

Bridging Advances with Horizons in Uncertainty Quantification and Explainable Artificial Intelligence for Weather and Climate Extremes

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Sc·AI·ence Café Series
11th September 2026





Contents

1. Introduction: AI for Weather and Climate Extremes
2. AI Methodologies for Detection and Forecasting
3. Model Calibration and Uncertainty Quantification
4. Explainable Artificial Intelligence and Process Understanding
5. Conclusion: Bridging Advances with Horizons

References

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References

Droughts, Heatwaves, Wildfires



Damage caused by the fire in the western mountains of Madrid. EFE/Rodrigo Jiménez.

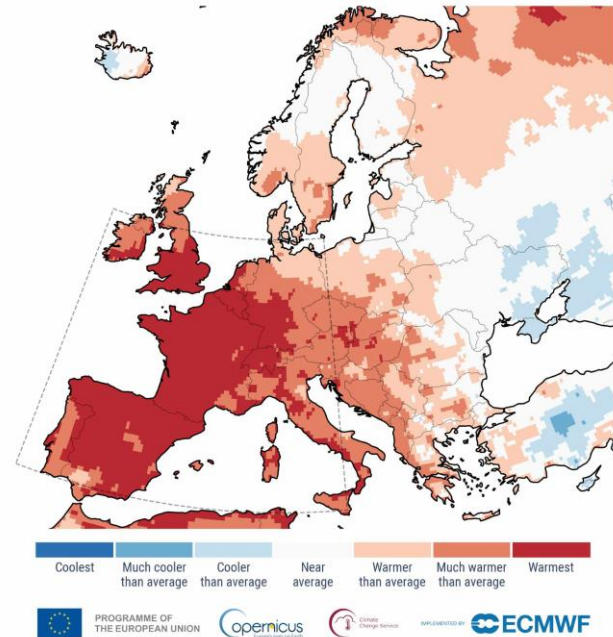
<https://sciencemediacentre.es/en/study-attributes-extreme-weather-conditions-fuelled-fires-spain-and-france-climate-change>



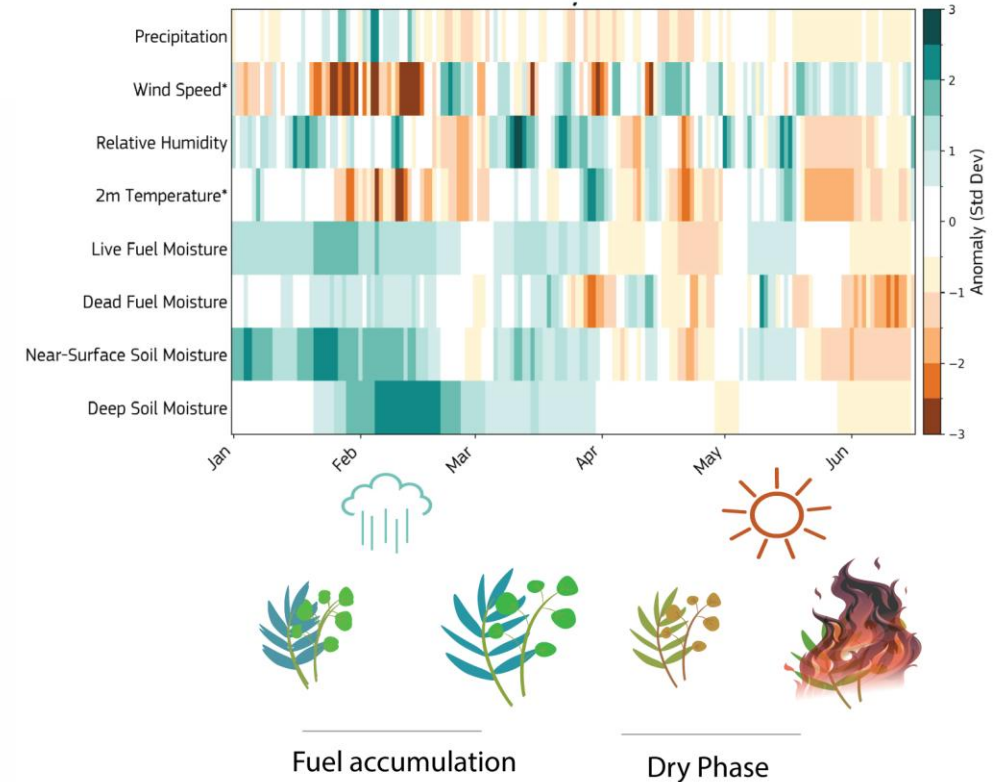
Fire in western Spain, 2022. This summer, an ongoing drought has spurred even more widespread fires. Copernicus Sentinel data. <https://eos.org/research-and-developments/climate-change-made-spain-wildfires-at-least-20-times-more-likely>

Anomalies and extremes in surface air temperature in June–July 2026

Data: ERA5 (1979–2025) • Reference period: 1991–2020 • Credit: C3S/ECMWF



Hydroclimatic Conditions for the Western Mediterranean in 2026

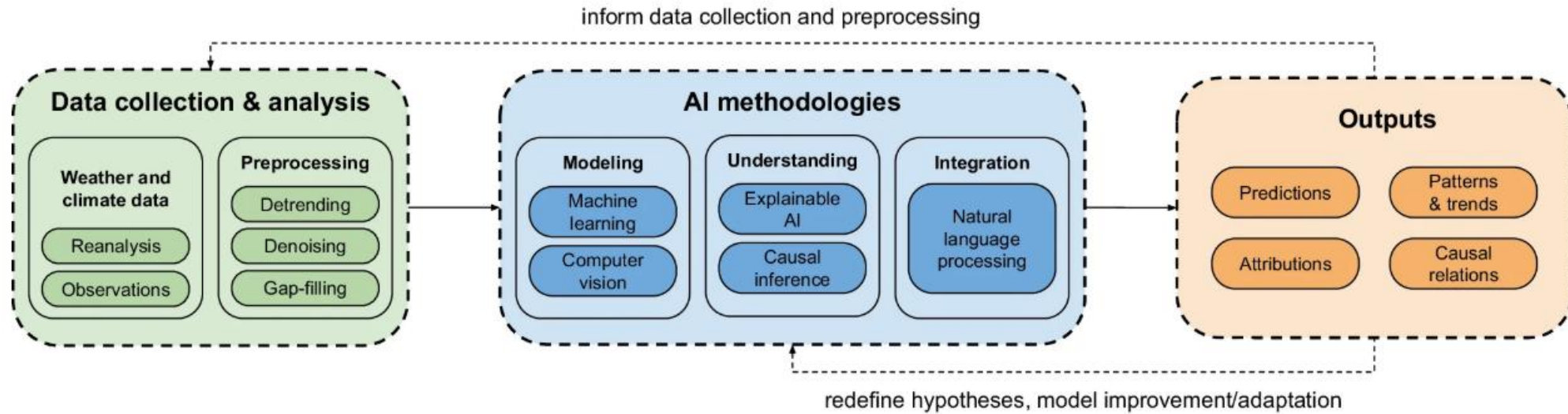


Sources, ERA5-Land, Sparky-fuel

Hydroclimatic conditions preceding the 2026 wildfire outbreak in the Western Mediterranean <https://stateofwildfires.com/news/understanding-spains-2026-wildfires-through-hydroclimatic-rebound/>

- Mediterranean region, a hotspot for compound drought-heatwave-wildfire events.
- Soil moisture deficits exacerbate extreme summer temperatures, directly driving wildfire risk.
- Move beyond isolated single-hazard detection to integrated multi-hazard early warning systems.

1 Introduction: AI for Weather and Climate Extremes



DETECTION



Space-time series
Underlying patterns

FORECASTING



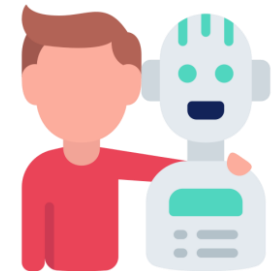
Anticipate
future extremes

IMPACTS



Social, economic, and
environmental consequences

XAI



Expert-comprehensive
Real deployment



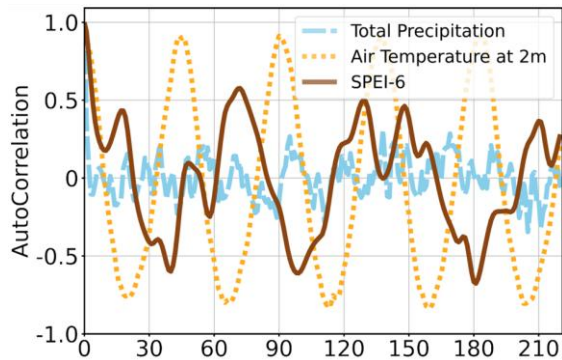
Contents

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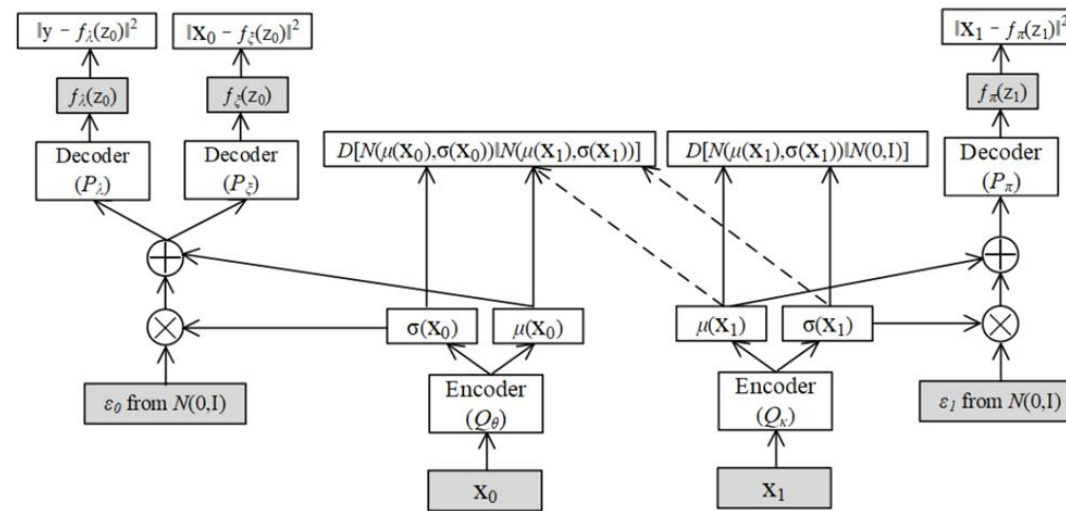
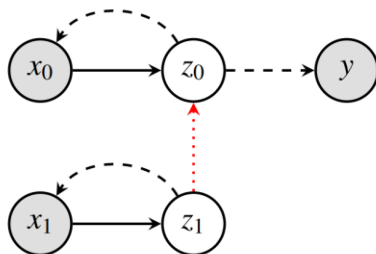
References

