipo \  
-Wl, --export-dynamic" f2py -c appname.pyf app_plugs.F90 libapp1.a \  
libapp2.a ... -lnetcdf -L/.../software/netcdf3/lib -L/.../openmpi/lib \  
--backend distutils
```

where the option “-no-ipo” closes out Interprocedural Optimization to minimize potential uncertainties due to optimization cross modules and the option “-Wl” ensures used functions linked to DLL. Note that here the openmpi/lib also needs to be recompiled with the tag “-fPIC.” Finally, as the above command is normally conducted without any error message, a complete DLL file called *appname.cpython-311-x86\_64-linux-gnu.so* is formed (automatically named by the compiling environment parameters), which is a Python-callable DDL “shared object” where all subroutines and functions are callable by PMC. All information about the logic structure of *appname.cpython-311-x86\_64-linux-gnu.so* is recorded in the signature file *appname.pyf*, which will be served as an import name in PMC, also serving as an efficient guideline for constructing PMC.



### 2.2.3 Fortran-callable Python (FCP) algorithms

140 To let the Fortran codes be able to call Python-coded algorithms, we need an interface (called *callback\_python.F90*, for instance) that translates the Python external functions into Fortran-callable public subroutines (called *python\_algorithm{1,2}* etc., for instance). At the same time, the *app\_plug.F90* shall include the definition of these external functions (called *python\_foo{1,2}* etc., for instance) which are transported from PMC into Fortran application at plug-ins in *app\_plug.F90* as arguments. This Fortran interface file *callback\_python.F90* shall be compiled with *app\_plug.F90* together by going through  
145 the procedure described above to join the signature file *appname.pyf*. Then, all subroutines representing python algorithms can be called in any Fortran application through a normal “use” statement.

## 2.3 The PMC’s structure and execution of Python-Fortran hybrid computation

### 2.3.1 The PMC’s structure

A PMC (called *appname\_main.py*, for instance) shall consist of three important parts: import statements, model integration  
150 conductor and AI algorithm interface as described before. The import statements must include “from *appname* import *module\_list*” (import selected Fortran modules from *appname* defined before) or simply “import *appname*” to import all modules in *appname*. The import statements may include any necessary modules that are used in PMC such as an MPI module which provides process-element identification (PE-id) etc. information, as well as defined AI algorithms and so on.

To minimize Python-recoding for the existed Fortran model, the PMC’s statements for conducting model integration usually  
155 remain simple as possible as Python AI algorithms are conveniently called by the Fortran model. In the example of climate model application of  $H_{2p}$ MDA, which will be described in **Sect. 3**, we implement an AI strongly-coupled data assimilation (SCDA) based on the existed Fortran-coded weakly-coupled data assimilation (WCDA). Due to the strongly-modular nature of existed Fortran codes, the AI algorithm trained by deep-learning is conveniently inserted at the atmosphere-ocean interface, we let PMC to take care of time integration loop (detailed in **Sect. 3.2**). However, in the example of  $H_{2p}$ MDA’s  
160 NWP model application described in **Sect. 4**, we implement AI DA in the 3<sup>rd</sup> domain downscaled from a recursive domain integration. In that circumstance, the PMC’s model integration conductor only consists of a single line, which will be elucidated in **Sect. 4.2**.

### 2.3.2 The execution of Python-Fortran hybrid computation

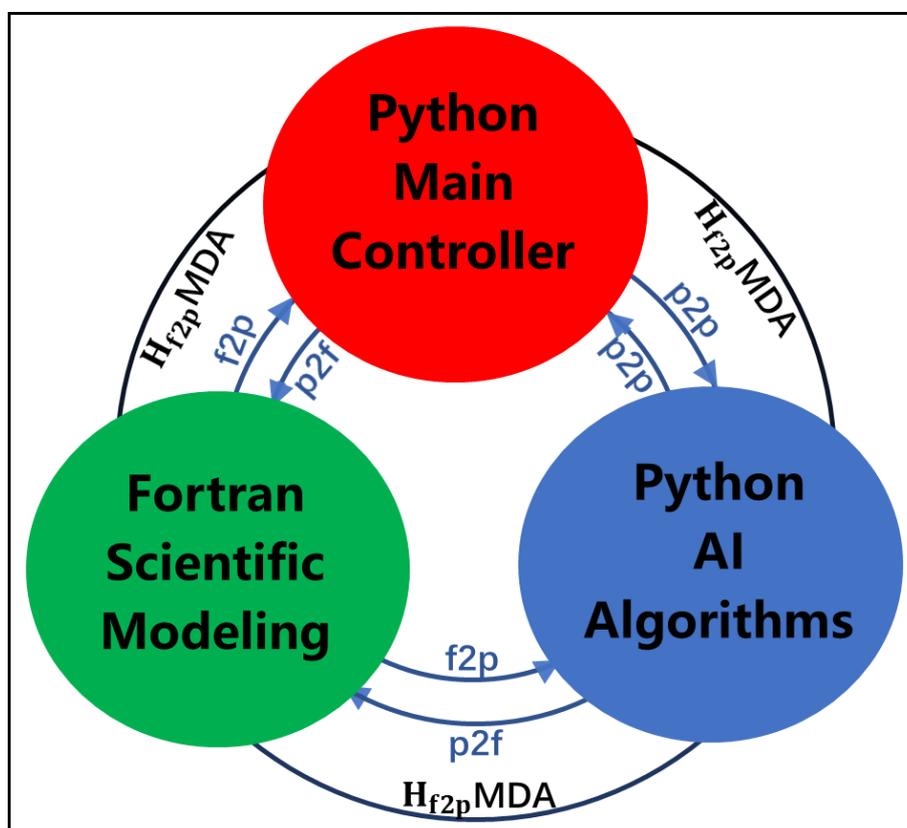
We can still use *mpirun* command to reflect the MPI nature of Python-Fortran hybrid computation as:

```
165 $ mpirun -n xx python appname_main.py > appname.log
```



where “xx” is the PE number required by the program, *appname.log* is the log file recording the log information during the program running. We may insert this run command line into the existed *run\_script* file of the Fortran model to let the  $H_{f2p}MDA$  run in a large scale of MPI usage by a *qsub* command to submit it to the back-end job queue.

170 Through the steps described above, the infrastructure of Python-Fortran hybrid modeling and data assimilation ( $H_{f2p}MDA$ ) can be constructed. As illustrated in **Fig. 2**, within the  $H_{f2p}MDA$  infrastructure, the scientific modeling and machine learning AI algorithms can be deeply incorporated. Next, we will use examples of climate model CDA and weather model high-precision DA to give specific implementation of  $H_{f2p}MDA$ .



175 **Figure 2:** A schematic illustration of the designed infrastructure of Python-Fortran hybrid modeling and data assimilation ( $H_{f2p}MDA$ ) for deep incorporation of scientific modeling and machine learning AI algorithms.



### 3 $H_{f2p}$ MDA applied to climate model

#### 3.1 The CM2 model and its WCDA system

The CM2 is a fully-coupled Earth system model consisting of the atmosphere, ocean, land and sea-ice components (Lin, 2004; Gnanadesikan et al., 2006; Winton, 2000), having been an important member of the Coupled Model Intercomparison Project (CMIP) (Delworth et al., 2006a; Randall, 2007; Taylor et al., 2012; Eyring et al., 2016). The version we used in this study has the atmosphere model with  $2^\circ$  latitude  $\times$   $2.5^\circ$  longitude horizontal resolution and 24 vertical levels, and the ocean with  $1^\circ \times 1^\circ$  horizontal resolution and 50 vertical levels, time stepping with 30 minutes and 2 hours for atmosphere and ocean as well as their coupling. As the first CGCM's CDA system, the first version of CM2-CDA was developed based on the ensemble Kalman filter (EnKF) (Zhang and Anderson, 2003; Zhang et al., 2007), implemented in a WCDA manner. However, an EnKF CDA system is very expensive and has a limitation on extracting low-frequency observational signals (Yu et al., 2019). To resolving this issue, based on scale disassembling of a long time series of single model solution and the EnKF's framework, a multiscale high-efficiency approximate EnKF (MSHea-EnKF) was designed (Yu et al., 2019) and implemented into the CM2 (Lu et al., 2020). Therefore, the current version of CM2-CDA employed in this study uses a sequential WCDA procedure which forwards on single CM2 coupled model integrated with atmosphere-ocean observations as they are available.

In a WCDA procedure, the atmosphere (ocean) observations only adjust the atmosphere (ocean) own itself state and observational information transfers cross the atmosphere and ocean by coupled model exchanged fluxes. Without direct observational adjustment between the atmosphere and ocean, imperfect coupling physics may still introduce errors into the coupled model and CDA remains in an incomplete fashion. The strongly-CDA (SCDA) has been pursued to fulfill sufficient balanced and coherent coupled state estimation in CDA (Zhang et al., 2020) but it keeps in difficulties (e.g. De Rosnay et al., 2022) imposed by the limitation of linear regression in traditional DA algorithms for such different characteristic scales cross the atmosphere and ocean. The natural nonlinear nature of machine deep learning AI algorithms makes SCDA feasible if it is inserted into a WCDA system as an additional term.

Next, we will describe how to apply the  $H_{f2p}$ MDA framework outlined in **Sect. 2** to the CM2-CDA to construct an  $H_{f2p}$ MDA-CM2<sub>CDA</sub> so that an AI SCDA scheme can be conveniently incorporated into CM2-CDA.

