Stable climate simulations using a realistic GCM with neural network parameterizations for atmospheric moist physics and radiation processes

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5

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Abstract. In climate models, subgrid parameterizations of convection and eloudclouds are one of the main reasons forcauses of the biases in precipitation and atmospheric circulation simulations. In recent years, due to the rapid development of data science, Machinemachine learning (ML) parameterizations for convection and clouds have been provendemonstrated to have the potential to perform better than conventional parameterizations. At present, most of the existingMost previous studies arewere conducted on aqua-planet and idealized models, and the problems of simulatedsimulation instability and climate drift still exist. In realistic configurated models, developing a machine learningDeveloping an ML parameterization scheme remains a challenging task- in realistically configured models. In this studypaper, a set of deep-residual deep neural networks (ResDNNs)

- 15 with <u>a</u> strong nonlinear fitting ability is designed to emulate a superparameterization (SP) with different types of outputs. Sensitivity tests show that high-outputs in a hybrid ML-physical general circulation model (GCM). It can sustain stable simulations for over 10 years under real-world geographical boundary conditions. We explore the relationship between the accuracy is necessary to develop a stable ML parameterization. Trialand stability by validating multiple deep neural network (DNN) and ResDNN sets in prognostic runs. In addition, there are significant differences in the prognostic results of the stable
- 20 <u>ResDNN sets. Therefore, trial-and-error is used to acquire the optimal ResDNN set for both high-performance-skill and long-term stability, named-which we name the NN-Parameterization. In offline validation, the NN-Parameterization emulatescan emulate the SP results far better than the conventional subgrid parameterizations. Then, in in mid- to high-latitude regions with a high accuracy. However, its prediction skill over tropical ocean areas still needs improvement. In the multi-year prognostic test, NN Parameterization reproduces reasonable climate mean states but still with some biases. Most importantly, NN</u>
- 25 parameterization successfully reproduces the climate variability in a superparameterizated GCM, with an over 30 time faster running speed. Under real geographical boundary conditions, the hybrid ML physical GCM well simulates the spatial distribution of boreal summerthe hybrid ML-physical GCM simulates the tropical precipitation well over land and significantly improves the frequency of the precipitation extremes, which is largelyare vastly underestimated in the Community Atmospheric Model version 5 (CAM5) with thea horizontal resolution of 1.9°×2.5°. Furthermore, the hybrid ML-physical
- 30 GCM simulates a stronger<u>the robust</u> signal of the Madden-_Julian oscillation with a more reasonable propagation speed than CAM5. <u>However</u>, there are still substantial biases with the hybrid ML-physical GCM in the mean states, including the temperature field in the tropopause and at high latitudes and the precipitation over tropical oceanic regions, which are larger

than those in CAM5. This study is a pioneer to achieve in achieving multi-year stable climate simulations using a hybrid ML-physical GCM inunder actual land-_ocean boundary conditions- that become sustained over 30 times faster than the target SP.

35 It demonstrates the emerging potential for<u>of</u> using machine learning<u>ML</u> parameterizations in climate simulations.

1 Introduction

The general General circulation models (GCMs) have been widely used for studyingto study climate variability, prediction, and projections. Despite decades of GCM development, most GCMs stillcontinue to suffer from many systematic biases, especially atin low-latitudes. A-latitude regions. The prominent tropical bias inof most current GCMs is referred to as the double intertropical convergence zone (ITCZ) syndrome, which is characterized by two parallel zonal bands of annual precipitation straddling the equator over the central and eastern Pacific (Lin, 2007; Zhang et al., 2019). Convectively coupled equatorial waves and the Madden-Julian Oscillationoscillation (MJO), featured which are characterized by eastward propagating convective cloud clusters, are also not well simulated in by GCMs (Ling et al., 2017; Cao and Zhang, 2017).

- Many studies have attributed most of these biases to the imperfection of deficiencies in the parameterization schemes for 45 atmospheric moist convection and cloud processes in the current GCMs (Zhang and Song, 2010; Cao and Zhang, 2017; Song and Zhang, 2018; Zhang and Song, 2019). Cloud-related processes span a large range of spatial scales, from micron-scale cloud nucleation, to meter-scale turbulence, to individual convective cells and organized convective systems, which are a few kilometers to hundreds of kilometers in size, and to tropical disturbances, which have a spatial scale of thousands of kilometers. They directly influence the radiation balance and hydrological cycle of the earth system and interact with the atmospheric
- 50 circulation, affecting the transport and distribution of energy (Emanual et al., 1994). Therefore, it is very important to simulate the cloud and convection processprocesses in GCMs correctly. However, the current-GCMs that are currently used for climate simulations have a horizontal resolution of ~100km100 km and a vertical hydrostatic coordinate. Thus, in most GCMs, besides in addition to parameterized cloud microphysics, convection and its influence on the atmospheric circulation are represented by convective parameterization schemes, which are usually based on simplified theories, limited observations,
- 55 and empirical relationships (Tiedtke, 1989; Zhang and McFarlane, 1995; Lopez-Gomez et al., 2020). Those These schemes regard convective heat and moisture transport as the collective effects of idealized individual kilometer-scale convective cells. They cannot represent the effects of many complicated convective structures, including organized convective systems, leading which leads to large uncertainties and biases in climate simulations (Bony et al., 2015).

Cloud Resolving Models (CRMs), on the other hand, In contrast, cloud resolving models (CRMs) have long been used to simulate convection. Because CRMs have higher horizontal and vertical resolutions and can explicitly resolve the thermodynamic processes <u>involved</u> in convection, they simulate convection more accurately, including convective organization (Feng et al., 2018). In recent years, CRMs have been used as <u>superparameterization for SuperParameterization</u> (SP) in low-resolution GCMs to <u>replaceand have replaced</u> conventional cumulus convection and cloud parameterization schemes. The most commonly used SP model is the superparameterized <u>version of the Community</u> Atmosphere Model

- 65 (SPCAM) developed by the National Center for Atmospheric Research (NCAR) (Grabowski and Smolarkiewicz, 1999; Grabowski, 2001, 2004; Khairoutdinov and Randall, 2001; Randall et al., 2003; Khairoutdinov et al., 2005). Compared with conventional cumulus convection and cloud parameterization schemes, SPCAM performs better in simulating mesoscale convective systems, diurnal eyeles of precipitation cycles, monsoons, the precipitation frequency distribution, and MJOsthe MJO (Khairoutdinov et al., 2005; Bretherton et al., 2014; Jiang et al., 2015; Jin et al., 2016; Kooperman et al., 2016). However,
- 70 when using 2Da 2-D CRM as for SP, the improvement on of the climate mean states is not obvious (Khairoutdinov et al., 2005). Also In addition, SPCAM requires far more computing resources (i.e., an order of magnitude or more) than a Community Atmosphere Model (CAM) with the same resolution CAM in 1 to 2 orders of magnitude according to the resolution of the CRM subdomain. Thus, the use of SPCAM in long-term climate simulations and ensemble prediction predictions is restricted by the current computing resources. Developing novel and computationally efficient schemes for high performance convection and cloud processes is still an open problem highly desired in GCM development.

In the last 5 years, the rapid development of machine learning (ML) technologiestechniques, especially deep learning technologiestechniques such as neural networksNeural Networks (NNs), has provided novel approaches to constructing parameterization schemes. Machine learning can identify and, discover, and model complex nonlinear relationships that exist in large data sets and model them.datasets. Several studies have used machine learningML methods to develop convection and cloud parameterization schemes (e.g., Gentine et al., 2018; Rasp et al., 2018). These studies followed a similar approach. The

first step is to derive a target dataset from a reference simulation, which is later used for machine learning to train the ML models training. Then, the trained machine learning ML models are often evaluated offline against other independent reference simulations, and finally, they are implemented in a GCM to replace the conventional parameterization schemes.

