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Observation-Based Initialization for Inverse Modeling of Atmospheric Temperature with Rossby-Constrained Transport

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Abstract

We consider a finite-dimensional inverse problem for atmospheric temperature transport from sparse satellite observations. A spectral stream function with Rossby dispersion defines the horizontal velocity, and a convection–diffusion equation maps its parameters to temperature measurements. The main methodological component is a regularized construction of the initial temperature and compatible latitudinal boundary values from the preceding day’s observations. A bounded latitude coordinate, a low-order background, and two longitudinal harmonics provide a smooth periodic initial field without using the assimilation day’s temperatures. Continuous piecewise-linear finite elements, implicit Euler stepping, and streamline upwind/Petrov–Galerkin stabilization solve the forward problem. An adaptive artificial bee colony algorithm identifies 28 flow parameters under a shared perturbation-speed constraint. For 105 nighttime Aura Microwave Limb Sounder measurements on 6 March 2011, the fine-mesh root-mean-square discrepancy is 5.129 K and the Pearson correlation is 0.660. The corresponding linear-initialization experiment gives 6.127 K and 0.373, respectively. The root-mean-square discrepancy therefore decreases by 16.3%. A static evaluation of the new initial field gives a correlation of 0.549, providing a reference for assessing the additional improvement obtained with optimized transport. The results support observation-based initialization for temperature reconstruction within the considered model and motivate further evaluation of predictive performance and flow identifiability.

Keywords: Inverse problem, Convection–diffusion equation, Finite element method, Rossby waves, Initial conditions, Satellite temperature data

Dedicated to Professor Ivan Egorovich Egorov on the occasion of his 75th anniversary

1 Introduction

Reconstruction from irregular measurements is a central problem in differential-equation-based modeling. In atmospheric applications, satellite observations provide broad coverage but do not specify a simultaneous continuous field. The measured temperature must therefore be connected to model variables through an explicit observation operator. Planetary Rossby waves offer a reduced description of large-scale horizontal motion, with propagation controlled by the latitudinal variation of the Coriolis parameter [1, 2]. Temperature, however, is not identical to the stream function: its response also depends on the transported background and on the initial and boundary data.

The Microwave Limb Sounder (MLS) on Aura measures atmospheric temperature profiles along a nearly polar orbit [3, 4]. At a selected vertical level, these data form sparse tracks in space and time. Direct harmonic approximation of temperature has been explored with artificial bee colony optimization [5, 6]. A transport formulation instead uses spectral flow parameters to generate a velocity and computes the temperature by solving a partial differential equation. This distinction is essential when interpreting inferred amplitudes and velocities.

Initial conditions are particularly influential in a weakly diffusive model. A prescribed linear latitude profile may create a meridional gradient that is poorly matched to the observed day. Conversely, replacing that profile by a nearly uniform temperature removes much of the mechanism by which horizontal advection generates temperature variations. The initial field must therefore represent both the latitude background and the longitudinal structure. Its continuation to unobserved latitudes must also agree with the imposed boundary values.

This paper combines a regularized, preceding-day initialization with a Rossby-constrained temperature transport inverse problem. The initial field uses a bounded latitude coordinate and a small number of longitudinal modes, selected by cross-validation with complete satellite passes withheld. A smooth envelope makes the longitudinal contribution vanish at the channel boundaries. The resulting initial and boundary data are fixed before the target-day flow inversion. A stabilized finite element solver [7, 8] and an adaptive artificial bee colony search [9] complete the computational framework.

The numerical study compares linear initialization, static evaluation of the observation-based initial field, and transport after parameter identification. All reported model–observation statistics use the same 105 target-day observations. This comparison assesses the sensitivity of the reduced inverse model to its temperature initialization. It also makes explicit the distinction between a better temperature fit and uniquely identifiable Rossby-wave dynamics.

2 Transport model and inverse problem

Let λ and φ be longitude and latitude in radians. Local angular coordinates centered at $\varphi_0 = 62^\circ\text{N}$ are

$$x = \cos \varphi_0 \lambda, \quad y = \varphi - \varphi_0, \quad X = R_E x, \quad Y = R_E y, \quad (1)$$

where $R_E = 6371000$ m. The computational channel is

$$\Omega = (-\pi \cos \varphi_0, \pi \cos \varphi_0) \times (\varphi_B - \varphi_0, \varphi_N - \varphi_0), \quad (2)$$

with $\varphi_B = 50^\circ\text{N}$ and $\varphi_N = 80^\circ\text{N}$. This is a local β -plane approximation over a full periodic longitude interval, not a spherical metric discretization. Its use across a 30-degree latitude band is a modeling approximation.

We prescribe

$$\psi(\mathbf{p}; x, y, t) = \sum_{m=0}^{M-1} A_m \cos(k_m x + l_m y - \omega_m t + \theta_m), \quad (3)$$

$$k_m = \frac{m}{\cos \varphi_0}, \quad \omega_m = \mathcal{U} k_m - \frac{\beta_a k_m}{k_m^2 + l_m^2}, \quad (4)$$

where $\beta_a = 2\Omega_E \cos \varphi_0 \simeq 6.84688 \times 10^{-5} \text{ s}^{-1}$, $\Omega_E = 7.292115 \times 10^{-5} \text{ s}^{-1}$, and $\mathcal{U} = U_{\text{phys}}/R_E$. For $k_m = l_m = 0$, the dispersive term is set to zero. The scaled stream function ψ and its amplitudes have units s^{-1} ; the dimensional stream function is $R_E^2 \psi$. The angular-coordinate velocity and physical perturbation velocity are

$$\mathbf{b} = (-\psi_y, \psi_x), \quad \mathbf{v}' = R_E \mathbf{b}, \quad \nabla \cdot \mathbf{b} = 0. \quad (5)$$

