Machine learning-based emulator for the physics-based simulation of auroral current system

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Abstract

Using a machine learning technique called echo state network (ESN), we have developed an emulator to model the physicsbased global magnetohydrodynamic (MHD) simulation results of REPPU (REProduce Plasma Universe) code. The inputs are the solar wind time series with date and time, and the outputs are the time series of the ionospheric auroral current system in the form of two-dimensional (2D) patterns of field-aligned current, potential, and conductivity. We mediated a principal component analysis for a dimensionality reduction of the 2D map time series. In this study, we report the latest upgraded Surrogate Model for REPPU Auroral Ionosphere version 2 (SMRAI2) with significantly improved resolutions in time and space (5 min in time, ~1 degrees in latitude, and 4.5 degrees in longitude), where the dipole tilt angle is also newly added as one of the input parameters to reproduce the seasonal dependence. The fundamental dependencies of the steady-state potential and field-aligned current patterns on the interplanetary magnetic field (IMF) directions are consistent with those obtained from empirical models. Further, we show that the ESN-based emulator can output the AE index so that we can evaluate the performance of the dynamically changing results, comparing with the observed AE index. Since the ESN-based emulator runs a million times faster than the REPPU simulation, it is promising that we can utilize the emulator for the real-time space weather forecast of the auroral current system as well as to obtain large-number ensembles to achieve future data assimilation-based forecast.

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14	Key Points:
15 16	• We developed machine learning-based emulator for surrogating the ionospheric outputs of a global MHD simulation called REPPU.
17 18	• The new emulator model SMRAI2 runs million times faster than the original physics- based simulation.
19 20 21	• The new emulator model SMRAI2 can be utilized for the real-time space weather forecast of auroral current system.

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- emulator to model the physics-based global magnetohydrodynamic (MHD) simulation results of
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- current system as well as to obtain large-number ensembles to achieve future data assimilation-
- 40 based forecast.

41 Plain Language Summary

42 Physics-based auroral simulations, such as Japanese REPPU code, are not practically fast enough

for the purpose of real-time space weather forecast, even using the designated super computers.

44 Here we developed a million-times-faster "emulator" to surrogate the outputs of the physics-

- 45 based simulation, using the machine-learning technique called Echo State Network. The newly
- 46 developed emulator, the surrogate model for REPPU auroral Ionosphere version 2 (SMRAI2)
- 47 enables us to realize the real-time forecast of the auroral current system.

48 **1 Introduction**

49 Forecasting the auroral current system in the polar regions has been one of the core parts

- of the operational space weather forecast because the auroral current system is the origin of the
- enhanced satellite drag via the Joule heat in the thermosphere. In recent years, such an
- 52 importance has been especially growing, and the spacecraft operations are getting more sensitive
- along the heavy utilization of the low-earth orbit. For example, it was remarkable that as many as
- 54 38 commercial satellites lost at the same time during moderate storms in February 2022 (e.g.,
- 55 Kataoka et al., 2022). The auroral current system, including auroral electrojet activities as known
- by the AE index, has been of fundamental importance for other various space weather aspects,
- 57 including geomagnetically induced currents (GIC) flowing along the ground-based
- infrastructures (e.g., Kataoka and Ngwira, 2016), and satellite charging and communicationsmalfunctions.
- 60 On the other hand, there is a long history of conducting physics-based simulations to (1 - understand the variable polar ioneenhere (Lyon et al. 1080). Only 0.000 (1086). Because of the
- understand the variable polar ionosphere (Lyon et al., 1980; Ogino, 1986). Because of the
- 62 nonlinear nature of the spatially complex evolution of auroral ovals and the magnetospheric
- 63 plasma flows as driven by the time-varying solar wind conditions, a global
- 64 magnetohydrodynamic (MHD) simulation with the input of the solar wind parameters is

65 necessary to reproduce the resultant auroral current system, as depicted by the ionospheric

- 66 conductivities, potential, and field-aligned currents. Among many sophisticated MHD
- 67 simulations, REPPU (REProduce Plasma Universe) has been known as one of the best models
- for resolving various space weather phenomena including auroral substorms (Ebihara et al.,
- 69 2015a; 2015b; Tanaka et al., 2017; 2018; 2022b). However, the major difficulty of REPPU and
- other simulation codes for the operational space weather forecast is that it is time-consuming to
- solve the MHD equations, even using the designated cluster computers.

This study shows that the latest development in machine learning techniques can help 72 solve this time-consuming issue. The very initial approach of such an emulator version 1.0 was 73 proposed by Kataoka et al. (2023), using the time-dependent machine learning model called echo 74 state network (ESN). In this study, we conducted a major upgrade of the ESN-based emulator by 75 training the emulator model using an order of magnitude larger amount of the REPPU simulation 76 outputs from that of ver1.0, as conducted by the long-term simulation runs (Nakamizo and 77 Kubota, 2021) under the space weather forecast operations at National Institute of Information 78 and Communications Technology (NICT). 79

In Section 2 we describe the REPPU simulation code and explain the technical details of the machine-learning model, especially focusing on how to emulate the REPPU simulation's ionospheric outputs. In Section 3, we show the primary results of the new emulator model. In Section 4, we discuss the performance and the limitation. Concluding remarks are briefly

summarized in Section 5.

85 2 Methods

86 2.1 Magnetohydrodynamic simulation code: REPPU

REPPU is an MHD simulation code developed for studying the global magnetosphere-87 ionosphere coupling (Tanaka, 1995; Tanaka, 2015). The REPPU code is characterized by an 88 excellent ionospheric reproduction of fundamental auroral phenomena such as substorms 89 (Ebihara and Tanaka, 2015a; 2015b), sun-aligned arcs (Tanaka et al., 2017), and the theta aurora 90 (Tanaka et al., 2018). In this study, we used an improved REPPU simulation code (Nakamizo 91 92 and Kubota, 2021), including the effects of a tilted dipole axis and seasonal changes of solar zenith angles. The total number of grid cells in the magnetosphere is 30722 (horizontal) $\times 240$ 93 94 (vertical), where the unstructured grid system (Moriguchi et al., 2008; Nakamizo et al., 2009) is employed. The number of grid cells in the ionosphere is 30722. In this study, for the training and 95 testing data, we took only the northern polar ionosphere, i.e. 30×80 pixels in latitude and 96 longitude, after applying the 2×4 binning in latitude and longitude. The ionospheric outputs of 97 the field-aligned current J//, conductivities Σxx (north-south), Σxy (off-diagonal), Σyy (east-98 west), and ionospheric potential Φ are saved every min, where the current continuity equation at 99 the two-dimensional height-integrated ionosphere (x: north-south, y: east-west) is satisfied as: 100

$$J_{\parallel} = \nabla \cdot \mathbf{J}_{\perp} = \nabla \cdot \left(\tilde{\Sigma} \cdot \mathbf{E} \right), \tag{1}$$

