

1 **Single-Column Emulation of Reanalysis of the**
2 **Northeast Pacific Marine Boundary Layer**

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5 **Key Points:**

- 6 • A new machine learning boundary layer parameterization, MARBLE, is developed
7 from ERA5 reanalysis data for the summertime Northeast Pacific.
- 8 • Used in a single-column model, MARBLE reproduces ERA5 thermodynamic struc-
9 ture and cloud properties over 7-day simulation periods.
- 10 • MARBLE reproduces the regional climatology of the stratocumulus to cumulus
11 transition.

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Abstract

An artificial neural network is trained to reproduce thermodynamic tendencies and boundary layer properties from ERA5 Hires reanalysis data over the summertime Northeast Pacific stratocumulus to trade cumulus transition region. The network is trained prognostically using 7-day forecasts rather than using diagnosed instantaneous tendencies alone. The resulting model, Machine Assisted Reanalysis Boundary Layer Emulation (MARBLE), skillfully reproduces the boundary layer structure and cloud properties of the reanalysis data in 7-day single-column prognostic simulations over withheld testing periods. Radiative heating profiles are well-simulated, and the mean climatology and variability of the stratocumulus to cumulus transition are accurately reproduced. MARBLE more closely tracks the reanalysis than does a comparable configuration of the underlying forecast model.

1 Introduction

Stratocumulus clouds cover over one-fifth of Earth's surface in the annual mean (Warren et al., 1986). These clouds strongly reflect incoming shortwave radiation and have little effect on outgoing longwave radiation, resulting in a strong cooling radiative effect on Earth's energy balance (Chen et al., 2000; Wood, 2012). Small changes in stratocumulus cover and thickness are sufficient to produce radiative effects comparable to the effects associated with increasing greenhouse gases (Slingo, 1990). Thus, climate model behavior in subtropical stratocumulus to cumulus transition regions such as the Northeast Pacific is critical in representing Earth's energy balance and cloud feedbacks on climate.

Significant biases and challenges persist in the representation of stratocumulus clouds in climate models (e.g. Hannay et al. (2009), Medeiros et al. (2012), Lin et al. (2014), Dal Gesso et al. (2015)). Traditional parameterizations have difficulty representing stratocumulus and their transition to cumulus, because the stratocumulus layer is thin, capped by a sharp inversion, and maintained by turbulent eddies unresolved at the grid scale of climate models. These eddies are strongly influenced by the clouds and their radiative effects, and may have a complex vertical structure. Turbulent entrainment through the sharp inversion is particularly important but subject to numerical errors as well as representational uncertainties.

43 The complexity of this problem and the relatively slow improvement of climate model
44 simulations of these cloudy boundary layers suggests the exploration of radically differ-
45 ent parameterization approaches, such as ‘ultraparameterization’ (Parishani et al., 2017)
46 or the use of machine learning to holistically represent the combined effect of all of the
47 interacting processes, the approach explored here.

48 Here we use machine learning to emulate reanalysis. Using reanalysis allows our
49 model to learn not only from the conventional parameterization used in the global fore-
50 cast model, but also from the observational update or ‘analysis increment’ applied in the
51 data assimilation cycle. This update provides a natural bias correction to the conven-
52 tional model, which can improve performance compared to the parameterization suite
53 of the forecast model used to create the reanalysis. In this study, we focus on the sum-
54 mertime Northeast Pacific, a particularly well-studied subtropical transition region (e.g.
55 Stevens et al. (2003); Zhou et al. (2015); Albrecht et al. (2019)) with large horizontal gra-
56 dients of sea-surface temperature (SST) and climatological low cloud cover. To speed
57 up training, we limit the domain size and the scope of the network to be able to suffi-
58 ciently sample the variability with a dataset that fits in the 4GB of memory available
59 on our GPU. However, there is no fundamental reason the same approach could not be
60 applied globally using computational resources sufficient to process the larger volume
61 of data, for example by using multiple GPUs training in parallel.

62 We use an artificial neural network (ANN) to predict the lower-tropospheric heat-
63 ing and moistening tendencies in each model grid column. An ANN is a nonlinear ma-
64 chine learning model trained by iteratively modifying a large number of model weights
65 to optimize a loss function. ANNs have been used successfully to emulate radiation in
66 a prognostic setting (Krasnopolsky et al., 2005) and to diagnose cloud fraction and pre-
67 cipitation (Krasnopolsky et al., 2013). More recently they have been used to represent
68 convection in a prognostic setting, using deep networks on superparameterization model
69 data (Rasp et al., 2018) and a novel approach to prognostic model training on near-global
70 cloud-resolving model data (Brenowitz & Bretherton, 2018).