The parameter vector is

$$\mathbf{p} = (l_0, A_0, \theta_0, \dots, l_{M-1}, A_{M-1}, \theta_{M-1}, \mathcal{U}). \quad (6)$$

In the reported implementation, $\mathcal{U}$ enters the dispersion relation only. The transport velocity in Eq. (5) contains the perturbation flow, without an added mean zonal velocity. Accordingly, U_{phys} is interpreted here as a phase-propagation parameter rather than an independently recovered total zonal wind. Mode $m = 0$ is stationary and zonally uniform; it is not a propagating longitudinal wave.

The admissible set consists of

$$0 \leq l_m \leq 4, \quad -\pi \leq \theta_m \leq \pi, \quad 0 \leq A_m \leq \frac{V_{\text{max}}}{R_E \sqrt{k_m^2 + l_m^2}}, \quad (7)$$

$$-20 \leq U_{\text{phys}} \leq 100 \text{ m/s}, \quad B(\mathbf{p}) := R_E \sum_{m=0}^{M-1} A_m \sqrt{k_m^2 + l_m^2} \leq V_{\text{max}}, \quad (8)$$

with $V_{\max} = 20$ m/s. The amplitude bounds limit each modal velocity contribution individually, while the shared constraint limits their combined contribution.

The shared constraint in Eq. (8) bounds the physical spectral perturbation velocity uniformly in space and time. Indeed, the m -th velocity contribution is $R_E A_m(l_m, -k_m) \sin(k_m x + l_m y - \omega_m t + \theta_m)$, whose magnitude is at most $R_E A_m \sqrt{k_m^2 + l_m^2}$. For every admissible parameter vector, the triangle inequality therefore gives $|\mathbf{v}'| \leq B(\mathbf{p}) \leq V_{\max}$ at every position and time.

This sufficient bound can be conservative because the modal velocities need not attain their individual maxima together. Candidates exceeding the bound are repaired by multiplying every amplitude by $V_{\max}/B(\mathbf{p})$, with a small inward numerical tolerance.

For fixed $\mathbf{p}$, the temperature T satisfies

$$\partial_t T + \mathbf{b}(\mathbf{p}) \cdot \nabla T - D \Delta T = 0 \quad \text{in } \Omega \times (0, t_f], \quad (9)$$

where

$$D = \frac{D_{\text{phys}}}{R_E^2} = 2.4636827904 \times 10^{-12} \text{ s}^{-1}, \quad D_{\text{phys}} = 100 \text{ m}^2/\text{s}. \quad (10)$$

The diffusivity is a fixed effective coefficient in this two-dimensional experiment, not an estimated physical eddy diffusivity. Temperature and diffusive flux are periodic in x . The remaining conditions are

$$T(x, y, 0) = T_0(x, y), \quad T(x, y_B, t) = T_B, \quad T(x, y_N, t) = T_N. \quad (11)$$

Section 3 constructs all three temperature data consistently.

The equation is a reduced horizontal transport model. It omits vertical advection, adiabatic temperature changes, radiative forcing, and the dynamical feedback of temperature on the flow. The stream function is a superposition of prescribed dispersive modes; no nonlinear barotropic vorticity equation is solved. These choices delimit the interpretation of the inverse problem.

For two solutions with the same $\mathbf{b}$, diffusivity, and boundary values, their difference w has homogeneous latitude traces. Periodicity and $\nabla \cdot \mathbf{b} = 0$ yield

$$\frac{1}{2} \frac{d}{dt} \|w\|_{L^2(\Omega)}^2 + D \|\nabla w\|_{L^2(\Omega)}^2 = 0. \quad (12)$$

Indeed, multiplication by w and integration by parts eliminate the advective and diffusive boundary terms. This gives uniqueness for the fixed-coefficient forward problem and a contraction with respect to its initial field. It does not imply rapid forgetting of that field when diffusion is weak. It also does not compare the two numerical experiments directly, since their boundary values and fitted velocities differ.

At the initial time,

$$\partial_t T|_{t=0} = -\mathbf{b} \cdot \nabla T_0 + D \Delta T_0. \quad (13)$$

With a zonally uniform T_0 , the advective temperature response comes entirely from its latitude gradient. An almost uniform replacement would therefore suppress this response unless longitudinal structure is supplied separately.

For observations d_j at positions $\mathbf{z}_j$ and times assigned to satellite passes, the discrete inverse problem is

$$\min_{\mathbf{p} \in \mathcal{P}} J_h(\mathbf{p}), \quad J_h(\mathbf{p}) = \frac{1}{N_{\text{obs}}} \sum_{j=1}^{N_{\text{obs}}} [H_j T_h(\mathbf{p}; \bar{t}_{q(j)}) - d_j]^2. \quad (14)$$

Here $\mathcal{P}$ is defined by Eqs. (7)–(8); H_j is specified in Section 4. The flow inversion uses an unweighted temperature discrepancy. The regularization introduced below applies to the initial field, not to J_h . With $M = 9$, the flow inversion has $3M + 1 = 28$ parameters.