103
$$\tilde{\Sigma} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ -\Sigma_{xy} & \Sigma_{yy} \end{pmatrix}, \qquad (2)$$

104
$$\mathbf{E} = \left(-\frac{\partial \Phi}{\partial x}\right)$$

$$= \left(-\frac{\partial\Phi}{\partial x}, -\frac{\partial\Phi}{\partial y}\right). \tag{3}$$

The interplanetary magnetic field (IMF) Bx, By, and Bz are defined in the GSM
(Geocentric Solar Magnetospheric) coordinate system. The real-time solar wind data (IMF Bx,
By, Bz, solar wind speed V, proton density Np, and temperature Tp) at 1 min resolution was
linearly interpolated if there was a data gap and used as the input time series to run the REPPU
simulations. The real-time solar wind data can differ from the finally calibrated solar wind data,
such as OMNI dataset. Nevertheless, it is essentially little problem for the machine-learning
model to learn the REPPU simulation results for variable input patterns.

NICT team has been operating the real-time simulation with the improved REPPU code for the space weather forecast (Nakamizo and Kubota, 2021). The REPPU simulation has been running on the High-Performance Computing System at NICT since August, 2020. The simulation-run basically works automatically. Still, it is sometimes manually stopped and restarted due to some failures of the computing system, such as the system maintenances and failures of the simulation. The saved results are, therefore, not necessarily continuous.

In this study, we selected major interplanetary shock events and other large-amplitude events since 2021, including both predominantly southward and predominantly northward IMF conditions to include both storm-time and non-storm-time, respectively, as shown in **Table 1**. We also selected the long-term non-stop runs from December 2020 to January 2021 to compensate for the winter-time training data. Another long-term results from June to July 2021 is also prepared as the testing time interval.

124 2.2 Machine-learning model: Echo state network

125 The basic flow of the development of Surrogate Model for REPPU Auroral Ionosphere version 2 (SMRAI2) and the relationship of REPPU simulation and ESN model is graphically 126 summarized in Figure 1. Firstly, we adopted the dimensionality reduction for the ionospheric 127 outputs as obtained from REPPU simulations, by applying the principal component analysis 128 (PCA) using the Python 3 scikit-learn/pca. Very similar method was used by Licata and Mehta 129 (2023) for different purpose (thermosphere model emulator). The time series of each parameter z130 = { Σxy , Φ , or J//}, at certain (latitude, longitude) position of the grid indices (i,j), can be 131 represented by the time averaged spatial pattern z_0 and the linear combination of time-dependent 132 PCA variables α and PCA component patterns U as follows: 133

134 135

$$z(i, j, t) = z_0(i, j) + z_1(i, j, t),$$

$$z_1(i, j, t) = \sum_{r=1}^{N_r} \alpha_r(t) U_r(i, j) .$$
(5)

(4)

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136

In this study, the numbers of PCA components Nr are selected to be 10 for Σxy and Φ , and 20 for J// to reconstruct >90% variance of the original features.

140 To those time-dependent PCA variables α , we employed essentially the same Echo State 141 Network model (Jaeger, 2001; Jaeger and Haas, 2004; Tanaka et al., 2019) as Kataoka et al. (2023) documented. In this study, we used the ESN module of Python 3 as developed by Tanaka
et al. (2022a) (See https://github.com/GTANAKA-LAB/DTS-ESN/).

144 The ESN model used in this study is described by the reservoir state vector \mathbf{x} and the 145 model output vector \mathbf{y} at t = n + 1 steps as follows:

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$$\mathbf{x}(n+1) = \tanh\left\{W^{in}\mathbf{u}(n+1) + W\mathbf{x}(n)\right\},\tag{6}$$

$$\mathbf{y}(n+1) = W^{out}\mathbf{x}(n+1). \tag{7}$$

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Here, the weight matrices W^{in} and W are multiplied by the input vector **u** (the solar wind time series) and the reservoir state vector **x**, respectively. We create the random and sparse node connections of W^{in} and W, where only 10% of the matrix elements are random values between -1.0 and 1.0, and the remaining 90% are zero. The weight matrices W^{in} and W are fixed, while only Wout is trained by the ridge regression with the regularization parameter $\beta = 10^{-3}$ to minimize the objective function F,

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$$F = \sum_{n=1}^{N} \left\| \mathbf{y}(n) - \mathbf{d}(n) \right\| + \frac{\beta}{2} \left\| W^{out} \right\|^{2},$$
(8)

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where **d** is a desired data vector consisting of the time series of the PCA variables of J//, Σxy , and Φ .

As the input vectors u, the solar wind speed and density are normalized as log_{10} V - 2.5, and log_{10} Np - 1.0, respectively, before training the ESN model because both the solar wind speed and density follow log-normal distributions (Burlaga and Lazarus, 2000). The IMF By and Bz components are also used as the input parameters. Further, the dipole tilt angle is newly introduced as the input to adopt the model for all seasons. The dipole tilt angle is calculated from the date and time by Python 3 pyspedas/geopack.

167 The emulator was trained by 107-day worth of outputs (30816 time steps) of REPPU 168 simulation results. The testing data is 52 days, including both quiet and active months. The 169 selection of training data and testing data was summarized in **Table 1**. The basic specifications 170 of ESN-based emulators ver1.0 and ver2.0 are summarized in **Table 2**.

We optimized the number of the nodes (elements of x) to be 400, 250, and 300 for J//, Φ , and Σxy , respectively, and the spectral radius (maximum eigenvalue of W) to be 0.99 for all J//,

173 Φ , and Σxy , by finding the minimum values of the normalized root-mean-square errors

174 (NRMSE) using the testing data for the first PCA variables. From these results, the constructed

emulator model has NRMSE of ~0.7, ~0.5, and ~0.8 to reconstruct the first PCA variables of J//, Φ , and Σxy , respectively.