71 We begin by discussing the reanalysis dataset (Section 2) and outline the MAR-
72 BLE model (Section 3). This is followed by an evaluation of MARBLE’s performance
73 over the Northeast Pacific (Section 4). Finally, we summarize key strengths of MARBLE

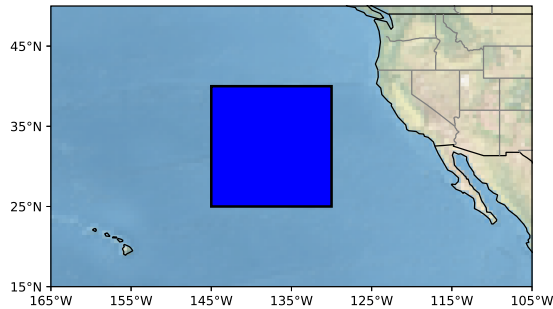


Figure 1. Study region used for model training and evaluation. The blue square indicates the region of study.

74 and discuss future extensions of this data-driven machine-learning parameterization ap-
 75 proach (Section 5).

76 **2 Dataset**

77 The European Center for Medium-Range Weather Forecasts (ECMWF) Reanal-
 78 ysis 5th Generation (ERA5) is a global reanalysis dataset, documented at [https://confluence.](https://confluence.ecmwf.int/display/CKB/ERA5+data+documentation)
 79 [ecmwf.int/display/CKB/ERA5+data+documentation](https://confluence.ecmwf.int/display/CKB/ERA5+data+documentation). In this study we use the high-
 80 resolution realization (HRES) run at 31km horizontal resolution, which provides hourly
 81 data on 31 model levels in the vertical domain we are modeling (from the surface to 3km).
 82 Our study uses reanalysis data for June-August 2008-2016 over the Northeast Pacific on
 83 a 0.5° grid from 230°W - 215°W and 25°N - 40°N , as shown in Figure 1.

84 MARBLE is trained and evaluated on hourly values in June, July, and August. For
 85 state quantities such as temperature, surface pressure, vertical wind, humidity, or mix-
 86 ing ratios, instantaneous values are used. For flux quantities such as surface precipita-
 87 tion or radiative fluxes, hourly mean values are used. Data from 2008 through 2014 are
 88 used for training, and validation is performed on 2015 data to determine a reasonable
 89 model configuration. Data from 2016 are used for evaluation once all model configura-
 90 tion has been determined, including number of neurons, depth of network, choice of ac-
 91 tivation function, etc.

3 Model Description

Following most conventional climate model parameterizations, we use a vertically nonlocal column-oriented approach. The diabatic heating and moistening tendencies at each height within a grid column are functions of conditions throughout that grid column, but not other grid columns. Other boundary conditions at the surface or top of our simulated tropospheric layer, e. g. surface fluxes of sensible and latent heat, are allowed to affect the entire vertical column in a single time step, reflecting possible rapid vertical transport in turbulent eddies.

We apply the multi-timestep training approach used by Brenowitz and Bretherton (2018) to vertically-resolved reanalysis data over the Northeast Pacific. This training approach generates a numerically stable and accurate model, whereas a model trained on tendencies at each timestep is numerically unstable. We call this approach Machine-Assisted Reanalysis Boundary Layer Emulation (MARBLE). MARBLE replaces all sub-grid and radiative heating parameterizations and resolved vertical advection within its domain. For simplicity, our implementation does not yet predict momentum tendencies.

3.1 Dimensionality Reduction

Rather than use the full resolution vertical profile of the ERA5 product, we reduce the dimensionality of the data using principal components on a constant height grid. Like the choice of a limited horizontal region, this is done to reduce the memory footprint of the training dataset. First, the ERA5 profiles are interpolated to an evenly spaced height grid of 20 points from the lowest model level to a height of 3km. The mean vertical profiles based on the training data (Figure S1) are removed. The time-height perturbations of each variable are separately decomposed into principal components. We keep enough components to explain 99% of the variability of the training data – 10 components for liquid water static energy (s_l) and total water mixing ratio (r_t) and 5 for vertical wind (Figure S2).

