Data-driven emulation of Modal Aerosol Microphysics via Neural Operator-Based Modeling

Zhe Bai and Damian Rouson

Lawrence Berkeley National Lab, Berkeley, CA 98195, United States
*zhebai@lbl.gov, rouson@lbl.gov

Supplementary information

Table S.1 lists the atmospheric parameters and aerosol variables used as the input physical variables of the surrogate models quantifying the modal aerosol microphysics process.

i_T	air temperature (K) input to aerosol microphysics
i_{pmid}	pressure input (Pa) to aerosol microphysics
i_{pdel}	pressure layer thickness (Pa) input to aerosol microphysics
i_{zm}	geopotential height (m) input aerosol microphysics
i_{pblh}	PBL height (m) input to aerosol microphysics
i_{qh2o}	specific humidity (kg/kg) input to aerosol microphysics
$i_{[a1,a2,a3,a4]\_dgnum}$	Mode $[a1,a2,a3,a4]$ dry diameter (m)
$i_{[a1,a2,a3,a4]\_dgnumwet}$	Mode $[a1,a2,a3,a4]$ wet diameter (m)
$i_{[a1,a2,a3,a4]\_wetdens}$	Mode $[a1,a2,a3,a4]$ wet density (kg/m^3)
$i_{vmr_{H_2SO_4}\,preAerMic}$	H_2SO_4 VMR ($mol/mol\text{-}air$) before aerosol microphysics
$i_{vmr_{SOAG}\,preAerMic}$	$SOAG$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{bc}\,[a1,a4]\,preAerMic}$	$bc_{[a1,a4]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{mom}\,[a1,a2,a4]\,preAerMic}$	$mom_{[a1,a2,a4]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{ncl}\,[a1,a2]\,preAerMic}$	$ncl_{[a1,a2]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{num}\,[a1,a2,a4]\,preAerMic}$	$num_{[a1,a2,a4]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{pom}\,[a1,a4]\,preAerMic}$	$pom_{[a1,a4]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{so_4}\,[a1,a2,a3]\,preAerMic}$	$so_{4\,[a1,a2,a3]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{soa}\,[a1,a2,a3]\,preAerMic}$	$soa_{[a1,a2,a3]}$ VMR ($mol/mol\text{-}air$)
$i_{vmr_{H_2SO_4}\,preGsChem}$	H_2SO_4 VMR ($mol/mol\text{-}air$) before gas-phase chemistry

Table S.1. Atmospheric parameters and input aerosol variables used as input to the surrogate models.

Figure S.1 compares relative $\mathscr{L}_1$ error of the performance of the four surrogate models in predicting the VMR tendency of aerosol mode variables. ADON and ADON-PCA show improved accuracy, and ADON-PCA has the best prediction performance for 16 out of 20 variable.

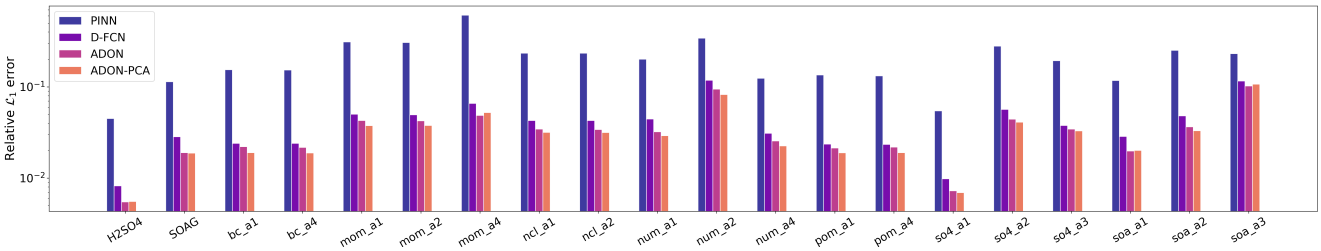

Figure S.1. Relative $\mathscr{L}_1$ error for the predictions of all aerosol mode variables using four surrogate models: PINN, D-FCN, ADON and ADON-PCA. ADON and its variant ADON-PCA show more accurate predictions with respect to the E3SM results among the surrogate models.

Figure S.2 illustrates the global view of VMR tendency of the number concentration of accumulation-mode aerosol particles from upper to lower atmosphere as a key component of the atmospheric aerosol population.