In this study, we independently constructed the emulators for J//, Σxy , and Φ maps.

178 However, the current continuity Eq. (1) relates these parameters, and any inconsistencies among

these parameters can therefore give hints to evaluate the deviations in the emulation results for

180 future applications.

181 It takes less than 10 s for the emulator to calculate a 1-day variation of auroral current 182 system using a single node. In contrast, it takes ~5 days for the REPPU simulation to calculate 183 the same 1-day variation using the 30-node cluster computer. Therefore, the computational cost 184 of the SMRAI2 is approximately a million times more efficient than the original physics-based 185 REPPU simulation.

186 **3 Results**

187 One of the major upgrades of SMRAI2 from the emulator ver1.0 (Kataoka et al., 2023) is 188 the dipole tilt angle dependence by learning the simulation outputs from different seasons. From 189 the steady state conditions for different tilt angles, **Figure 2** shows that the trained model learned 190 the tilt angle dependence of the Hall conductivity Σxy . Notably, the dayside conductivity is high 191 in the summer season, while the nightside conductivity is low in the summer. The obtained 192 tendency of the nightside conductivity is consistent with the results of Newell et al. (2010).

193 Figure 3 shows the IMF clock angle dependence of the Region-1 and Region-2 fieldaligned current system (Iijima and Potemra, 1978). The IMF clock angle is defined as the angle 194 195 made in the By-Bz space, i.e., atan(By/Bz). We picked up the steady-state conditions of SMRAI2 results for each input parameter to make this figure. The overall IMF clock angle 196 dependence and the amplitude of J// are reasonable, and consistent with empirical models such as 197 Weimer (2001a). Further, we can see the IMF By dependent cusp current system in the higher 198 199 latitude region than the Region 1 currents (Fujii and Iijima, 1980), especially during the northward IMF conditions. 200

Figure 4 shows the IMF clock angle dependence of the ionospheric potential, almost the 201 same with the results from the emulator ver1.0 (Kataoka et al., 2023), consistent with empirical 202 models such as Weimer-2K model (Weimer, 2001b) as shown in Figure 5. Comparing Figures 4 203 and 5, the IMF By dependent appearances of the crescent- and round-shaped cells are clearly 204 captured. However, the amplitude of cross-polar cap potential is only ~60% compared to the 205 empirical models. Such an underestimating tendency is naturally expected, as we adopted the 206 coarse-graining of ionospheric potential such as the binning and PCA analysis. We will come 207 back to this point later. 208

209 4 Discussions

210 One way to examine the performance of the SMRAI2 using the open data is to calculate 211 the AE index (https://wdc.kugi.kyoto-u.ac.jp/aedir/index.html) from the emulator and compare it 212 with the observed values. In this study, we calculate the AU/AL indices (AE = AU - AL) from 213 the emulator results with the electric field as estimated by the spatial derivatives of Φ map using 214 the central difference,

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- 216

$$\left(\frac{\partial\Phi}{\partial x},\frac{\partial\Phi}{\partial y}\right) = \left(\frac{\Phi_{i+1} - \Phi_{i-1}}{2\Delta x},\frac{\Phi_{j+1} - \Phi_{j-1}}{2\Delta y}\right),\tag{9}$$

217 where *i* and *j* are the indices of latitude and longitude, respectively, and the Δx (north-218 south) and Δy (east-west) are calculated from the colatitude θ , longitude φ , and the Earth radius 219 R_E as

221
$$(\Delta x, \Delta y) = \left(\frac{\Delta \theta}{360} 2\pi R_E, \frac{\Delta \varphi}{360} 2\pi R_E \sin \theta\right).$$
 (10)

The ionospheric Hall current vectors are then calculated as

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$$\mathbf{J}_{Hall} = \left(\Sigma_{xy}E_{y}, -\Sigma_{xy}E_{x}\right) = \left(-\Sigma_{xy}\frac{\partial\Phi}{\partial y}, \Sigma_{xy}\frac{\partial\Phi}{\partial x}\right).$$
(11)

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We then applied the so-called equivalent current theorem (Maeda, 1955; Fukushima, 1969; 1976) where the east-west component of the Hall current in the unit of A km⁻¹ is nearly equal to the north-south component of the magnetic field at the ground in the unit of nT to calculate the AU/AL indices from the envelopes of the emulator outputs. The magnetic latitude range for the AU/AL calculation is selected from 60° to 70°.

The resultant AU and AL indices are shown in **Figure 6** for the one-month time interval, using the 5-min OMNI solar wind data. The data gaps of the OMNI 5-min data were filled by the forward interpolation using the Python 3 pandas/fillna/ffill method. **Figure 7** shows the 2D histogram for the 15-year results, indicating that the ESN-based emulator tends to underestimate the AE index. The cross-correlation coefficients between observed and emulated indices for the 15-year data are 0.592, 0.596, 0.666 for AU, AL, and AE indices, respectively.

There are multiple causes for this underestimation of the AE index. First, it is natural to 238 expect that the coarse-graining of ionospheric potential, such as the binning and PCA analysis 239 must give smaller values than the original simulation results, as we pointed out at the end of 240 Section 3. Also, the finite difference of **Equation 9** can further give the underestimation of the 241 electric field, which was used to calculate the Hall current and the AE index. Therefore, having 242 such a smaller AE index estimation by the ESN-based emulator is not surprising. Instead, we can 243 use the SMRAI2 results as the fair values for the AE index prediction with the possible errors, as 244 shown in **Figure 7**. 245

Since the AE index roughly represents the macroscopic energy release in the polar 246 ionosphere, we can diagnose some hidden characteristics of the new SMRAI2 via inputting the 247 synthetic solar wind data. We prepared the synthetic solar wind data to pick up the peak values 248 of the predicted AE index during the 80 min time interval after the southward IMF turnings from 249 the steady state of the northward IMF Bz = 1.0 nT, changing the IMF amplitude, solar wind 250 speed, and density. Ebihara and Tanaka (2019) showed, using the REPPU simulations, that the 251 positive density dependence of the auroral electrojet intensity is clear during weakly southward 252 IMF, while it is not likely the same during strongly southward IMF. Similarly complex tendency 253 for the density appeared in the results from the emulator ver2.0, as shown in the right panel of 254 Figure 8. In contrast to the density, the dependence of the AE peak intensity on the solar wind 255 speed is relatively simple, as linearly correlating with the product of southward IMF Bz and solar 256 wind speed V, which was seen in both Ebihara and Tanaka (2019) as well as in the left panel of 257 Figure 8. 258