Tendencies are decomposed using the principal components of their respective prognostic variable (for example, clear-sky radiative heating rates are decomposed using the basis for s_l). All vertically-resolved quantities are input and output as principal components. All inputs and outputs are additionally normalized so that their values in the training dataset have a mean of 0 and variance of 1. After training, computed outputs

123 are re-scaled and transformed back to a constant height grid for plotting and error eval-
 124 uation.

125 **3.2 Neural Network Design**

126 The core of MARBLE is a feed-forward neural network for supervised learning. The
 127 loss functions being iteratively minimized during training are weighted sums of mean squared
 128 errors of the model outputs, as described below. They do not include any regularization
 129 terms, as L1 and L2 regularization were found not to significantly affect model gener-
 130 alization.

131 MARBLE is trained while integrating forward 7 days with a one-hour forward Eu-
 132 ler timestep, as shown in Figure 2. Training with a significantly shorter period of 2 days
 133 was found to produce a model that is numerically unstable within a few days, whereas
 134 after training over periods of 7 days we did not observe instability in the model even af-
 135 ter a month-long forecast. Figure 2b shows the internal structure of the neural network,
 136 which has three layers and uses the rectifier linear activation function (ReLU), defined as

$$137 \quad \text{ReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} \quad (1)$$

138 The input, internal, and output layers contain 33, 128, and 51 neurons, respectively.
 139 Figure 2a shows in detail how the neural network is used to compute the next model state
 140 in the course of training. The components are color coded to show their role in model
 141 training. Input forcings from the ERA5 dataset include surface latent and sensible heat
 142 flux, sea surface temperature, surface pressure, mid and high cloud fractions, downwelling
 143 shortwave fluxes at top-of-atmosphere and top-of-domain, top-of-domain rainwater mix-
 144 ing ratio, and the vertical structure of vertical wind decomposed into its principal com-
 145 ponents. The input to the network also includes the principal components of s_l and r_t
 146 output from the previous timestep, which on the first timestep are taken from the ERA5
 147 dataset. These inputs include all relevant top and bottom-of-domain forcings.

148 The neural network produces a set of diagnostic outputs, a clear-sky radiative heat-
 149 ing rate which is optimized to match its ERA5 counterpart, and unconstrained "resid-
 150 ual" tendencies for s_l and r_t . This includes effects of surface fluxes, analysis increments,
 151 cloud radiative effects, and turbulence. At the inversion, there is usually substantial com-