- Krasnopolsky et al. (2013) first proposed a proof-of-concept for developing convection parameterization based on the NN technique. Specifically, an ensemble of shallow NNs was applied to learn <u>the</u> convective temperature and moisture tendencies, <u>withand the</u> training data <u>from for the</u> CRM simulations <u>was</u> forced <u>byusing</u> observations in the tropical western Pacific. The resulting convective parameterization scheme was able to simulate the main features of <u>eloudthe clouds</u> and precipitation in the NCAR CAM4 diagnostically. However, the key issue of prognostic validation in 3-D GCMs <u>washas</u> not <u>been</u> addressed. Recent studies have investigated ML parameterizations in prognostic mode in simplified aqua-planet GCMs.
- 90 For example, Rasp et al. (2018) developed a deep-fully connected deep_NN (DNN) to predict convection and clouds, which was trained with theusing data from an aqua-planet SPCAM. The NNDNN-based parameterization was then implemented in the corresponding aqua-planet CAM and produced multi-year prognostic results that were close to the SPCAM data. For this NNDNN-based parameterization, Rasp (2020) found that minor changes, either to the training dataset or into the input/output vectors, can lead to model integration instabilities. Brenowitz and Bretherton (2019) fitted a DNN for convection and clouds
- 95 to the coarse-grained data from a near-global aqua-planet cloud-resolving simulation using the System for Atmospheric Modeling (SAM). The NN scheme was then tested prognostically in a coarse-grid SAM. Their results showed that there were unphysicalnon-physical correlations were learned by the network, and the information in the upper levels obtained from the input vectordata had to be removed to produce stable long-term simulations. Rather than using NNs, Yuval and O'Gorman

(2020) used the random forest algorithm to develop an ML parameterization based on the training data from a high-resolution

idealized 3-D model with a setup of<u>on the</u> equatorial beta plane. They used two independent random forests to <u>separately</u> emulate <u>the</u> different processes <u>separately</u> and ensured<u>the</u> physical constraints by predicting subgrid fluxes instead of tendencies. Later, Yuval et al. (2021) completed the same task <u>withusing</u> NNs. Both <u>worksmethods</u> achieved stable simulations <u>infor</u> coarse resolution aqua-planet GCMs. <u>To determine why some methods can achieve stable prognostic simulations and others cannot</u>, Brenowitz et al. (2020) proposed methods to <u>interpretfor interpreting</u> and <u>stabilizestabilizing</u> ML
 parameterization <u>offor</u> convection. In their <u>workstudy</u>, a wave spectra analysis tool was introduced to explain why the ML

coupled GCMs blew up.

In real-world climate models with variedvarying underlying surfaces, convection and clouds are more diverse under different climate backgrounds, which makes the task of developing ML-based parameterizations more complicated. A few early works have shown earlier studies demonstrated the feasibility of using neural networks fitting cloud processes

- 110 in real-world models. Han et al. (2020) used a 1-D deep residual convolutional neural network (ResNet) to emulate moist physics in SPCAM. This ResNet-based parameterization fitted fit the targets with a high accuracy and iswas successfully implemented in a single column model. Mooers et al. (2021) gotdeveloped a high-skill DNN viausing an automated machine learningML technique and forced an offline land model withusing DNN emulated atmospheric fields. However, neither of these studies have-tested their NNs prognostically for long-term simulations. Similar to the idea of using several NNs for
- 115 different processes in proposed by Yuval and O'Gorman (2020), in this study-uses, a set of NNs was used to emulate convection and cloud processes in SPCAM with anthe actual global land-ocean distribution. We useused the residual connections inof Han et al. (2020) to acquire super deep neural networks with a great nonlinear fitting ability. Furthermore, we conductconducted systematic trial-and-error analysis to filter out unstable NN-parameterizations-Parameterizations and getto obtain the best residual deep neural network (ResDNN) set within terms of both accuracy and long-term stability. The NN
- 120 parameterization_Parameterization scheme iswas then implemented in thea realistically configurated configured CAM to obtain long-term stable simulations. Technically, NNs are commonly implemented viausing high-level programming languages such as Python and deep learning libraries. However, GCMs are mainly written in Fortran, making integrating them with deep learning algorithms inconvenient. Therefore, we introduceintroduced an NN-GCM coupling platform in which NN models and GCMs can interact through data transmission. This coupling strategy can facilitatefacilitates the development of ML-
- 125 physical hybrid models with <u>a high flexibility</u>. Under real-<u>geography geographic</u> boundary conditions, <u>our work achieveswe</u> <u>achieved</u> more than 10-year-long stable climate simulations in Atmospheric Model Intercomparison Project (AMIP)-style experiments by-using a hybrid ML-physical GCM. The simulation results <u>may showexhibited</u> some biases in <u>the mean</u> climate <u>mean-fields</u>, but <u>they</u> successfully <u>reproducereproduced the</u> variability in SPCAM. To our knowledge, this is the first time a decade-long stable real-world climate simulation is has been achieved with ausing an NN-based parameterization.
- 130 The remainder of this paper is organized as follows. Section 2 briefly describes the model, the experiments, the <u>DNNNN</u> algorithm, and the <u>DNNNN</u>-GCM coupling platform. Section 3 <u>analyses analyzes</u> the simulation stability of NNCAM. Section 4 presents the offline validation of the <u>DNNNN</u> scheme, focusing on the output temperature and moisture tendencies.

<u>Results</u> The results of the multi-year simulations, employing the DNN parameterization conducted using the NN-Parameterization scheme, are shownpresented in Section 5. A summary and the conclusions are presented in Section 6.

135 2 Methods and dataData

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In this study, we <u>choosechose</u> SPCAM as the reference model to generate <u>the</u> target simulations. A set of NNs <u>iswas</u> trained <u>withusing</u> the target simulation data <u>usingand</u> optimized hyperparameters. Then, they <u>arewere</u> organized as a subgrid physics emulator and <u>were</u> implemented into the superparameterized version of Community Atmospheric Model (in SPCAM)₇₂ replacing both the CRM-<u>-</u>based SP and the radiation effects of the CRM. This NN-enabled GCM is <u>hereinafter</u> referred to as NNCAM-hereafter.

2.1 SPCAM setup and data generation

The GCMs used in this study arewere the CAM5.2 developed by the National Center for Atmospheric Research and its superparameterized version SPCAM (Khairoutdinov and Randall, 2001; Khairoutdinov et al., 2005). A complete description of CAM5 ishas been given by Neale et al. (2012). The dynamic core of CAM5 has a horizontal resolution of 1.9°×2.5° and 30 vertical levels with a model top at about 2 hPa. To represent moist processes, CAM5 adopts a plume-based treatment offor shallow convection (Park and Bretherton, 2009), a mass-flux parameterization scheme for deep convection (Zhang and McFarlane, 1995), and an advanced two-moment representation of eloud<u>for</u> microphysical cloud processes (Morrison and Gettelman, 2008; Gettelman et al., 2010). In the AMIP experiments we conducted, CAM5 iswas coupled to a land surface model the Community Land Model version 4.0 land surface model (Oleson et al., 2010) and uses the prescribed sea surface

150 temperatures and sea ice concentrations-<u>were used.</u>

In this study, SPCAM iswas used to generate the training data. In SPCAM, a two-dimensional (2-D) CRM iswas embedded in each grid column of the host CAM as the SP. The 2-D CRM hascontained 32 grid points in the zonal direction and 30 vertical levels that arewere shared with the host CAM. The CRM handleshandled the convection and cloud microphysics to replace the conventional parameterization schemes, and the. The radiation iswas calculated on the CRM subgrids in order to include the cloud-radiation interactioninteractions at the cloud scale (Khairoutdinov et al., 2005). Under a realistic configuration, the planetary boundary layer processprocesses, orographic gravity wave drags, and the dynamic core arewere computed on the CAM grid. One conceptual advantage of using SPCAM as the reference simulation is that the subgrid and grid-scale processes are clearly separated, makingwhich makes it easy to define the parameterization task for an ML algorithm (Rasp, 2020).

160 2.2 NN-Parameterization

2.2.1 Data sets Datasets

The NN-Parameterization is a deep learning emulator of the SP and its cloud-scale radiation effects in SPCAM. Therefore, the inputs of this emulator are borrowed from the SP input variables, such as the grid-scale state variables and forcings, including the specific humidity q_v , temperature T, largescale water vapor forcing $\left(\frac{\partial q_v}{\partial t}\right)_{ls}$, and temperature forcing $\left(\frac{\partial T}{\partial t}\right)_{ls}$. Additionally, we selectselected the surface pressure P_s and solar insolation (SOLIN) at the top of the model from the radiation module. The outputs of the NN-Parameterization are subgrid-scale tendencies of the moisture $\left(\frac{\partial q_v}{\partial t}\right)$ and of temperature $\left(\frac{\partial T}{\partial t}\right) dry$ static energy $\left(\frac{\partial s}{\partial t}\right)$ at each model level as well as. It should be noted that $\left(\frac{\partial s}{\partial t}\right)$ is the sum of the heating from the moist processes in the SP and the heating from the SP radiation (shortwave heating *qrs* plus longwave heating *qrl*). To complete the emulation of the cloud radiation process, apart from the commonly used net shortwave and longwave radiative fluxes at both the surface and the <u>Top of the Atmosphere (TOA. This heating is composed of moist heating in the SP and the GCM grid averaged SP radiative heating. Also, (Rasp et al., 2018; Mooers et al., 2021), it is importantessential to include direct and diffuse</u>

downwelling solar radiation fluxes as output variables <u>in order</u> to force the coupled land surface model. Specifically, they are <u>the</u> solar downward visible direct to surface (SOLS), solar downward near infrared direct to surface (SOLL), solar downward visible diffuse to surface (SOLSD), and solar downward near infrared diffuse to surface (SOLLD). <u>fluxes.</u> In the end, the
 precipitation is derived from column integration of <u>the</u> predicted moisture tendency to <u>keepensure</u> basic water conservation.