2 AI Methodologies (I): Domain Knowledge-Driven Detection

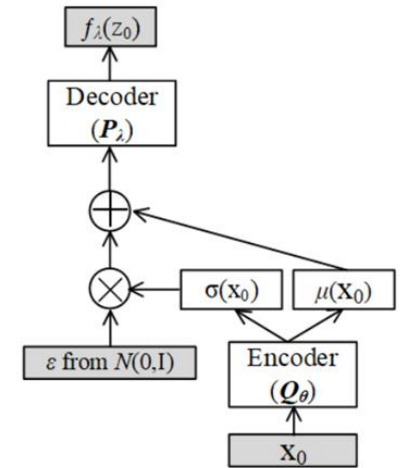
- **DK-VRN**: Novel hybrid variational recurrent neural network (LSTM-based) for **drought detection**
- Combines **observational data** (precipitation, air temperature 2m; x_0) and **domain knowledge** (multi-scalar SPEI, x_1)
- **Kullback-Leibler divergence** loss term as a regularization, enhancing generalization and robustness
- Estimated expectation of **drought probability and uncertainty** computed by means of importance sampling (K generated outputs)



Graphical model of DK-VRN

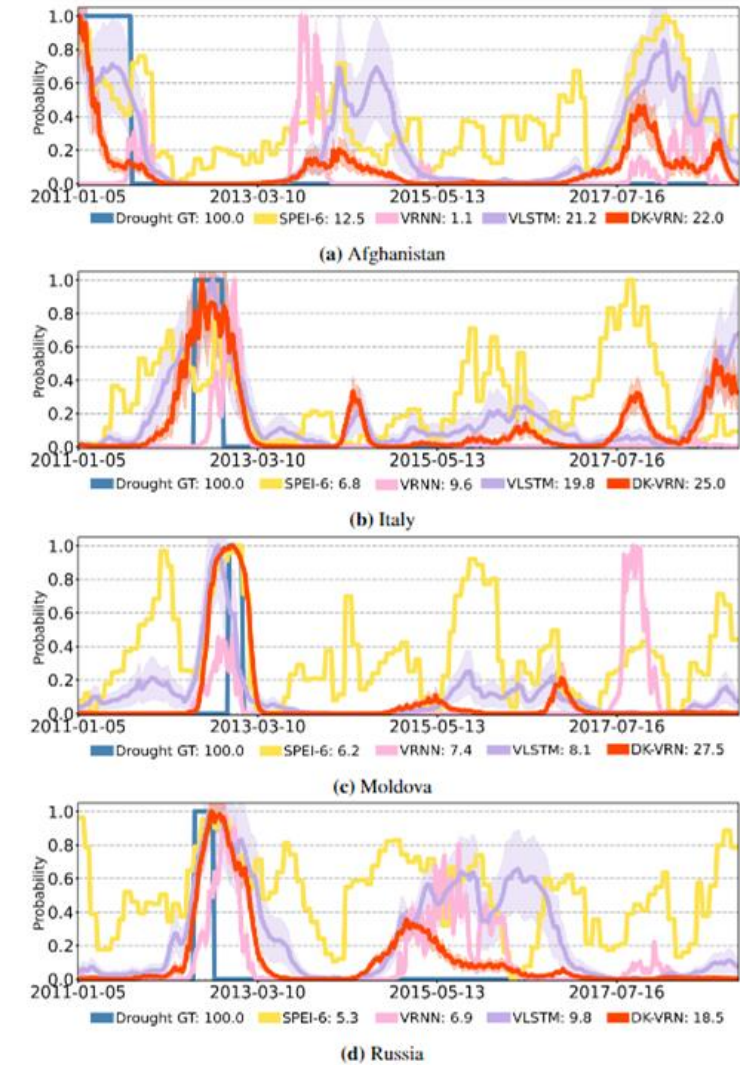
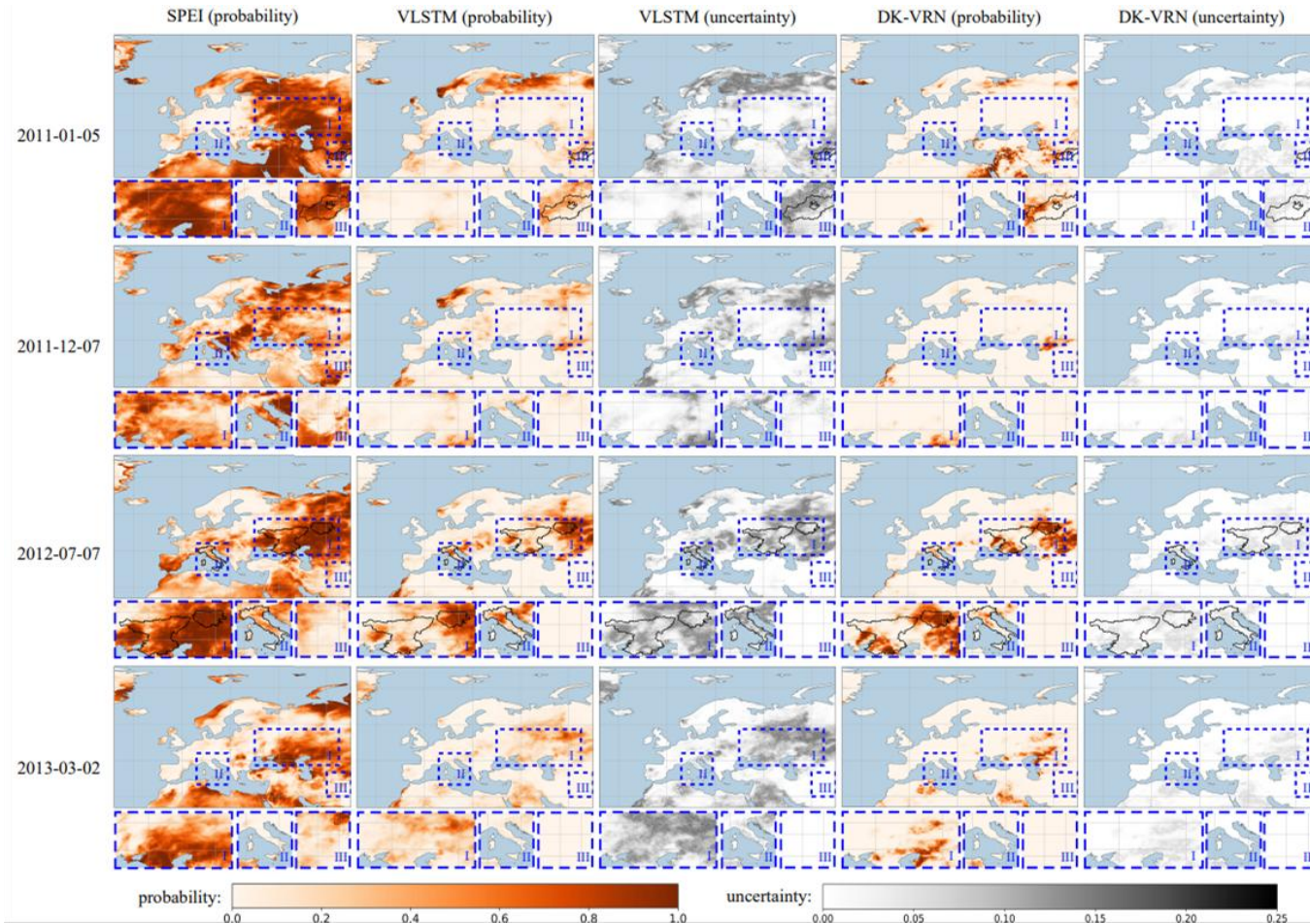