The global view of VMR tendency of the mass concentration of accumulation-mode black carbon and sulfate aerosol particles in the model layer closest to the earth surface is presented in Figure S.3.

Figure S.4 shows the global view of the number concentration of accumulation mode aerosol particles of the ML emulation result using the trained ADON-PCA model versus the E3SM simulation for the Aitken mode aerosol particle concentrations Δnum_a2, where distinct discrepancy is observed in the middle troposphere layer.

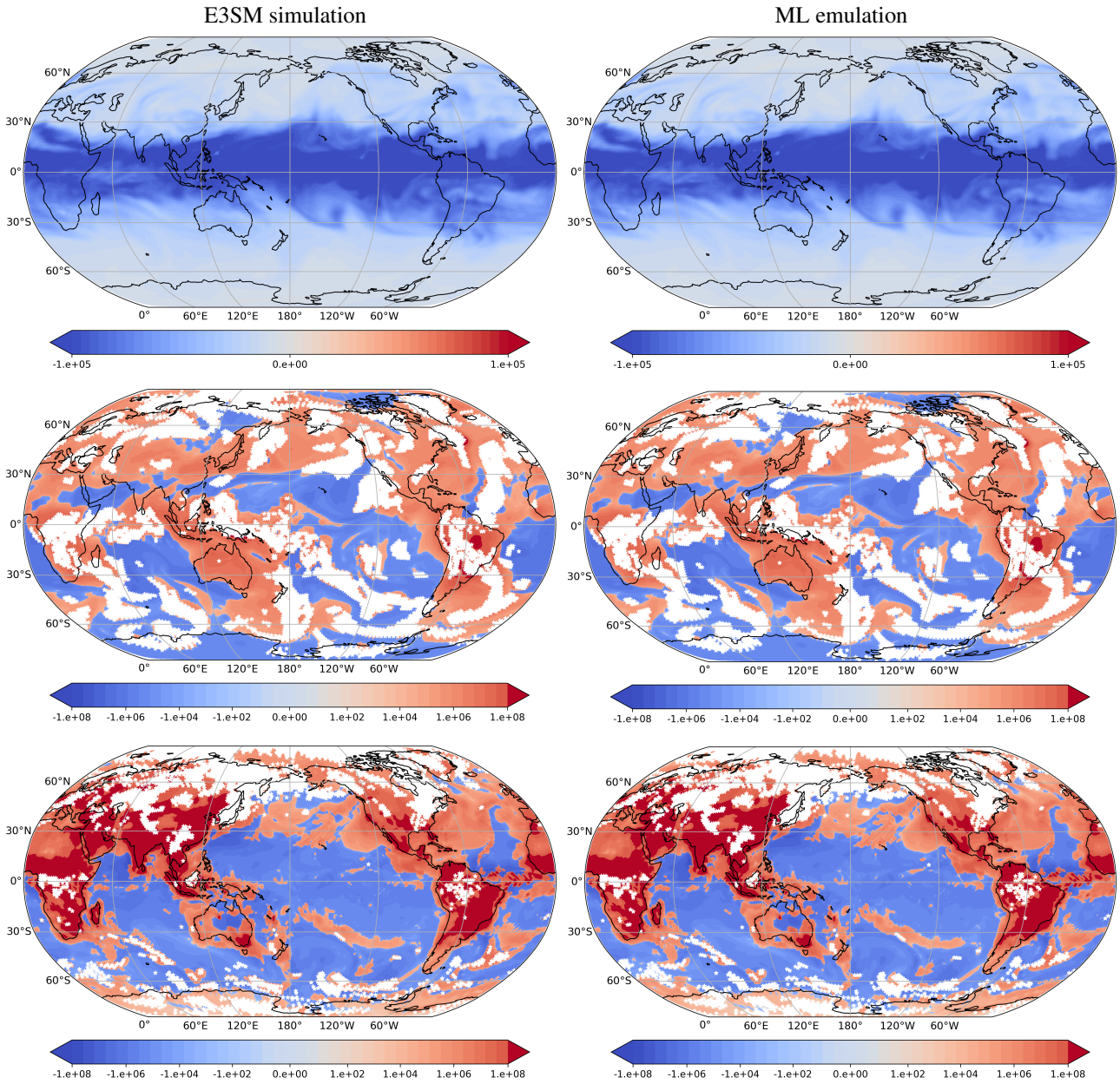

Figure S.2. Global view of VMR tendency of the number concentration of accumulation-mode aerosol particles from upper to lower atmosphere, a key component of the atmospheric aerosol population. (Left) VMR tendency Δnum_a1 collected from the E3SM simulation output of aerosol physics distribution at 00:30:00 UTC on on 12/30/2010. (Right) ADON-PCA prediction results emulating the solver of E3SM taking the input at 00:00:00 UTC on 12/30/2010.