#### 3.2 Design of modular $H_{f2p}$ MDA-CM2<sub>CDA</sub>

##### 3.2.1 The environment requirement

Beside the general environment described in **Sect. 2.2.1**, we need to use *openmpi* for MPI application in this  $H_{f2p}$ MDA-CM2<sub>CDA</sub> case. We need to recompile *openmpi* package with added “-fPIC” tag and “make install”. Then we *source* a file of command list containing the following 3 lines to add the *openmpi* application to the environment *myf2p*:



```
export PATH=".../openmpi/bin:$PATH"  
export LIBRARY_PATH=".../openmpi/lib:$LIBRARY_PATH"  
export LD_LIBRARY_PATH=".../openmpi/lib:$LD_LIBRARY_PATH"
```

Again, the *openmpi* directory shall be in the specific application directory for  $H_{f2p}$ MDA-CM2<sub>CDA</sub> so that this *openmpi* setting  
210 does NOT influence any other applications.

### 3.2.2 Recompiling of CM2-CDA all static libraries

In general, the CM2 model has a very clear modular feature, in which the atmosphere and ocean components have relatively-independent structure, with land as atmospheric boundary processes and sea-ice being the interface of atmosphere and ocean. The main controller *coupler\_main* organizes all interfaces between model components and loops time integration as every  
215 half hour for the atmosphere and every two hours for the ocean and atmosphere-ocean coupling. The weakly CDA conducts atmosphere (ocean) DA computation within the atmosphere (ocean) component and it therefore does not change the basic logic structure of *coupler\_main*. The entire CM2-CDA package of codes consists of 4 static libraries: *libfms.a*, *libland.a*, *libecda.a* and *libcoupler.a*. Here *libfms.a* contains all the lowest shared information such as MPI and remapping functions etc. and *libland.a* is a relatively-independent application package for land model based on *libfms.a*, while *libecda.a* includes  
220 all atmosphere and ocean model components as well as CDA subroutines beside land model. Finally, *libcoupler.a* is the highest infrastructure to connect all parts above together by *coupler\_main*. To make all Fortran modules in these static libraries becoming PCF modules, we first partition the main controller *coupler\_main.F90* as two parts, *cm2\_cda\_mainsubs.F90* and *cm2\_cda\_plugs.F90*. The *cm2\_cda\_mainsubs.F90* is basically a modified version of *coupler\_main.F90*, in which the main program is disassembled into a list of subroutines such as *cm2\_cda\_maininit()*,  
225 *atmos\_step()* and *ocean\_step()* etc. as module initialization and single step model integration. The *cm2\_cda\_plugs.F90* simply organizes various model component integration of single step as plug-ins (*tool\_atmos\_step()* and *tool\_ocean\_step()* etc., for instance) for PMC.

Following the procedure described in Sect. 2.2.2, we first recompile 4 static libraries *libfms.a*, *libland.a*, *libecda.a* and *libcoupler.a* by adding “-fPIC” option tag. Then we use *f2py* to combine *cm2\_cda\_plugs.F90* with these 4 static libraries  
230 together to create the signature file *cm2\_cda.pyf* and DLL *cm2\_cda.python-311-x86\_64-linux-gnu.so*. Finally, the DLL *cm2\_cda.python-311-x86\_64-linux-gnu.so* to work directory where *cm2\_cda\_main.pyis* stored.

### 3.2.3 $H_{f2p}$ MDA-CM2<sub>CDA</sub>'s PMC and its execution

Based on the guideline of PMC's structure described in Sect. 2.3.1, we construct the python main controller of  $H_{f2p}$ MDA-CM2<sub>CDA</sub>, called *cm2\_cda\_main.py*. In this case, as arranging time integration of the coupled model, *cm2\_cda\_main.py* also  
235 takes in charge of connecting the atmosphere-ocean interface with the AI SCDA algorithm implemented by latent space



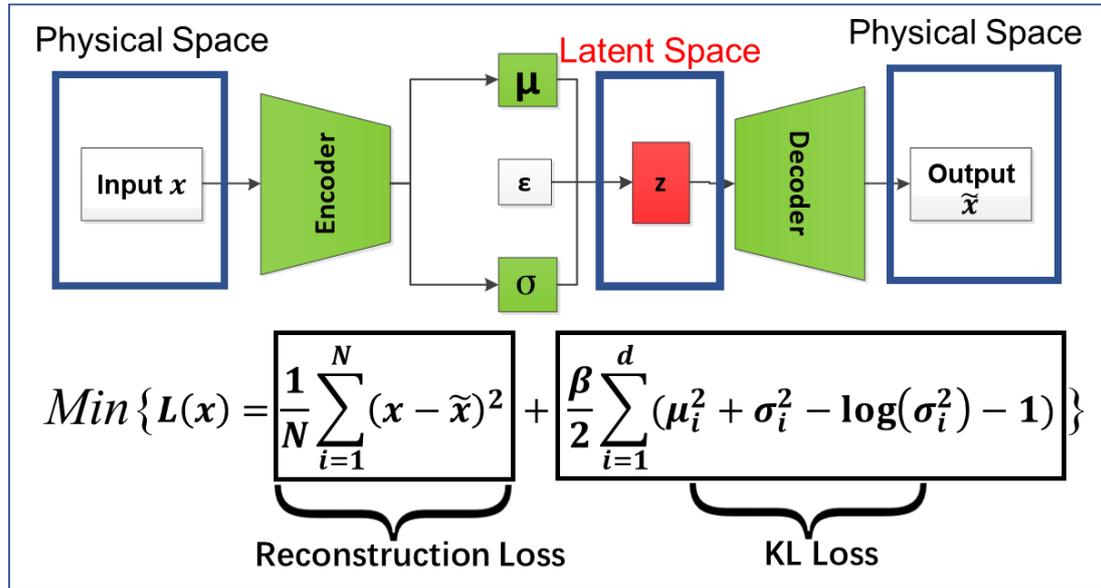
variational autoencoder, which will be described in the next section. Then following the procedure described in **Sect. 2.3.2**, we can run *cm2\_cda\_main.py* to complete the process of  $H_{2p}MDA-CM2_{CDA}$ 's design and execution.

### 3.3 A latent space VAE SCDA algorithm within $H_{2p}MDA-CM2_{CDA}$

240 Since the PMC *cm2\_cda\_main.py* conducts the coupled model time integration and it explicitly controls the evolution of coupling interface between the atmosphere and ocean, we can conveniently insert SCDA into the model integration. What follows describes a latent space variational autoencoder (VAE) SCDA algorithm, which consists of VAE latent space transformation and latent space minimization (Cheng et al., 2022).

#### 3.3.1 VAE latent space transformation

245 The VAE refers to a class of deep generative models that combines artificial neural network and variational Bayesian methods (Cheng et al., 2024; Fan et al., 2025). We can use **Fig. 3** to illustrate the transformation process of between the physical and latent spaces by VAE used in this study. Unlike a basic autoencoder architecture, we here use a version including a Gaussian distribution constraint of latent space so that the minimized total loss includes the Kullback-Leibler (KL) loss which ensures the distribution of induced tensor in latent space close to a Gaussian (Solera-Rico et al., 2024; Lin et al., 2025), called  $\beta$ -VAE. The principle of the used algorithm is to induce a reduced-order tensor in the latent space (denoted as  $z$  in the upper panel of **Fig. 3**) by minimizing the total loss  $L(x)$  consisting of reconstruction and KL losses (shown in the lower panel of **Fig. 3**). We set the value of parameter  $\beta$  as  $10^{-6}$  to seek a relatively compact representation of the latent space while maintaining the reconstruction accuracy. While the detailed description of the algorithm can be referred to Lin et al. (2025), we will outline the data-training process of transformation between the physical and latent spaces below.



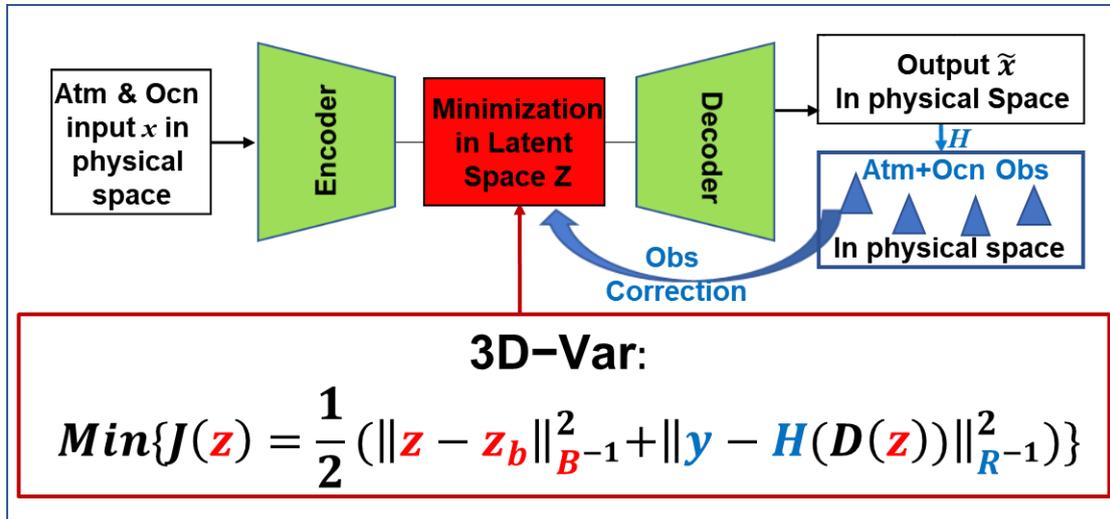
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**Figure 3:** A schematic illustration of the principle of transformation between physical and latent spaces in which the loss function includes reconstruction loss and Kullback-Leibler (KL) loss weighted by a  $\beta$  value (called  $\beta$ -VAE). The reconstruction loss measures the accuracy of VAE reconstruction while the KL loss measures the distance between the generated probability distribution and Gaussian distribution. The algorithm is implemented by data-trained machine learning.