—The large-scale forcings are commonlywere often not included in previous studies with<u>that used an</u> aqua-planet configuration. However, under <u>a</u> realistic configuration, such forcings are composed of the dynamics and the planetary boundary layer diffusion, thereby carryingand thus, they carry critical information about the complex background circulations and surface conditionconditions. Similarly, thosethe downwelling solar radiation fluxes with <u>direct</u> separation of <u>direct</u> versus diffusion recordsrecord the received solar energy received by the coupled surface model with<u>for</u> different land cover types and processes (Mooers et al., 2021). If <u>they are</u> not included, the land surface is not heated up by the sun, therefore, which seriously weakingweakens the sea and land breeze and monsoon circulations. In this study, we used the vertical integration of the NN predicted moisture tendency as an approximation of the surface precipitation, which has also been used in previous studies (e.g., O'Gorman et al., 2018; and Han et al., 2020). In the offline validation test, we observed negative precipitation events

185 (27% occurrence in 1 year of results). Nonetheless, 93% of the negative precipitation events had a magnitude of less than 1 mm/day. In the online prognostic runs, reasonable rainfall results (more details will be provided in Section 5) were achieved using this approximation scheme.

Table 1 lists the input and output variables and their normalization factors. There are 30 model levels for each profilevariables/variable.Therefore, the input vector consists of 122 elements for 4 profile variables and 2 scalars, while the 68-190element output vector is madecomposed of 2 profiles and 8 scalars. All of the input and output variables are normalized to
ensure that they are inof the same magnitude before they are putinput into the NN-parameterizationParameterization for the

training, testing, <u>modeland</u> prognostic <u>model</u> validation. <u>It should be noted that each variable is normalized as a whole at all levels.</u> The normalization factor for each variable shown in the <u>supplemented</u> codebase <u>iswas</u> determined by the maximum of its absolute <u>values</u>. <u>value</u>.

The training dataset used by all <u>of the considered NNs isconsisted of 40% of the temporally randomrandomly</u> sampled <u>data</u> from the 2-year SPCAM simulation from January 1, 1997, to December 31, 1998. Notably, <u>It should be noted that</u> random sampling iswas only done in the time dimension, but not in <u>the latitude and longitude dimensions</u>, including all 13,824 samples from <u>the global grid points</u> for each selected time step. To avoid any <u>mixmixing</u> or temporal connection between the training set and <u>the offline validation set</u>, we <u>random samplerandomly sampled</u> 40% <u>timestepsof the time steps</u> from the SPCAM simulation in <u>the vear-2000 as-to produce the offline validation set</u> in used for the sensitivity test.

2.2.2 A ResDNN Setset

InDuring the development of the NN-Parameterization scheme, it iswas found that when different variables are used as the output of the neural network, the training difficulty of the training is quite different. EspeciallyIn particular, the neural network's ability to fit the radiation heating and scalar fluxes is significantly stronger than the tendencies variables. This is also

- 205 found in Gentine et al. (2018), in which) also reported this, and they found that the coefficient of determination (R²) of the radiative heating tendency is was higher than that of the moisture tendency at most model levels. We believethink that using a single NN with one targetoutput to train all of the variables, (i.e., the moisture tendency, temperaturedry static energy tendency, and radiation fluxes, inevitably causes) is possible to cause mutual interference. Since gradient descending is applied to optimize the network induring the training, mutual interference between different targets is expected tooutputs will cause the
- 210 cancel out of gradient directions used for <u>the descending (Crawshawto cancel out (Yu</u> et al., 2020; <u>Zhang and Yang., 2021)</u> and), which will ultimately affect the convergence of the network. <u>We use Thus, we used three</u> different neural networks <u>with</u> <u>the same hyperparameters</u> to train
 - (1) the tendency of the moisture and temperature, and ;
 - (2) the tendency of the dry static energy; and
- 215 (3) the radiation fluxes at the surface and TOA.

It should be noted that the radiation fluxes include the net shortwave and longwave radiative fluxes at the surface (FSNS and FLNS, respectively-) and at the TOA (FSNT and FLNT, respectively) and four solar radiation fluxes (SOLS, SOLL, SOLSD, and SOLLD). By doing so, we avoidavoided the gradient cancellation between multiple targets and improve and improved the convergence speed and fitting accuracy when training the network. As will be described in Section 3.1, when using the same

220 network configuration, <u>the</u> radiation fluxes are trained <u>much easier with more easily and have a higher accuracy than the</u> tendencies of <u>the</u> moisture and temperature. We admit that putting <u>the</u> heating and moistening <u>raterates</u> in two different NNs arbitrarily <u>eutcuts the</u> physical connections between them. <u>ButHowever</u>, this separation is <u>surely doingmakes the</u> training <u>more easily</u>easier in the <u>developing</u>development stage.

- In this study, to mimic the column-independent SP and its radiation effects, the input and output of <u>the</u>_NN-225 Parameterization have to be both <u>had to be</u> 1-D vectors. This means that the <u>data</u>-input and output of <u>the</u>_NN-Parameterization are much simpler than those in <u>the</u>-existing mainstream <u>machine learningML</u> problems, such as image recognition and textspeech recognition, so. <u>Thus</u>, it is impossible to <u>directly</u> apply most of the existing complex neural networks <u>directly</u>. <u>Taking</u> the convolutional neural network CNN as an example, the study of Albawi et al. (2017) shows that CNN has more advantages than DNN in the learning of large scale images. The problem we face is that the input is a 122-dimensional vector stitched by
- 230 multiple different physical quantities with only 4 30 element 1D profiles plus 2 scalars, which cannot meet the requirements of "large-scale" (generally at least 32×32 two-dimensional images). So, there is no need to use CNN.. Hornik et al. (1989) proved<u>demonstrated</u> that a single-layer neural network can approximate any function. Although the problem that NN-Parametrization needs to deal with is highly nonlinear, from the point of view of machine learning, it is essentially a mapping problem from a 122-element 1D-vector to a 1D-vector with a length of 68. According to the universal approximation theorem,
- 235 DNNit is feasible- for a DNN to map from a 122-element 1-D vector to a 1-D vector with a length of 68, which is what the NN-Parameterization does. Therefore, when constructing the NN-Parametrization, we first tried to use a DNN for the fitting, and introduced residual connections to extend the DNN in to a ResDNN.

After numerous experiments, we <u>gotobtained</u> the best hyperparameters <u>offor the</u> DNN and ResDNN. When training a <u>Fullyfully</u> connected DNN, the hidden layer width of the network should be set to 512, and the network's depth should not

- 240 exceed 7₅ otherwise it will affect, the convergence of the DNN- will be affected. In order to make the neural network capture more non-linear information, enhance the fitting ability- was enhanced. We introduce skip connections to extend the 7-layer DNN to a 14-layer ResDNN. The network structure of the ResDNN is shown in Figure 1. In the training process, both the DNN and ResDNN use an initial learning rate of 0.001 and a learning rate decaying strategy asfor the cosine annealing (Loshchilov et al., 2016) without dropout and L2 regularization. Adam (Kingma and Ba, 2014) iswas chosen as the optimizer
- 245 to minimize the mean squared square errors (MSEs). The results in The specific hyperparameter searching space of the DNN and ResDNN is documented in Table S1.

Figure 2 showshows that the ResDNN can fit fits the data is significantly better than the DNN, with details described in Section 3.1. At the same time, the sensitivity tests in section 3 also prove that no DNN model can ensure the stable simulation of NNCAM. So, we we chose ResDNNsResDNN sets as stable candidates to build the NN-Parameterization. After obtaining
all-well-fit ResDNN sets, the next step is to couple the candidates into NNCAM one by one for the prognostic tests and to find the sets that can support a stable simulation. To complete this extremely challenging task, we have more than 50 prognostic tests. All of the experiments and analyses onrelated to the stability will be introduced in section 3-as well.

2.2.3 Implementation of NN-Parameterization

The NN-Parameterization is implemented into SPCAM to replace both the CRM-based superparameterization and its radiation effects <u>based</u> on the <u>basisaverage</u> of <u>the</u> coarse grid-average. In. At the beginning of each <u>timesteptime step</u>, NNCAM calls the NN-Parameterization and predict predicts the moisture tendency $\left(\frac{\partial q_v}{\partial t}\right)^{-1}$ the temperature dry static energy tendency $\left(\frac{\partial x}{\partial t}\right)^{\frac{\partial s}{\partial t}}$ from the moist physics and radiative heating, and all of the radiation fluxes- at the surface and the TOA. Then, the DNN predictions are returned to NNCAM, updating the model states and radiation fluxes are updated. Additionally, the surface total surface precipitation is derived from the column integration of the predicted moisture tendency. The near-surface conditions of the atmosphere and the downwelling radiation fluxes are transferred to the land surface model. After the coupling of the-land surface model and the prescribed Sea Surface Temperature (SST) are coupled, the host CAM5 performs the planetary boundary layer diffusion and letlets its dynamic core complete a timesteptime step integration (Figure 1). In the next timesteptime step, the dynamic core returns the new model states to the NN-Parameterization as inputs again. During the whole entire process, the NN-Parameterization and GCM will-constantly update each other's status. HowDetermining a way to couple the NN-Parameterization with the GCM and to run them efficiently and effectively is the key to the implementation of NNCAM. To solve these problems, we developed the NN-GCM coupler-that, which integrates the NNs into NNCAM, which. This process will be introduced in the following next section.