3 Observation-based initial and boundary data

The initialization uses only nighttime observations from 5 March 2011. The flow parameters are subsequently fitted to 6 March. Both days contain 105 selected observations in 15 passes. The preceding-day latitude range is 58.994° – 67.515° N, substantially narrower than the computational channel.

To control continuation outside this interval, introduce the bounded latitude coordinate

$$\eta(\varphi) = \tanh\left(\frac{\varphi - \varphi_c}{s_\varphi}\right), \quad \varphi_c = 63.254^\circ, \quad s_\varphi = 5^\circ. \quad (15)$$

The ratio uses the same angular units in numerator and denominator. The center is the midpoint of the observed latitude range. The scale s_φ is a chosen smoothing parameter. Boundedness prevents polynomial growth far outside the data, but introduces a prior tendency toward a flatter background; it is not an atmospheric law.

For L longitudinal harmonics, define

$$\bar{T}_0(\varphi) = c_0 + c_1 \eta + c_2 P_2(\eta), \quad P_2(\eta) = \frac{1}{2}(3\eta^2 - 1), \quad (16)$$

$$W_0(\varphi, \lambda) = \sum_{r=1}^L [(a_r + b_r \eta) \cos(r\lambda) + (d_r + e_r \eta) \sin(r\lambda)]. \quad (17)$$

All coefficients have units K. These temperature modes are distinct from the stream-function modes in Eq. (3). The index r prevents confusion between the two expansions.

Let $\mathbf{c} = (c_0, c_1, c_2, a_1, d_1, b_1, e_1, \dots)$ and let B_L be the design matrix evaluated at the preceding-day observation positions. The coefficient vector minimizes

$$\|B_L \mathbf{c} - \mathbf{d}_0\|_2^2 + \alpha \mathbf{c}^\top \Lambda_L \mathbf{c}, \quad \alpha = 1, \quad (18)$$

where

$$\text{diag } \Lambda_L = (0, 0.2, 3, 1^2, 1^2, 2 \cdot 1^2, 2 \cdot 1^2, \dots, L^2, L^2, 2L^2, 2L^2). \quad (19)$$

Table 1 Initial-field model selection using only 5 March 2011. Errors are in K; the validation column holds out complete satellite passes

L	Coefficients	Training RMSE	Pass-grouped RMSE
0	3	6.293	6.368
1	7	5.997	7.401
2	11	3.053	4.473
3	15	2.942	4.521
4	19	2.681	4.718

Thus the intercept is unpenalized, whereas curvature, higher longitudinal orders, and latitude modulation receive stronger penalties. The numerical weights are fixed modeling choices. The solution is

$$\mathbf{c}^* = (B_L^\top B_L + \alpha \Lambda_L)^{-1} B_L^\top \mathbf{d}_0. \quad (20)$$

For $\alpha > 0$ and at least one observation, the regularized problem in Eq. (18) has a unique minimizer. Indeed, for any $\mathbf{z} \neq 0$, the quadratic form of the coefficient matrix $B_L^\top B_L + \alpha \Lambda_L$ is $\|B_L \mathbf{z}\|_2^2 + \alpha \mathbf{z}^\top \Lambda_L \mathbf{z}$. Both terms are nonnegative. If the second term vanishes, only the intercept component can be nonzero. Since the first design column consists of ones and there is at least one observation, the first term is then strictly positive. The coefficient matrix is therefore positive definite.

The order L is selected among $0, \dots, 4$ using five folds of complete passes. Number passes from zero and assign pass q to fold $q \bmod 5$. Each fold holds out three entire passes; the prediction errors from all folds are pooled. Fixed coordinate and penalty choices are used throughout. The result is a source-day model-selection diagnostic, not an independent validation error for the subsequent transport inversion.

Table 1 favors $L = 2$. Adding further harmonics lowers the training error but does not lower the grouped validation error. The difference between $L = 2$ and $L = 3$ is small, so the selected order should not be interpreted as proof of a unique atmospheric spectrum.

Let φ_- and φ_+ be the smallest and largest preceding-day observed latitudes. Define

$$S(z) = \begin{cases} 0, & z \leq 0, \\ 3z^2 - 2z^3, & 0 < z < 1, \\ 1, & z \geq 1, \end{cases} \quad g(\varphi) = S\left(\frac{\varphi - \varphi_B}{\varphi_- - \varphi_B}\right) S\left(\frac{\varphi_N - \varphi}{\varphi_N - \varphi_+}\right). \quad (21)$$

The initial field and boundary temperatures are

$$T_0(\varphi, \lambda) = \bar{T}_0(\varphi) + g(\varphi)W_0(\varphi, \lambda), \quad T_B = \bar{T}_0(\varphi_B), \quad T_N = \bar{T}_0(\varphi_N). \quad (22)$$

Since $g = 1$ throughout the observed latitude interval, the taper preserves the fitted field values at all observation locations. At both boundaries, $g = 0$, so the initial