(a) Training stage



(b) Test stage

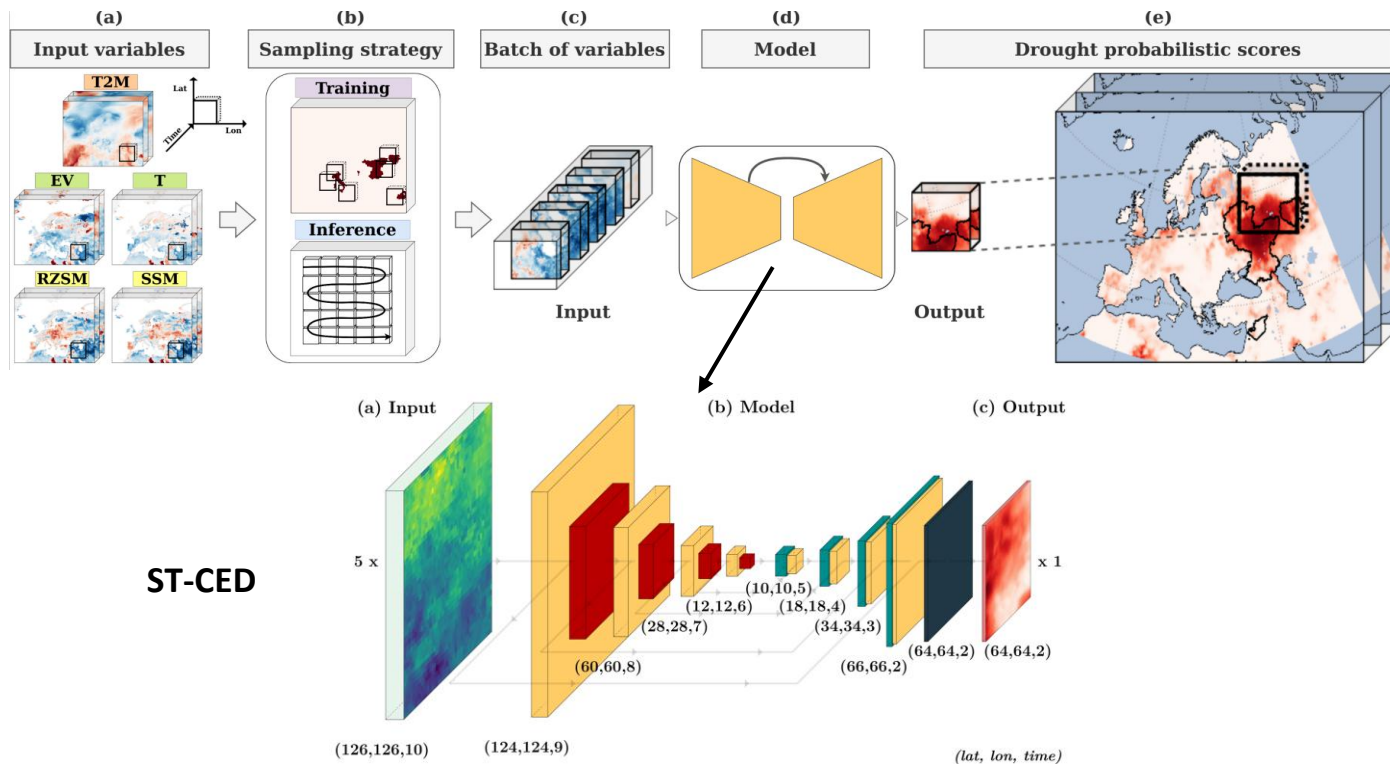
AI Methodologies (I): Domain Knowledge-Driven Detection



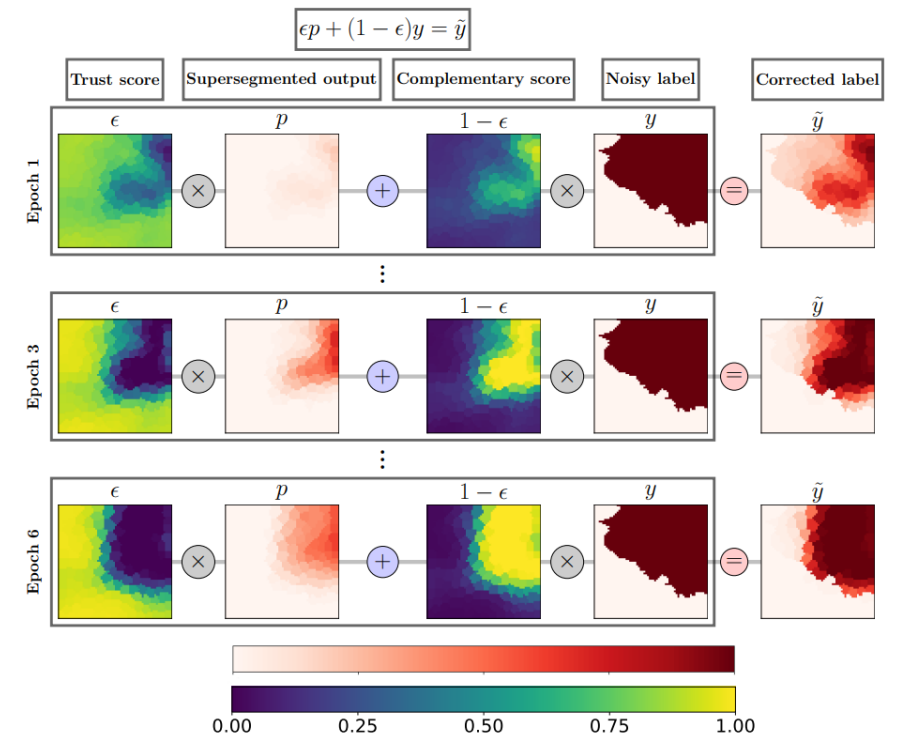
- Lower number of false alarms than SPEI
- DK-VRN captures drought events with lower uncertainty than VLSTM
- Better generalization for unseen locations

2 AI Methodologies (II): Detection and Noisy Labels

- **ST-CED**: Spatio-temporal convolutional encoder-decoder for drought detection
- 3D architecture that models spatio-temporal dependencies
- Strategies for **robust learning with noisy labels (NL)**, such as the ones available in **EM-DAT/GDIS databases**
- Novel **superpixel-based label self-correction method (SPLSC)**

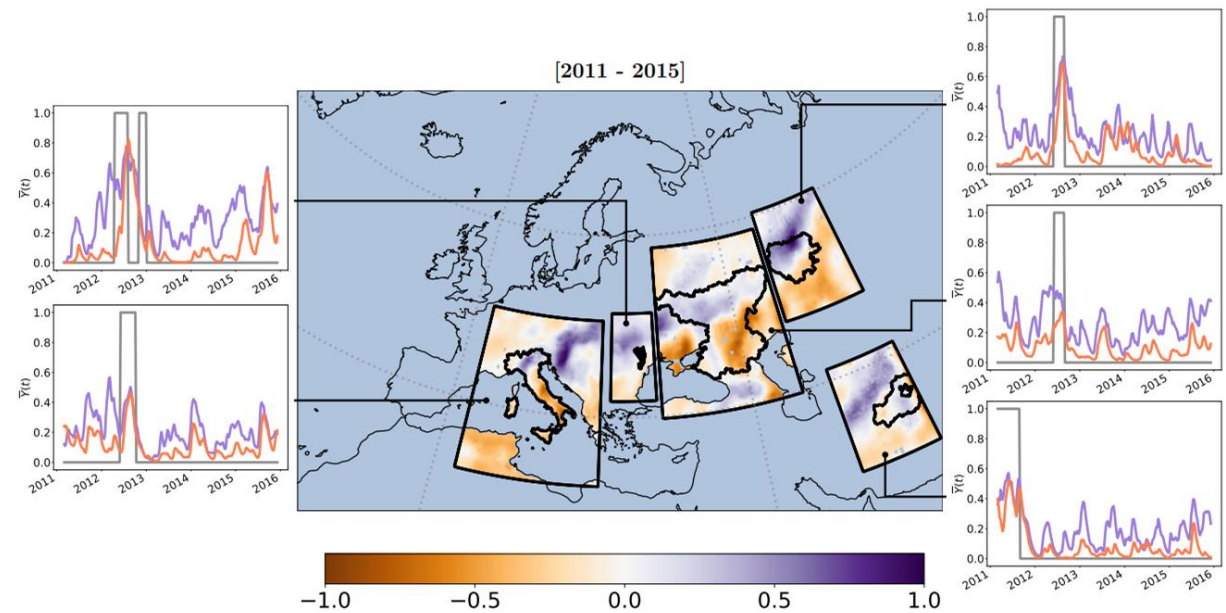
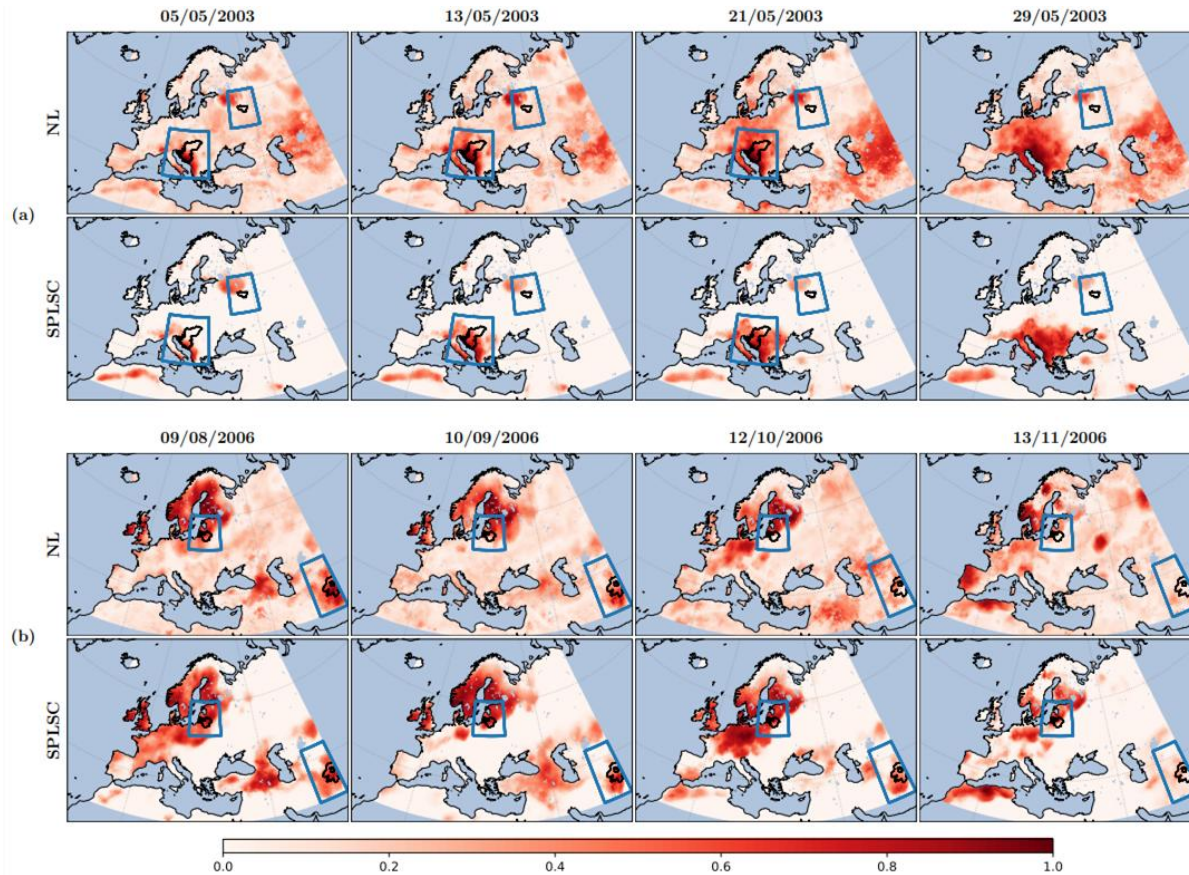


