AviaSafe: A Physics-Informed Data-Driven Model for Aviation Safety–Critical Cloud Forecasts

Supplementary Material

1. Mathematical Formulation and Implementation of CNOP

To investigate the physical sensitivity of our model, we compute the Conditional Nonlinear Optimal Perturbation (CNOP). The CNOP represents the initial perturbation $\delta\mathbf{x}_0^*$ that maximizes the forecast error at optimization time T within a target region, subject to an initial energy constraint.

1.1. Moist Energy Norm

The magnitude of the perturbation is measured using the moist total energy norm:

$$\|\mathbf{x}'\|^2 = \frac{1}{2}\int_D \Big(u'^2 + v'^2 + \frac{c_p}{T_r}T'^2 + R_a T_r \left(\frac{p'_s}{p_r}\right)^2 + \frac{L^2}{c_p T_r} q'^2 \Big)\, dD \tag{1}$$

where u', v' represent the zonal and meridional wind perturbations, and T', p'_s, q' denote perturbations in temperature, surface pressure, and specific humidity, respectively. The constants are defined as: specific heat at constant pressure $c_p = 1004\,\mathrm{J\,K^{-1}kg^{-1}}$, latent heat of condensation $L = 2.5 \times 10^6\,\mathrm{J\,kg^{-1}}$, and dry air gas constant $R_a = 287\,\mathrm{J\,K^{-1}kg^{-1}}$. The reference values are set to $T_r = 270\,\mathrm{K}$ and $p_r = 1000\,\mathrm{hPa}$. This norm enforces physically meaningful perturbations.

1.2. Optimization Algorithm

We employ the Spectral Projected Gradient (SPG) method combined with the Barzilai-Borwein (BB) step size strategy to solve the constrained optimization problem efficiently.

The optimization process involves the following steps:

1. **Gradient Calculation:** Computing the gradient of the cost function J with respect to the initial state using the adjoint mechanism (via automatic differentiation).
2. **Spectral Step Size:** Updating the step size α_k using the BB formula $\alpha_k = \frac{\mathbf{s}_{k-1}^T\mathbf{s}_{k-1}}{\mathbf{s}_{k-1}^T\mathbf{y}_{k-1}}$, where $\mathbf{s}_{k-1}$ is the state difference and $\mathbf{y}_{k-1}$ is the gradient difference from the previous iteration.
3. **Non-monotone Line Search:** Performing a line search to ensure global convergence while allowing occasional increases in the objective function (controlled by memory depth M) to escape local optima.
4. **Projection:** Projecting the updated perturbation onto the constraint ball defined by the moist energy norm $\|\delta\mathbf{x}_0\| \le \xi$.

Algorithm 1 CNOP Calculation via Spectral Projected Gradient (SPG)

Require: Pre-trained Model $\mathcal{M}$, Initial State $\mathbf{x}_0$, Constraint ξ, Max Iterations K_{max}, Memory M.
Ensure: Optimal Perturbation $\delta\mathbf{x}^*$.

Initialize perturbation $\delta\mathbf{x}_0 \leftarrow$ random noise, projected to $\|\delta\mathbf{x}_0\| \le \xi$.
Initialize step size α_0, memory $\mathcal{H} = \{-\infty\}$.
Compute initial gradient $\mathbf{g}_0 = \nabla J(\delta\mathbf{x}_0)$ via backpropagation.
Apply spatial smoothing: $\mathbf{g}_0 \leftarrow \mathrm{Smooth}(\mathbf{g}_0)$.
for $k = 0$ to $K_{max} - 1$ **do**
  1. Descent Direction:
    $\mathbf{d}_k = \mathcal{P}_\xi(\delta\mathbf{x}_k + \alpha_k\mathbf{g}_k) - \delta\mathbf{x}_k$ ▷ Projected gradient direction
  2. Line Search:
    Find step $\lambda \in (0, 1]$ satisfying Armijo condition w.r.t $\max(\mathcal{H})$.
    $\delta\mathbf{x}_{k+1} = \delta\mathbf{x}_k + \lambda\mathbf{d}_k$
  3. Update Gradient:
    Compute forecast and loss $J(\delta\mathbf{x}_{k+1})$.
    Compute raw gradient $\hat{\mathbf{g}}_{k+1}$.
  4. Update Step Size:
    $\mathbf{s}_k = \delta\mathbf{x}_{k+1} - \delta\mathbf{x}_k$
    $\mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$
    $\alpha_{k+1} = \mathrm{clip}\left(\frac{\mathbf{s}_k^T\mathbf{s}_k}{\mathbf{s}_k^T\mathbf{y}_k}, \alpha_{min}, \alpha_{max}\right)$
  Update memory $\mathcal{H}$ with current loss J.
  if $\|\mathbf{d}_k\| < \epsilon$ **then** break
end for
return $\delta\mathbf{x}^* = \delta\mathbf{x}_{final}$

1.3. Hyperparameter Settings

To facilitate reproducibility, we detail the specific hyperparameters used in our CNOP experiments. The optimization is performed over a forecast window of $T = 72$ hours, targeting the region spanning 21°N to 30°N and 105°E to 121°E.

Optimization Constraints. The radius of the initial perturbation constraint ball is set to $\xi = 0.6$. The optimization is bounded by a maximum of $K_{max} = 50$ iterations. For the non-monotone line search, we set the memory depth to $M = 10$. The step size α is dynamically updated within the range $[10^{-3}, 50]$.