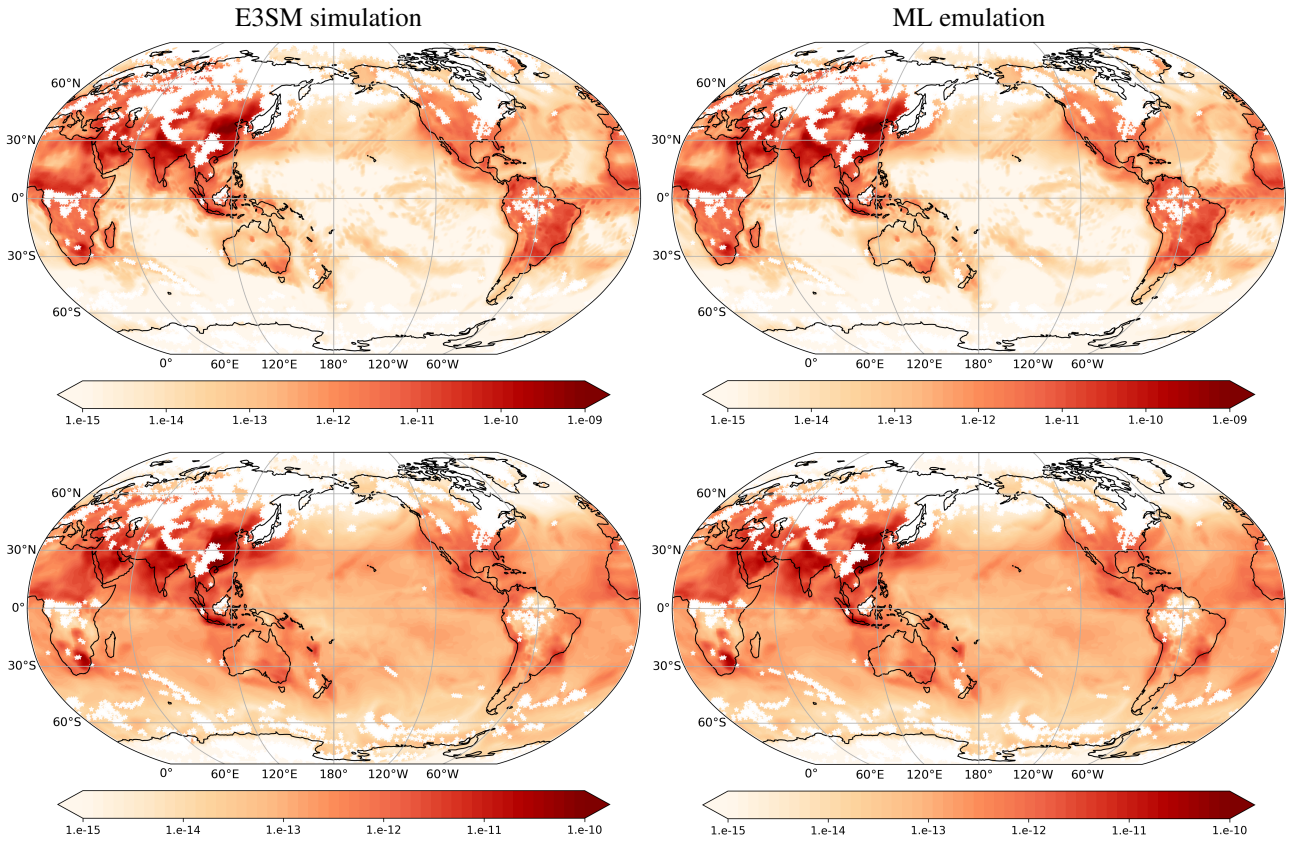

Figure S.3. Global view of VMR tendency of the concentration of accumulation-mode black carbon and sulfate aerosol particles in the model layer closest to the earth surface. (Left) VMR tendency Δnum_a1 collected from the E3SM simulation output of aerosol physics distribution at 00:30:00 UTC on on 12/30/2010. (Right) ADON-PCA prediction results emulating the solver of E3SM taking the input at 00:00:00 UTC on 12/30/2010.