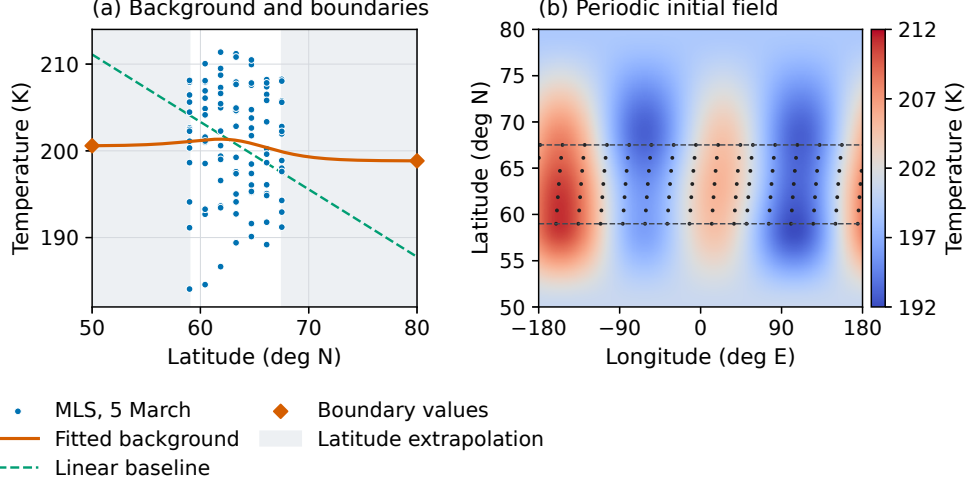


Fig. 1 Observation-based initialization. (a) Preceding-day MLS measurements (blue points), fitted latitude background (orange curve), linear baseline (dashed green curve), and new boundary values (orange diamonds). Light-gray shading marks unobserved latitude intervals. (b) Periodic initial field on a blue-to-red temperature scale, with dark measurement positions and dashed limits of the observed latitude band

latitude traces equal the constant Dirichlet data for every longitude. The resulting initial field is periodic and continuously differentiable.

For the selected $L = 2$, the fitted field is

$$\bar{T}_0 = 200.715693 - 0.864651\eta - 1.016909P_2(\eta), \quad (23)$$

$$W_0 = (-1.911918 + 0.439597\eta) \cos \lambda + (-1.940367 + 1.503594\eta) \sin \lambda \\ + (4.808989 - 0.470116\eta) \cos 2\lambda + (4.819606 + 0.343831\eta) \sin 2\lambda, \quad (24)$$

in K. The unrounded coefficients are retained in the accompanying machine-readable data. The compatible boundary values are

$$T_B = 200.584963 \text{ K}, \quad T_N = 198.843769 \text{ K}. \quad (25)$$

They are extrapolated values, since no selected observations lie at 50° or 80° N. Figure 1 illustrates the fitted background and complete initial field.

The measurements collected during 5 March are combined into one spatial field. This daily composite is assigned at the beginning of the 6 March transport calculation; it is not a simultaneous snapshot at that instant. No within-day phase propagation or intervening evolution from 5 March is applied in the initialization stage. This temporal approximation is an explicit part of the experiment.

The control initialization is

$$T_0^{\text{lin}}(\varphi) = 250 - 70 \frac{\varphi}{\pi/2} \text{ K}, \quad (26)$$

with its own compatible traces 211.111 K at 50°N and 187.778 K at 80°N. Thus the comparison changes both the initial field and its latitude boundary values. It does not isolate their separate effects.

4 Finite element reconstruction and optimization

4.1 Forward discretization and observation operator

Let $V_{\text{per}} \subset H^1(\Omega)$ contain functions with matching longitude traces, V_0 impose zero latitude traces, and V_g impose the two temperatures in Eq. (11). The weak problem is

$$(\partial_t T, v) + (\mathbf{b} \cdot \nabla T, v) + D(\nabla T, \nabla v) = 0 \quad \forall v \in V_0, \quad (27)$$

where $(\cdot, \cdot)$ is the $L^2(\Omega)$ inner product.

Continuous piecewise-linear finite elements are used on a triangular mesh. Periodic degrees of freedom are identified. The stream function is interpolated into the same scalar space, $\psi_h^{n+1} = I_h \psi(\mathbf{p}; t_{n+1})$, and

$$\mathbf{b}_h^{n+1} = (-\partial_y \psi_h^{n+1}, \partial_x \psi_h^{n+1}). \quad (28)$$

This elementwise constant curl is used directly in the transport equation. Its normal component is continuous across mesh faces because the tangential derivative of the continuous linear trace of ψ_h is single-valued. It therefore retains divergence freedom in the distributional sense. A projection into a continuous quadratic vector space is made only for visualization, not for advection.

For $\Delta t_n = t_n - t_{n-1}$, find $T_h^n \in V_{h,g}$ such that

$$\begin{aligned} (T_h^n - T_h^{n-1}, v_h) + \Delta t_n (\mathbf{b}_h^n \cdot \nabla T_h^n, v_h) + \Delta t_n D(\nabla T_h^n, \nabla v_h) \\ + \Delta t_n \sum_K \tau_K (R_K^n, \mathbf{b}_h^n \cdot \nabla v_h)_K = 0, \quad v_h \in V_{h,0}, \end{aligned} \quad (29)$$

$$R_K^n = \frac{T_h^n - T_h^{n-1}}{\Delta t_n} + \mathbf{b}_h^n \cdot \nabla T_h^n, \quad \tau_K = \frac{h_K}{2\sqrt{|\mathbf{b}_h^n|^2 + \epsilon_b}}. \quad (30)$$

Here h_K is the element diameter, and ϵ_b is the small numerical regularizer used in the code to avoid division by zero. The implemented stabilization parameter includes the convection contribution only; temporal and diffusive contributions are not included in τ_K . The residual omits $D\Delta T_h^n$ because that term vanishes inside a linear element. Equations (29)–(30) define the SUPG formulation used in this study [7, 8]. The initial finite element temperature is the nodal interpolant of Eq. (22). Implementation uses FEniCS/DOLFIN [10].