Although it is improved from ver1.0 (Kataoka et al., 2023), the temporal resolution of 5 min still gives the major limitation of the SMRAI2. For example, we cannot discuss the highly dynamic phenomena such as the substorm onset and sudden commencement, in which all 262 ionospheric parameters drastically evolve in a short time scale of less than 5 min. Those rapid

- variation can cause large-amplitude GIC events, which is one of the important targets of the
- operational space weather forecast. One of the future works, therefore, include improving of the
- temporal resolution to 1 min since the ESN method can be applied to diverse temporal scales
- (Tanaka et al., 2022a). Caveat should also be made here that it may not so simply work to solve
- the substorm-onset-related problems by improving the temporal resolution because there is an essential difficulty in reproducing the variation just before and after the substorm onsets, as
- coming from the probabilistic nature of the substorm onsets (Nakano and Kataoka, 2022; Nakano
- et al., 2023).

Therefore, another natural next step would be the data assimilation of the SMRAI2 emulator to correct the exact timing of the substorm onset and the amplitude via the observation data. The million-times faster SMRAI2 emulator has a significant advantage in this direction, compared to the physics-based simulation, because it is essential to increase the ensemble number necessary for data assimilation. For realizing the data assimilation-based forecast, it would be reasonable to use any partial data or point data which is available for real-time use via

applying the cutting-edge data assimilation techniques (Nakano et al., 2020).

278 **5 Conclusions**

We showed that SMRAI2 emulator model is ready-to-use for the real-time space weather 279 forecast of the auroral current system for both the northern and southern hemispheres. We 280 developed the latest upgraded version 2.0 of the ESN-based emulator for the REPPU 281 simulation's ionospheric outputs of the field-aligned current, potential, and conductivity, which 282 runs a million times faster than the REPPU code. The resolutions of the latest ESN-based 283 emulator ver2.0 are significantly improved in time, latitude, and longitude, compared to the 284 ver1.0, and the dipole tilt angle is also newly introduced as one of the input parameters, in 285 addition to IMF By, Bz, V, and Np, thanks to an order of magnitude larger training dataset. We 286 confirmed that the IMF clock-angle dependence of the auroral current system is consistent with 287 that obtained from empirical models. New functions of the ESN-based emulator ver2.0 includes 288 automatic OMNI solar wind data input and the AE index output by indicating the date only. 289

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301 **Open Research**

The OMNI solar wind data with the AE/AU/AL indices are publicly available at https://omniweb.gsfc.nasa.gov/ow_min.html. The Python 3 codes and the training/testing datasets for the ESN-based emulator model, SMRAI2, used in this study are open to the public at https://github.com/ryuhokataoka/REPPU-ESN2 (v2.0.0 was released at

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410

Figure 1. Block diagram of SMRAI2 development to graphically summarize the relationshipamong the REPPU, PCA, and ESN.



411 **Figure 2**. The tilt angle dependence of Σxy . Steady-state conditions of SMRAI2 are shown,

fixing the solar wind parameters By = 0.0 nT, Bz = 5.0 nT, Np = 5/cc, and Vsw = 400 km/s.



414 **Figure 3**. The IMF clock angle dependence of field-aligned current in the northern hemisphere.

- Steady-state conditions from the SMRAI2 are shown, fixing the tilt angle = 0.0, B = 5.0 nT, Np
- 416 = 5/cc, and Vsw = 450 km/s.



418 **Figure 4**. The IMF clock angle dependence of ionospheric potential in the northern hemisphere.

Steady-state conditions from the SMRAI2 are shown, fixing the tilt angle = 0.0, B = 5.0 nT, Np = 5/cc, and Vsw = 450 km/s.



421

422 **Figure 5**. The IMF clock angle dependence of ionospheric potential in the northern hemisphere

423 as obtained from the Weimer2K empirical model, with the tilt angle = 0.0, B = 5.0 nT, Np =

424 5/cc, and Vsw = 450 km/s.



Figure 6. Example of the calculation of AU/AL indices by SMRAI2, compared with the

427 observed values, for the one-month time interval from October 1, 1999.





430 **Figure 7**. 2D histogram for the AE index as predicted by SMRAI2 against the observed AE

431 index for the 15-year time interval from January 1, 2000.



Figure 8. Heat map analysis of the SMRAI2-predicted AE peak intensity in the (left) IMF Bz-V
space and in (right) IMF Bz-Np space.

Start	End	# of days	Notes
2021/05/10	2021/05/15	5	Shock, moderate storm
2021/05/31	2021/06/03	4	Shock
2021/07/26	2021/07/29	4	northward IMF
2021/09/09	2021/09/12	4	northward IMF
2021/10/11	2021/10/14	4	Shock
2021/11/01	2021/11/06	6	Shock, intense storm
2021/11/25	2021/11/29	5	Shock
2022/01/30	2022/02/03	5	Shock
2022/03/11	2022/03/15	5	Shock
2022/03/28	2022/04/1	5	Shock
2022/08/15	2022/08/19	5	Shock
2021/12/01	2022/01/24	55	Long run for training
2022/06/10	2022/07/31	52	Long run for testing

Table 1. List of the selected events for training and testing the ESN model.

Table 2. Specifications of SMRAI emulators version 1.0 (Kataoka et al., 2023) and version 2.0 (this study).

Parameters	SMRAI1	SMRAI2
Time resolution	10 min	5 min
Latitude resolution	~2 deg	~1 deg
Longitude resolution	11.25 deg	4.5 deg
Input solar wind parameters	By, Bz, Np, Vsw	Tilt, By, Bz, Np, Vsw
Training dataset	~10 days worth	~100 days worth
Hemisphere	North only	North and south

1	Machine learning-based emulator for the physics-based simulation of auroral current system
Ζ	current system
3	
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13	
14	Key Points:
15 16	• We developed machine learning-based emulator for surrogating the ionospheric outputs of a global MHD simulation called REPPU.
17 18	• The new emulator model SMRAI2 runs million times faster than the original physics- based simulation.
19 20 21	• The new emulator model SMRAI2 can be utilized for the real-time space weather forecast of auroral current system.