### 260 3.3.2 A SCDA algorithm in latent space minimization

Based on the technology of VAE latent space transformation described above, as shown in **Fig. 4**, Latent Data Assimilation (LDA) further introduces a minimization process in the latent space, which includes an observational term (see lower panel of **Fig. 4**) in the loss function being minimized, to implement data assimilation (Cheng et al., 2024). Note that the utilization error covariance matrices  $B$  and  $R$  (also serving as scaling factors for the background and observational terms respectively) makes the loss function non-dimensional in minimization for which we choose 3-dimensional variational (3D-Var) for simplicity in this study (although 4D-Var could also be used).

The explicit minimization process (will be outlined in **Sect. 3.3.3**) to implement LDA is very fast since the size of states in the latent space is quite small due to its reduced-order nature. It is convenient to include atmosphere and ocean model variables in the physical space vector  $x$  (input in **Fig. 4**) and atmosphere and ocean observational observations (see **Fig. 4**) at the air-sea interface. Then, the final decoded physical space vector  $\tilde{x}$  is an updated model state that incorporates the atmosphere and ocean observations. The LDA illustrated by **Fig. 4** therefore implements SCDA in which the atmosphere (ocean) observations realize instantaneous and direct adjustment for the ocean (atmosphere) state. Since the encoding and decoding process is done by machine deep learning that consisting of nonlinear activation functions, such SCDA is nonlinear although a minimization process is used to incorporate observational data into the latent space (Lin et al., 2025).



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Figure 4: A schematic illustration of the strongly-coupled data assimilation (SCDA) principle of observational correction of atmosphere-ocean fields by latent space minimization i.e. 3-dimensional variational (3D-Var) working on the atmospheric and oceanic observations.  $\mathbf{B}$  and  $\mathbf{R}$  are error covariance matrices for the latent space state background and observations, also serving as the normalization (scaling) factor of the loss function being minimized. Such an SCDA algorithm is implemented by a high-efficient machine learning process described in Sect. 3.2.3.

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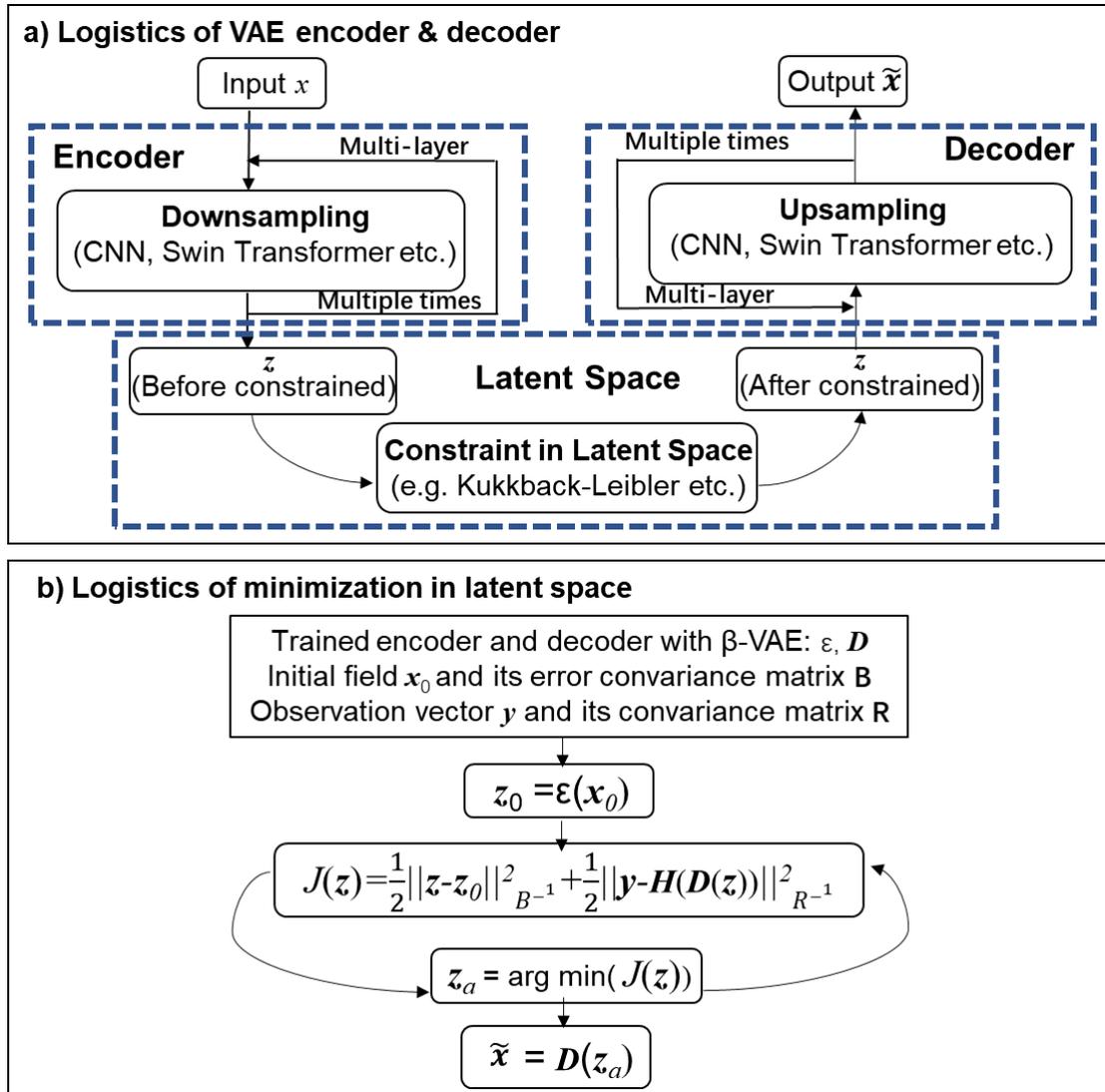
### 3.3.3 The VAE's data-training and latent space minimization

This section gives programming comments on VAE training and latent space minimization of SCDA in  $H_{f2p}MDA-CM2_{CDA}$ , serving as a guideline on concrete coding. For VAE training, on the one hand, the basic procedure of transformation between physical and latent spaces by VAE encoder and decoder is very simple and standardized as illustrated by Fig. 5a. In general, it only consists of downsampling, upsampling and latent space constraint (if necessary), three or even two parts. On the other hand, the training process for a specific application could be very unique in selections of parameters and loop levels as well as neural networks etc. To that end, we will provide the specific procedure descriptions when we present the experiment results for CM2-SCDA in Sect. 3.4 and WRF-DA within the  $H_{f2p}MDA$  in Sect. 4.3.

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In contrast to VAE training, in all applications, latent space minimization is conducted in a quite uniform way as shown in Fig. 5b. Once the training process of VAE encoder  $\mathcal{E}$  and decoder  $\mathcal{D}$  is done, a joint atmosphere-ocean state vector  $x$  and a latent space state vector  $z$  can be transformed back and forth very high-effiviently by the trained  $\mathcal{E}$  and  $\mathcal{D}$ . Due to the order of state vector  $z$  in the non-dimensional latent space is reduced to a necessarily-small size, the minimization can be conducted in a very fast way. As the error criterion in prior is satisfied, the assimilation solution  $\tilde{x}$  is ready.

290



295 **Figure 5: Logistics of VAE latent space data assimilation in Hf2pMDA. a) A general implementation flow-chart of encoder and decoder for transformation between physical and latent spaces as principally illustrated in Fig. 3 for a  $\beta$ -VAE. b) A general implementation flow-chart of minimization in latent space.**

### 3.4 Preliminary results of SCDA by Hf2pMDA-CM2CDA

#### 3.4.1 The VAE reconstruction of physical variables at air-sea interface

300 In the Hf2pMDA-CM2CDA system, to produce SCDA results, we first train the encoder and decoder to reconstruct the reduced-order state in latent space using the atmosphere and ocean state variables at the air-sea interface. High-efficiently



reconstructing the latent space with necessary accuracy is the core of training scheme which consists of various selections on parameters and loop levels as well as neural networks etc. For the CM2-SCDA, we set the input vector  $x_0$  consisting of the atmosphere surface wind, temperature and pressure ( $U_s, V_s, T_s, P_s$ ), and ocean surface currents, temperature and height (SSU, SSV, SST, SSH). The concrete training process is shown in details by Fig. 6. As summarized by Fig. 5a, the most part of encoder (decoder) conducts a training of downsampling (upsampling). However, it's worth to mention that different from a general case in which the physical state usually only includes information within a component of multi-sphere geofluid, in this SCDA case, the physical state being transformed consists of atmospheric and oceanic information with different characteristic scales. Under this circumstance, the VAE training process therefore includes a Cross Attention step which consists of mixing and its inverse (separation). Apart from this point, the VAE still follows a pretty general training procedure for downsampling and upsampling.