Label self-correction using SPLSC



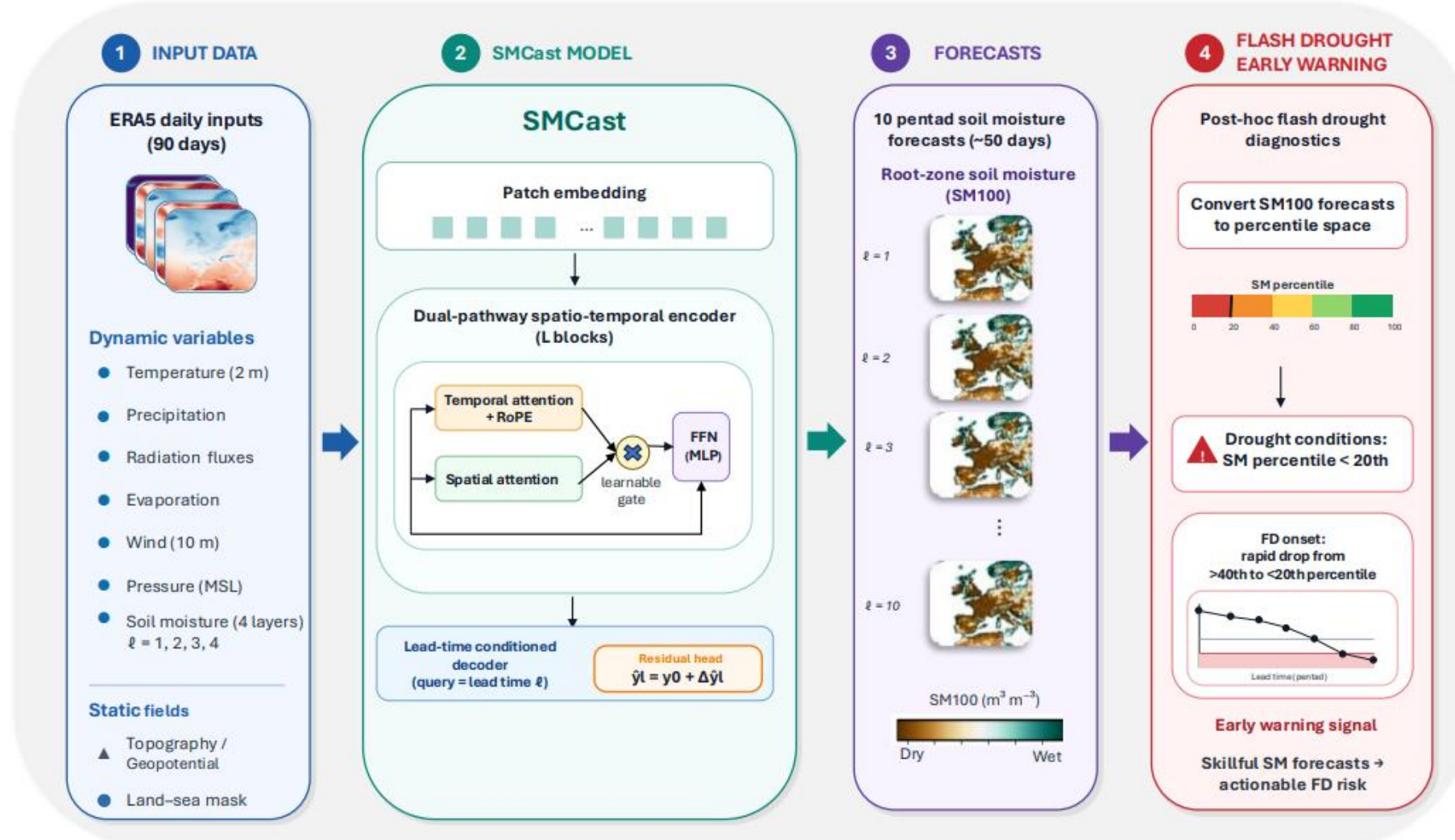
2 AI Methodologies (II): Detection and Noisy Labels

NL: Model trained with noisy labels (purple); SPLSC: Model trained with label self-correction (orange)



- ST-CED significantly outperforms well-known drought indices (SPEI, EnSMA, CDI)
- Higher precision and fewer false alarms for most events when training with label self-correction

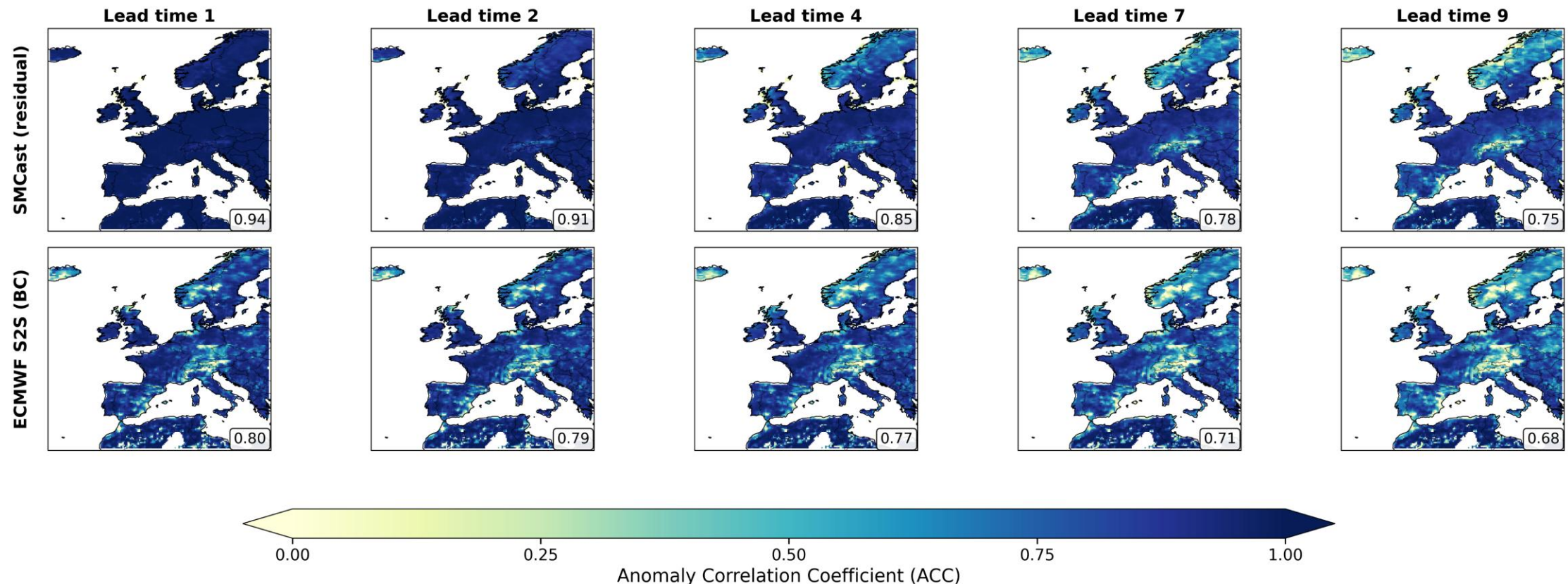
2 AI Methodologies (III): Flash Drought Forecasting



- **SMCast**: Dual-pathway, spatio-temporal Vision Transformer (ViT)
- Temporal land-surface memory and spatial hydroclimatic co-variability
- **90-day daily input**
- **10 future pentad forecasts (~50 days)** in a single pass using horizon-specific learnable embeddings
- Predict **target deviations relative to the latest observed state**
- **Quantile-head decoder**

2 AI Methodologies (III): Flash Drought Forecasting

- 2021–22 test: Highest skill for **SMCast**, outperforming persistence, raw/bias-corrected ECMWF S2S, and DL baselines
- Forecast skill decreases with increasing lead time in both models
- Lowest ACC values observed over northern and central Europe



2 AI Methodologies (III): Flash Drought Forecasting

- Transforming SM100 predictions post-hoc into climatological percentiles yields strong **drought detection**
- SMCast improves Yuan onset criterion and Flash Drought Intensity Index (FDII) errors
- However, **event-based multi-pentad rapid onset detection remains a challenge** across all S2S models

