

Supplementary Information

for

Automated Optimization of Solar Energetic Particle Acceleration and Transport Parameters Against Five-Spacecraft Observations of the 9 October 2021 Event

Hiroyuki Tako Ishikawa^{1,*}, Naho Fujita¹, Yuta Kato^{1,2}, Miki Kurihara^{1,3}, Takashi Minoshima⁴, Daikou Shiota^{5,2}, Kazumasa Iwai², Marco Pinto⁷, António Pessanha Gomes^{7,8}, Go Murakami⁶, Kanya Kusano², and Chihiro Mitsuda^{1,2}

¹Space Data Frontiers Research Center, Fujitsu Research, Fujitsu Limited, Japan

²Institute for Space–Earth Environmental Research, Nagoya University, Japan

³Graduate School of Science, Department of Astronomy, The University of Tokyo, Japan

⁴Center for Mathematical Science and Advanced Technology, Japan Agency for Marine–Earth Science and Technology, Japan

⁵Radio Research Institute, National Institute of Information and Communications Technology, Japan

⁶Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, Japan

⁷Laboratory of Instrumentation and Experimental Particle Physics, Lisboa, Portugal

⁸Instituto Superior Técnico, Universidade de Lisboa, Portugal

*ishikawa.h.tako@fujitsu.com

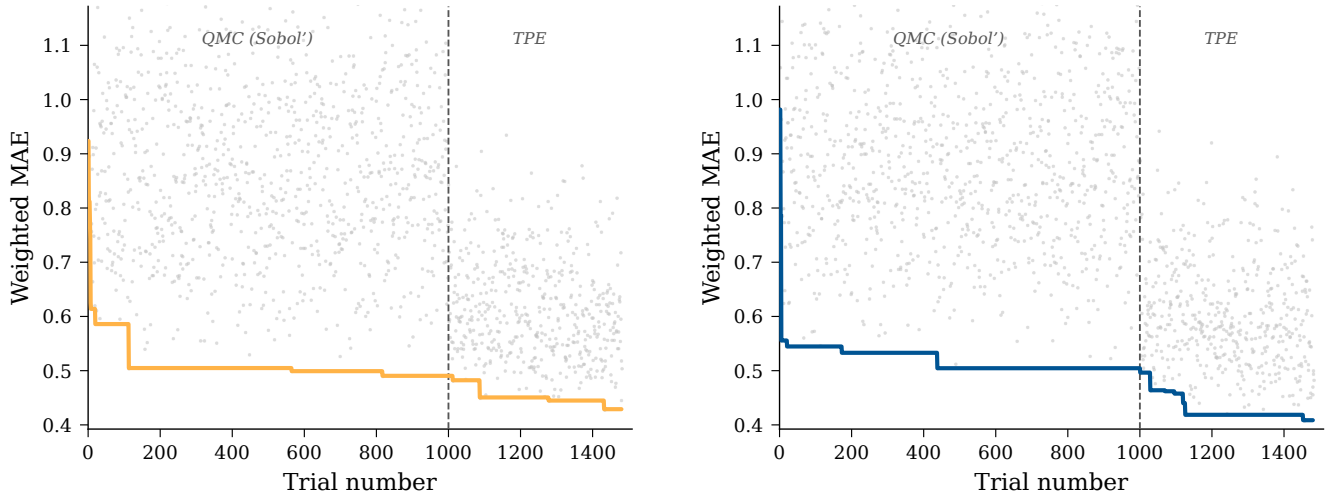


Figure S1. Optimization history for the RUN1 (left) and RUN2 (right) MHD configurations. Each point represents the objective function value (the weighted MAE of the main-text equation for $\mathcal{L}$, in $\log_{10}$ space) of a single trial; the solid curve traces the running best. The vertical dashed line at trial 1000 marks the transition from QMC (Sobol') sampling to TPE.