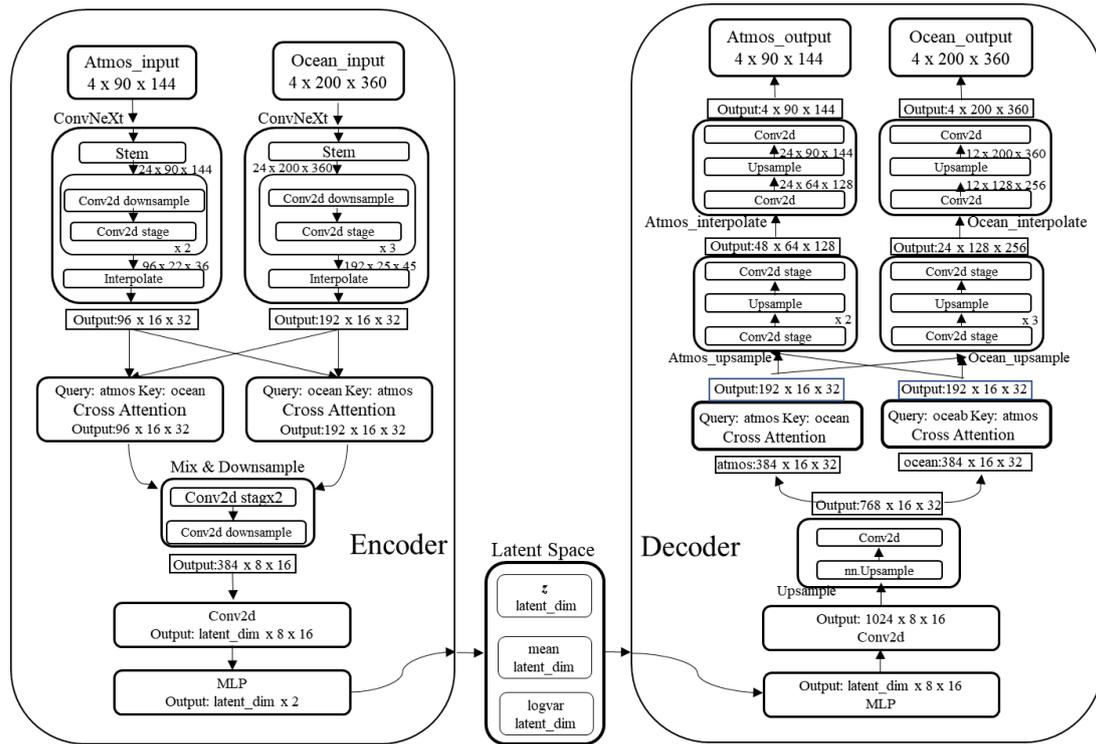
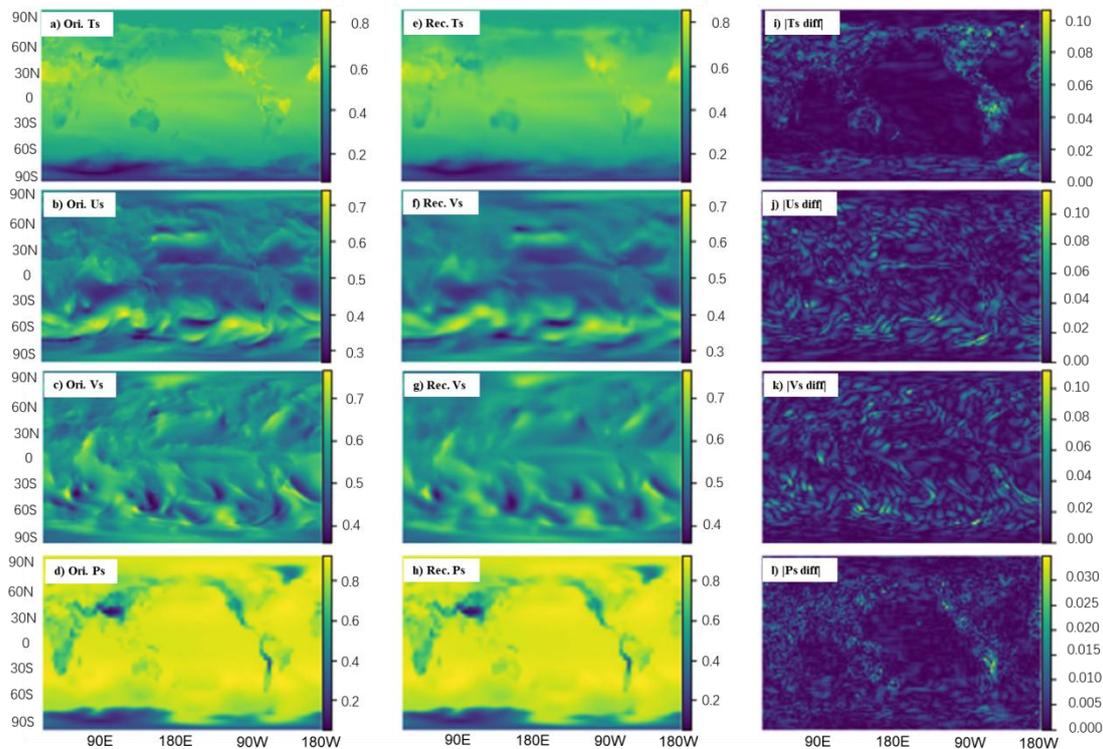


Figure 6: The training process of VAE encoder (left) and decoder (right) in physical-latent space transformation of SCDA in Hf2pMDA-CM2<sub>CDA</sub> as a specific implementation of general VAE logistics shown in Fig. 5a. In this case, we set the latent\_dim as 20480. The denotation “×N” at the lower right corner of some box means repeating this operation by N times.

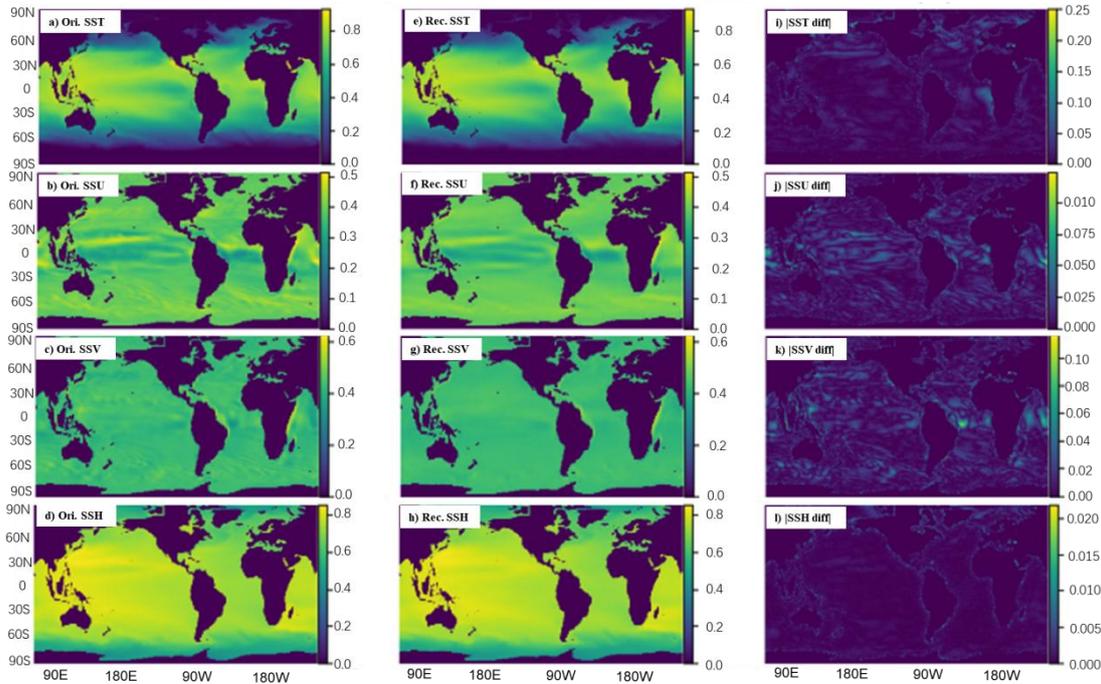
After simply conducting normalization on each variable of  $U_s, V_s, T_s, P_s, SSU, SSV, SST$  and  $SSH$  using the difference of its maximum and minimum values, we form the input vector  $x$  and go through the training procedure shown by Fig. 6 with a dataset of 50-year time series with 3-hour intervals (totally 144540 samples in time) to obtain the latent space vector  $z$ . The



320 reconstruction accuracy for each variable is presented in **Figs. 7 and 8**. From there, we can see that the reconstructed fields  
(**Figs. 7e-h**) are visually nearly-identical to the original physical fields (**Figs. 7a-d**). The absolute errors of the reconstruction  
always remain in an order of  $10^{-2}$  (**Figs. 7i-l**). Although the reconstructed fields still show a little smoother than the original  
physical fields, the accuracy of reconstruction shall be sufficient for the first time practicing on climate SCDA issues.



325 **Figure 7:** The typical VAE reconstruction accuracy for atmosphere surface *a-e*) temperature  $T_s$ , *b-f*) u-component  $U_s$ , *c-g*) v-  
component  $V_s$  and *d-h*) pressure  $P_s$ . The time slide is randomly taken from a 5-year validation set. The leftmost (panels *a-d*) is the  
input  $x$ , the middle (panels *e-h*) is the reconstructed  $\tilde{x}$  through decoding from  $z$ , the rightmost (panels *i-l*) is the absolute values of  
their differences.



330 **Figure 8:** Same as Fig. 7 but for sea surface *aei*) temperature SST, *bff*) u-component SSUs *cgk*) v-component SSV and *dhl*) height SSH.

