Supplementary Information B (SB): Dynamic Topology of Expansion in CMIP6 Ensembles of Ecological Niche Models

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This document establishes the analytical framework for projecting the spatio-temporal kinematics of a biological invasion front. It transitions from static suitability projections to continuous dynamic systems analysis using discrete-time signal theory, characterizing the attractors in the climate suitability phase space based on the final computational implementation.

1 Mathematical Definition and Ecological Masking

In the context of ecological niche modeling using raster images, the continuous geographical space is discretized into a matrix $\mathbf{R} \in \mathbb{R}^{H \times W}$. Likewise, continuous time t is replaced by the discrete domain nT, where n is the future sample or climatic scenario number ($n = 0, 1, 2, \dots$) and T is the constant sampling interval (e.g., $T = \Delta t$ in years).

The ensemble median habitat suitability sequence is denoted as $\mathbf{R}[n]$. To ensure the kinematic analysis evaluates only ecologically probable occurrences rather than marginal habitats, a dynamic binary mask $\mathbf{M}[n]$ is applied to each projected period utilizing the 10th-percentile training presence threshold (τ_{10}):

$$\mathbf{M}[n] = \begin{cases} 1 & \text{if } \mathbf{R}[n] \geq \tau_{10} \\ \text{NA} & \text{if } \mathbf{R}[n] < \tau_{10} \end{cases} \tag{1}$$

2 Matrix Kinematics via Finite Differences

To characterize the SDM dynamics within the masked optimal habitat, we apply finite difference operators over the sequence. To prevent boundary truncation artifacts and arithmetic NA propagation along the dynamic edge of the invasion front, finite difference calculations ($V[n]$ and $A[n]$) were evaluated across continuous suitability layers prior to applying the dynamic binary mask $M[n]$. Element-wise matrix operations strictly omitted non-evaluable nullities outside the calibration domain while preserving continuous numerical gradients across transitional boundary pixels crossing the τ_{10} threshold.

2.1 Average Discrete Velocity ($\mathbf{V_{avg}}$)

The velocity represents the suitability rate of change matrix. To center the kinematic evaluation around a specific instant n, we compute the average velocity bridging the preceding and subsequent intervals:

$$\mathbf{V}_{\text{avg}}[n] = \frac{1}{2}\left(\frac{\mathbf{R}[n] - \mathbf{R}[n-1]}{T} + \frac{\mathbf{R}[n+1] - \mathbf{R}[n]}{T}\right) \tag{2}$$

Note: To evaluate the pure magnitude of expansion regardless of its direction, the absolute intensity $|\mathbf{V}_{avg}[n]|$ *is used.*

2.2 Discrete Acceleration ($\mathbf{A}_{\text{cent}}$)

Acceleration represents the matrix change in velocity. Using the Central Finite Difference method, which provides higher mathematical precision (truncation error $\mathcal{O}(T^2)$) by avoiding directional bias in the derivative:

$$\mathbf{A}_{\text{cent}}[n] = \frac{\mathbf{R}[n+1] - 2\mathbf{R}[n] + \mathbf{R}[n-1]}{T^2} \tag{3}$$

3 Properties and Practical Limitations: State Space

Modeling through discrete state variables allows us to analytically project future habitat suitability by assuming kinematic conservation. In matrix form, the state update equation is expressed as:

$$\mathbf{R}[n+1] = \mathbf{R}[n] + T \cdot \mathbf{V}_{\text{avg}}[n] + \frac{1}{2}T^2 \cdot \mathbf{A}_{\text{cent}}[n] \tag{4}$$

This property is fundamental for geographical interpolation or extrapolation to intermediate periods not directly simulated by GCMs.

To ensure numerical stability during matrix computation (via the `terra` package):

- **Spatial Alignment:** Operations require strict topological congruence (CRS, extent, and resolution). Divergences mandate prior bilinear resampling.
- **Handling Nullities:** Element-wise calculations omit `NA` cells. Due to the dynamic mask $\mathbf{M}[n]$, calculations are strictly confined to the ecologically relevant invasion front.
- **Irregular Intervals:** If the sampling interval is not constant, the strict T^2 model is relaxed to a mean temporal interval $\overline{T} = \frac{T_1+T_2}{2}$ to prevent arithmetic discontinuities.

4 Topological Classification of Regimes ($\mathcal{R}$)

By defining a strict asymptotic stability threshold $\epsilon = 1 \times 10^{-6}$ and a discriminator function $S(\cdot) \in \{-1, 0, 1\}$, the dynamic state in each pixel is classified by evaluating the velocity and acceleration tensor $[S(\mathbf{V}_{\text{avg}}[n]), S(\mathbf{A}_{\text{cent}}[n])]$:

Phase Space $[S(\mathbf{V}), S(\mathbf{A})]$	Class $\mathcal{R}$	Ecological Denomination (Front Dynamics)
$[1, 1]$	$\mathcal{R}_{++}$	**Runaway Expansion:** Increase in suitability with positive acceleration. Aggressive expansion.
$[1, -1]$	$\mathcal{R}_{+-}$	**Asymptotic Saturation:** Suitability increases, but at a decreasing rate. Approaching climatic carrying capacity.
$[-1, 1]$	$\mathcal{R}_{-+}$	**Reactivation / Damping:** Suitability loss is slowing down, suggesting an ecological floor or a future recovery pulse.
$[-1, -1]$	$\mathcal{R}_{--}$	**Continuous Retraction:** Progressive and accelerated collapse of the species' original suitability.
$[0, 0]$	$\mathcal{R}_0$	**Metastable Equilibrium:** Variables are null or below ϵ. Propagation within a constant niche.

5 Temporal Consistency and Statistical Evaluation

Instead of quantifying epistemic uncertainty across independent climate models (which is handled through the ensemble median), this framework quantifies the **temporal stability** of the invasion dynamics across evaluated periods.

5.1 Likelihood-Ratio G-Test

Shifts in the spatial proportions of the five dynamic regimes across different time instants $(t_1, \ldots, t_N)$ were statistically evaluated using a likelihood-ratio G-test of independence. This metric identifies whether the invasion front exhibits significant evolutionary phase shifts over the course of the century.

5.2 Temporal Agreement Index

The temporal consensus of the invasion regime per pixel is defined by the empirical mode across time $\mathcal{C}^* = \mathrm{Mo}(\mathcal{R}_{t_1}, \ldots, \mathcal{R}_{t_N})$. The stability of this regime is mapped as the Temporal Agreement Percentage (U_{time}):

$$U_{\mathrm{time}} = \left(\frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(\mathcal{R}_{t_i} = \mathcal{C}^*) \right) \times 100 \tag{5}$$

where $\mathbb{I}$ is the indicator function. High values indicate a highly conserved trajectory (e.g., persistent runaway expansion), whereas lower values highlight volatility in local climate suitability trends.