

# Supplementary Material

## DATA AVAILABILITY

Supporting information (Movies S1 - S4 and Data sets S1 - S4) are archived and available online (via https://doi.org/10.5281/zenodo.5542601). In addition, raw simulation data are preserved on the Cheyenne supercomputer and can be made available upon request.

#### **1 SUPPLEMENTARY DATA**

#### Data Sets S1-S3

Data Set S1 contains a randomly chosen sample of  $N_p = 2.5 \times 10^3$ , of the  $2 \times 10^7$  total, example test particle trajectories taken from the GCRC run. Data Sets S2 and S3 contain the same sample taken from PRC and HRC, respectively, i.e. the test particles in each of the data sets have matching initial conditions but are evolved using different particle mass.

These data are in the <code>H5Part1</code> particle data format, built on <code>HDF52</code>, and can be loaded into commonlyused visualization tools like <code>VisIt3</code> or <code>Paraview4</code>. Data is grouped into temporal slices, <code>Step#N</code>, refers to the  $n^{th}$ -output, with output cadence  $\Delta t = 5$  seconds. For each time slice, particle variables are stored as size  $N_p$  arrays. For instance, <code>Step#20/K</code>, is a size  $N_p$  array storing energies of each test particle at time  $T = 20 * \Delta t = 100$  seconds.

For each test particle we store the following variables:

- •"x"  $[R_E]$ : Particle position, SM-X.
- •"y"  $[R_E]$ : Particle position, SM-Y.
- •"z"  $[R_E]$ : Particle position, SM-Z.
- •"Xeq"  $[R_E]$ : Particle equatorial projection, SM-X.
- •"Yeq"  $[R_E]$ : Particle equatorial projection, SM-Y.
- •"Keq" [keV]: Particle energy in the  $E \times B$  frame of the equatorial projection.
- •"Aeq" [degrees]: Equatorial pitch angle of particle, i.e. particle is projected to the equator and conservation of the first invariant is assumed.
- •"id": Particle identifier, integer from  $[0, N_p]$ .
- •"T0" [seconds]: Particle activation time, when this particle is "born". Prior to this time, the particle is not meaningful and data is merely stored as a placeholder.
- •"isIn" [Boolean]: Whether or not particle is active. Inactive (isIn=0) particles either haven't yet been created, i.e. time is before T0in, or have been lost from the simulation domain. Otherwise particle is active (isIn=1).

<sup>&</sup>lt;sup>1</sup> http://dav.lbl.gov/archive/Research/AcceleratorSAPP

<sup>&</sup>lt;sup>2</sup> https://www.hdfgroup.org

<sup>&</sup>lt;sup>3</sup> https://wci.llnl.gov/simulation/computer-codes/visit/

<sup>&</sup>lt;sup>4</sup> https://www.paraview.org

A simple, example Python script is shown below to demonstrate reading and plotting data from the collection of test particle trajectories.

```
1 #Example Python script to use Dataset S1-S3, H5Part test particle data
 2 #Displays trajectories of first N0 test particles projected to the equatorial plane
 3 #S1: GCRC
 4 #S2: PRC
 5 #S3: HRC
 6
7 import numpy as np
 8 import h5py
9 import matplotlib.pyplot as plt
10
11 NO = 10 #Number of particles to display, starting at first
12
13 fIn = "DatasetS1.h5part" #Name of input dataset
14 with h5py.File(fIn, 'r') as hf:
15
     gIDs = [str(grp.name) for grp in hf.values()] #Group IDs
     Nt = len([stp for stp in gIDs if "/Step#" in stp]) #Number of time slices
16
17
18
    X = np.zeros((Nt, N0))
19
    Y = np.zeros((Nt, N0))
20
    for i in range(Nt):
21
     gID = "Step#%d"%(i)
22
       X[i,:] = hf[gID]["xeq"][0:N0]
23
       Y[i,:] = hf[gID]["yeq"][0:N0]
24
25 plt.figure()
26 for n in range (N0):
27
     plt.plot(X[:,n],Y[:,n])
28
29 plt.axis('equal')
30 plt.show()
31
32
```

Listing 1. Example Python visualization using test particle trajectories

#### Data Set S4

A randomly selected subset of the tuples (Equation 5 of main text) derived from the GCRC test particle ensemble in the manner described in Section 2.3. This data set contains  $N = 10^6$  points out of the  $\approx 10^9$ mined from the simulation data.