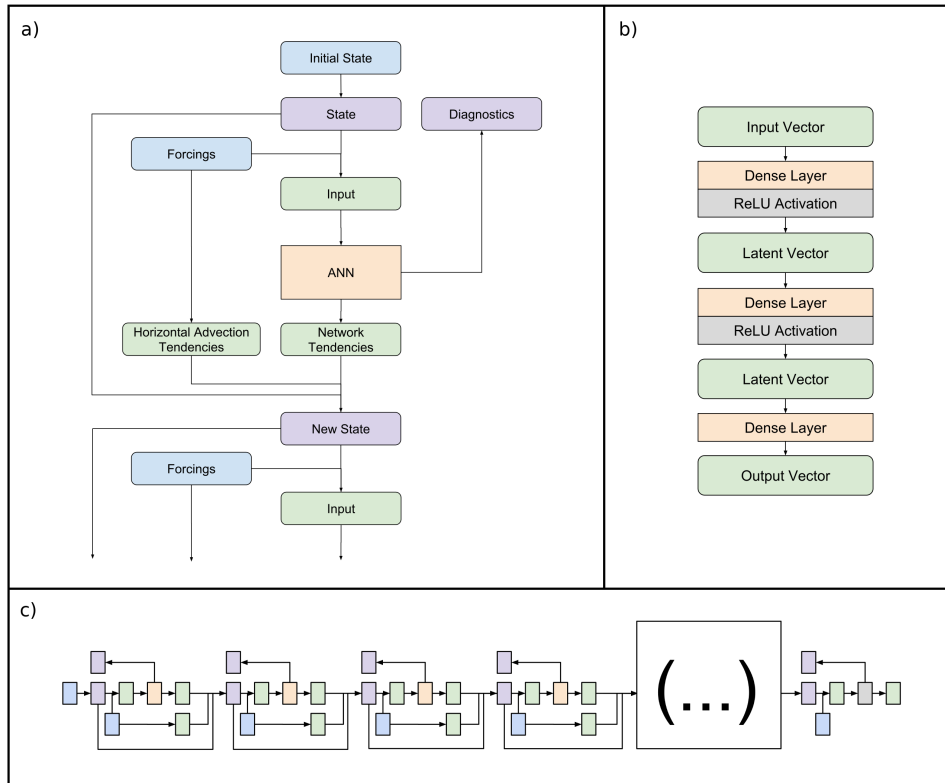


Figure 2. Artificial neural network structure and training approach, showing a) how components are connected in the first timestep, b) the internal structure of the ANN component, and c) how those components are chained together to train over multiple timesteps. Orange represents operations with trainable weights, grey represents static operations without trainable weights, purple represents output vectors whose values are included in the optimized loss function, green represents internal vectors used by the model, and blue represents data collected from ERA5 used as input to the model. At each timestep in c) the ANN uses the same weights. Network tendencies include both clear-sky radiative heating and residual tendencies.

152 compensation between vertical advection (which is imperfectly represented by the reduced-
 153 dimension basis used by MARBLE) and entrainment contributions to the residual ten-
 154 dency. Hence, we also fold vertical advection into the residual tendency.

155 These tendencies, together with clear-sky radiative heating and ERA5-derived hor-
 156 izontal advection of heat and moisture by the mean wind, are then added to the previ-
 157 ous model state, producing a state at the next time step. The residual tendencies are
 158 not optimized to directly match any value in the ERA5 dataset. However, the model *is*
 159 optimized to produce thermodynamic states that match the states in ERA5, and the only
 160 way it can do this is by learning the correct form of tendency to add to the model state.

161 Figure 2c shows the full structure of the system being optimized. While not pic-
 162 tured, a total of 168 time units are used to step the model state forward a total of 7 days
 163 in 1-hour increments. In training, the system is considered as a single neural network
 164 whose optimized output includes diagnostic values and model state at every timestep (in-
 165 dicated by purple boxes).

166 The full equations for the tendencies at each timestep can be written as:

$$\begin{aligned}
 \frac{ds_l}{dt} &= \frac{ds_l}{dt}_{hadv} + \mathbf{W}_{sl} \cdot ReL(\mathbf{W}_2 \cdot ReL(\mathbf{W}_3 \cdot \vec{x}_{in} + \vec{b}_3) + \vec{b}_2) + \vec{b}_{sl} \\
 \frac{dr_t}{dt} &= \frac{dr_t}{dt}_{hadv} + \mathbf{W}_{rt} \cdot ReL(\mathbf{W}_2 \cdot ReL(\mathbf{W}_3 \cdot \vec{x}_{in} + \vec{b}_3) + \vec{b}_2) + \vec{b}_{rt}
 \end{aligned} \quad (2)$$

169 where the subscript 'hadv' denotes a prescribed horizontal advective tendency, \vec{x}_{in} is
 170 a vector containing the normalized inputs, \mathbf{W} represents trained weight matrices, and
 171 \vec{b} represents trained bias vectors. *ReL* is the rectified linear activation function as de-
 172 fined in Equation 1.

173 \vec{x}_{in} includes all inputs to the neural network as previously described in this sec-
 174 tion, concatenated into one vector. Horizontal advective fluxes are intentionally not in-
 175 cluded in \vec{x}_{in} to avoid the model learning the inversion height from the vertical struc-
 176 ture of the ERA5 advective forcings, an approach that might go wrong in a three-dimensional
 177 simulation.

178 Using normalized outputs, the loss function being minimized is

$$\begin{aligned}
 E &= \frac{1}{N_s N_t} \sum_{sample} \sum_{timestep} \left(\frac{1}{z_t} \int_{z=0}^{z=z_t} \left(\frac{1}{4} [(s_l^m - s_l^a)^2 + r_t^m - r_t^a]^2 \right) \right. \\
 &\quad + \frac{1}{14} [(r_c^m - r_c^a)^2 + (r_r^m - r_r^a)^2 + (C^m - C^a)^2 + (R_{cs}^m - R_{cs}^a)^2] dz \\
 &\quad \left. + \frac{1}{14} [(C_{lo}^m - C_{lo}^a)^2 + (P_s^m - P_s^a)^2 + (\mathcal{L}^m - \mathcal{L}^a)^2] \right)
 \end{aligned} \quad (3)$$

182 where subscript m and a refer to model and actual values respectively, N_t is num-
 183 ber of timesteps, N_s is the number of training samples, and z_t is the height of the model
 184 domain. The remaining terms represent model outputs, as listed in the following section
 185 in Table 4.2. The weighting in the loss function is defined such that half of the weight
 186 is evenly distributed between the two prognostic terms, and the other half between di-
 187 agnostic outputs.