22 Abstract

- Using a machine learning technique called echo state network (ESN), we have developed an
- emulator to model the physics-based global magnetohydrodynamic (MHD) simulation results of
- 25 REPPU (REProduce Plasma Universe) code. The inputs are the solar wind time series with date
- and time, and the outputs are the time series of the ionospheric auroral current system in the form
- of two-dimensional (2D) patterns of field-aligned current, potential, and conductivity. We
- 28 mediated a principal component analysis for a dimensionality reduction of the 2D map time
- series. In this study, we report the latest upgraded Surrogate Model for REPPU Auroral
- 30 Ionosphere version 2 (SMRAI2) with significantly improved resolutions in time and space (5 31 min in time, ~1 degrees in latitude, and 4.5 degrees in longitude), where the dipole tilt angle is
- min in time, ~1 degrees in latitude, and 4.5 degrees in longitude), where the dipole tilt angle also newly added as one of the input parameters to reproduce the seasonal dependence. The
- fundamental dependencies of the steady-state potential and field-aligned current patterns on the
- interplanetary magnetic field (IMF) directions are consistent with those obtained from empirical
- 35 models. Further, we show that the ESN-based emulator can output the AE index so that we can
- ³⁶ evaluate the performance of the dynamically changing results, comparing with the observed AE
- 37 index. Since the ESN-based emulator runs a million times faster than the REPPU simulation, it is
- promising that we can utilize the emulator for the real-time space weather forecast of the auroral
- current system as well as to obtain large-number ensembles to achieve future data assimilation-
- 40 based forecast.

41 Plain Language Summary

42 Physics-based auroral simulations, such as Japanese REPPU code, are not practically fast enough

for the purpose of real-time space weather forecast, even using the designated super computers.

44 Here we developed a million-times-faster "emulator" to surrogate the outputs of the physics-

- 45 based simulation, using the machine-learning technique called Echo State Network. The newly
- 46 developed emulator, the surrogate model for REPPU auroral Ionosphere version 2 (SMRAI2)
- 47 enables us to realize the real-time forecast of the auroral current system.

48 **1 Introduction**

49 Forecasting the auroral current system in the polar regions has been one of the core parts

- of the operational space weather forecast because the auroral current system is the origin of the
- enhanced satellite drag via the Joule heat in the thermosphere. In recent years, such an
- 52 importance has been especially growing, and the spacecraft operations are getting more sensitive
- along the heavy utilization of the low-earth orbit. For example, it was remarkable that as many as
- 54 38 commercial satellites lost at the same time during moderate storms in February 2022 (e.g.,
- 55 Kataoka et al., 2022). The auroral current system, including auroral electrojet activities as known
- by the AE index, has been of fundamental importance for other various space weather aspects,
- 57 including geomagnetically induced currents (GIC) flowing along the ground-based
- infrastructures (e.g., Kataoka and Ngwira, 2016), and satellite charging and communicationsmalfunctions.
- 60 On the other hand, there is a long history of conducting physics-based simulations to (1 - understand the variable polar ionegrhere (Lyon et al. 1080). Oging 1086). Because of the
- understand the variable polar ionosphere (Lyon et al., 1980; Ogino, 1986). Because of the
- 62 nonlinear nature of the spatially complex evolution of auroral ovals and the magnetospheric
- 63 plasma flows as driven by the time-varying solar wind conditions, a global
- 64 magnetohydrodynamic (MHD) simulation with the input of the solar wind parameters is

65 necessary to reproduce the resultant auroral current system, as depicted by the ionospheric

- 66 conductivities, potential, and field-aligned currents. Among many sophisticated MHD
- 67 simulations, REPPU (REProduce Plasma Universe) has been known as one of the best models
- for resolving various space weather phenomena including auroral substorms (Ebihara et al.,
- 69 2015a; 2015b; Tanaka et al., 2017; 2018; 2022b). However, the major difficulty of REPPU and
- other simulation codes for the operational space weather forecast is that it is time-consuming to
- solve the MHD equations, even using the designated cluster computers.

This study shows that the latest development in machine learning techniques can help 72 solve this time-consuming issue. The very initial approach of such an emulator version 1.0 was 73 proposed by Kataoka et al. (2023), using the time-dependent machine learning model called echo 74 state network (ESN). In this study, we conducted a major upgrade of the ESN-based emulator by 75 training the emulator model using an order of magnitude larger amount of the REPPU simulation 76 outputs from that of ver1.0, as conducted by the long-term simulation runs (Nakamizo and 77 Kubota, 2021) under the space weather forecast operations at National Institute of Information 78 and Communications Technology (NICT). 79

In Section 2 we describe the REPPU simulation code and explain the technical details of the machine-learning model, especially focusing on how to emulate the REPPU simulation's ionospheric outputs. In Section 3, we show the primary results of the new emulator model. In Section 4, we discuss the performance and the limitation. Concluding remarks are briefly

summarized in Section 5.

85 2 Methods

86 2.1 Magnetohydrodynamic simulation code: REPPU

REPPU is an MHD simulation code developed for studying the global magnetosphere-87 ionosphere coupling (Tanaka, 1995; Tanaka, 2015). The REPPU code is characterized by an 88 excellent ionospheric reproduction of fundamental auroral phenomena such as substorms 89 (Ebihara and Tanaka, 2015a; 2015b), sun-aligned arcs (Tanaka et al., 2017), and the theta aurora 90 (Tanaka et al., 2018). In this study, we used an improved REPPU simulation code (Nakamizo 91 92 and Kubota, 2021), including the effects of a tilted dipole axis and seasonal changes of solar zenith angles. The total number of grid cells in the magnetosphere is 30722 (horizontal) $\times 240$ 93 94 (vertical), where the unstructured grid system (Moriguchi et al., 2008; Nakamizo et al., 2009) is employed. The number of grid cells in the ionosphere is 30722. In this study, for the training and 95 testing data, we took only the northern polar ionosphere, i.e. 30×80 pixels in latitude and 96 longitude, after applying the 2×4 binning in latitude and longitude. The ionospheric outputs of 97 the field-aligned current J//, conductivities Σxx (north-south), Σxy (off-diagonal), Σyy (east-98 west), and ionospheric potential Φ are saved every min, where the current continuity equation at 99 the two-dimensional height-integrated ionosphere (x: north-south, y: east-west) is satisfied as: 100

$$J_{\parallel} = \nabla \cdot \mathbf{J}_{\perp} = \nabla \cdot \left(\tilde{\Sigma} \cdot \mathbf{E} \right), \tag{1}$$