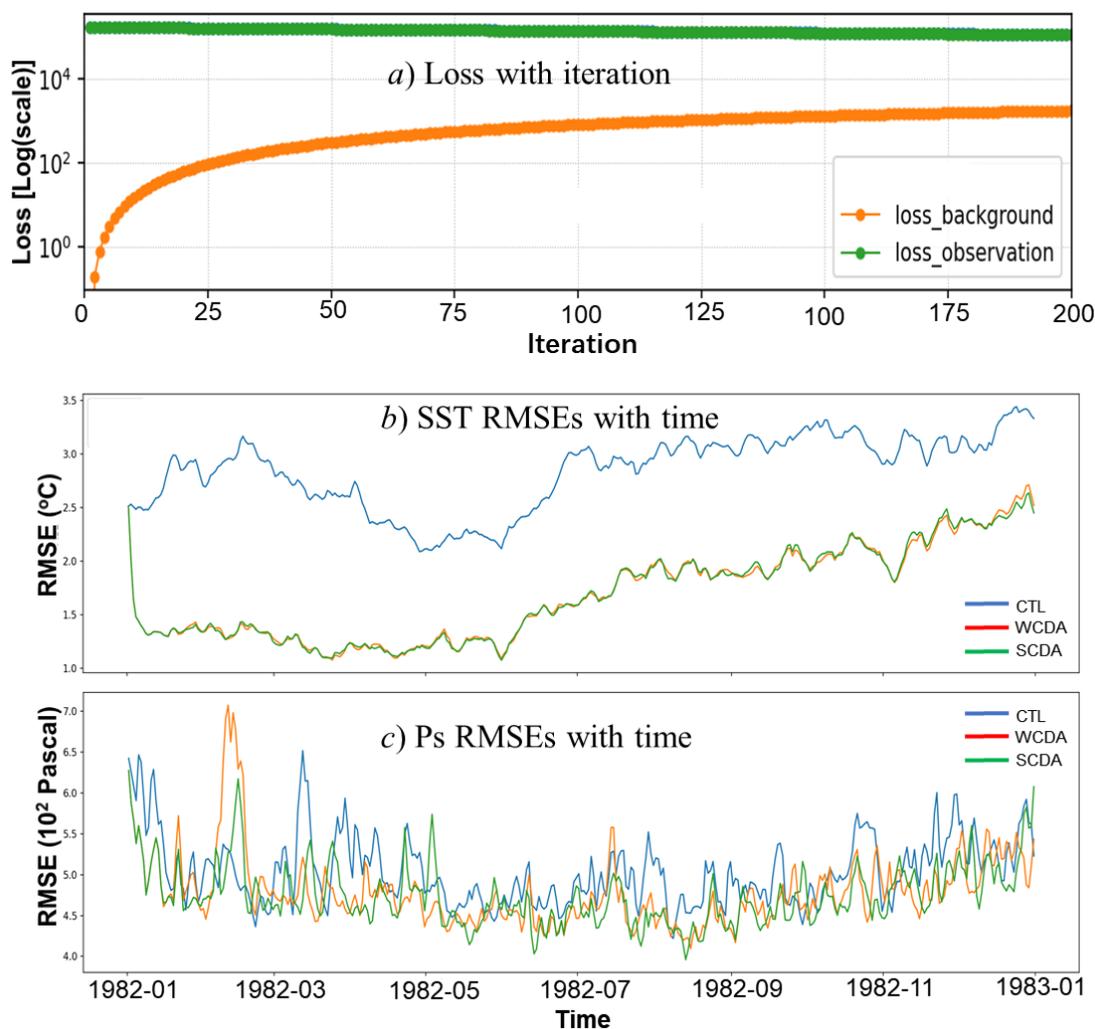
### 3.4.2 The SCDA results

In the case of  $H_{f2p}MDA-CM2_{CDA}$ , through the VAE training, we establish a latent space which is transformed from the air-sea interface space so that we can efficiently conduct minimization to blending atmospheric and oceanic observations into the model space. Here while the size of coupled state vector in physical space is 343,296, through space transformation, the state vector size in the latent space becomes 20480 with a reduction rate of 94%, which makes fast and efficient minimization feasible. Next, we will show that although only 6% of physical space vector size is used in latent space minimization, the reconstruction fields are reasonably to represent the background physical information for extracting observational information.

340 In this test case, we use the ERA5 (5<sup>th</sup> generation atmospheric reanalysis of European Centre for Medium-Range Weather Forecasts) surface pressure  $P_s$  (with a 25 km horizontal resolution) and OISST (NOAA 1/4°Daily Optimum Interpolation Sea Surface Temperature) as atmospheric and oceanic observations respectively. We run the  $H_{f2p}MDA-CM2_{CDA}$  system on the whole 1982 and present a typical minimization process in Fig. 9a and the whole year verification results in Figs. 9b-c. The latent space can be comprehended as a reduced-order holographic space that represents all nonlinear complex relationships of physical variables. In this space, as minimization proceeds, when the observation loss decreases (brown curve in Fig. 9a, the latent space state vector  $z$  gets adjusted as the background loss increases (green curve in Fig. 9a) so that

the observations are coherently incorporated into the background at the convergent point that the background and observation reach equilibrium.

From **Figs. 9b-c**, we can see that due to the low-frequency and quasi-linear nature of ocean motions, both WCDA and SCDA make the model SST quickly converged to observations and keep in nearly identical root mean squared errors (RMSEs) in most of the time. In the contrary, because of strong internal variability of the atmosphere, the curves of Ps RMSEs in WCDA and SCDA quickly separate after a few days, but SCDA does not show his merit within a few months. After about 4~5 months, SCDA starts to show a little smaller RMSEs. In terms of a 6-month mean in July to December, SCDA reduces the WCDA's RMSE by roughly 4%, in which SCDA's RMSE is 4.62 out of 4.81 of WCDA's.



355

**Figure 9:** *a)* Variations of the background loss (brown) and observation loss (green) by the iteration in the latent space minimization as shown in Fig. 5b for carrying out SCDA, and *bc)* the time series of root mean squared errors (RMSEs) of SST and



**Ps in free model control simulation (CTL) (blue), and WCDA (brown) as well as SCDA (green) produced by Hf2pMDA-CM2<sub>CDA</sub> at the 200<sup>th</sup> iteration of minimization. The WCDA is a multiscale high-efficient approximate filter (MSHea-EnKF).**

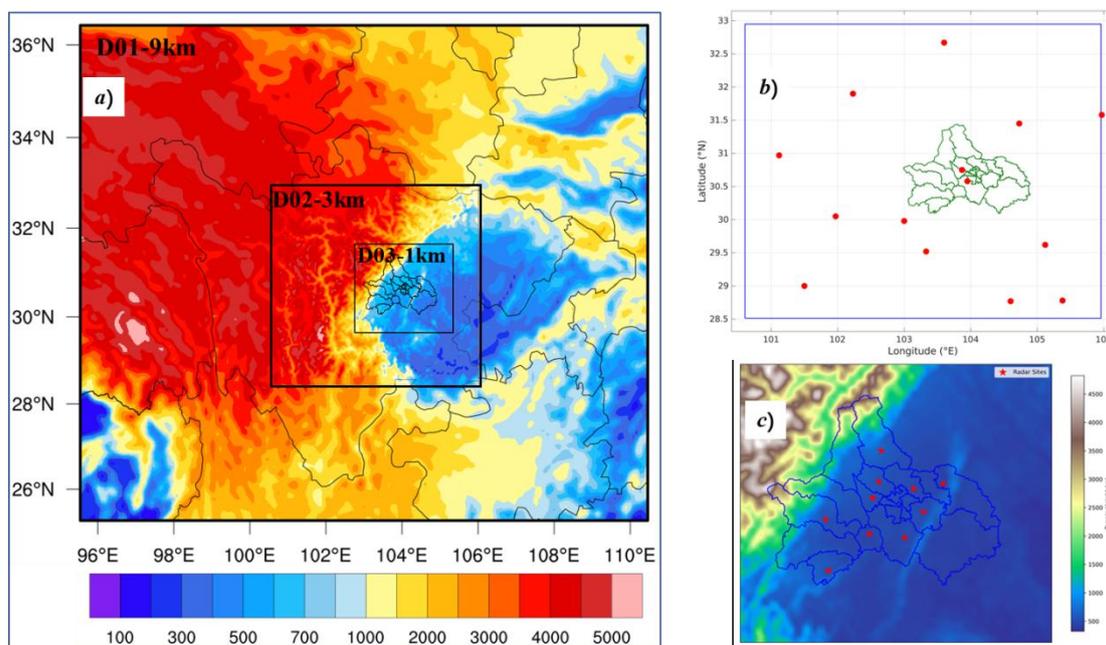
360 It's worth to mention that in this Hf2pMDA-CM2<sub>CDA</sub> case, the model resolution is pretty low (~200 km for the atmosphere  
and ~100 km for the ocean). Under the circumstance, the coupled model dynamics in general is quasi-linear (Perlwitz et al.,  
2017), and it is possible that WCDA can extract the most of observational information into the coupled model. However, our  
preliminary results using Hf2pMDA-CM2<sub>CDA</sub> exhibits the promise that after a sufficient time scale, SCDA can create  
additional values to the CDA system. This may become critically-important as the model attempts to resolve fine-scale and  
365 frequent air-sea coupling processes as a tropical cyclone or mesoscale eddy passes by.