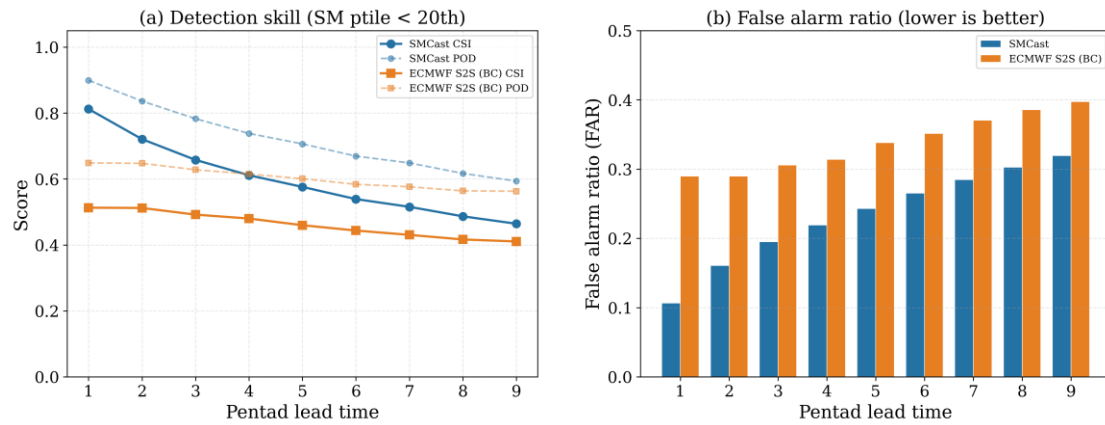
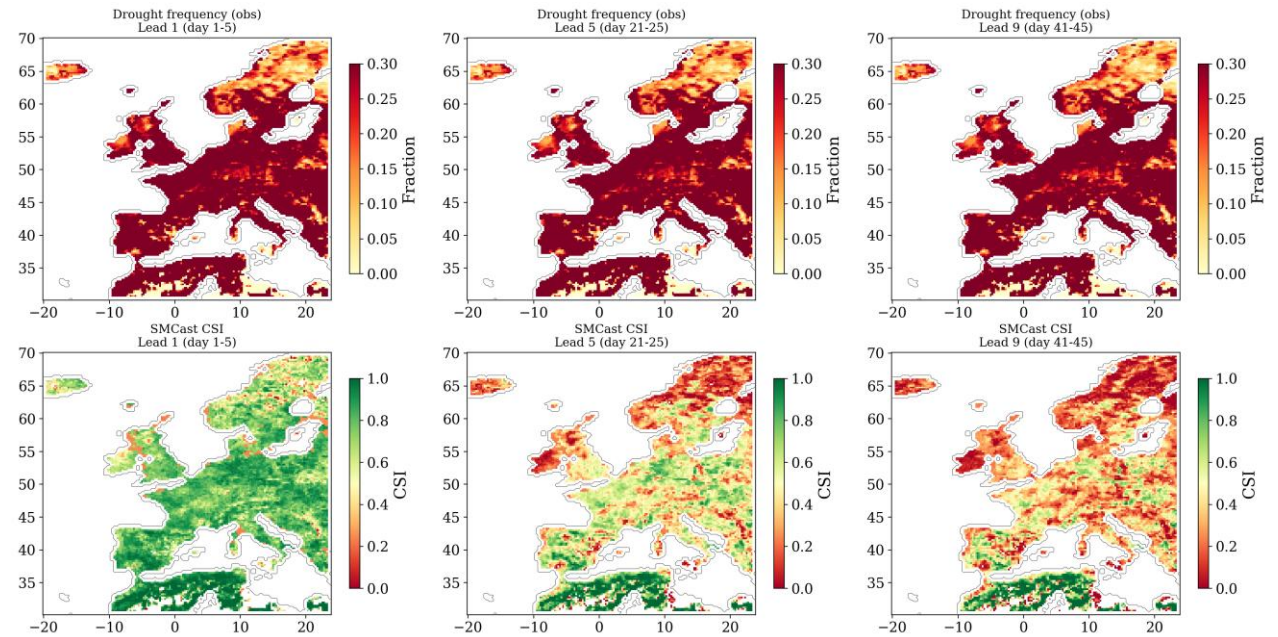


Table 4 Event-based flash drought skill at selected lead times, for both SMCast (left) and ECMWF S2S (BC) (right). Both the Yuan onset criterion [5] and the FDII binary detection ($FDII > 0$) yield near-zero CSI, reflecting the difficulty of resolving rapid intensification within a bounded forecast window. SMCast nonetheless shows higher precision (lower FAR) and lower continuous FDII error (FDII MAE) than ECMWF S2S (BC).

Lead	Yuan onset		FDII (>0)		FDII MAE
	CSI	FAR	CSI	FAR	
5 (d 21–25)	0.04 / 0.02	0.84 / 0.95	0.02 / 0.02	0.88 / 0.95	0.24 / 0.35
7 (d 31–35)	0.05 / 0.03	0.80 / 0.93	0.04 / 0.04	0.85 / 0.92	0.42 / 0.66
9 (d 41–45)	0.05 / 0.04	0.81 / 0.92	0.04 / 0.05	0.85 / 0.90	0.33 / 0.46

Critical Success Index (CSI)



Bridge A: Advances and Horizons in Detection and Forecasting

- **Advances:**

- **Hybrid and Probabilistic Detection:** Embedded SPEI domain priors into variational recurrent networks to quantify predictive uncertainty and reduce false alarms
- **Learning with Noisy Labels:** Implemented spatio-temporal label self-correction to train reliably on noisy natural disaster records
- **Subseasonal Forecasting:** Resolving multi-pentad forecasting for fast-developing extreme events like flash droughts

- **Horizons:**

- **Overcoming Rapid-Onset Bottlenecks:** Improve multi-pentad onset detection for rapid-developing events like flash droughts
- **Multi-Hazard Foundation Models:** Scaling specialized models into unified foundation architectures that maintain physical consistency across compound/cascading extremes

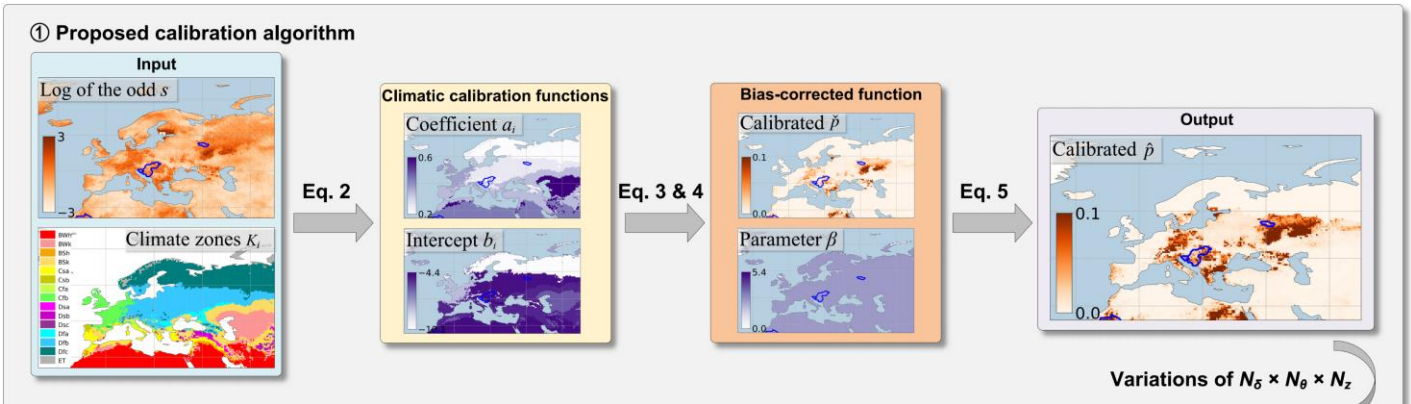
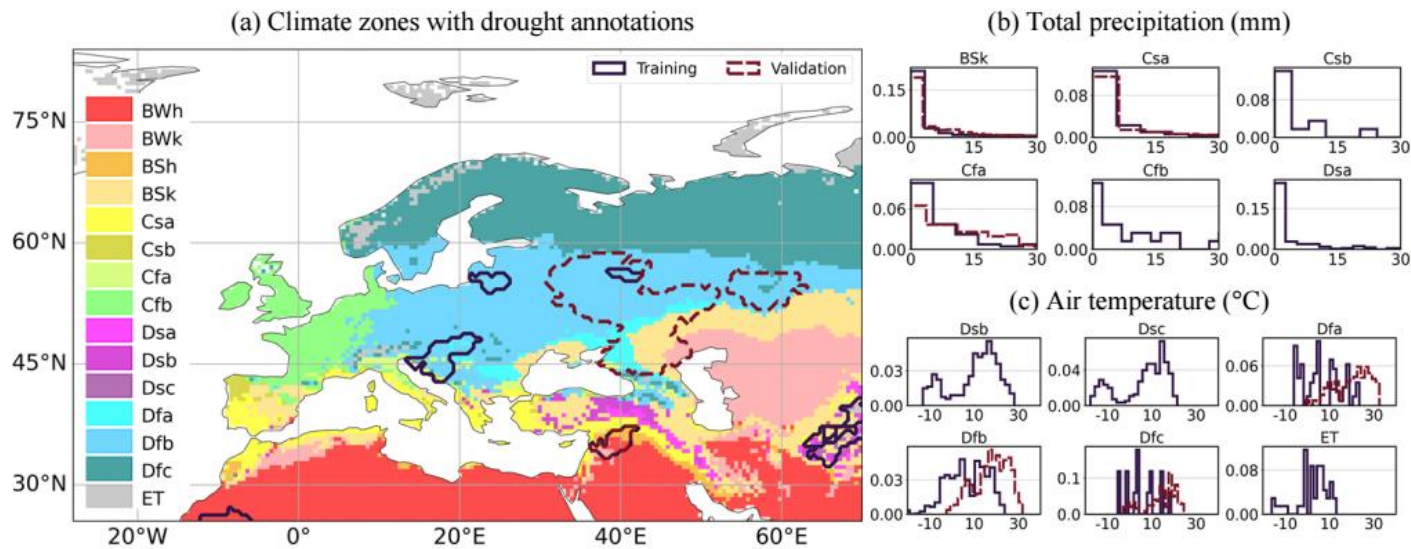


Contents

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3 Drought Detection and Model Calibration



- Uncalibrated outputs due to 2 main shifts:
 - Label prior shift: Event scarcity and training undersampling
 - Likelihood shift: Variability in climate variables conditioning on droughts
- Two-Step Calibration Strategy:
 - Climatic calibration, dividing Europe into Köppen-Geiger climate zones
 - Bias-corrected function: Non-linear transformation on the validation set to rectify likelihood shifts

Overall calibration errors (%) for different parametric calibration algorithms in the test subset, given the DK-VRN model.