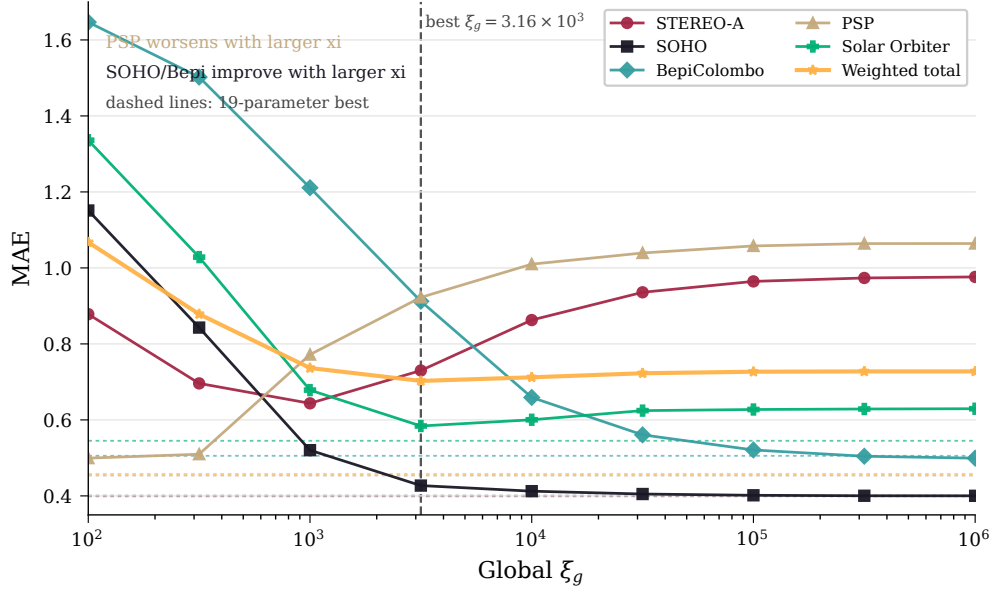


Figure S2. Response of the objective function to collapsing the seven free mean free path coefficients onto a single global value ξ_g , with the twelve injection efficiencies held at the RUN1 best-fit values. The horizontal axis is ξ_g on a logarithmic scale; the vertical axis is the mean absolute error. Curves show the per-spacecraft MAE for the five observers and the weighted total. The horizontal dashed line marks the objective value of the 19-parameter best-fit solution and the vertical dashed line marks the best global value, $\xi_g = 3.2 \times 10^3$. PSP, the only spacecraft magnetically connected to the eastern field lines, degrades monotonically as ξ_g increases, whereas SOHO and BepiColombo improve monotonically, so that no single value satisfies all five observers simultaneously.

Table S1. Shock parameters passed from the coupling module to SEPIF. All shock-surface quantities listed below are functions of heliolongitude ϕ on the shock front. When evaluating the source term Q_j acting on field line j , these quantities are sampled at $\phi_j(t)$, the heliolongitude where field line j intersects the shock at time t .

Quantity	Symbol used in this paper	Role in SEPIF
Time coordinate	t	Time axis for transport and injection
Heliolongitude on shock surface	ϕ	Field-line–shock intersection $\phi_j(t)$ and bin mapping $k(j, t)$
Shock radius	R_{shk}	Shock position along each magnetic field line
Radial shock speed	V_{shk}	DSA source term in Q_j
Upstream speed in shock frame	V_{up}	Injection momentum and spectral index
Downstream speed in shock frame	V_{down}	Compression and spectral index
Upstream density	n_{up}	Source normalization in Q_j
Compression ratio	$s = V_{\text{up}}/V_{\text{down}}$	$\beta = 3s/(s - 1)$
Magnetic-field magnitude	$ B $	Transport coefficients and flux conversion
Shock obliquity angle	θ_B	Injection/acceleration efficiency terms

Table S2. Parameter bounds and scaling for the 19-parameter optimization.