#### **4 Hf2pMDA applied to an NWP model**

##### **4.1 Brief description of WRF and its DA system in multi-layer nesting**

###### **4.1.1 A multi-layer nesting WRF model**

Here we use a version of Weather Research and Forecasting (WRF, v3.7.1) model configured as 3-layer nesting at 9, 3 and 1  
370 km horizontal resolutions for the West of China (D01), Central Sichuan Province (D02) and Chengdu City (D03)  
respectively as shown in **Fig. 10a**. The WRF model is divided into 50 vertical levels from the surface to the model top at 50  
hPa. The model includes most of the primary physics such as the Kain-Fritsch convection parameterization (Kain, 2004),  
Rapid Radiative Transfer Model for GCMs (RRTMG) longwave and shortwave radiations (Clough et al., 2005) and Yonsei  
University (YSU) boundary layer (Hu et al., 2013) as well as WRF single-moment 3-class (WSM3) microphysics (Hong et  
375 al., 2004) etc. The initial and boundary conditions are drawn from the ERA5 reanalysis dataset in this study. The original  
purpose of this WRF configuration is to study the impact of lidar observations on the Chengdu City. Here we employ it to  
exhibit the capability to conveniently carry out parallel experiments using Hf2pMDA conducting traditional DA and AI LDA.



380 **Figure 10: The configurations of a) 3-layer nesting model domain at 9, 3 and 1 km horizontal resolutions for the West China (D01), Central Sichuan Province (D02) and Chengdu City (D03), b) conventional observation stations in D02, and c) Lidar stations deployed in Chengdu City D03.**

#### 4.1.2 A multi-scale WRF DA system

Same as the CM2-CDA described in Sect. 3.1, a multiscale high-efficiency approximate EnKF (MSHea-EnKF) (Yu et al., 2019) data assimilation algorithm is used in this multi-layer nesting WRF to carry out multiscale observational information extraction (Wang et al., 2024). To do that, we conduct the large scale “observational” constraint in D01 using ERA5’s wind and temperature, local data constraint in D02 and D03 using the conventional observations shown in Fig. 10b (in D02) as well as additional Lidar observations shown in Fig. 10c (in D03). In this study, once the  $H_{f2p}$ MDA-WRF<sub>DA</sub> system (will be described in the next section) is set, we use it to conduct parallel assimilation experiments in the 1 km resolution Chengdu City core domain by the classic MSHea-EnKF and VAE LDA to test validation of the  $H_{f2p}$ MDA-WRF<sub>DA</sub>.

### 390 4.2 Design of $H_{f2p}$ MDA-WRF<sub>DA</sub>

#### 4.2.1 Code modification and recompiling of WRF and its multiscale DA system

Unlike the CM2 model which is highly modularized, the WRF model uses a recursive function called *integrate* to perform downscaling simulations by inputting differently-defined domain as its argument. Under this circumstance, we adopt a strategy in which the WRF main program is changed to a module containing subroutine *wrf* and the whole model and its DA



395 codes are packed as an entity that is used by *wrfda\_plug.F90*. In this case, the *wrfda\_plug.F90* only defines a subroutine  
called *call\_wrf\_main* which calls the subroutine *wrf* and defines an *external\_python\_foo* before the subroutine call. The  
*python\_foo* is passed in by the *call\_wrf\_main* as an argument from the PMC that will be described in **Sect. 4.2.2**. The  
external *python\_foo* is a trained LDA algorithm which is used by *callback\_python.F90* where a *python\_da* interface is  
defined as a Fortran subroutine which is public to any Fortran module if applicable.