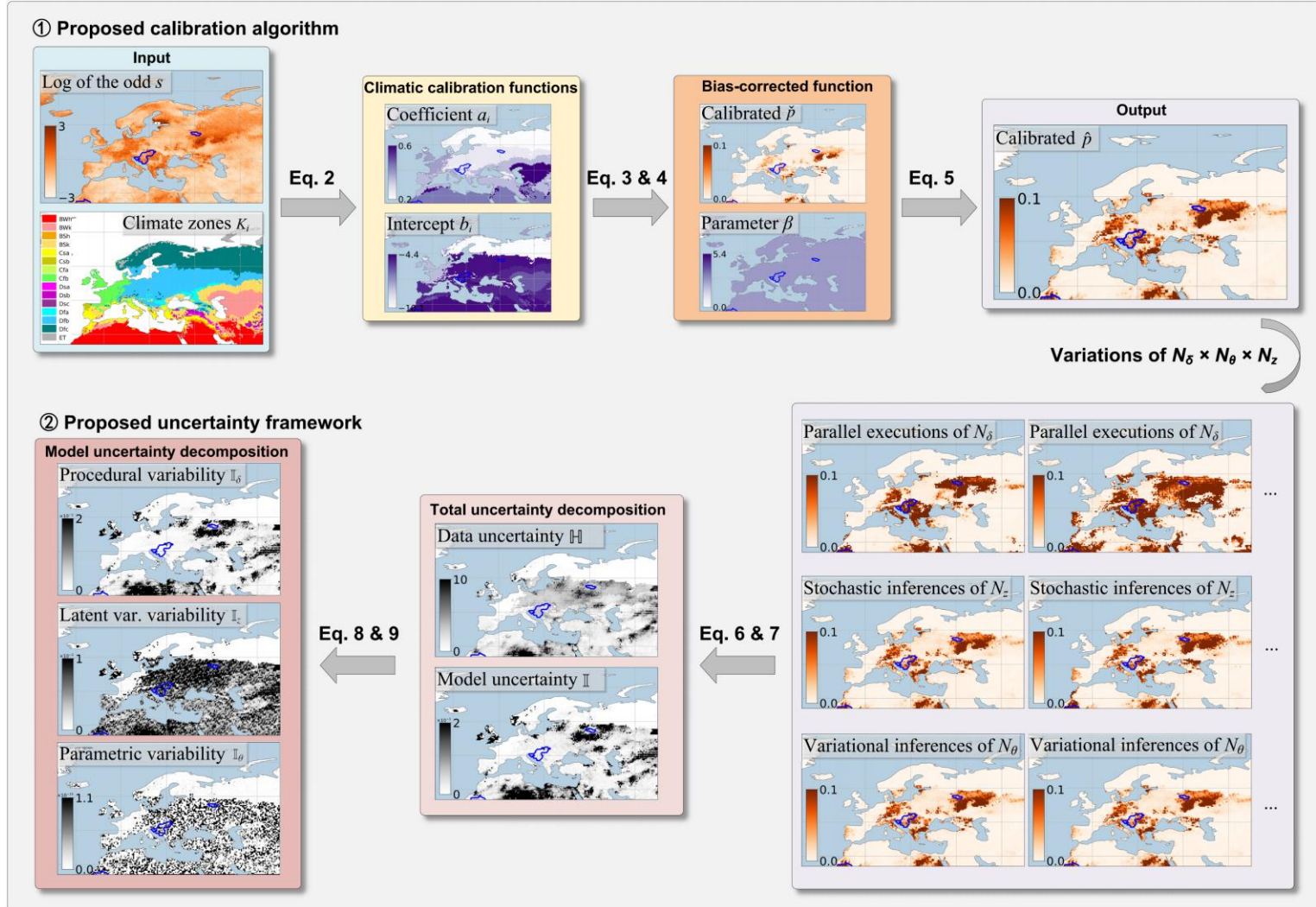
	Uncalibrated	Temp	Platt	Poly	Proposed
ECE	4.06	3.64	0.40	0.35	0.31
RMSCE	3.40	2.48	0.32	0.28	0.23
Training (s)	–	17.8	30.41	3.17	72.0
Inference (s)	–	0.07	0.07	0.03	0.07

Results (%) in the test subset for the ablation study conducted on the different components of the proposed calibration algorithm, given the DK-VRN model.

Climatic calibration	Bias-corrected	ECE	RMSCE
✗	✗	4.06	3.40
✗	✓	3.98	3.34
✓	✗	0.31	0.26
✓	✓	0.31	0.23

✗: not applied, ✓: applied.

Drought Detection and Uncertainty Quantification



- Entropy-based UQ framework
- Predictive uncertainty decomposition:
 - **Data Uncertainty** ($\mathbb{I}_H$): Aleatoric noise inherent in ERA-5 variables
 - **Procedural Variability** ($\mathbb{I}_\delta$): Model training randomness, sampled over N_δ initial random seeds
 - **Parametric Variability** ($\mathbb{I}_\theta$): NN weight uncertainty, approximated via N_θ Monte Carlo Dropout passes
 - **Latent Variable Variability** ($\mathbb{I}_z$): Stochasticity in VAE latent space, sampled via N_z variational draws

$$\mathbb{I}(Y; (\delta, \theta, z)) = \underbrace{\mathbb{I}(Y; (\delta, \theta, z)) - \mathbb{I}(Y; (\theta, \delta) | z^*)}_{\text{latent variable variability } \mathbb{I}_z} + \underbrace{\mathbb{I}(Y; (\theta, \delta) | z^*) - \mathbb{I}(Y; \delta | z^*, \theta^*)}_{\text{parametric variability } \mathbb{I}_\theta} + \underbrace{\mathbb{I}(Y; \delta | z^*, \theta^*)}_{\text{procedural variability } \mathbb{I}_\delta},$$

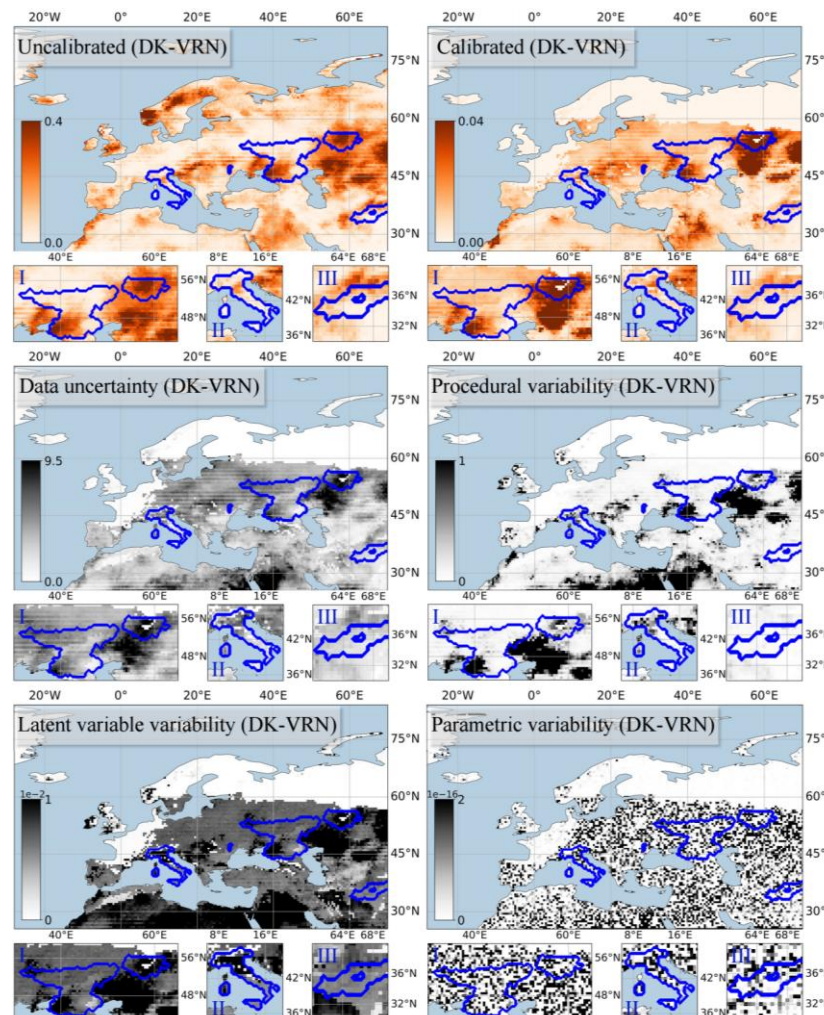
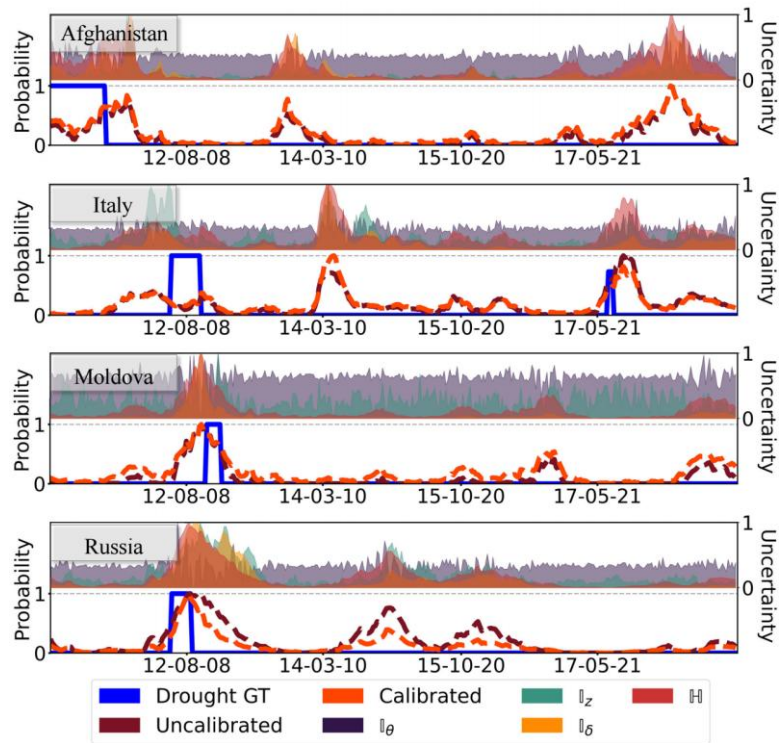
3

Decision-Making and Rejection Strategies for Trustworthy Decisions

- Quantified uncertainties
- Ensemble predictions
- Rejecting uncertain positive/negative predictions
- From expert systems to human-in-the-loop

Quantified uncertainties of the DK-VRN model for the test subset (%).