Consecutive observations are assigned to different passes when their time gap exceeds 1000 s. For observation indices $\mathcal{I}_q$ in pass q , define

$$\bar{t}_q = \frac{1}{|\mathcal{I}_q|} \sum_{j \in \mathcal{I}_q} t_j^{\text{obs}}. \quad (31)$$

During optimization, the solver advances successively to the 15 pass-mean times. Each measurement retains its individual spatial position. The maximum shift from its actual time to the pass mean is 74.714 s. This grouping assumes temperature varies slowly over the approximately 150-s passage across the selected latitude band.

For each point $\mathbf{z}_j$, let $\mathbf{z}_{j1}, \mathbf{z}_{j2}, \mathbf{z}_{j3}$ be the three nearest mesh nodes in the coordinates of Eq. (1). Barycentric weights solve

$$\sum_{a=1}^3 w_{ja} = 1, \quad \sum_{a=1}^3 w_{ja} \mathbf{z}_{ja} = \mathbf{z}_j, \quad H_j T_h = \sum_{a=1}^3 w_{ja} T_h(\mathbf{z}_{ja}). \quad (32)$$

This describes the program's nearest-three-node operator. It does not assert that these nodes form the mesh element containing the point. Noncollinearity is required, and weights can be negative if the point lies outside their triangle. An element-search operator would be a natural refinement, but is not part of the reported run.

The final solution is saved at 100 uniformly spaced times with $\Delta t = 832.12$ s. For evaluation at a pass mean between two saved times, the model nodal fields are linearly interpolated in time before applying Eq. (32). At the first pass this uses the interpolated initial field at $t = 0$. The measured temperatures and observation coordinates are not interpolated in time. Thus the search objective and final statistics correspond to distinct spatial and temporal discretizations.

4.2 Adaptive constrained search

The Two-Strategy adaptive Artificial Bee Colony (TSaABC) method combines exploratory and best-directed mutations [9, 11]. The implementation maintains $SN = 3$ candidates. For a randomly chosen coordinate j , two proposal formulas are

$$\tilde{p}_j = p_j^{r_1} + \xi(p_j^{r_1} - p_j^{r_2}), \quad (33)$$

$$\tilde{p}_j = \frac{1}{2}(p_j^{r_1} + p_j^{r_2}) + \xi(p_j^{r_1} - p_j^{r_2}) + \zeta(p_j^{\text{best}} - p_j^{r_1}), \quad (34)$$

where ξ is uniform on $[-1, 1]$, ζ is uniform on $[0, 1]$, and eligible distinct population indices are selected at random. Other coordinates initially retain the current candidate values. Every proposal is clipped to the parameter box and repaired to satisfy Eq. (8). It replaces the current candidate only if J_h decreases.

If s_1, s_2 count successful proposals of the two strategies during a search phase, the probability p_f of the best-directed strategy is updated by

$$p_f \leftarrow 0.95p_f + 0.05 \frac{s_1}{s_1 + s_2} \quad (s_1 + s_2 > 0), \quad p_f(0) = 0.5. \quad (35)$$

The counters are reset after this update. Two mutation/selection phases visit each candidate; the second allows a best-centered version of the exploratory proposal with probability 0.2. Candidates with more than 100 failed proposals are reinitialized and repaired. The best solution over the complete history is retained. These details specify the implemented adaptive variant; no global optimality guarantee is claimed.

The recorded budget is 1000 continuation cycles after an initial search call. Because that call also performs one internal cycle, the notebook executes 1001 internal cycles when completed. The supplied convergence figure follows the notebook’s displayed 1000-cycle history. The complete random state was not archived, so the saved parameter vector and fields, rather than an identical stochastic search path, define the reproducible result.

5 Numerical experiment and discussion

5.1 Data and computational configuration

The numerical assessment uses 105 nighttime measurements of 6 March 2011 selected by local solar time less than 10 h and latitude between 50° and 80°N . The selected observations occupy approximately 58.994° – 67.515°N and comprise seven points per pass. The experiment uses Aura MLS temperature observations at the 0.002 hPa pressure level, together with the corresponding geographic coordinates and measurement times. These measurements provide a common dataset for comparing the initialization strategies. Recommended MLS screening criteria and pressure-dependent retrieval characteristics are described in the instrument documentation [12].

Time is measured from the first target-day observation, with observation times truncated to integer seconds, and $t_f = 83212$ s. The mesh has N latitude subdivisions and

$$N_x = \text{round}\left(N \frac{2\pi \cos \varphi_0}{\varphi_N - \varphi_B}\right) \quad (36)$$

longitude subdivisions; each rectangle is divided into two triangles. Identification uses 90×16 cells, or 2880 triangles, and the pass-mean time steps. The final recomputation uses 270×48 cells, or 25920 triangles, and 100 uniform steps. The saved visualization mesh has 13279 vertices, including duplicated periodic-edge positions. This two-resolution workflow combines parameter estimation on the coarse mesh with a more detailed final representation of temperature evolution.

The linear-initialization control uses the same spectral flow representation, search implementation, diffusivity, shared speed bound, and fine-mesh observation evaluation. Each transport experiment uses its corresponding initial field and compatible boundary values, with flow parameters determined in a separate stochastic optimization run. A static control evaluates Eq. (22) at the target-day positions and provides a reference for the temperature structure inherited from the preceding day. The static field is evaluated analytically, while the transport calculations use the finite element observation operator described in Section 4.