The data contains the following arrays, each of size N, with each tuple given by a fixed array index over each of the arrays. For the quantites  $\Delta R_{EQ}$  and  $\Delta K$ , the change in radial projection and energy respectively, these changes are over the sampling cadence  $\Delta t = 5s$ .

- •"Xeq"  $[R_E]$ : Particle equatorial projection, SM-X.
- •"Yeq"  $[R_E]$ : Particle equatorial projection, SM-Y.
- •"K" [keV]: Particle energy.
- •"Aeq" [degrees]: Particle equatorial pitch angle,  $\alpha_{EQ}$ .
- •"dR"  $[R_E]$ : Change in radius of equatorial projection,  $\Delta R_{EQ}$ .
- •"dK" [keV]: Change in particle energy in the local  $E \times B$  frame,  $\Delta K$ .

- •"Lb"  $[R_E]$ : Magnetic lengthscale,  $L_{\nabla B}$ , defined by Equation 4.
- •"dS" : Local buoyancy,  $\delta S$ , defined by Equation 2.

A simple, example Python script is shown below to demonstrate reading and plotting data, in this case a 2D histogram comparing local buoyancy and radial transport, from the data set.

```
1 #Example Python script to use Dataset S4, H5 correlation data as described in main text
 2 #Display 2d histogram plot of dR (equatorial change in radius) versus dS (local buoyancy)
 3
4 import numpy as np
 5 import h5py
6 import matplotlib.pyplot as plt
7 import matplotlib as mpl
8
9 fIn = "DatasetS4.h5" #Name of input dataset
10 with h5py.File(fIn, 'r') as hf:
    dR = hf["dR"] [...] #Radial displacement
11
    dS = hf["dS"] [...] #Local buoyancy
12
13
    dK = hf["dK"] [...] #Change in energy
14
    K = hf["K"] [...] #Energy
15
    Xeq = hf["Xeq"][...] #Equtorial X
    Yeq = hf["Yeq"][...] #Equtorial Y
16
17
    W = hf["W" ] [...] #Test particle weights
18
19 #Make histogram
20 V = mpl. colors. LogNorm(1.0e-3, 10)
21 plt.figure()
22 plt.hist2d(dS,dR,bins=(250,250),density=True,weights=W*K,norm=V)
23 plt.xlim([-0.6,0.6])
24 plt.ylim([-1,1])
25 plt.colorbar()
26 plt.axhline(y=0.0, color='red')
27 plt.axvline(x=0.0, color='red')
28 plt.show()
29
30
```

Listing 2. Example Python histogram using correlation data.

#### 2 SUPPLEMENTARY MOVIES

Movie S1: Animation of integrated flux tube entropy in the format of Figure 2 of the main text.

- Movie S2: Animation of combined MHD and test particle simulation data for GCRC in the format of Figure 1 of the main text.
- Movie S3: Animation of combined MHD and test particle simulation data for PRC in the format of Figure 1 of the main text.
- Movie S4: Animation of combined MHD and test particle simulation data for HRC in the format of Figure 1 of the main text.

### **3 SUPPLEMENTARY FIGURES**



**Figure S1.** Example of the "local buoyancy", defined by Equation 2 in the main text, plotted in the equatorial plane. Blue regions correspond to "bubbles", regions with depleted entropy relative to the background. Solid lines depict contours of constant magnetic field strength.



**Figure S2.** Local buoyancy, defined by Equation 2 in the main text, plotted as a function of time and MLT, measured in degrees with  $180^{\circ}$  corresponding to midnight, for selected values of radius.



**Figure S3.** Distribution of magnetic lengthscale, defined by Equation 4 of the main text, for two categories of bubbles: "all bubbles",  $\delta S < -0.075$ , and "deeply depleted bubbles",  $\delta S < -0.2$ . The quantity  $\delta S$ , the local buoyancy, is defined by Equation 2 in the main text.



**Figure S4.** Resolution study of the magnetic lengthscale, defined by Equation 4 in the main text, in the same format as Figure 5 of the main text.



**Figure S5.** Comparison of the evolution of GCRC (panel a), PRC (panel b), and HRC (panel c) in the same format as Figure 1 of the main text. State of the MHD and test particles are shown at T = 0, the time at which injection of new test particles is stopped after an hour of continuous test particle seeding.