Parameter	N_{free}	Min	Max	Scale
ξ (mean free path coefficient)	7	1	10^6	log
ξ_{shk} (shock MFP coefficient)	0 (fixed)		1.0	—
e_0 (injection efficiency)	12	10^{-4}	3×10^{-2}	log

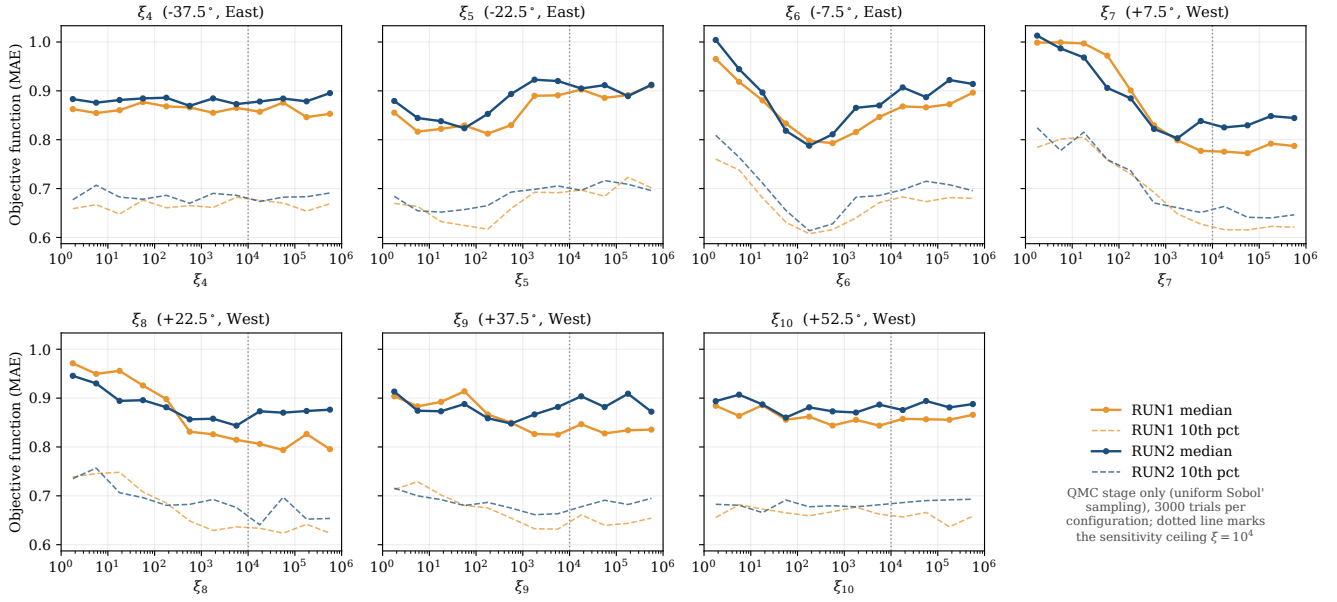


Figure S3. Marginal response of the objective function to each free mean free path coefficient. Each panel shows, for one coefficient ξ_j , the median objective value among all trials falling in a given logarithmic bin of ξ_j (solid, circles) and the corresponding 10th percentile (dashed), for RUN1 (orange) and RUN2 (blue). Only the QMC stage is used, so that the trials are a uniform Sobol' sample of the 19-dimensional search space and the marginal is not biased by the adaptive sampling of the TPE stage; each configuration contributes 3000 trials. The dotted vertical line marks the sensitivity ceiling $\xi = 10^4$. The eastern coefficients ξ_5 and ξ_6 show interior optima, ξ_7 and ξ_8 decrease monotonically and then plateau above the ceiling, and ξ_4 and ξ_{10} are flat across the entire search range. Values are marginalized over the remaining 18 parameters, so a flat curve indicates that the objective does not respond to that parameter on average, not that it is unconstrained under every configuration of the others.