5.2 Numerical results

Observation-based initialization improves the agreement with target-day temperatures while retaining the existing 28-parameter flow representation. The optimization produces the best recorded coarse-mesh objective

$$J_h(\mathbf{p}^*) = 32.0553687 \text{ K}^2, \quad \sqrt{J_h(\mathbf{p}^*)} = 5.661746 \text{ K}. \quad (37)$$

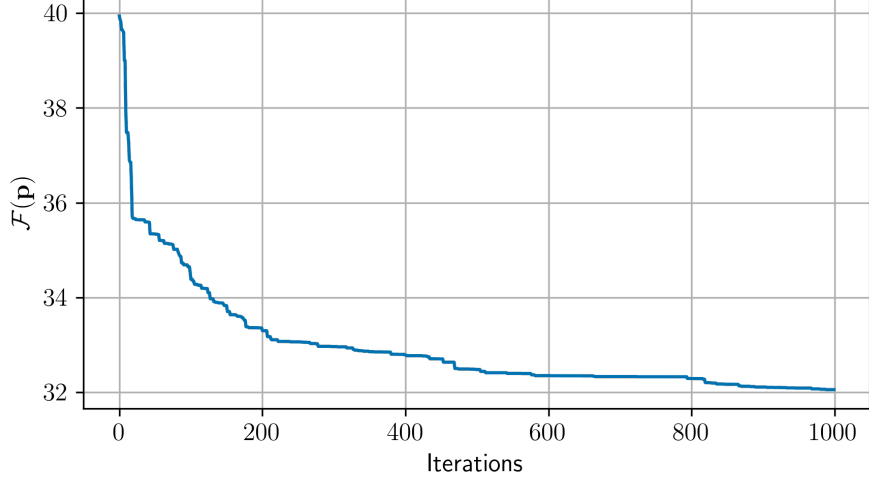


Fig. 2 Convergence history for the observation-based initialization (blue curve)

Table 2 Target-day comparison for the same 105 observed temperatures. Transport rows use the fine-mesh recomputation. The static row evaluates the analytic initial field without temperature evolution

Model	MSE (K ²)	RMSE (K)	r	ε_{rel} (%)
Linear initialization, transport	37.5415	6.127	0.373	3.078
MLS initial field, static	34.6208	5.884	0.549	2.955
MLS initialization, transport	26.3019	5.129	0.660	2.576

Figure 2 records the progress of the best retained objective. A rapid initial reduction is followed by smaller improvements over the remaining search cycles.

For the final recomputation, define

$$\text{RMSE} = \left[\frac{1}{n} \sum_{j=1}^n (M_j - d_j)^2 \right]^{1/2}, \quad r = \frac{\sum_j (M_j - \bar{M})(d_j - \bar{d})}{\sqrt{\sum_j (M_j - \bar{M})^2 \sum_j (d_j - \bar{d})^2}}, \quad (38)$$

$$\varepsilon_{\text{rel}} = 100 \frac{\text{RMSE}}{\bar{d}}, \quad \bar{d} = 199.0850985 \text{ K}. \quad (39)$$

Here M_j is the final model estimate at an observation point, and the relative error expresses RMSE as a percentage of the mean observed absolute temperature. The target-day statistics quantify agreement with the observations used to identify the flow parameters. The source-day pass-grouped validation in Table 1 separately assesses the construction of the initial field.

The fine-mesh RMSE decreases from 6.127 to 5.129 K, a reduction of 16.3% relative to the linear control (Table 2). The Pearson correlation increases from 0.373 to

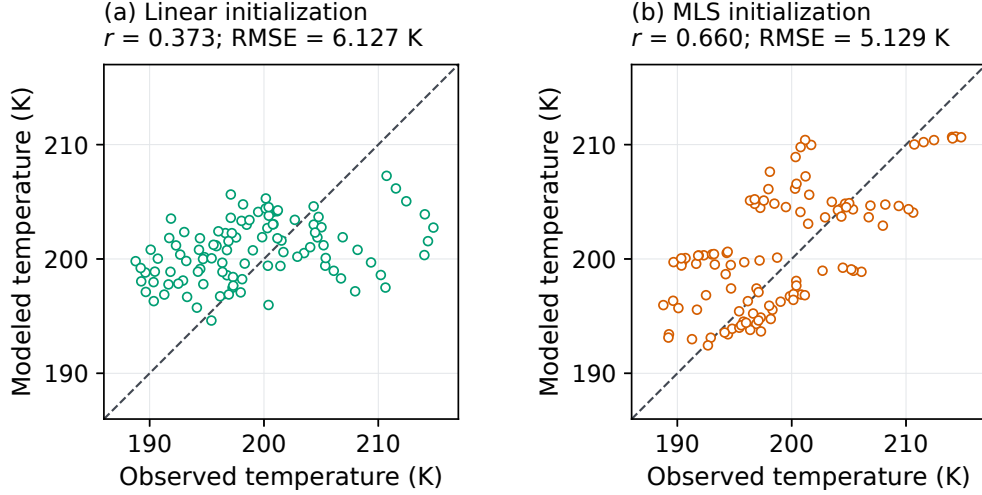


Fig. 3 Modeled versus observed temperatures for all 105 target-day pairs: (a) linear initialization (green circles) and (b) MLS initialization (orange circles). Dashed gray lines denote exact agreement; both panels have the same axis limits

0.660. These improvements are accompanied by a closer representation of the observed temperature variability. The population standard deviation of the modeled samples increases from 2.607 to 5.184 K, compared with 6.354 K for the observations. Figure 3 illustrates the broader range of modeled temperatures: the MLS-initialized samples span 192.442–210.700 K, while the observed range is 188.775–214.818 K.