400 Once the preparation described above is done, we follow the procedures described in **Sects. 2.2.1 and 2.2.2** to complete  
environment setting and Fortran codes compiling. At this point, the signature file *wrfda.pyf* and the “shared object”  
*wrfda.cpython-311-x86\_64-linux-gnu.so* are ready for being imported to PMC.

#### 4.2.2 The PMC of H<sub>2p</sub>MDA-WRF<sub>DA</sub> and its execution

In this case, the PMC *wrfda\_main.py* is very concise. After importing necessary Fortran and Python modules including some  
405 interfaces and utilities for usage of LDA, the *wrfda\_main.py* directly makes a Python call to *call\_wrf\_main* as  
*wrfda.wrfda\_plug.call\_wrf\_main(transpond)*. Here the *transpond* is the function that will become external *python\_foo* in the  
subroutine *call\_wrf\_main* by argument passing. Following the procedure described in **Sect. 2.3.2**, we can execute the  
H<sub>2p</sub>MDA-WRF<sub>DA</sub> system.

#### 4.3 Preliminary results of H<sub>2p</sub>MDA-WRF<sub>DA</sub>

##### 410 4.3.1 The VAE reconstruction of WRF D03

We use ERA5 dataset to create boundary and initial conditions and conduct 3-layer nesting downscaling simulations as  
described in **Sect. 4.1.1**. Each case is run for 36 hours with hourly output in D03. We discard the first 12 hours as  
downscaling spinup and connect all data in last 24 hours of these cases in 2022-2024 to form a 3-year hourly dataset (totally  
8760 samples in time) for the VAE reconstruction training as shown in **Fig. 11**. It’s worth to mention that in this case,  
415 pursuing 1 km resolution high-precision expression, we particularly concern local small scale information, and therefore we  
set a relatively large latent\_dim (196608) with only a reduction rate of roughly 25%.

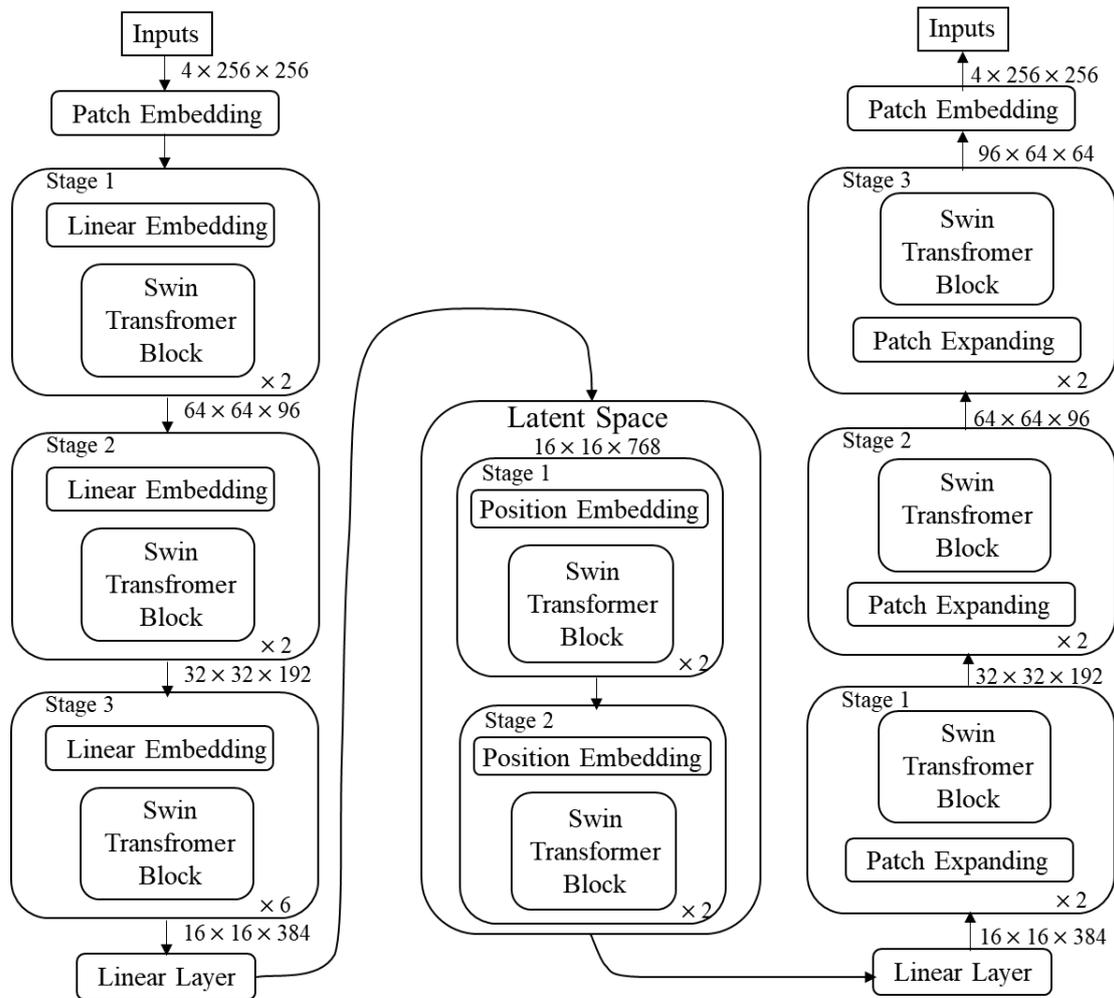
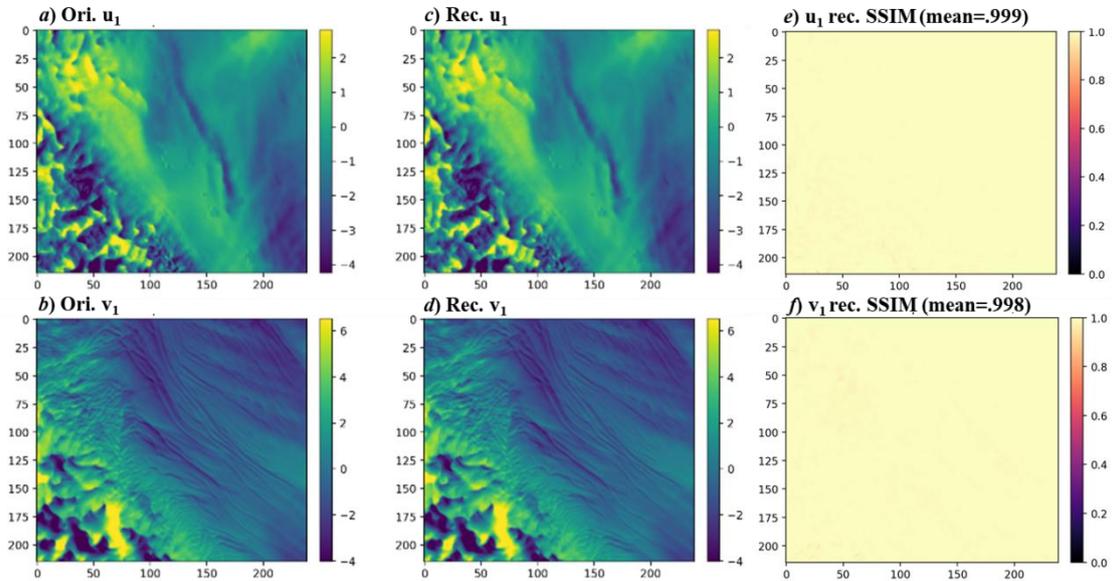
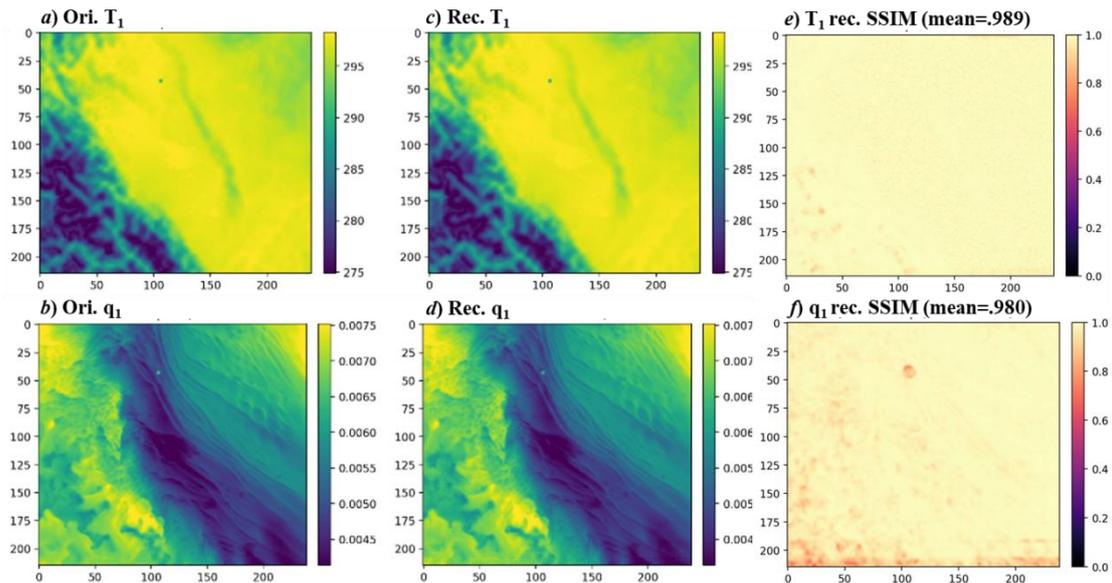


Figure 11: Same as Fig. 6 but for WRF DA of Hf2pMDA-WRF<sub>DA</sub> in D03. In this case, we set the latent\_dim as 196608.

In this test case, we only assimilate the surface observations as shown in Figs. 10b-c. We first show the reconstruction accuracy. As examples, the reconstructed surface wind ( $u_1, v_1$ ), temperature ( $T_1$ ) and moisture ( $q_1$ ) fields at 00UTC on 23 June 2025 are shown in Figs. 12 and 13, which are randomly drawn from a 1-month validation dataset of June 20 - July 20, 2025, for which we will conduct parallel MSHea-EnKF and LDA experiments using Hf2pMDA-WRF<sub>DA</sub> in D03. From Figs. 12 and 13, we can see that the VAE encoder and decoder reconstructed fields (Figs. 12c-d, 13c-d) represent these physical variables (Figs. 12a-b, 13a-b) very accurately, with a nearly-perfect SSIM (Structure Similarity Index Measure  $\approx 0$ ) (Figs. 12e-f, 13e-f). Note that the shown quantity is normalized values by the difference of maximum and minimum of corresponding physical variable.



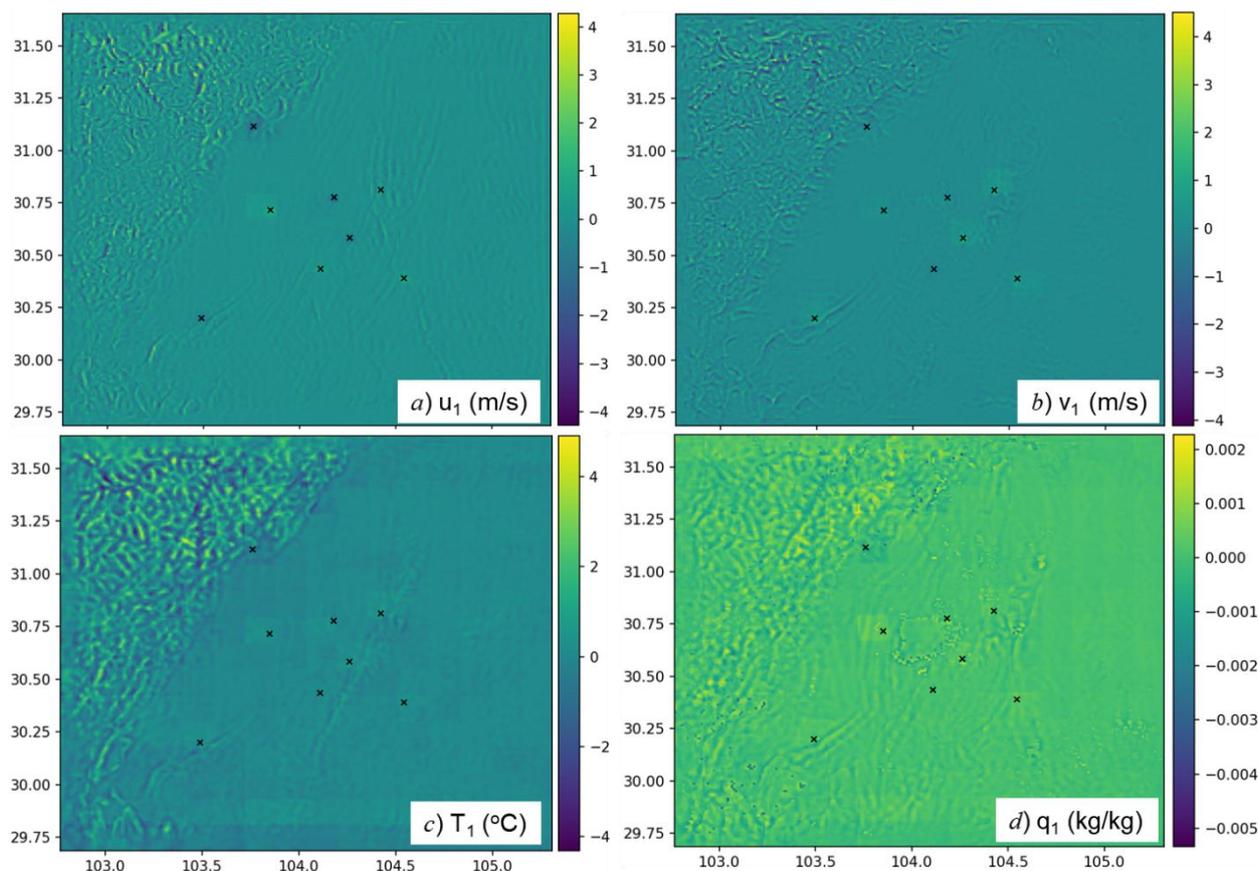
430 **Figure 12:** The typical VAE reconstruction accuracy for surface wind *ace*) u-component  $u_1$ , *bdf*) v-component  $v_1$ . The time slide is at 00UTC on 23 June 2025, randomly taken from a 1-month validation dataset for 20 June - 20 July, 2025. The leftmost panels *a-b* are the input  $x$ , the middle panels *c-d* are the reconstructed  $\tilde{x}$  through decoding from  $z$ , the rightmost panels *e-f* are the Structure Similarity Index Measure (SSIM) for the corresponding reconstruction.