103
$$\tilde{\Sigma} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ -\Sigma_{xy} & \Sigma_{yy} \end{pmatrix}, \qquad (2)$$

104
$$\mathbf{E} = \left(-\frac{\partial \Phi}{\partial x}\right)$$

$$= \left(-\frac{\partial\Phi}{\partial x}, -\frac{\partial\Phi}{\partial y}\right). \tag{3}$$

The interplanetary magnetic field (IMF) Bx, By, and Bz are defined in the GSM
(Geocentric Solar Magnetospheric) coordinate system. The real-time solar wind data (IMF Bx,
By, Bz, solar wind speed V, proton density Np, and temperature Tp) at 1 min resolution was
linearly interpolated if there was a data gap and used as the input time series to run the REPPU
simulations. The real-time solar wind data can differ from the finally calibrated solar wind data,
such as OMNI dataset. Nevertheless, it is essentially little problem for the machine-learning
model to learn the REPPU simulation results for variable input patterns.

NICT team has been operating the real-time simulation with the improved REPPU code for the space weather forecast (Nakamizo and Kubota, 2021). The REPPU simulation has been running on the High-Performance Computing System at NICT since August, 2020. The simulation-run basically works automatically. Still, it is sometimes manually stopped and restarted due to some failures of the computing system, such as the system maintenances and failures of the simulation. The saved results are, therefore, not necessarily continuous.

In this study, we selected major interplanetary shock events and other large-amplitude events since 2021, including both predominantly southward and predominantly northward IMF conditions to include both storm-time and non-storm-time, respectively, as shown in **Table 1**. We also selected the long-term non-stop runs from December 2020 to January 2021 to compensate for the winter-time training data. Another long-term results from June to July 2021 is also prepared as the testing time interval.

124 2.2 Machine-learning model: Echo state network

125 The basic flow of the development of Surrogate Model for REPPU Auroral Ionosphere version 2 (SMRAI2) and the relationship of REPPU simulation and ESN model is graphically 126 summarized in Figure 1. Firstly, we adopted the dimensionality reduction for the ionospheric 127 outputs as obtained from REPPU simulations, by applying the principal component analysis 128 (PCA) using the Python 3 scikit-learn/pca. Very similar method was used by Licata and Mehta 129 (2023) for different purpose (thermosphere model emulator). The time series of each parameter z130 = { Σxy , Φ , or J//}, at certain (latitude, longitude) position of the grid indices (i,j), can be 131 represented by the time averaged spatial pattern z_0 and the linear combination of time-dependent 132 PCA variables α and PCA component patterns U as follows: 133

134 135

$$z(i, j, t) = z_0(i, j) + z_1(i, j, t),$$

$$z_1(i, j, t) = \sum_{r=1}^{N_r} \alpha_r(t) U_r(i, j) .$$
(5)

(4)

137

136

In this study, the numbers of PCA components Nr are selected to be 10 for Σxy and Φ , and 20 for J// to reconstruct >90% variance of the original features.

140 To those time-dependent PCA variables α , we employed essentially the same Echo State 141 Network model (Jaeger, 2001; Jaeger and Haas, 2004; Tanaka et al., 2019) as Kataoka et al. (2023) documented. In this study, we used the ESN module of Python 3 as developed by Tanaka
et al. (2022a) (See https://github.com/GTANAKA-LAB/DTS-ESN/).

144 The ESN model used in this study is described by the reservoir state vector \mathbf{x} and the 145 model output vector \mathbf{y} at t = n + 1 steps as follows:

146

147

$$\mathbf{x}(n+1) = \tanh\left\{W^{in}\mathbf{u}(n+1) + W\mathbf{x}(n)\right\},\tag{6}$$

$$\mathbf{y}(n+1) = W^{out}\mathbf{x}(n+1). \tag{7}$$

149

Here, the weight matrices W^{in} and W are multiplied by the input vector **u** (the solar wind time series) and the reservoir state vector **x**, respectively. We create the random and sparse node connections of W^{in} and W, where only 10% of the matrix elements are random values between -1.0 and 1.0, and the remaining 90% are zero. The weight matrices W^{in} and W are fixed, while only Wout is trained by the ridge regression with the regularization parameter $\beta = 10^{-3}$ to minimize the objective function F,

156

157

$$F = \sum_{n=1}^{N} \left\| \mathbf{y}(n) - \mathbf{d}(n) \right\| + \frac{\beta}{2} \left\| W^{out} \right\|^{2},$$
(8)

158

where **d** is a desired data vector consisting of the time series of the PCA variables of J//, Σxy , and Φ .

As the input vectors u, the solar wind speed and density are normalized as log_{10} V - 2.5, and log_{10} Np - 1.0, respectively, before training the ESN model because both the solar wind speed and density follow log-normal distributions (Burlaga and Lazarus, 2000). The IMF By and Bz components are also used as the input parameters. Further, the dipole tilt angle is newly introduced as the input to adopt the model for all seasons. The dipole tilt angle is calculated from the date and time by Python 3 pyspedas/geopack.

167 The emulator was trained by 107-day worth of outputs (30816 time steps) of REPPU 168 simulation results. The testing data is 52 days, including both quiet and active months. The 169 selection of training data and testing data was summarized in **Table 1**. The basic specifications 170 of ESN-based emulators ver1.0 and ver2.0 are summarized in **Table 2**.