2.3 The NN-GCM Coupler coupler

Deep learning research mainly uses <u>machine learningML</u> frameworks based on Python interfaces to train neural network models, and <u>deploy themthey are deployed</u> through C++ or Python programs. <u>While GCM isIn contrast, GCMs are</u> mainly developed in Fortran, <u>which makes it is a</u>-very challenging <u>work</u>-to call a neural network model based on<u>a</u> Python/C++ interface in GCM codes written in Fortran. Solving the problem of code compatibility between <u>the</u> NN and GCM can significantly help develop NN-_based <u>Parameterizationsparameterizations</u> for climate models.

To implement an NN-based Parameterization parameterization in the current climate modelmodels, which isare mostly developed in Fortran, many researchers tryhave attempted to getobtain the network parameters (e.g., the weight, and bias) from the machine learningML models and implement the NN models (e.g., DNNs) withusing hard coding in Fortran. At the runtime, NNCAM will call an NN-parametrization as a function (Rasp et al., 2018; Brenowitz and Bretherton, 2019). Recently, some researchers have developed a Fortran-neural network interface that can be used to deploy DNNs into GCMs (Ott et al., 2020). This interface can import neural network parameters from outside of the Fortran program, and the Fortran-based implementation ensures that it can be flexibly deployed in GCMs. However, embedding an NN-parameterization-Parameterization in NNCAM is still a troublesome task-with, and there is no existing coupling framework to support many of the latest network structures. This problem will restrict developersprevents researchers from building more powerful NNs and deploying them in NNCAM.

We <u>develop thedeveloped a</u> coupler to bridge <u>the</u> NN-Parameterization with the host CAM5. Through this coupler, the neural network can communicate with the dynamic core and other physical schemes in NNCAM in each time step. When NNCAM is running, as shown in (1) in Figure 5,3), the coupler receives the state and forcing output from <u>the</u> dynamic core in the Fortran-based CAM5. For each input variable, we use used the native Message Passing Interface (MPI) interface in CAM5 to gather the data offor all of the processes to into the master process into a tensor. Then, as shown in (2) of Figure 5, the coupler will transmittransmits the gathered tensor through the data buffer to the NN-Parameterization running on the same

- 290 node as the master process. (2) in Figure 3). The NN-Parameterization gets obtains the input, infers the outputs, and transmits them back to the coupler. As shown in (3) of in Figure 53, the coupler will first write writes these tendencies and radiation fluxes back to the master process, and then-broadcast, it broadcasts the data to the CAM5 processes running on the computing nodes through the MPI transmission interface. Therefore, other parameterizations getobtain the predictions from the NN-Parameterization to complete the follow-up procedures ((4) in Figure 5). 3).
- 295 In practice, the NN-GCM Coupler coupler introduces a data buffer that supports a system-level interface, which is accessible by both the Fortran--based GCM and the Python-based NN without supplementary foreign codes. This can avoid code compatibility issues when building Machine Learning ML coupled numerical models. It supports all mainstream machine learning ML frameworks, including native PyTorch and TensorFlow. Based on Using the coupler, one can efficiently and flexibly deploy the Deep Learning Model deep learning model in NNCAM, and can even take advantage of the latest developed 300 neural networks.

All neural network models deployed through using the NN-GCM Coupler can support a Graphics Processing Unit (GPU) accelerated inference to achieve excellent computing performance. In this study, we ran SPCAM and NNCAM on 192 CPU cores, NNCAM also used 2two GPUs for acceleration. During the NNCAM runtime, each time step of NNCAM requires the NN-Parameterization to complete an inference and conduct data communication with NNCAM. This is a typical high-305 frequency communication scenario. We evaluated the amount of data (about 20MB20 MB for CAM5 with thea horizontal resolution of $1.9^{\circ} \times 2.5^{\circ}$) that needs to be transmitted for each communication- and determined decided to establish a data buffer on a high-speed solid-state drive to ensure a balance of between performance and compatibility. It takes about 1x10⁻² seconds to access the data buffer in each time step, which is enough to support the efficient simulation of NNCAM. The Simulation Years simulation years per Dayday (SYPD) of NNCAM based on the NN-GCM Coupler has coupler represents an impressive 310 performance improvement. when using 192 Intel CPU cores, the SYPD of SPCAM is 0.3, the SYPD of CAM5 is 20, and the SYPD of NNCAM is 10. It is worth noting should be noted that. NNCAM based on the NN-GCM coupler uses an additional GPU to accelerate the NN-Parameterization. When the NN-GCM Couplercoupler is not used, the NN-

is 1.5.

315 **3 A Road to Stability**

3.1 Sensitivity Tests and Trial-and-error

To develop a stable NN-parameterization Parameterization, we propose a ResDNN set, where the use of a set of three ResDNNs, in which each neural network is responsible for predicting a class of variables (see section Section 2.2.2). One may wonder

Parameterization is implemented by using Fortran and is accelerated by the Fortran-based Math Kernel Library, and the SYPD

whether the ResDNN architecture is necessary and whether offline accuracy of NNs matters in Ott et al. (2020) demonstrated

320 <u>that there is a negative correlation between the offline MSE and online stability. This section tries to deal with the questions</u> via a series of sensitivity tests.

To prove the necessity of the ResDNN architecture, we use the 7-layer DNN when using tendencies as the control group. We do not include other types of ML architecture, since random forest is less likely to perform as accurately as neural networks and cannot be implemented outputs in GPUs (Yuval et al., 2021), and 1D CNN is not widely aqua-planet simulations. Since we

- 325 <u>also</u> used <u>tendencies as outputs</u> in other studies except Han et al. (2020) with unknown prognostic performance. The prognostic tests of the real-world simulations, we conclude that an NN-based parameterization begin at 1998-01-01 as that can support long-term integration should have a startup.high accuracy regarding training and validation. As initialization, ealling the SPwas described in SPCAM at the Section 2.2.2, we tried DNNs first step is required to generate the correct largescale forcings as the input for NN, and then, we extended the DNNs to ResDNNs to achieve a high offline accuracy
- 330 (Figure 2). Even through more accurate ResDNNs have a higher probability of becoming stable parameterizations (Figure 4), we still do not have a way to determine the stability a priori. Therefore, we still used the trial-and-error method to filter out unstable ones and then selected the best ResDNN set that could reduplicate the total energy time evolution of SPCAM with the least deviation, i.e., the NN-Parameterization.

3.2 Sensitivity tests

- 335 We conducted prognostic runs of all three neural networks in each NN set using the NN-GCM coupler. To demonstrate the reality behind the relationships between the offline accuracy and online stability under a real-world configuration, we conducted sensitivity tests using 10 DNN sets and dozens of ResDNN sets and conducted the training and evaluation using the settings described in Section 2.2.2. In the sensitivity tests, we freezeconducted prognostic runs (see details in Section 3.2) using all three neural networks in each NN set using the NN-GCM coupler.
- 340 First, we selected the best ResDNN for the 8 radiation fluxes to simplify the neural network choices, at the surface and the TOA that was shared in every NN set since their offline validation is extremely was exceptionally accurate with -R² above 2 0.98 over 50 training epochs (Figure 2b). Different fromIn contrast to the accurately trained radiation fluxes, the tendencies of temperature the dry static energy and moisture are less accurate and can hypothetically affect the prognostic performance. To evaluate the tendency of moistening and heating in those two tendencies using one metric, we introduced the MSE
- 345 of the rate of change of the moist static energy changing rate $(dh = C_p dT ds + L_v dq_v)$ as:):

$$MSE_h = \left\| \frac{1}{g} (dh_{NN} - dh_{SPCAM}) \Delta p \right\|_2,$$
(1)

where g is the <u>acceleration due to gravity constant</u>, C_p refers to is the heat capacity of air, L_v is the latent heat of water vapor, and Δp is the layer thickness. Multiple ResDNN pairs for dq_v and dT and DNN pairs are for dq_v and ds were trained from $\frac{1}{2}$ five epochs to 50 epochs, earryingresulting in different offline validation accuracy. accuracies. We used the maximum number of

350 steps until the model crashed to measure the prognostic performance.