188 Within MARBLE, r_t and s_l are prognostic. All other outputs are purely diagnos-
 189 tic and are determined directly from r_t , s_l , and model inputs. Because these diagnos-
 190 tic outputs are trained over the course of many timesteps in MARBLE, they can be ac-
 191 curately diagnosed from the kind of model state that MARBLE produces. In contrast,
 192 were we to train a diagnostic model using only ERA5 data as input, the model might
 193 perform poorly if MARBLE drifts away from ERA5-like states. We found that training
 194 a neural network to diagnose clear-sky radiative heating directly on ERA5 often produced
 195 unphysically high radiative heating rates when run prognostically in MARBLE, even at
 196 night.

197 Training was done using the AMSGrad variant (Reddi et al., 2018) of the Adam
 198 optimizer (Kingma & Ba, 2015) implementation in Keras, with a learning rate of 0.002
 199 and training batches of 4096 7-day single-column samples, initialized every 5 days. The
 200 ANN was trained for 500 epochs.

201 4 Evaluation

202 To evaluate the model, we integrate the state forward 7 days in a single-column mode
 203 using the specified ERA5 forcings for each given testing location, initialized every 5 days.
 204 We compare with the corresponding ERA5 state and a baseline forecast, both projected
 205 onto the same reduced basis.

206 4.1 Baseline Model

207 The fidelity of the ERA5 reanalysis relies heavily on the skill of the underlying ECMWF
 208 forecast model. Thus, a suitable single-column-like configuration of that forecast model
 209 provides a baseline for assessing whether any skill is added by MARBLE.

210 To this end, we used the first 12 hours of the short-term ECMWF forecasts avail-
 211 able as part of ERA5. To make a 7 day 'baseline' forecast in any grid column, we ac-

212 cumulate the tendencies of s_l and r_t from 14 successive 12-hour forecasts, but not the
 213 differences between each 12 hour forecast and the initialization of the next forecast (which
 214 we interpret as approximating the analysis increments). This baseline is not useful for
 215 clouds and precipitation, which MARBLE treats as diagnostic variables.

216 Each time step we also re-project onto the 20-point evenly spaced vertical grid and
 217 perform physical adjustments, setting negative values of r_t to zero and mixing any su-
 218 peradiabatic lapse rates to the dry adiabat, before projecting back into principal com-
 219 ponents. When performing dry adiabatic adjustment we neglect differences in layer mass
 220 for simplicity. This process of projection and adjustment increases baseline model squared
 221 correlation coefficients (R^2) of s_l and r_t against vertical profiles from the testing data
 222 by about 4% in the latter half of 7-day simulations.

223 Since the advective forcings from the short-range forecasts are almost identical to
 224 those in the ERA5 analysis, this baseline provides an analogue to the ECMWF model
 225 performance in single-column mode forced similarly to MARBLE. The most obvious way
 226 MARBLE can improve on the skill of this baseline is by learning the analysis increments.

227 4.2 Results

228 It is illuminating to inspect one such single column model run. We selected a sim-
 229 ulation from the testing data at random for this purpose (Figure 3).

230 MARBLE does a remarkably good job of reproducing the evolution of ERA5 bound-
 231 ary structure and cloud properties in this 7-day period. In contrast to the baseline sim-
 232 ulation, there is remarkably little apparent degradation of the forecast with time. We
 233 attribute this to the strong control of the boundary-layer depth and evolution by the ver-
 234 tical motion and horizontal advective forcings, a form of 'slow-manifold' behavior (Bretherton
 235 et al., 2010). Directly comparing the residual tendency produced by the ANN with its
 236 ERA5 counterpart, we see that MARBLE not only does very well at the inversion where
 237 tendencies are strongest, but also reproduces features in the tendency profile within the
 238 boundary layer and free troposphere. Inter-forecast tendencies produced every 12 hours
 239 in the analysis dataset are smoothed over longer periods in MARBLE. The clear-sky ra-
 240 diative heating profiles closely match the diurnal cycle of radiative heating and the im-
 241 pact of vertical thermodynamic structure on radiative heating rates seen in the ERA5
 242 heating profiles.