We optimized the number of the nodes (elements of x) to be 400, 250, and 300 for J//, Φ , and Σxy , respectively, and the spectral radius (maximum eigenvalue of W) to be 0.99 for all J//,

173 Φ , and Σxy , by finding the minimum values of the normalized root-mean-square errors

174 (NRMSE) using the testing data for the first PCA variables. From these results, the constructed

emulator model has NRMSE of ~0.7, ~0.5, and ~0.8 to reconstruct the first PCA variables of J//, Φ , and Σxy , respectively.

In this study, we independently constructed the emulators for J//, Σxy , and Φ maps.

178 However, the current continuity Eq. (1) relates these parameters, and any inconsistencies among

these parameters can therefore give hints to evaluate the deviations in the emulation results for

180 future applications.

181 It takes less than 10 s for the emulator to calculate a 1-day variation of auroral current 182 system using a single node. In contrast, it takes ~5 days for the REPPU simulation to calculate 183 the same 1-day variation using the 30-node cluster computer. Therefore, the computational cost 184 of the SMRAI2 is approximately a million times more efficient than the original physics-based 185 REPPU simulation.

186 **3 Results**

187 One of the major upgrades of SMRAI2 from the emulator ver1.0 (Kataoka et al., 2023) is 188 the dipole tilt angle dependence by learning the simulation outputs from different seasons. From 189 the steady state conditions for different tilt angles, **Figure 2** shows that the trained model learned 190 the tilt angle dependence of the Hall conductivity Σxy . Notably, the dayside conductivity is high 191 in the summer season, while the nightside conductivity is low in the summer. The obtained 192 tendency of the nightside conductivity is consistent with the results of Newell et al. (2010).

193 Figure 3 shows the IMF clock angle dependence of the Region-1 and Region-2 fieldaligned current system (Iijima and Potemra, 1978). The IMF clock angle is defined as the angle 194 195 made in the By-Bz space, i.e., atan(By/Bz). We picked up the steady-state conditions of SMRAI2 results for each input parameter to make this figure. The overall IMF clock angle 196 dependence and the amplitude of J// are reasonable, and consistent with empirical models such as 197 Weimer (2001a). Further, we can see the IMF By dependent cusp current system in the higher 198 199 latitude region than the Region 1 currents (Fujii and Iijima, 1980), especially during the northward IMF conditions. 200

Figure 4 shows the IMF clock angle dependence of the ionospheric potential, almost the 201 same with the results from the emulator ver1.0 (Kataoka et al., 2023), consistent with empirical 202 models such as Weimer-2K model (Weimer, 2001b) as shown in Figure 5. Comparing Figures 4 203 and 5, the IMF By dependent appearances of the crescent- and round-shaped cells are clearly 204 captured. However, the amplitude of cross-polar cap potential is only ~60% compared to the 205 empirical models. Such an underestimating tendency is naturally expected, as we adopted the 206 coarse-graining of ionospheric potential such as the binning and PCA analysis. We will come 207 back to this point later. 208

209 4 Discussions

210 One way to examine the performance of the SMRAI2 using the open data is to calculate 211 the AE index (https://wdc.kugi.kyoto-u.ac.jp/aedir/index.html) from the emulator and compare it 212 with the observed values. In this study, we calculate the AU/AL indices (AE = AU - AL) from 213 the emulator results with the electric field as estimated by the spatial derivatives of Φ map using 214 the central difference,

- 215
- 216

$$\left(\frac{\partial\Phi}{\partial x},\frac{\partial\Phi}{\partial y}\right) = \left(\frac{\Phi_{i+1} - \Phi_{i-1}}{2\Delta x},\frac{\Phi_{j+1} - \Phi_{j-1}}{2\Delta y}\right),\tag{9}$$

217 where *i* and *j* are the indices of latitude and longitude, respectively, and the Δx (north-218 south) and Δy (east-west) are calculated from the colatitude θ , longitude φ , and the Earth radius 219 R_E as

221
$$(\Delta x, \Delta y) = \left(\frac{\Delta \theta}{360} 2\pi R_E, \frac{\Delta \varphi}{360} 2\pi R_E \sin \theta\right).$$
 (10)

The ionospheric Hall current vectors are then calculated as

223 224

$$\mathbf{J}_{Hall} = \left(\Sigma_{xy}E_{y}, -\Sigma_{xy}E_{x}\right) = \left(-\Sigma_{xy}\frac{\partial\Phi}{\partial y}, \Sigma_{xy}\frac{\partial\Phi}{\partial x}\right).$$
(11)

226

225

We then applied the so-called equivalent current theorem (Maeda, 1955; Fukushima, 1969; 1976) where the east-west component of the Hall current in the unit of A km⁻¹ is nearly equal to the north-south component of the magnetic field at the ground in the unit of nT to calculate the AU/AL indices from the envelopes of the emulator outputs. The magnetic latitude range for the AU/AL calculation is selected from 60° to 70°.

The resultant AU and AL indices are shown in **Figure 6** for the one-month time interval, using the 5-min OMNI solar wind data. The data gaps of the OMNI 5-min data were filled by the forward interpolation using the Python 3 pandas/fillna/ffill method. **Figure 7** shows the 2D histogram for the 15-year results, indicating that the ESN-based emulator tends to underestimate the AE index. The cross-correlation coefficients between observed and emulated indices for the 15-year data are 0.592, 0.596, 0.666 for AU, AL, and AE indices, respectively.

There are multiple causes for this underestimation of the AE index. First, it is natural to 238 expect that the coarse-graining of ionospheric potential, such as the binning and PCA analysis 239 must give smaller values than the original simulation results, as we pointed out at the end of 240 Section 3. Also, the finite difference of **Equation 9** can further give the underestimation of the 241 electric field, which was used to calculate the Hall current and the AE index. Therefore, having 242 such a smaller AE index estimation by the ESN-based emulator is not surprising. Instead, we can 243 use the SMRAI2 results as the fair values for the AE index prediction with the possible errors, as 244 shown in **Figure 7**. 245