Figure 4 shows the offline validation MSE_h versus the <u>maximum</u> prognostic steps. <u>First, The</u> DNN-_parameterizations (blue triangles) are <u>systematically</u> less accurate than <u>the</u> ResDNN-<u>ones</u>-<u>parameterizations</u> (blue dots and black inverted triangles), which is consistent with Figure 2a. They <u>eannot run stably</u><u>could not sustain half a year of simulation</u> in <u>the</u> prognostic tests with the best DNN-_parameterization-<u>to sustain half a year of simulation</u>. For the ResDNNs, the less well-

trained ones with high <u>MSE crash for a shorterMSEs also crashed after short</u> simulation <u>period than DNNs-periods</u>. However, when the offline MSE <u>decreasesdecreased</u> to a certain level (e.g., 290 W^2/m^4), <u>some10</u> of the ResDNN--parameterizations <u>arewere</u> stable for extremein long-term simulations, while others remain unstable.

Generally, a NN parameterization of over 10 years (black inverted triangles). We speculate that ean support long-term integration should have both good generalization abilities and high accuracy for training and validation. Above all, sufficient accuracy is necessary for all neural networks. From Figure 4, it can be interpreted that a vague threshold exists in the validation MSE. ResDNNs can be trained for higher accuracy since they are much deeper than DNNs with much higher model capacity. So, they are the more competentaccurate ResDNN sets have a higher probability of becoming stable NN-Parameterizations since all of the stable NN-Parameterizations are ResDNNs.

- A few unstable ResDNN sets are equally or more accurate than DNNs in this job. On the other hand, the stable ones. 365 Previous studies showed have shown that high-capacity (more hidden layers and more weights and biases) models are harder to train and <u>are more likely to overfit produce overfitting</u> (Goodfellow et al., 2016). Thus, the prognostic stability differences between less well-trained ResDNNs and the well-trained ones are drastic compared with DNNs. Also, some<u>Some</u> overly trained ResDNNs with lowest validation loss are speculated to <u>overfit. Thoseproduce</u> overfitting<u>models</u>, and therefore, they are less likely to generalize to unknown backgrounds caused by accumulated errors in the ML-GCM system, <u>ending up model</u> 370 erashes. However, those are just intuitive experiences but not guarantee ways for stability causing the model to crash.
- In the time evolution of the <u>globalglobally</u> averaged total energy (Figure 5). The), the system energy grows exponentially and then blows up for unstable ResDNN-_parameterizations (the red and orange lines). In contrast, the stable ones can keep the total energy at a certain level and reproduce the annual cycle <u>of</u> fluctuations in SPCAM. Among the stable ResDNN schemessets, some can get nearly a perfect reproduction of<u>almost perfectly reproduce</u> the total energy evolution of SPCAM (the blue line), <u>while</u>). <u>However</u>, some inaccurately simulate the climate state with a <u>largesignificant</u> deviation (green line). Therefore, among the accurate ResDNN parameterizations (e.g., offline validation $MSE_{h} < -290 W^{2}/m^{4}$), we still have to use the trial-and-error to filter out unstable ones and then select the best ResDNN pair for moistening and heating rate that can reduplicate the total energy time evolution of SPCAM with the least deviation. We name this best<u>Apart from global averages</u>, the prognostic results of the 10 stable ResDNN pair together with the ResDNN in charge of radiation fluxes the NN-380 Parameterization. This NN GCM coupled model is called NNCAM and is later evaluated for climate mean states and variabilitysets vary from each other in terms of the global distribution. Figure S1 shows the precipitation spread across all of

the stable NN sets for the prognostic simulation from 1999 to 2003. The obvious standard deviation centers coincide with the heavy tropical precipitation areas.

3.23 Gravity Wave Diagnosis wave diagnosis

- 385 It is still a question of unclear why unstable NN-parameterizations <u>Parameterizations</u> blow up models. The fast-growing energy of the unstable runs indicates a possible underlying unrealistic energy amplifying mechanism in the <u>NN-GCM</u>-coupled <u>NN-GCM</u> system. Brenowitz et al. (2020) offered <u>several</u> interpretations. When an unstable NN-parameterization<u>Parameterization</u> is coupled with dynamics, it tends to amplify any unrealistic <u>perturbation perturbations</u> caused by emulation errors and <u>to pass</u> it to the entire system through gravity waves. In contrast, the stable NN-parameterizations tend to dump all
- 390 of the perturbsperturbations quickly. This is was found to be true in our study with for the realistic configuration. Such unstable gravity waves are were observed in the prognostic simulation of an unstable ResDNN (the real line in Figure 5). The animation in Movie S1 records the first unrealistic wave, and Movie S2 documents the more intense waves afterward with a perfectly round shape. after this point in time. Additionally, we found that our instable waves mostly occurred in the tropics, which is different from the mid-latitude instability that occurs when using ML parameterizations in aqua-planet simulations (Brenowitz

395 et al., 2020).

<u>Brenowitz et al.</u> (2020) also introduced an analysis tool that calculates <u>the</u> wave energy spectra of a hierarchy model that couples the <u>linear response functions</u><u>Linear Response Functions</u> (LRF) of <u>an</u> NN-<u>based</u> parameterization to a simplified two-dimensional linear dynamic system, <u>wherein which</u> perturbations can propagate in 2D2-D gravity waves. We <u>applyapplied</u> the tool in <u>ourthis</u> study and <u>detectdetected</u> similar results of<u>in the</u> unstable mode for the unstable ResDNN with <u>a</u> positive energy growth rate across all wave numbers at phase <u>speed betweenspeeds of</u> 5-m/s to <u>-</u>20 m/s (Figure <u>S1b</u>). <u>WhileS2b</u>). In contrast, the stable ResDNN <u>showsexhibited</u> a stable mode <u>withfor</u> the growth rate of nearly all wave numbers and phases below zero (Figure <u>S1a</u>S2a).

4 Offline Validation of NN-Parameterization

- Before evaluating the prognostic results, <u>demonstration of the</u> offline performance with geographic information is <u>neededneeds</u> 405 <u>to be demonstrated</u> for the following purposes: 1) <u>Toto</u> show how well our NN-Parameterization emulates the SP <u>infor a</u> realistic configuration compared with <u>the</u> baseline CAM5 physics and <u>with</u>-previous studies<u>-; and</u> 2) <u>Toto</u> reveal the <u>strengthstrengths</u> and <u>weaknessweaknesses</u> of <u>the</u> NN emulations with <u>the</u> correct input, <u>give</u> and to provide clues to the analysis of <u>the</u> prognostic results in the following section. We performed offline testing <u>withusing</u> a realistically <u>configuratedconfigured</u> SPCAM from January <u>1st1</u>, 1999, to December <u>31st31</u>, 2000, <u>wherein which the</u> NN-Parameterization
- 410 iswas diagnostically run paralleledparallel to the SP, and so doeswas the CAM5 physics. The results overfor the entire second year of the simulation period arewere chosen for evaluation, which was completely independent from the training dataset. Following the conventions inof Han et al. (2020) and Mooers et al. (2021), we choose used the mean fields and the coefficient

of determination (R^2) as the two<u>evaluation</u> metrics for evaluations. It should be noted that the NN-Parameterization was tuned to emulate the SP, and the CAM's parameterization was tuned to obtain close results to the observations. The latter is merely

415 <u>introduced as a baseline.</u>

The mean diabatic heating and drying rates produced by convection-and, large-scale condensation, and cloud radiation effects in SPCAM and the NN-Parameterization are in close agreement. Figure 6 shows the latitude-height cross-sections of the annual mean heating and moistening rates in SPCAM and the corresponding NN-Parameterization. At 5 °N, SPCAM showsexhibits the maximum latent heating in the deep troposphere, corresponding to the deep convection atin the ITCZ. In the subtropics, there is heating and moistening occur in the lower troposphere, corresponding to the stratocumulus and shallow convection in the subtropics. In the midlatitudesmid-latitudes, there is a secondary heating maximum below 400 hPa due to midlatitudethe mid-latitude storm tracks. All of these features are well reproduced by the NN-Parameterization. NoteIt should be noted that in the midtropospheremid-troposphere, the ITCZ peak in the drying rates rate in the ITCZ is slightly weaker in

the NN-Parameterization eompared with that of than in SPCAM (Figure Figures 6c and 6d).

- In addition to the mean fields, the high prediction skill of <u>the NN-Parameterization</u> is also shown indemonstrated by the spatial distribution of <u>the R^2 -values</u>. To demonstrate-illustrate the R^2 forvalues of the 3D3-D variables such as <u>the</u> diabatic heating and moistening, same as following Mooers et al. (2020),2021), the zonal averages arewere calculated in advance before the R^2 calculation for each location in the pressure-latitude cross-section. For <u>the</u> diabatic heating, <u>the R^2 value</u> is above ≥ 0.7 overthroughout the entire mid to lowmiddle and lower troposphere, and the high skill regions with R^2 values of greater than
- 430 0.9 concentrates are concentrated in the low levels but are extended to extend into the mid-troposphere in the storm tracks (Figure 7a). As forFor the moistening rate, the high skill zones concentrate are concentrated in the mid tomiddle and upper troposphere (Figure 7b), leavingwith low skill areas below. Those The regions with low accuracy lower accuracies are generally located in the mid-to-low-middle and lower troposphere in the tropics and subtropics, corresponding which correspond to the deep convection at the ITCZ and the shallow convection in the subtropics. Nonetheless, the tendencies from of the diagnostic
- 435 CAM5 parameterization hardly draw any similarity are not similar to those simulated by the SP, except for a few locations in the mid tomiddle and upper troposphere in the tropics and polar regions (Figure Figures 7c & and 7d).