	Corrected samples			Erroneous samples		
	TP+TN	TP	TN	FP+FN	FP	FN
I_z	5.4e-3	2.7e-2	5.4e-3	3.7e-2	3.8e-2	7.4e-3
I_θ	2.5e-5	4.0e-16	2.5e-5	1.8e-3	1.9e-3	9.2e-17
I_δ	3.7e-2	3.3e+0	3.4e-2	3.1e+0	3.2e+0	6.2e-2
H	1.7e+0	2.8e+1	1.7e+0	1.4e+1	1.5e+1	3.6e+0
Total	1.74	31.33	1.74	17.14	18.24	3.77



Classification performance of VLSTM and DK-VRN for different decision-making strategies, given the test subset (%).

	VLSTM		DK-VRN	
	ROC-AUC	PR-AUC	ROC-AUC	PR-AUC
Uncalibrated	66.39	0.91	72.27	2.29
Calibrated	66.39	0.91	72.27	2.29
Uncalibrated ensemble	69.96	1.32	73.61	2.45
Calibrated ensemble	69.52	1.99	74.06	2.59

ROC-AUC: Receiver Operating Characteristic Area Under the Curve.

PR-AUC: Precision-Recall Area Under the Curve.

These two metrics measure the accuracy of drought detection (classification).

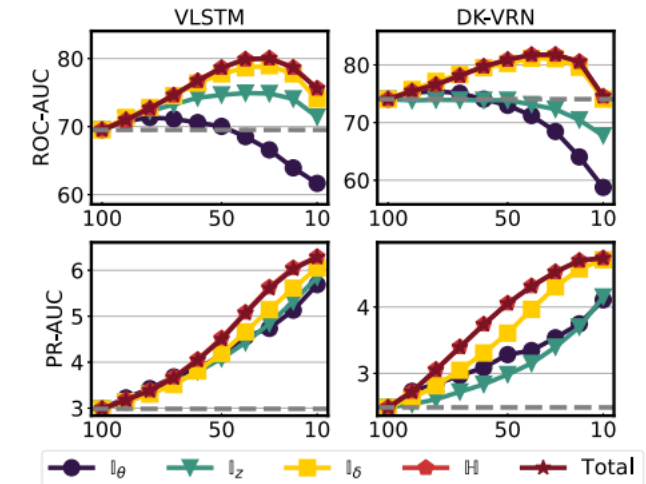


Fig. 4. Accuracy-rejection curves (%) for the VLSTM and DK-VRN models, given uncertain negative samples in the test subset. The x-axis denotes the keeping rate from 100% to 10%. For example, 80% keeping rate here represents rejecting the top 20% negative samples with higher uncertainty. The y-axis denotes the classification accuracy (ROC-AUC or PR-AUC). The calculation processes of metrics are included in the supplementary material. The dashed gray line denotes the raw results (without rejection).

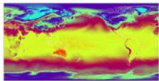
3

Evaluating Global AI Weather Models and Uncertainty Quantification

Data: T2m, TP6hr, Z500, T850 + AIWP input variables

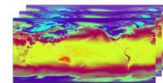
ERA5 [C3S, 2018]

- Ground truth dataset
- From ERA5 ARCO [Carver and Merose, 2023]



IFS ENS [ECMWF, 2016]

- SOTA ensemble NWP, $m = 50$ members
- From WeatherBench [Rasp et al., 2024]



Models: SOTA, open source & forecasting precipitation

FuXi [Chen et al., 2023]

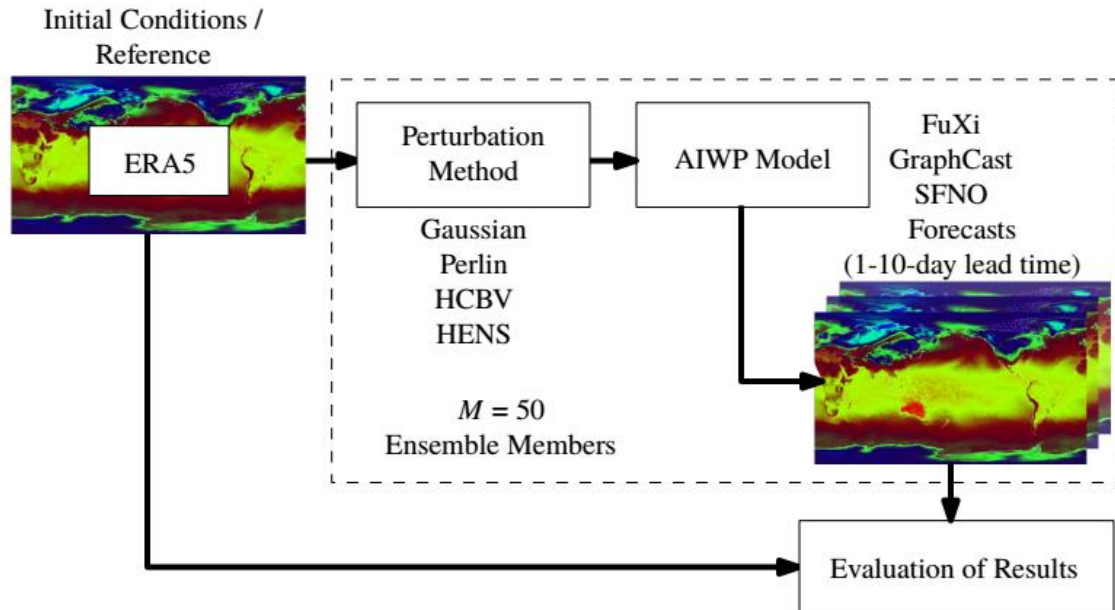
- Transformer
- Cascading (short, medium, long)

GraphCast [Lam et al., 2023]

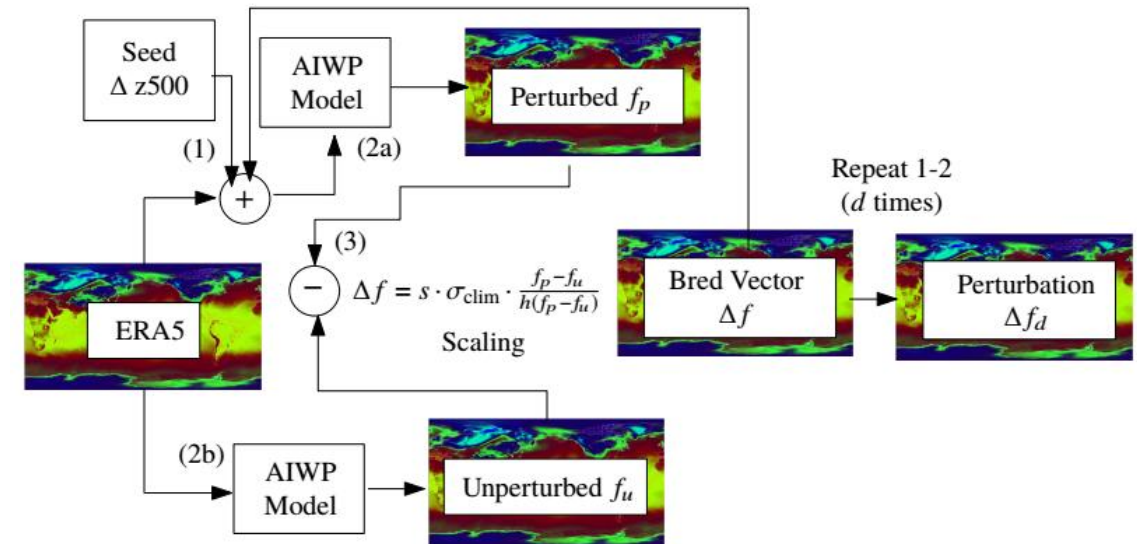
- Graph Neural Network (GNN)
- Top deterministic metrics

SFNO [Bonev et al., 2023]