Table S3. Energy channels and observation selection windows used for each spacecraft. The window end times were chosen to terminate before or near the local CME-driven shock passage at each observation point and therefore differ from the intervals adopted in other studies of this event (e.g., Palmerio et al. (2024, J. Space Weather Space Clim. 14, 3)). The windows listed here define the interval from which the observations are drawn. The objective function is evaluated on the time axis common to the observations and the simulation, and the simulated output begins only when the reconstructed shock reaches the inner boundary of the transport domain; the earliest sample that can therefore contribute lies between 06:55 and 07:35 UT on 9 October depending on the spacecraft, so no sample earlier than that enters the objective even though the windows nominally start at 00:00 UT. The last column gives the viewing direction of the data used: *integrated* denotes a direction-integrated product, *single* a single-aperture instrument, and the remaining entries the telescope selected.

Spacecraft	Instrument(s)	Energy channels (MeV)	Observation selection window (UTC, 2021)	Viewing direction
STEREO-A	LET, HET	4.0–4.5, 4.5–5.0, 5.0–6.0, 14.9–17.1, 29.5–33.4, 40.0–60.0	Oct 9 00:00 – Oct 12 00:15	integrated
SOHO	COSTEP/EPHIN	4.3–7.8, 7.8–25, 25–40.9, 40.9–53.0	Oct 9 00:00 – Oct 12 00:52	single
BepiColombo	BERM	1.5–5.9, 5.9–9.1	Oct 9 00:00 – Oct 9 23:46	anti-sunward
PSP	IS $\odot$ IS/EPI-Hi	13.5–16.0, 26.9–32, 45.3–53.8	Oct 9 00:00 – Oct 11 08:05	HET, A
Solar Orbiter	EPD/EPT, HET	5.83–6.13, 14.6–15.7, 29.4–32.0, 49.1–53.4	Oct 9 00:00 – Oct 11 01:52	sunward

ξ_g	STEREO-A	SOHO	BepiColombo	PSP	Solar Orbiter	Weighted total	N
$10^{2.0}$	0.878	1.151	1.647	0.499	1.336	1.068	9538
$10^{2.5}$	0.696	0.843	1.502	0.510	1.028	0.878	10129
$10^{3.0}$	0.644	0.520	1.211	0.772	0.678	0.737	10171
$10^{3.5}$	0.730	0.427	0.912	0.922	0.584	0.703	9975
$10^{4.0}$	0.863	0.412	0.659	1.010	0.600	0.712	9857
$10^{4.5}$	0.936	0.405	0.561	1.039	0.624	0.723	9820
$10^{5.0}$	0.965	0.402	0.521	1.058	0.627	0.727	9808
$10^{5.5}$	0.974	0.400	0.504	1.064	0.629	0.728	9803
$10^{6.0}$	0.976	0.400	0.499	1.064	0.629	0.728	9801
19-parameter best	0.399	0.401	0.505	0.454	0.545	0.458	10480

Table S4. Objective function of the spatially uniform baseline, in which the seven free mean free path coefficients ξ_4 – ξ_{10} are replaced by a single global value ξ_g while the twelve injection efficiencies are held at the RUN1 best-fit values. Columns 2–6 give the per-spacecraft MAE, defined as the mean over that spacecraft’s energy channels; column 7 gives the weighted mean over the five spacecraft using the weights adopted in the optimization (unity for STEREO-A, SOHO, PSP and Solar Orbiter, 0.7 for BepiColombo); column 8 gives the total number of channel-time points that pass the evaluation mask. The grid is logarithmic with a half-decade spacing. The row in bold is the best global value. The last row repeats the 19-parameter best-fit solution of the RUN1 representative session for reference; a re-evaluation of that solution reproduced the objective value recorded by the optimizer, 0.42896826316091, exactly; the value of 0.458 listed here is the same solution scored with the Solar Orbiter EPT channel corrected, as described in the Objective Function subsection of the Methods. A confirmatory run in which the three fixed far-eastern coefficients ξ_1 – ξ_3 were also set to ξ_g at the best global value returned identical per-spacecraft and total values and an identical N , confirming that those field lines do not contribute to the objective function. Note that N varies across the grid because the evaluation mask depends on the simulated intensity; the poorer fits have more points removed, so the degradation relative to the 19-parameter solution is if anything understated.