The static initial field gives RMSE 5.884 K and $r = 0.549$, showing that the preceding-day temperature structure provides an informative starting point for the reconstruction. Subsequent optimized transport further reduces RMSE to 5.129 K and increases the correlation to 0.660. Thus, the combined initialization-and-transport calculation achieves the closest agreement among the three cases, with the initial field supplying large-scale structure that the fitted evolution adapts to the target-day observations.

Figure 4 provides complementary views of this improvement. The pass means show better reproduction of the broad variability along the sampled satellite tracks. The latitude means show a substantial reduction of the strong negative gradient present in the linear-initialization control, bringing the modeled meridional variation closer in magnitude to that of the observations. Since the satellite passes sample changing longitude and time together, the pass comparison characterizes their joint contribution to the observed variability.

Table 3 reports the retained flow parameters and their individual contributions $V_m = R_E A_m \sqrt{k_m^2 + l_m^2}$ to the analytical speed bound. For the zero-amplitude mode $m = 1$, the velocity is independent of its phase and meridional wavenumber; the stored phase is therefore omitted.

The retained solution uses the prescribed analytical speed budget, with $B(\mathbf{p}^*) = 20.000$ m/s to the reported precision. The largest contributions come from modes $m =$

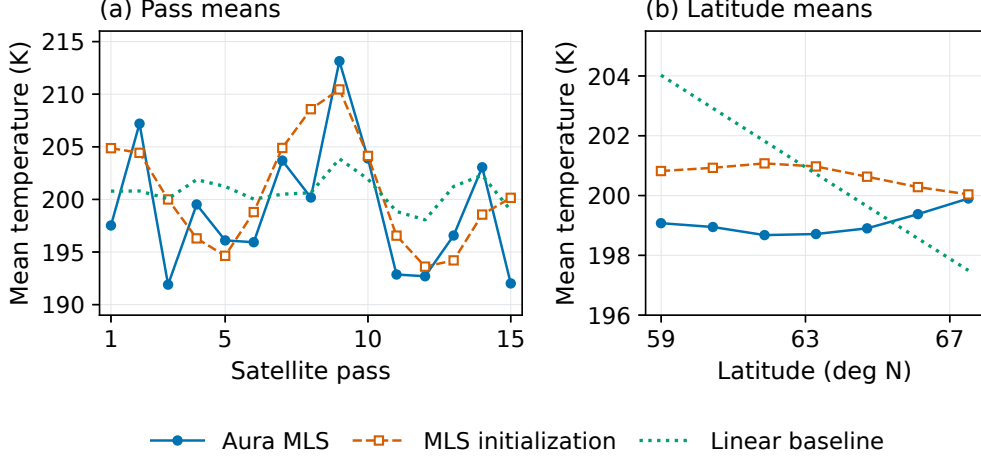


Fig. 4 Structure of the model-observation comparison. (a) Mean temperature of each seven-point pass. (b) Mean temperature at each of the seven latitude slots, averaged over passes. Blue filled circles denote Aura MLS, orange open squares with dashed lines denote MLS-initialized transport, and dotted green lines denote the linear-initialization control

Table 3 Flow parameters for MLS-initialized transport. The stationary zonal component is $m = 0$. A dash denotes the phase of an inactive mode

m	l_m	A_m (10^{-8} s^{-1})	θ_m/π	V_m (m/s)
0	2.239712	1.419939	0.055681	0.202614
1	0.000000	0.000000	—	0.000000
2	4.000000	12.914443	-0.991767	4.808053
3	1.854284	1.577503	0.398144	0.668721
4	1.368854	0.761589	-1.000000	0.418710
5	4.000000	3.239873	0.326464	2.348282
6	0.000000	0.673199	-0.801742	0.548142
7	4.000000	10.910109	-0.581068	10.730414
8	1.854781	0.251876	0.567362	0.275064

7 and $m = 2$, accounting for approximately 53.7% and 24.0% of this bound, respectively. The meridional upper bound is active for $m = 2, 5, 7$. These values describe how the constrained optimization distributes the available modal contributions within the selected spectral representation.

The fitted phase-propagation parameter is

$$\mathcal{U} = -1.0922929111 \times 10^{-7} \text{ s}^{-1}, \quad U_{\text{phys}} = -0.695900 \text{ m/s}. \quad (40)$$

Across the 100 saved times, the maximum physical speed of the elementwise advective curl, recomputed from the saved linear stream function, is 17.423 m/s. The maximum