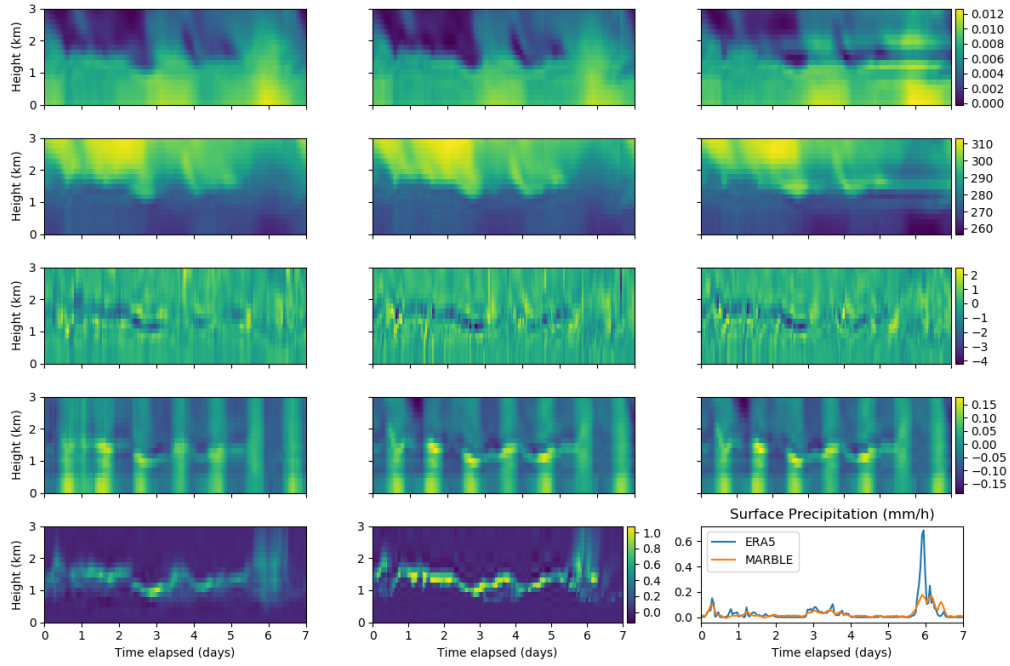


Figure 3. Randomly selected seven-day single-column prognostic simulation timeseries forced using withheld testing data, with comparison to ERA5 and baseline model. Initialized at 7:00 UTC on June 11, 2016 at 30°N, 133.5°W. Residual s_l and r_t tendencies have been modified by subtracting vertical advective tendencies diagnosed by centered differencing, leaving only the diabatic contributions.

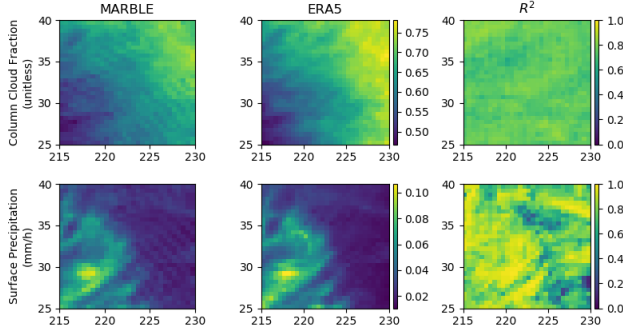


Figure 4. Horizontally-resolved mean values and correlation coefficients of key quantities, averaged across the last 3.5 days of 7-day simulations for the 2016 Northeast Pacific.

243 Some values can be unphysically negative, such as cloud fraction and mixing ratios.
 244 This is due in part to the use of principal components, where the projection of the
 245 real profiles onto their components can give negative values even in the training data.
 246 For the diagnostic outputs, this can be rectified by limiting the values. For total water
 247 mixing ratio, limiting may have unforeseen negative effects since it is not active during
 248 model training.