The global distribution of <u>the R^2 forvalues of</u> the precipitation predictions is shown in Figure 8. Our NN-Parameterization shows a great prediction skill globally produced excellent predictions in most of the in mid- and high-latitude regions, especially in the <u>midlatitude</u> storm tracks. <u>The However, the</u> prediction skill is relatively low in many <u>of the ocean</u> areas between 30°S

- 440 toand 30°N and in some midlatitude mid-latitude areas over continents (Figure 8a), in). In particular, the results are not ideal in the ITCZ deep convection regions. Moreover, for shallow convection in Subtropical along the equatorial regions, in the subtropical Eastern Pacific, and Subtropical in the subtropical Eastern Atlantic, the precipitation prediction skill hits bottom, corresponding to the subtropical. These areas correspond to the low skill zones for of the moistening rate (Figure 6b). On the other hand in the middle and lower troposphere from the equator to the subtropics (Figure 7b). As a baseline, the total
- 445 precipitation simulated by using the CAM5 parameterizations is much less analogous to the SP than the NN-Parameterization

with<u>and has</u> a systematically lower accuracy globally. <u>The CAM5 precipitation can reachachieve</u> a relatively high accuracy along the mid-latitude storm tracks, but <u>failit fails in</u> most regions in the tropics-<u>(Figure 8b)</u>.

Generally, <u>the NN-Parameterization performsperformed</u> far better than <u>the CAM5</u> parameterization in the 1-year <u>period</u> in the offline testing, and shows similar it had an accuracy assimilar to that of the DNN inused by Mooers et al. (20202021).

- 450 The <u>use of real-geography geographic</u> data can significantly decrease the emulation skill of a deep learning model (Mooers et al., 2021), where). This is because the convection backgrounds <u>of real geographic data</u> are much more complex with meridional and zonal asymmetric and <u>seasonal variated seasonally varying</u> circulations, not to mention. In addition, the <u>orographorography</u> and various types of underlying land <u>surface</u>. In that <u>surfaces also add complexity</u>. In this case, the ResDNN is a valuable NN architecture that <u>can bring good performanceperforms well</u> as the<u>an</u> automated hyperparameter tuning algorithm without
- 455 searchingthat does not need to search for hundreds of NN candidates. Still, our NN-Parameterization is exposed toproduced low accuracy predictions in subtropical shallowalong the equator over the oceans where the convection areas, a great challenge for machine learning emulation of moistening rate and precipitation. In those regions, the local variance/std-is close to zero. But the NNs in our study are trained in the loss function of mean squared error, which complex and vigorous and in subtropical ocean areas where the convection is not sensitive to small values.

460 5 Long-term Prognostic Validation

weak and concentrated at low levels. This indicates that the NN-Parameterization is selected forstill inadequate in rems of its emulation skill when simulating various types of deep and shallow convection in the tropics.

<u>5 Long-Term Prognostic Validation</u>

The NN-Parameterization produced the best prognostic performance in Section 3.1. It iswas coupled in the realistic configurated realistically configured SPCAM to replace the SP and its cloud-scale radiation effects. This coupled model is called referred to as NNCAM afterwardshereinafter and is compared with SPCAM and CAM5. All-The start time of all three model starts atwas January 1st1, 1998 as start up. They arewere all run for 6 years with the first year for spin up and the next 5 years from (January 1st1, 1999, to December 31st31, 2003) for evaluation and comparison. Later, the simulation of NNCAM iswas extended for another 5 years to December 31st31, 2008, to showdemonstrate its stability. Due to the excessive computing resources eonsumptionrequired, the SPCAM simulation of SPCAM iswas not get extended. In the analysis of the prognostic results, the following arewere selected for demonstration of to demonstrate the multi-year climatology and variability: multi-year

- cur
 - (1) The mean fields of temperature and humidity; fields;
 - (2) The mean precipitation, field;
- 475 (3) The precipitation frequency distribution; and the

(4) The Madden-_Julian Oscillation.

As was mentioned in the introduction section, SPCAM, which uses the 2-D SAM as the SP, does not simulate better mean climate states than its host coarse-grid model CAM5, but it excels in climate variability. What is remarkable about NNCAM is not its performance in simulating the mean climate, but its ability to achieve a stable multi-year prognostic simulation under

480 <u>a real-world global land-ocean distribution. The advantages and problems of this study will provide important references for</u> future research on NN-based stable long-term model integrations.

5.1 Climatology

5.1.1 Vertical profiles of temperature and humidity

- In this section, we first-evaluate the vertical structures of the mean temperature and humidity fields. Figure 9 shows the zonally averaged vertical profiles of the air temperature and specific humidity as-simulated by theusing NNCAM and the CAM5, in contrast compared to the SPCAM simulations. Overall, the NNCAM simulatesimulated reasonable thermal and moisture structures. However, it is shown that NNCAM has some biases in the multi-year mean fields of temperature and humiditymoisture fields produced by NNCAM are more biased than those produced by CAM5, which is shown as reflected by the larger root mean squaredsquare errors (RMSEs) or (Figure 9) and larger differences than compared to those of CAM5 (Figure S2).-10). The larger deviations are temperature biases in the tropopause, where. In this region, the cold-point region is thinner and warmer in NNCAM than in SPCAM and CAM5. In addition, there are cold biases above 200 hPa and warm biases blow over the polar regions in NNCAM. For the humidity field, there are slight dry biases over the equator and wet biases
- elsewhere in NNCAM. Even with thethese biases, the mean climate mean states are consistent with those in the last 5-year years of the simulation for NNCAM (Figure S3), which indicates almost nothat the climate driftstates simulated by NNCAM
 are constant in the long-term simulation.

5.1.2 Precipitation

- Figure <u>1011</u> shows the spatial distributions of <u>the</u> winter (December-January-February) and summer (June-July-August) mean precipitation simulated <u>byusing</u> SPCAM, NNCAM, and CAM5. The SPCAM simulation results are regarded as <u>the</u> reference precipitation. In SPCAM (<u>Figure 10aFigures 11a</u> and <u>10b11b</u>), massive precipitation can be <u>foundobserved</u> in <u>regions of the</u>
- 500 Asian monsoon region and midlatitudethe mid-latitude storm tracks over the northwest Pacific and Atlantic oceans. In the tropics, the primary peaks of <u>in the</u> rainfall <u>areoccur</u> in the eastern Indian Ocean and Maritime Continent regions. FurthermoreIn addition, two zonal precipitation bands are located at 0°-10°N in the equatorial Pacific and Atlantic oceans, constituting the northern ITCZ. The southern South Pacific Convergence Zone (SPCZ) is mainly located <u>at</u> around 5°S-10°S near the western Pacific warm pool region and experiences a southeast tilt<u>tilts southeastward</u> as it extends eastward into the central Pacific. The main spatial patterns of <u>the</u> SPCAM precipitation elimatology are properly reproduced by both NNCAM and CAM5. InFor
- NNCAM, the strong rainfall centers are well simulated over the tropical land regions overof the Maritime Continent, the Asian

monsoon region, and South America, and Africa (Figure 10eFigures 11c and 10d11d). In addition, the heavy summertime precipitation over the Northwestern Pacific simulated by SPCAM is well represented inby NNCAM (Figure 10aFigures 11a and 10e). In11c). For CAM5, there is too little precipitation over that this area (Figure 10e11e). Moreover, NNCAM ean

510 <u>maintainmaintained</u> the spatial pattern and global average of <u>the</u> precipitation in the next 5-<u>year years of the</u> simulation, <u>reassuring</u>demonstrating its long-term stability (Figure S4).