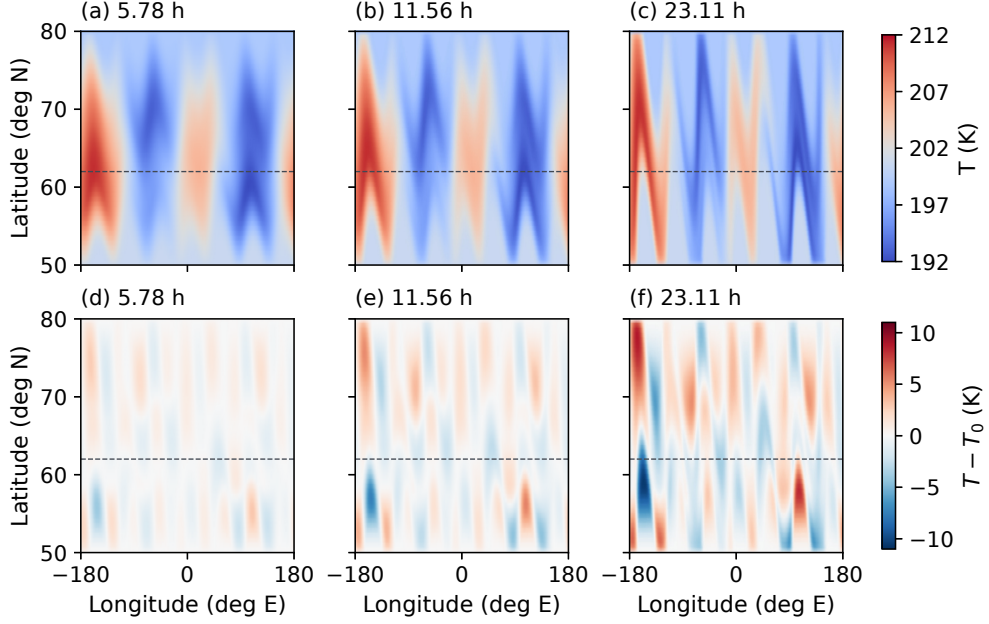


Fig. 5 Temperature evolution on the fine mesh. Panels (a)–(c) show absolute temperature at 5.78, 11.56, and 23.11 h on a common blue-to-red scale. Panels (d)–(f) show the difference from the initial finite element temperature at the same times: blue denotes cooling, red denotes warming, and white denotes zero change. The difference scale is centered at zero and spans -11 to 11 K. Dashed gray lines mark 62°N ; each row shares a color bar

nodal speed in the projected visualization field is 17.271 m/s. Both sampled maxima lie below the prescribed 20 m/s bound. The analytical estimate in Eq. (8) and these discrete maxima provide complementary descriptions of the continuous spectral velocity and its numerical representations.

Figure 5 illustrates the temperature evolution at 5.78, 11.56, and 23.11 h, together with the change from initialization. Across all saved mesh vertices and times, temperature ranges from 191.995 to 211.181 K. The initial low-order longitudinal structure remains recognizable as advection redistributes temperature and develops additional spatial variability. The calculation provides a temperature field throughout the periodic channel. Beyond the sampled latitude band, this field represents a model-based continuation determined by the fitted flow, taper, and boundary data.

5.3 Discussion

The results demonstrate the value of observation-based initialization for the considered temperature reconstruction. A latitude background and two longitudinal temperature harmonics improve agreement while retaining the 28-dimensional flow inversion. This highlights the benefit of incorporating measured temperature structure into the initial and boundary data before increasing the spectral complexity of the velocity field. The comparison considers each initial field together with its compatible boundary values; controlled variants could further quantify their individual contributions.

The preceding-day composite supplies a spatially structured prior, while the bounded latitude coordinate and taper provide a smooth continuation beyond the measured band. The corresponding boundary temperatures are extrapolated from this fit. Their influence, together with that of the smoothing choices, can be characterized through sensitivity experiments. The present formulation focuses on horizontal temperature transport; consistent inclusion of mean advection, vertical motion, and temperature forcing offers directions for extending the forward model and the associated parameter identification.

The assessment concerns a one-day reconstruction with a separately optimized flow for each transport case. Multiday experiments with withheld target observations would extend the evaluation to predictive performance, while repeated random starts and sensitivity to the admissible parameter ranges would characterize the variability and identifiability of the fitted flow. The coarse-to-fine change in discrepancy combines spatial refinement, smaller time steps, and temporal interpolation of the saved fields. Separate spatial and temporal refinement, together with comparison of the nearest-node and containing-element observation operators, would quantify these numerical contributions.

The temperature residual provides a combined diagnostic whose potential sources include retrieval uncertainty, sampling effects, initialization, and the representation of atmospheric transport. Additional contributions may arise from unresolved tides and gravity waves, whose interactions are relevant in the middle and upper atmosphere [13]. Native MLS uncertainty and screening metadata [12], together with additional observations, would support a more detailed error budget and physical interpretation of the remaining variability. Such analyses would build on the improved temperature agreement obtained with the observation-based initial field.

6 Conclusions

Observation-based initialization was integrated with a stabilized finite element inverse model of Rossby-constrained temperature transport. A regularized preceding-day fit supplies a latitude background, two longitudinal temperature harmonics, and compatible boundary values. The spectral flow is identified under a shared analytical speed bound.

For 105 nighttime Aura MLS measurements, the fine-mesh RMSE is 5.129 K (2.576% of the mean observed temperature) and the correlation is 0.660, compared with 6.127 K and 0.373 for linear initialization. Static evaluation of the new initial field gives 5.884 K and 0.549. Thus initialization contributes substantially to the final agreement, and optimized transport further improves it.

The results support the combined use of observation-based initialization and constrained transport for temperature reconstruction from sparse satellite data. Multiday experiments with independent observations would extend this assessment to predictive performance and the identifiability of the inferred flow.

Statements and Declarations

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Competing interests. The authors declare that they have no competing interests.

Data availability. The Aura MLS Level 2 temperature observations (version 4.2x) used in this study were obtained from NASA’s Goddard Earth Sciences Data and Information Services Center (GES DISC), dataset MLS/Aura Level 2 Temperature V004 (ML2T), <https://doi.org/10.5067/Aura/MLS/DATA2021>. The analysis uses observations from 5–6 March 2011 at the 0.002 hPa pressure level.

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