249 Having seen an example timeseries, we statistically evaluate MARBLE’s overall per-
 250 formance averaged over all NE Pacific locations and initialization times in the testing
 251 dataset. For this evaluation we use the second half of these simulations (Days 3.5-7) to
 252 avoid inheriting skill from the initial state. When we inspect model skill as a function
 253 of simulation timestep, we see the skill for s_t and r_t deteriorates gradually and levels off
 254 by 3.5 days (Figure S3).

255 MARBLE does very well at representing the thermodynamic structure and cloud
 256 properties of ERA5 over this region during the second half of the 7-day single-column
 257 forecasts, outperforming the baseline by a considerable margin. Despite its reduced ver-
 258 tical resolution, MARBLE has learned to improve upon the parameterized heating and
 259 moistening tendencies of the baseline ECMWF forecast model. The bias, root mean squared
 260 error, and fraction of explained variance for several quantities are listed in Table 1. As
 261 was seen in Figure 3, the largest errors are seen in vertically-resolved cloud fraction, which
 262 still shows good performance.

Table 1. MARBLE performance for 2016 Northeast Pacific. Simulations described in Section 4. Evaluation is performed over the last 3.5 days of each 7-day simulation. The training mean at each height is subtracted before calculating the squared correlation coefficient R^2 . Baseline values are computed from the baseline model described in Section 4.1. Liquid water static energy is normalized by the heat capacity of dry air at constant pressure.

Quantity	Mean Bias	RMSE	R^2	Baseline R^2
liquid water static energy (s_l/C_{pd})	-0.05 K	2.8 K	0.90	0.73
total water mixing ratio (r_t)	0.065 g/kg	0.9 g/kg	0.90	0.74
clear-sky radiative heating rate (R_{cs})	0.01 K/hr	0.04 K/hr	0.73	
vertically-resolved cloud fraction (C)	-0.0030	0.12	0.69	N/A
cloud water mixing ratio (r_c)	-1.3e-3 g/kg	3.4e-2 g/kg	0.65	N/A
rain water mixing ratio (r_{rain})	7.0e-5 g/kg	2.4e-3 g/kg	0.96	N/A
column low cloud fraction (C_{low})	-0.033	0.18	0.77	N/A
surface precipitation (P_s)	9.8e-3 mm/h	8.5e-2 mm/h	0.86	N/A
column cloud water (\mathcal{L})	-0.0046 kg/m ²	0.026 kg/m ²	0.85	N/A

263 The horizontally-resolved mean 'climate' for JJA 2016 is shown in Figure 4. De-
 264 spite not receiving any information about the spatial location of each sample other than
 265 sea surface temperature, MARBLE skillfully represents ERA5's stratocumulus to cumu-
 266 lus transition. There do exist small wave-like artifacts in the machine learning output,
 267 which would likely be smoothed if the columns could communicate in the horizontal. The
 268 third column in Figure 4 shows that the model does a good job of reproducing the vari-
 269 ability of ERA5 throughout the domain.

270 MARBLE also reproduces ERA5's mean diurnal variability of low cloud fraction
 271 and precipitation across the NE Pacific (Figure S4). It produces both a thickening of low
 272 cloud and increase in precipitation during the night, with thinner cloud and lower pre-
 273 cipitation during the day when cloud-top shortwave heating reduces turbulent mixing
 274 from cloud-top longwave cooling in this region.

275 5 Conclusions

276 We have shown that an ANN trained over many timesteps as in Brenowitz and Brether-
 277 ton (2018) does a remarkably good job of matching the thermodynamic evolution and
 278 boundary layer properties of the ERA5 reanalysis dataset over the summertime North-
 279 east Pacific in a single column model. We have created a machine learning model, MAR-
 280 BLE, that learns not only to reproduce the effects of the physical parameterizations in
 281 the underlying weather forecast model, but also to add the systematic impacts of anal-
 282 ysis increments from data assimilation on the reanalysis. This serves as a natural form
 283 of model bias correction. In this study, MARBLE was trained and applied to a partic-
 284 ular region and season. We have also successfully trained a version of MARBLE for sum-
 285 mertime boundary layer parameterization over the southern U. S. Great Plains, and it
 286 is being tested as the lower tropospheric diabatic process parameterization for regional
 287 boundary-forced three-dimensional simulations with a mesoscale model. If this proves
 288 successful, we will try to generalize MARBLE to work globally.

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 296 may be accessed at <http://atmos.washington.edu/~mcgibbon/mb19/>.

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