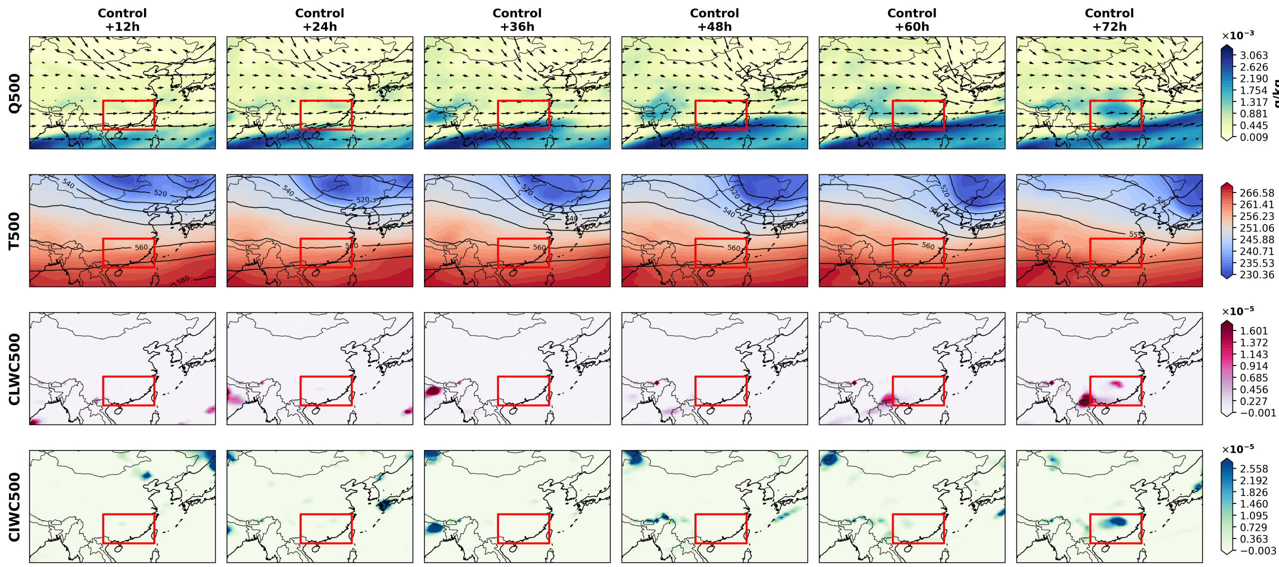

Figure 1. **Spatiotemporal evolution of the control forecast at 500 hPa.** This figure displays the 72-hour forecast trajectory starting from the unperturbed initial state. The columns represent forecast lead times from +12h to +72h. The rows, from top to bottom, illustrate: specific humidity (Q500) overlaid with wind vectors, temperature (T500) with geopotential height contours, cloud liquid water content (CLWC500), and cloud ice water content (CIWC500). The red bounding box highlights the target region for verification. This baseline evolution serves as the reference for assessing the impact of initial state perturbations.

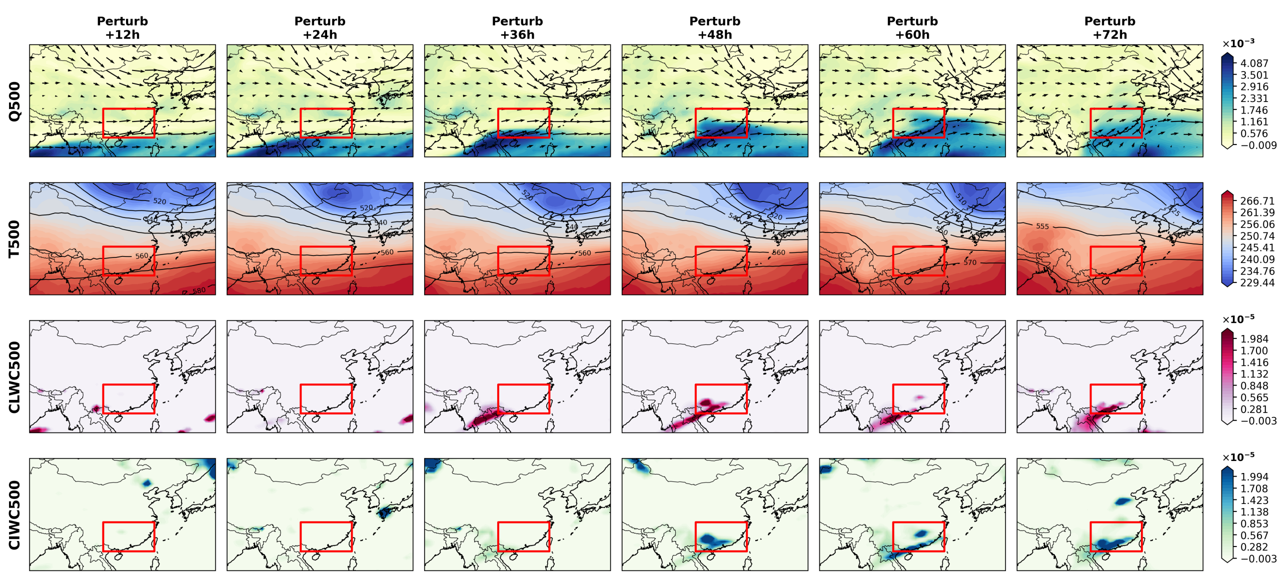

Figure 2. **Spatiotemporal evolution of the CNOP-perturbed forecast at 500 hPa.** This figure shows the forecast results initialized with the CNOP-perturbed state ($\mathbf{x}_0 + \delta\mathbf{x}_0^*$), using the same variable layout and time intervals as the control forecast.