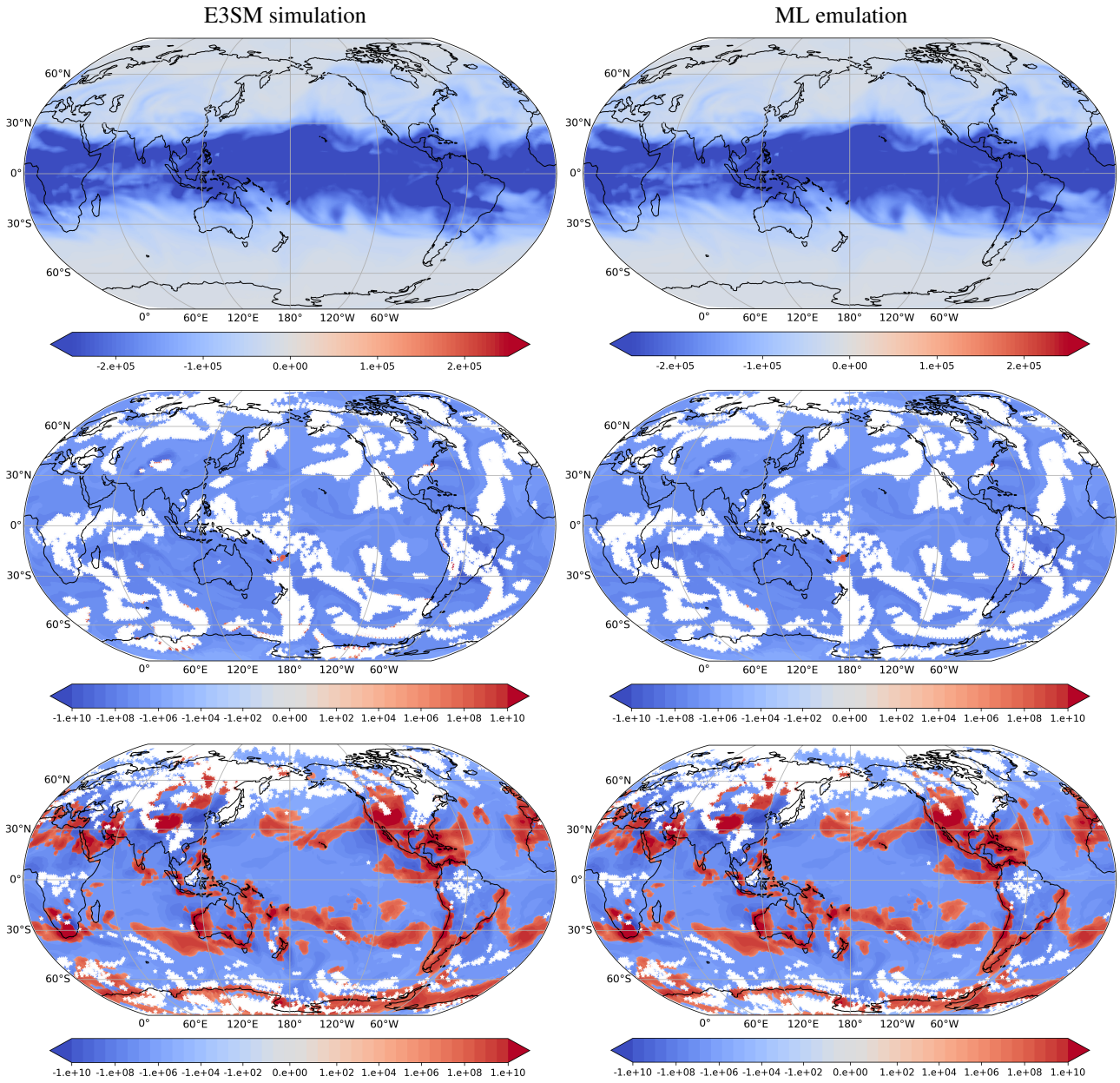

Figure S.4. Global view of the VMR tendency of Aitken-mode aerosol particle concentrations, from upper to lower atmosphere. (Left) VMR tendency Δnum_a2 collected from the E3SM simulation output of aerosol physics distribution at 00:30:00 UTC on on 12/30/2010. (Right) ADON-PCA prediction results emulating the solver of E3SM taking the input at 00:00:00 UTC on 12/30/2010.