Since the AE index roughly represents the macroscopic energy release in the polar 246 ionosphere, we can diagnose some hidden characteristics of the new SMRAI2 via inputting the 247 synthetic solar wind data. We prepared the synthetic solar wind data to pick up the peak values 248 of the predicted AE index during the 80 min time interval after the southward IMF turnings from 249 the steady state of the northward IMF Bz = 1.0 nT, changing the IMF amplitude, solar wind 250 speed, and density. Ebihara and Tanaka (2019) showed, using the REPPU simulations, that the 251 positive density dependence of the auroral electrojet intensity is clear during weakly southward 252 IMF, while it is not likely the same during strongly southward IMF. Similarly complex tendency 253 for the density appeared in the results from the emulator ver2.0, as shown in the right panel of 254 Figure 8. In contrast to the density, the dependence of the AE peak intensity on the solar wind 255 speed is relatively simple, as linearly correlating with the product of southward IMF Bz and solar 256 wind speed V, which was seen in both Ebihara and Tanaka (2019) as well as in the left panel of 257 Figure 8. 258

Although it is improved from ver1.0 (Kataoka et al., 2023), the temporal resolution of 5 min still gives the major limitation of the SMRAI2. For example, we cannot discuss the highly dynamic phenomena such as the substorm onset and sudden commencement, in which all 262 ionospheric parameters drastically evolve in a short time scale of less than 5 min. Those rapid

- variation can cause large-amplitude GIC events, which is one of the important targets of the
- operational space weather forecast. One of the future works, therefore, include improving of the
- temporal resolution to 1 min since the ESN method can be applied to diverse temporal scales
- (Tanaka et al., 2022a). Caveat should also be made here that it may not so simply work to solve
- the substorm-onset-related problems by improving the temporal resolution because there is an essential difficulty in reproducing the variation just before and after the substorm onsets, as
- coming from the probabilistic nature of the substorm onsets (Nakano and Kataoka, 2022; Nakano
- et al., 2023).

Therefore, another natural next step would be the data assimilation of the SMRAI2 emulator to correct the exact timing of the substorm onset and the amplitude via the observation data. The million-times faster SMRAI2 emulator has a significant advantage in this direction, compared to the physics-based simulation, because it is essential to increase the ensemble number necessary for data assimilation. For realizing the data assimilation-based forecast, it would be reasonable to use any partial data or point data which is available for real-time use via

applying the cutting-edge data assimilation techniques (Nakano et al., 2020).

278 **5 Conclusions**

We showed that SMRAI2 emulator model is ready-to-use for the real-time space weather 279 forecast of the auroral current system for both the northern and southern hemispheres. We 280 developed the latest upgraded version 2.0 of the ESN-based emulator for the REPPU 281 simulation's ionospheric outputs of the field-aligned current, potential, and conductivity, which 282 runs a million times faster than the REPPU code. The resolutions of the latest ESN-based 283 emulator ver2.0 are significantly improved in time, latitude, and longitude, compared to the 284 ver1.0, and the dipole tilt angle is also newly introduced as one of the input parameters, in 285 addition to IMF By, Bz, V, and Np, thanks to an order of magnitude larger training dataset. We 286 confirmed that the IMF clock-angle dependence of the auroral current system is consistent with 287 that obtained from empirical models. New functions of the ESN-based emulator ver2.0 includes 288 automatic OMNI solar wind data input and the AE index output by indicating the date only. 289

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301 **Open Research**

The OMNI solar wind data with the AE/AU/AL indices are publicly available at https://omniweb.gsfc.nasa.gov/ow_min.html. The Python 3 codes and the training/testing datasets for the ESN-based emulator model, SMRAI2, used in this study are open to the public at https://github.com/ryuhokataoka/REPPU-ESN2 (v2.0.0 was released at

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410

Figure 1. Block diagram of SMRAI2 development to graphically summarize the relationshipamong the REPPU, PCA, and ESN.



411 **Figure 2**. The tilt angle dependence of Σxy . Steady-state conditions of SMRAI2 are shown,

fixing the solar wind parameters By = 0.0 nT, Bz = 5.0 nT, Np = 5/cc, and Vsw = 400 km/s.



414 **Figure 3**. The IMF clock angle dependence of field-aligned current in the northern hemisphere.

- Steady-state conditions from the SMRAI2 are shown, fixing the tilt angle = 0.0, B = 5.0 nT, Np
- 416 = 5/cc, and Vsw = 450 km/s.



418 **Figure 4**. The IMF clock angle dependence of ionospheric potential in the northern hemisphere.

Steady-state conditions from the SMRAI2 are shown, fixing the tilt angle = 0.0, B = 5.0 nT, Np = 5/cc, and Vsw = 450 km/s.



421

422 **Figure 5**. The IMF clock angle dependence of ionospheric potential in the northern hemisphere

423 as obtained from the Weimer2K empirical model, with the tilt angle = 0.0, B = 5.0 nT, Np =

424 5/cc, and Vsw = 450 km/s.



Figure 6. Example of the calculation of AU/AL indices by SMRAI2, compared with the

427 observed values, for the one-month time interval from October 1, 1999.





430 **Figure 7**. 2D histogram for the AE index as predicted by SMRAI2 against the observed AE

431 index for the 15-year time interval from January 1, 2000.



Figure 8. Heat map analysis of the SMRAI2-predicted AE peak intensity in the (left) IMF Bz-V
space and in (right) IMF Bz-Np space.

Start	End	# of days	Notes
2021/05/10	2021/05/15	5	Shock, moderate storm
2021/05/31	2021/06/03	4	Shock
2021/07/26	2021/07/29	4	northward IMF
2021/09/09	2021/09/12	4	northward IMF
2021/10/11	2021/10/14	4	Shock
2021/11/01	2021/11/06	6	Shock, intense storm
2021/11/25	2021/11/29	5	Shock
2022/01/30	2022/02/03	5	Shock
2022/03/11	2022/03/15	5	Shock
2022/03/28	2022/04/1	5	Shock
2022/08/15	2022/08/19	5	Shock
2021/12/01	2022/01/24	55	Long run for training
2022/06/10	2022/07/31	52	Long run for testing

Table 1. List of the selected events for training and testing the ESN model.

Table 2. Specifications of SMRAI emulators version 1.0 (Kataoka et al., 2023) and version 2.0

439 (this study).

Parameters	SMRAI1	SMRAI2
Time resolution	10 min	5 min
Latitude resolution	~2 deg	~1 deg
Longitude resolution	11.25 deg	4.5 deg
Input solar wind parameters	By, Bz, Np, Vsw	Tilt, By, Bz, Np, Vsw
Training dataset	~10 days worth	~100 days worth
Hemisphere	North only	North and south