**Figure 13:** Same as Fig. 12 but for surface *ace*) temperature  $T_1$ , and *bdf*) moisture  $q_1$ .

### 4.3.2 The LDA results in D03

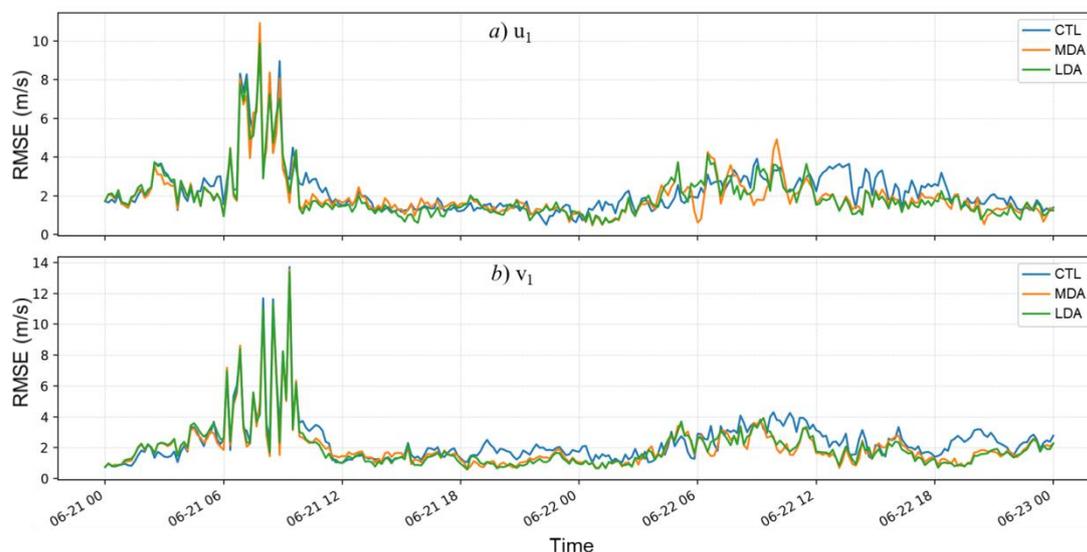
435 We insert the VAE encoder and decoder trained in Sect. 4.3.1 into the  $H_{f2p}MDA-WRF_{DA}$  system designed in Sect. 4.2 and employ the latent space minimization described in Sect. 3.3.2 to replace the D03 DA procedure. In this way, we can perform DA experiments with classic multiscale MSHea-EnKF and new VAE-LDA within the  $H_{f2p}MDA-WRF_{DA}$  framework in a parallel fashion. We run the system from 00UTC 21 June 2025 to 00UTC July 21 2025 with initial and boundary conditions remapped from ERA5 reanalysis, in which the WRF model with 9/3 (1) km resolutions in D01/D02 (D03) assimilate  
 440 conventional surface station (Lidar) observations shown in Figs. 10b-c. We first show the distribution of analysis increments at the first step assimilation in Fig. 14. We see very local  $u_1$  and  $v_1$  adjustments that distribute around Lidar locations (Figs. 14a-b), and although the Lidar only provides wind measurements in this case, the temperature and moisture also get consistent adjustments (Figs. 14c-d) under this VAE-LDA multivariate nonlinear assimilation framework.



445 **Figure 14:** The distributions of analysis increments (the analysis minus the first guess from background) of the first model level *a*)  $u_1$  and *b*)  $v_1$  and *c*) temperature  $T_1$  as well as *d*) specific humidity  $q_1$  at the minimization convergent point of the first assimilation step in D03 LDA of  $H_{f2p}MDA-WRF_{DA}$ . The  $H_{f2p}MDA-WRF_{DA}$  system is run from 00UTC 21 June

2025 to 00UTC July 21 2025 with initial and boundary conditions remapped from ERA5 reanalysis. The black asterisks denote the locations of 8 Lidars.

450 Then, we present the time series of RMSEs of the first model level (near surface) u-component (called  $u_1$ ) and v-component (called  $v_1$ ) produced by the classic multiscale DA (denoted by MDA) and new VAE-LDA (denoted by LDA) in Fig. 15. Within the  $Hf2pMDA-WRF_{DA}$  it is very convenient to perform traditional DA and newly-developed AI DA in a parallel fashion. We see that except for the period of 06UTC-10UTC 21 June, in most of the time, both the MDA and LDA reduce the RMSEs from the CTL. However, we also see that the VAE-LDA gives equivalent results of classic MDA. Since the  
 455 model version used in this study does still not resolve turbulence-featured extreme events (1 km horizontal resolution and 100 m vertical resolution in planetary boundary layer in this case), when one of 8 Lidars measures out a local gust event at 06UTC-10UTC 21 June, either MDA or LDA does not capture this event. This leads to large RMSEs during this period for all of CTL, MDA and LDA. Follow studies will first detect the sensitivities of these DA schemes on model horizontal and vertical resolutions, and then perform deep research on VAE-LDA to get optimal results, serving for low-altitude economy  
 460 environment safety insurance.



465 **Figure 15: The time series of root mean squared errors (RMSEs) of the first model level u-component ( $u_1$ ) and v-component  $v_1$  in free model control simulation (CTL) (blue), and multiscale high-efficient approximate filter (MSHea-EnKF) data assimilation (MDA, brown) as well as VAE latent data assimilation (LDA, green) produced by  $Hf2pMDA-WRF_{DA}$  in the D03 domain. Both MDA and LDA experiments are conducted under the configuration of multi-layer nested downscaling shown in Fig. 10a in which the WRF model with 9/3 (1) km resolutions in D01/D02 (D03) assimilate conventional surface station (Lidar) observations shown in Figs. 10b-c. What are shown here are the results of the first two days in the one month test period of 00UTC 21 June 2025 to 00UTC July 21 2025.**



## 5 Summary and discussions

470 Based on the f2py protocol, a Fortran-Python hybrid programming infrastructure platform called  $H_{f2p}MDA$  has been developed for deep incorporation of AI and scientific modeling and data assimilation. In this  $H_{f2p}MDA$  framework, any Python-coded (Fortran-coded) AI (scientific) algorithm (scheme) can be used by a scientific modeling and data assimilation module (machine learning procedure). As two typical application examples of  $H_{f2p}MDA$ , the implementations with a coupled global climate model CM2 with modularized Fortran structures and a multi-layer nesting downscaling weather model WRF  
475 featured as recursive Fortran integration, have been presented in details. The CM2's (WRF's)  $H_{f2p}MDA$  implementation establishes a nonlinear strongly-coupled (high-precision) climate (weather) data assimilation system called  $H_{f2p}MDA-CM2_{CDA}$  ( $H_{f2p}MDA-WRF_{DA}$ ). Test results of  $H_{f2p}MDA-CM2_{CDA}$  ( $H_{f2p}MDA-WRF_{DA}$ ) show that while the  $H_{f2p}MDA$  conveniently inserts an AI latent DA algorithm into the  $CM2_{CDA}$  ( $WRF_{DA}$ ) system and fulfills global strongly-CDA (regional high-precision DA), it readily improves the assimilation quality from a traditional DA method. Except for deeply evaluating  
480 scientific values in  $H_{f2p}MDA-CM2_{CDA}$  and  $H_{f2p}MDA-WRF_{DA}$ , follow-up studies also include incorporating more advanced AI DA algorithms into  $H_{f2p}MDA$ , for example, the generative assimilation and prediction (GAP) (Yang et al., 2025) based on image recognition technology.

More generally, the  $H_{f2p}MDA$  designed in this study is a high-efficient infrastructure platform for deep-incorporation of AI and science since it only requires a minimum change on legacy Fortran codes of sciences that have a long persistently-  
485 developing history. Following the procedure of  $H_{f2p}MDA$ , on the one hand, it is feasible to incorporate data-driven machine deep learning algorithms to improve scientific modeling. For example, there are urgent demands of new parameterization schemes for high-resolution (HR) Earth system model (e.g. Chang et al., 2020) or even resolving the challenging problems of HR Earth system modeling (e.g. Gou et al., 2025). On the other hand, the rich achievements on scientific modeling from long time development over more than a half century since 1950s can directly advance development of science-guided AI  
490 algorithms (e.g. Hao et al., 2025). In that sense, while the  $H_{f2p}MDA$  has a very wide scope of applications, it requires more efforts to optimize its structure and deepen its infrastructure development so that it can be more conveniently plugged in any application scenario.

### Code and data availability

The ERA5 dataset (Hersbach et al., 2020) can be obtained from <https://doi.org/10.24381/cds.adbb2d47>.

495 The OISST v2.1 sea surface temperature dataset (Huang et al., 2021) can be obtained from <https://www.ncei.noaa.gov/products/optimum-interpolation-sst>.

The CM2.1 model (Delworth et al., 2006a) can be obtained from <https://github.com/mom-ocean/MOM5> and the CM2.1 model version with DA modules is also archived on Zenodo (<https://doi.org/10.5281/zenodo.18883209>; Delworth et al., 2006b).



500 The Weather Research and Forecasting model version 3.7.1 (WRF v3.7.1; Skamarock et al., 2008) can be obtained from [https://www2.mmm.ucar.edu/wrf/users/download/get\\_source.html](https://www2.mmm.ucar.edu/wrf/users/download/get_source.html).

The model code for Hf2pMDA-CM2CDA and Hf2pMDA-WRFDA developed in this study is archived on Zenodo at <https://doi.org/10.5281/zenodo.18800167> (Zhu et al., 2026b). The observational datasets used in the experiments are available at <https://doi.org/10.5281/zenodo.18799861> (Zhu et al., 2026a).

### 505 **Author contributions**

XZ and ZLin are co-first authors who contributed equally to this work. Both of them conduct all test work on Python-Fortran hybrid programming as well as VAE and latent minimization and join the paper edits. SZ is the corresponding author who proposes the idea, designs and organizes the research project, writes and edits the paper. ZLu participates the test experiments on WRF multiscale data assimilation and joins the discussions. SW and XH manage the Leice Transient team and OUC team respectively, and join the discussions and make comments on the research work. ZX participates the test experiments on WRF VAE training experiments and joins the discussions. ZR, JL, JX, YG, RH, XY and ML contribute to this research by joining the discussions and making comments on the research and manuscript.

### **Competing interests**

The authors declare that they have no conflict of interest.

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## Review statement

- 525 The review statement will be added by Copernicus Publications listing the handling editor as well as all contributing referees according to their status anonymous or identified.

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