Generally, <u>the NNCAM drawsresults are</u> more <u>similaritysimilar</u> to SPCAM than <u>the CAM5 results in terms of the spatial</u> distribution of <u>the summertime multiyear multi-year</u> precipitation, with smaller <u>RMSERMSEs</u> and <u>globalglobally</u> averaged biases. However, <u>in theon a</u> difference plot (Figure <u>HS5</u>), NNCAM moderately underestimates <u>the precipitation</u> along the

- 515 equator, in the Indian monsoon region, and maritime continentover the Maritime Continent in the summer (Figure 11aS5a). In the boreal winter, NNCAM simulates a weak andSPCZ that is excessively separated SPCZ-from the ITCZ, with both precipitation centers shiftingshifted away from each other. As a result, we detect-underestimation occurs in the equatorial regions of the maritime continent as well asMaritime Continent and in the SPCZ-but, while overestimation onoccurs to the north of the equator in the WestWestern Pacific (Figure 11b), which makesS5b), and thus, NNCAM less resembles
- 520 SPCAM <u>less</u> than CAM5 in this season. This simulation biases in NNCAM are speculated linked to the weaker drying tendencies of the ITCZ midtroposphere from the NN parameterization and low accuracyunderestimation of NNCAM predictions the precipitation along the equator can also be observed in the zonal mean multi-year precipitation plots (Figure 12). There is a more significant minimum zone in the equatorial precipitation near the equator compared with in SPCAM and CAM5 for the annual average (Figure 12a) and the boreal winter average (Figure 12c).
- 525 <u>In contrast to the oceanic rainfall, NNCAM predicts the precipitation over the land surfaces with good skill in the tropics</u> (land fraction equal to 1), which resembles the tropical land rainfall intensity of SPCAM and Tropical Rainfall Measuring <u>Mission (TRMM) observations of the annual and boreal summer averages (Figures 12d and 12e). According to Kooperman et</u> <u>al. (2016), SPCAM predicts the Asian and African Monsoon activity better, which leads to the more accurate land rainfall in such areas. This is related to the stronger convective variability in the SP than the conventional parameterizations. As an emulator of SPCAM, NNCAM inherits this strength.</u>

5.2 Variability

5.2.1 Frequency Distribution distribution of Precipitation precipitation

Moreover, NNCAM <u>showsexhibited a</u> better performance in simulating <u>the precipitation extremes</u>. Figure 1213 shows the probability <u>densities_density</u> function of <u>the simulated daily precipitation</u> in the tropics ($30^{\circ}S-30^{\circ}N$) with a precipitation

535 intensity interval of 1 mm day⁻¹. InFor CAM5, the heavy precipitation events exceeding 20 mm day⁻¹ are greatly underestimated. In addition, for CAM5, the light to moderate precipitation events between (2–20 mm day⁻¹) are overestimated, with an unreal probability peak around 10 mm day⁻¹ in CAM5, which is a typical simulation bias found in simulations with parameterized convection but not inand no explicitly resolved convectionsconvection (Holloway et al., 2012). Compared with CAM5, the

spectral distribution of the precipitation infor NNCAM is much closer to that of SPCAM. The heavy rainfall events are 540 substantially enhanced, and the overestimated moderate precipitation $\frac{1}{2} - 20 \text{ mm dav}^{-1}$ is reduced, with no spurious peak at around 10 mm day⁻¹.

5.2.2 The MJO

The MJO is a crucial tropical intraseasonal variability at the that occurs on a time scale of 20–100 days (Wheeler and Kiladis, 1999). Figure 1314 presents the wavenumber and frequency spectra for the daily equatorial precipitation daily anomalies 545 from for SPCAM, NNCAM, and CAM5 in 4 four consecutive boreal winterwinters from 1999 to 2003. SPCAM shows widespread power signals over zonal number of zones 1-4 and periods between of 20-100 plusdays, as well as a peak around at zonal zone numbers of 1-3 and periods of 70-100-day days for the eastward propagation (Figure $\frac{13a}{14a}$). Similarly, infor NNCAM, there is a spectral peak at the-wavenumbers of 1-2 and periods of 50-80 days for east the eastward propagation (Figure $\frac{13b}{14b}$), exhibiting intense intraseasonal signals. -For CAM5 (Figure $\frac{13c}{14c}$), the spectral power is concentrated 550 around 30-day days and exhibits more extended periods (greater than 80 days) at a wavenumber of 1 for the eastward propagation. In addition, CAM5 also shows signals of westward propagation around with a 30-day period. Compared with CAM5, NNCAM showsexhibits stronger intraseasonal power and resembles SPCAM better. To quantify this similarity, we ealculated the coefficient coefficients of determination R^2 of for the precipitation spectrum inspectra of NNCAM and CAM5₇ using the spectrum inof SPCAM as the target value. The R^2 value of the precipitation spectrum $\frac{R^2}{100}$ in NNCAM (0.51) is much higher than that $\frac{1}{10}$ for CAM5 (0.40).

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The MJO is characterized by the eastward propagation of deep convective structures along the equator. Generally, it generally forms over the Indian Ocean, strengthens over the Pacific, and weakens inover the eastern Pacific due to interactioninteractions with cooler SSTs (Madden and Julian, 1972). Figure 1415 presents the longitude-time lag evolution offor the 10°S-10°N meridional averaged daily anomalies of the intraseasonal (filtered withusing a 20-100-day bandpass)

- precipitation and 200 hPa zonal wind (U200) in the boreal winter. The results show that both SPCAM and NNCAM reasonably 560 reproduce the eastward propagating propagation of the convection from the Indian Ocean across the Maritime Continent toand into the Pacific (Figure 14aFigures 15a and 14b), 15b). This is confirmed by both the precipitation field and U200 field. Therefore, we conclude that NNCAM captures the key MJO propagation simulated inby SPCAM. In contrast, the time lag plot offor CAM5 depicts an unpleasant westinaccurate westward propagation. Same as Similar to the precipitation spectrum, the
- 565 R^2 value of the time lag coefficient is shown to quantify the resemblance similarities between the simulations. The time lag coefficient of the U200 infield for NNCAM is much closer to that for SPCAM than CAM5, with a waymuch higher $-R^2_{\tau}$ value, indicating that the NN-Parameterization successfully emulates the convection variability of the SP-and reflects it, which is reflected in the dynamic fields.

6 Summary and Conclusions

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- 570 ThisIn this study-investigates, the potential of deep neural network-_based parameterizations in SPCAM to reproduce long-term climatology and climate variability-<u>was investigated.</u> We presentdeveloped an NN-Parameterization, via a ResDNN set, to emulate the SP with a 2D2-D CRM and its cloud scale radiation in effects in for a realistic configurated realistically configured SPCAM with a true land-ocean distribution and orography. The input variables to the NN-Parameterization include the specific humidity, temperature, largescale water vapor and temperature forcings, surface pressure, and solar
- 575 insolation. The output variables of the NN-Parameterization consist of include the subgrid tendencies of the moisture and temperature, net dry static energy and the radiation fluxes at the top of the model and surface, and solar radiation fluxes down to the surface. We proposed propose a set of 14-layer deep residual neural networks, in which each NN is in charge of one typegroup of output variable variables. With such a design, we gain thegained a best emulation accuracy for each predictor. Via a Through systematic trial-and-error searching procedure, we are were able to firstly select sets of ResDNNs that support
- 580 stable prognostic climate simulations, and then <u>choose</u>, we chose the best set with <u>the</u> lowest climate errors as the formal NN-Parameterization. Moreover, <u>athe</u> mechanism of <u>the</u> unreal perturbation amplification <u>is foundwas identified</u> in <u>the</u> GCM simulations with unstable NN-parameterizations with_Parameterizations using the spectrum diagnostic tool invented <u>inby</u> Brenowitz et al. (2020).

The offline test showstests demonstrated the greatgood skills of the NN-Parameterization in emulating the SP outputs and itsthe cloud scale radiation effects inof SPCAM. The overall diabatic heating and drying rates in the NN-Parameterization and SPCAM are in close agreement. When implemented in the host SPCAM to replace its time-consuming SP and its radiation effects, the NN-Parameterization successes insuccessfully produced an extensive stable long-term stable prognostic simulation and predictspredicted reasonable mean vertical structures in temperature and humidity, structures and the precipitation distributions. Compared with the SPCAM target simulation, NNCAM still produces some biases in the mean fields, such as a warmer troposphere over the polar regions and in the tropopause and underestimation of strong precipitation underestimation in the equatorial regions. On the other handIn addition, the better climate variability inof SPCAM overcompared to CAM5 is wellwas learned well by our NN-Parameterization and was reproduced inby NNCAM, with better frequency infor extreme rainfall, and a similar MJO spectrum and, propagation direction, and speed. Although withDespite the current biases in the climate states so far, NNCAM can still be regarded as thea first attempt to prognostically-couple a NN-based parameterization in realistic configurated 3Dand a realistically configured 3-D GCM.

Many previous studies have well-studied machine learninginvestigated ML parameterizations implemented in aquaplanet configurated 3D GCM.configured 3-D GCMs. Some faced instability problems in coupled simulations (Brenowitz and Bretherton, 2019), while someothers succeeded in producing stable long-term stable prognostic simulations with deep fullyconnected neural networks (Rasp et al., 2018; Yuval et al., 2021)), as well as random forest algorithms (Yuval and O'Gorman, 2020). In contrast to aqua-planet simulations, the spatial heterogeneity is prominent over the land in GCMs, which are configurated with configured using real-geography geographic boundary conditions. In this case, a plain fully connected neural networks the SP output (Mooers et al., 2021). The convection, clouds, and interactions with the interacted radiation of in the CRM together with and the real-geography geographic boundary conditions are without a doubt far more complicated than in idealized models. To meet the new demand underfor realistic configuration configurations, we design designed a ResDNN with

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sufficient depth to further improve the nonlinear fitting ability of the NN-Parameterization. With the skip connections, the 7layer DNN models can be extended to 14 layers, therefore, significant thereby significantly improving the offline accuracy. In the prognostic tests, a fewdozen ResDNN--parameterizations can support supported a stable long-term stable-run, while all of the DNN-parameterizations are so fartested were found to be unstable.

Trial-and-error is still theour only way to find stable NN-based parameterizations. SoThus far, we have not come up withdeveloped an a priori mothed method that guaranteed guarantees stability. However, we dodid find some clues in the 610 sensitivity tests. We believe sufficient offline accuracy is essential for online stability and can be achieved by confirming all of the inaccurate NN-parameterizations -- Parameterizations as unstable. On the other handIn addition, some of the highly accurate ones still crash the prognostic simulation, where we find rapid increasing. In this case, the total energy, was found to increase rapidly. This mechanism is that unstable NNs cannot damp the neural network emulation errors-but, and they amplify 615 and propagate them to the entire system through gravity waves.

The prognostic biases inof the mean fields in are speculated as to be a result of by the combined effect of the emulation errors of all of the NN-Parameterization prediction fields. Further study is required. Still, it earmay be related to the spatially non-uniform accuracy of the NN-Parameterization, such as the relatively low fitting accuracy in the tropical deep convective regions and the shallow subtropical convection and stratiform cloud regions. Such problems have also been reported in previous studies (Gentine et al., 2018; Mooers et al., 2021). We believe that an NN-parameterization-Parameterization with 620 heterogeneous characteristics across different regions, rather than a globally uniform scheme, can further improve the fitting accuracy in thisthese tropical and subtropical regionregions.

Embedding deep neural networks into Fortran-based atmospheric models is still a handicap. Before this study, researchers mainly used hard coding to build neural networks (Rasp et al., 2018; Brenowitz and Bretherton, 2019). An easier waymethod 625 is to use Fortran--based neural network libraries that can flexibly import network parameters (Ott et al., 2020). These methods have been used to successfully implemented NN implement NNs in GCMGCMs, but they can only support dense, layer-based NNNs. As a result, developers cannot take advantage of the most advanced neural network structures, such as convolution, shortcut, self-attention, and variational autoencoder, etc., structures, to build powerful DNN-ML-based Parameterizations. Just this research, throughstudy, using an NN-GCM Coupler, the NN-

Parameterization eancould support the mainstream GPU-enabled machine learningML frameworks. Thanks to the simple and 630 effective implementation of the DNNNN-GCM Coupler our NNCAM achieves achieved an SYPD 30 times SYPD compared to that of SPCAM by using a ResDNN set in and NN-Parameterization, although even though these DNNs are much deeper than the previous state-of-the-art fully- connected NNs in this field.

635 Code and data availability. The original training and testing data can be accessed at https://doi.org/10.5281/zenodo.5625616. The source codes of SPCAM version 2 and NNCAM have been archived, and made publicly available for downloading from https://doi.org/10.5281/zenodo.5596273.

Competing interests. The authors declare no conflict of interest.

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- 765 **Table 1**. Input and output variables. For the inputs, $q_v(z)$ is the vertical water vapor profile. T(z) is the temperature profile. $dq_{v\,l.s.}(z)$ and $dT_{l.s.}$ are the large scale forcings of the water vapor and temperature, respectively. P_s is the surface pressure; and *Solin* is the TOA solar insolation. For the outputs, $dq_v(z)$ and ds(z) are the tendencies of the water vapor and dry static energy due to moist physics and radiative processes calculated using the NN-Parameterization. The net longwave and shortwave fluxes at the surface and the TOA are the surface net longwave flux (FLNS), surface net shortwave flux (FLNT),
- 770 TOA net longwave flux (FLNT), and TOA net shortwave fluxes (FSNT). The four downwelling shortwave solar radiation fluxes are the solar downward visible direct to surface (SOLS), solar downward near infrared direct to surface (SOLL), solar downward visible diffuse to surface (SOLSD), and solar downward near infrared diffuse to surface (SOLLD) fluxes reaching the surface.

Inputs	Outputs
$q_{v}(z), T(z), dq_{vls}(z), dT_{ls}(z), P_{s}, Solin$	$dq_{\nu}(z)$, $ds(z)$, FLNS, FSNS, FLNT, FSNT, SOLS, SOLL,
	SOLSD, SOLLD

Figures 1 – 15



Figure 1. Schematic diagram of the structure of the ResDNN. It consists of seven residual blocks, each of which (dashed box)
contains two 512 node-wide dense (fully connected) layers with an ReLU as the activation and a layer jump. The inputs and outputs are discussed in Section 2.2.2.



Figure 2. Fitting accuracies (R^2) of both the proposed ResDNN (solid orange lines) and the DNN (dashed blue lines) for different outputs. (a) The R² of the moist static energy changing rate (dh) versus the training epochs; and (b) the fitting accuracy of the average R^2 for the eight radiation fluxes. Note: the R^2 values are calculated for both space and time in the validation dataset.



Figure 3. A flow chart of NNCAM, including the NN-GCM coupler. NNCAM runs in the direction of the arrow, and each box represents a module. Among them, the NN-GCM coupler is indicated by the pink box. The NN-Parameterization is shown in the box on the right. ① The dynamic core transmits data to the NN-GCM coupler; ② and ③ the data communication between the NN-GCM coupler and the NN-Parameterization; and ④ the host GCM accepts the results from the NN-Parameterization.



Figure 4. The mean square error of the offline moist static energy vs. the prognostic steps. The black inverted triangles (10 in total but some overlap due to their close MSE_h values) denote stable NN coupled prognostic simulations that last for more than 10 years. The blue dots denote unstable simulations, and the blue triangles denote unstable DNNs. The dots with colored outlines are shown in Figure 5 for the time evolution of the globally averaged energy.



Figure 5. Time evolution of the globally averaged column of the integral total energy of NNCAM with different ResDNNparameterizations (marked with the same colors as in Figure 4), SPCAM target (black line), and CAM5 control run (grey dashed line). The blue line indicates the stable and accurate ResDNN, the green line indicates the stable but deviating ResDNN, and the orange and red lines indicate unstable ResDNNs.



Figure 6. Latitude-pressure cross sections of the annual and zonal mean heating (top) and moistening (bottom) due to moist physics during the year 2000 for (a, c) SPCAM simulations, and (b, d) the offline test using the NN-Parameterizations.



Figure 7. Latitude-pressure cross sections of the coefficient of determination (R^2) for the zonally averaged heating (left panels) and moistening (right panels) predicted using (a & b) the NN-Parameterization in the offline one-year SPCAM run, and (c & d) the offline CAM5 parameterizations. Both were evaluated at a 30-min time step interval. Note: the areas where R^2 is greater than 0.7 are contoured in pink, and the areas where R^2 is greater than 0.9 are contoured in orange.



825 **Figure 8.** Latitude-pressure cross sections of the coefficient of determination (R^2) for the time sequence at each location for (a) the derived precipitation predicted using the NN-Parameterization and (b) the total precipitation from the CAM5 parameterization compared to the offline one-year SPCAM run. The predictions and SPCAM targets are for a 30 min time step interval. Note: the areas where R^2 is greater than 0.7 are contoured in pink, and the areas where R^2 is greater than 0.9 are contoured in orange.



Figure 9. Latitude-pressure cross sections of the zonal mean temperature (left panels) and specific humidity (right panels) averaged from 1999 to 2003 predicted using (a, b) SPCAM, (c, d) NNCAM, and (e, f) CAM5.



Figure 10. Latitude-pressure cross-section of the zonal and annual mean differences in the temperature (left panels) and specific humidity (right panels) between (a & c) NNCAM and SPCAM and (b & d) CAM5 and SPCAM. The simulation period for all of the models was from 1999 to 2003.



Figure 11. The mean precipitation rate (mm day⁻¹) averaged from 1999 to 2003 for June-July-August (left panels) and December-January-February (right panels) predicted using (a, b) SPCAM, (c, d) NNCAM, and (e, f) CAM5.



Figure 12. The zonal mean precipitation rate (mm/day) averaged from 1999 to 2003 for (a, d) the annual mean, (b, e) June-July-August, and (c, f) December-January-February. The black, blue, and red solid lines denote SPCAM, NNCAM, and CAM5, respectively. The dark green dashed line denotes the averaged results of the TRMM 3B42 daily rainfall product.



Figure 13. Probability densities of the daily mean precipitation in the tropics (30°S–30°N) obtained from the three model simulations. The black, blue, and red solid lines denote SPCAM, NNCAM, and CAM5, respectively.



Figure 14. The wavenumber-frequency spectra for the daily precipitation anomalies at 10°S–10°N for (a, b) SPCAM, (c, d) NNCAM, and (e, f) CAM5 simulations in boreal winter.