- Spherical Fourier Transform-based
- Evolution of FourCastNet

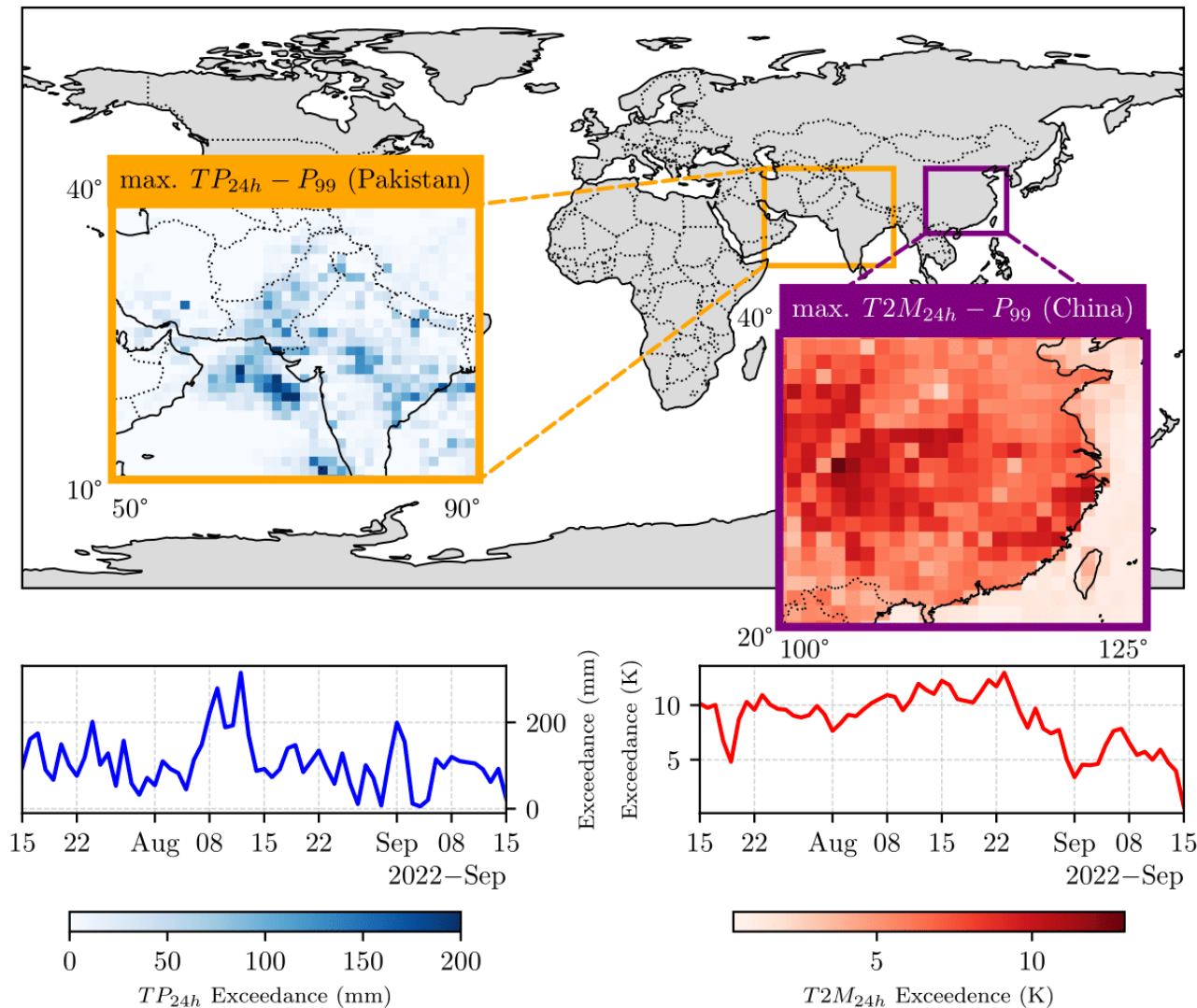


Hemispheric Centered Bred Vectors (HCBV)



3

Global AI Weather and UQ: Case Studies



2 case studies in August 2022:

1) Pakistan Flooding

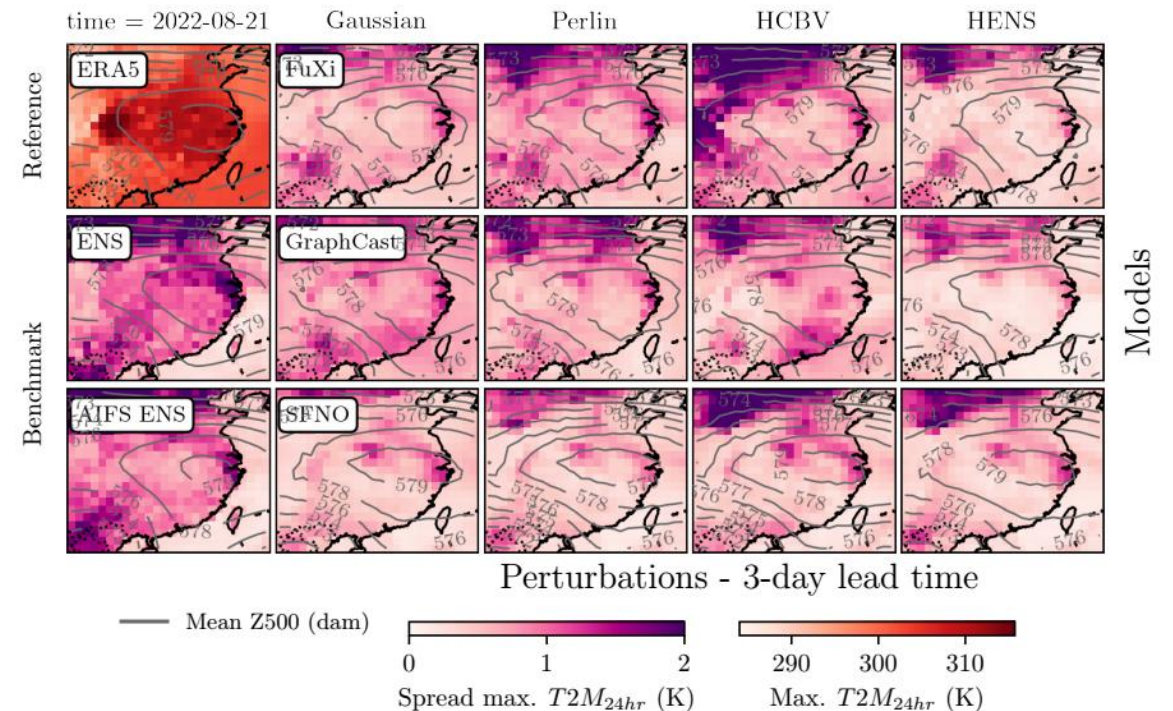
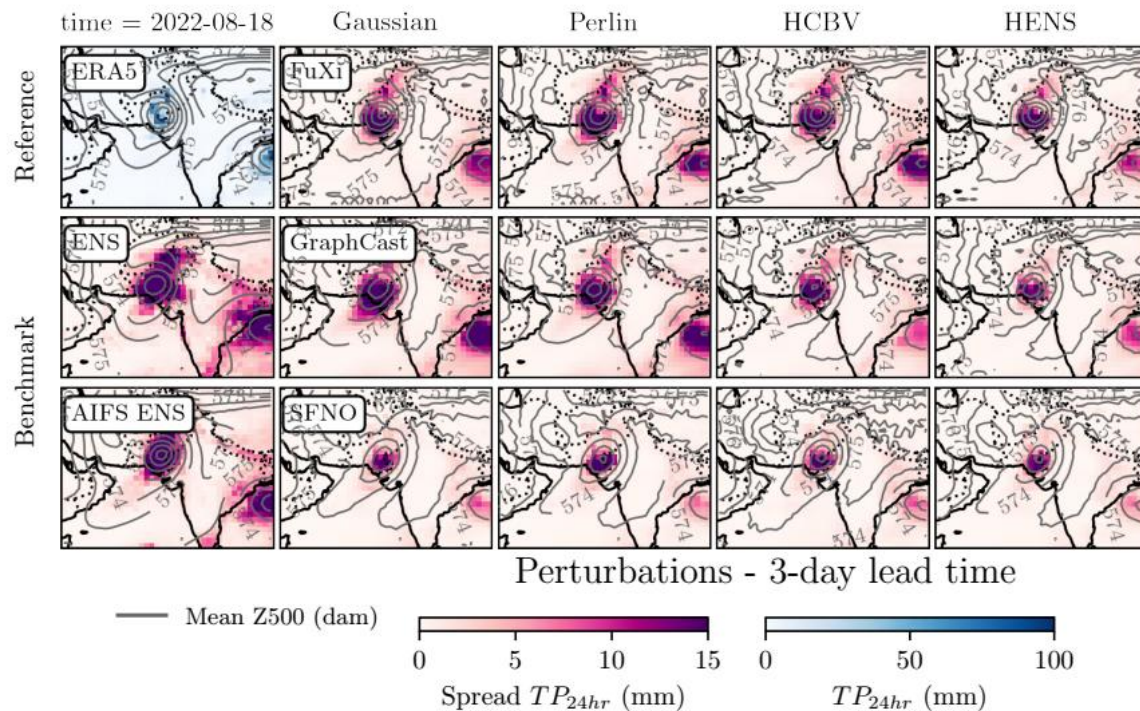
- Extreme monsoon rains
- Thousands of deaths
- 30 million people displaced
- **Total Precipitation (TP)**

2) China Heatwave

- Unprecedented heat and drought
- ~50,000 deaths
- Energy crisis and historical lows in the Yangtze River
- **2m Temperature (T2M)**

3 Evaluating Global AI Weather Models and Uncertainty Quantification

- Native probabilistic AI models match/exceed ECMWF ENS performance, whereas perturbed deterministic models still fall slightly short
- Model architecture is the primary driver of ensemble performance, outweighing the impact of the specific perturbation technique used
- Gaussian and Perlin noise reliably model realistic spread, offering a computationally efficient alternative to complex perturbation methods



3

Bridge B: Advances and Horizons in Uncertainty Quantification

- **Advances:**

- **Multi-Component UQ and Post-Hoc Calibration:** Established a two-step parametric calibration and entropy-based framework to quantify uncertainty
- **Uncertainty-Guided Decision Making:** Rejecting the top 20% most uncertain predictions directly boosts overall detection accuracy
- **Global AI Weather Model Benchmarking:** Benchmarks show model architecture impacts ensemble performance significantly more than the perturbation method used

- **Horizons:**

- **Native Probabilistic Models:** Moving beyond basic input perturbations toward natively probabilistic architectures
- **Variable-Dependent Skill Gaps:** Tailoring UQ to fix performance disparities across physical variables (e.g., strong performance on thermal extremes vs. weaker on precipitation)

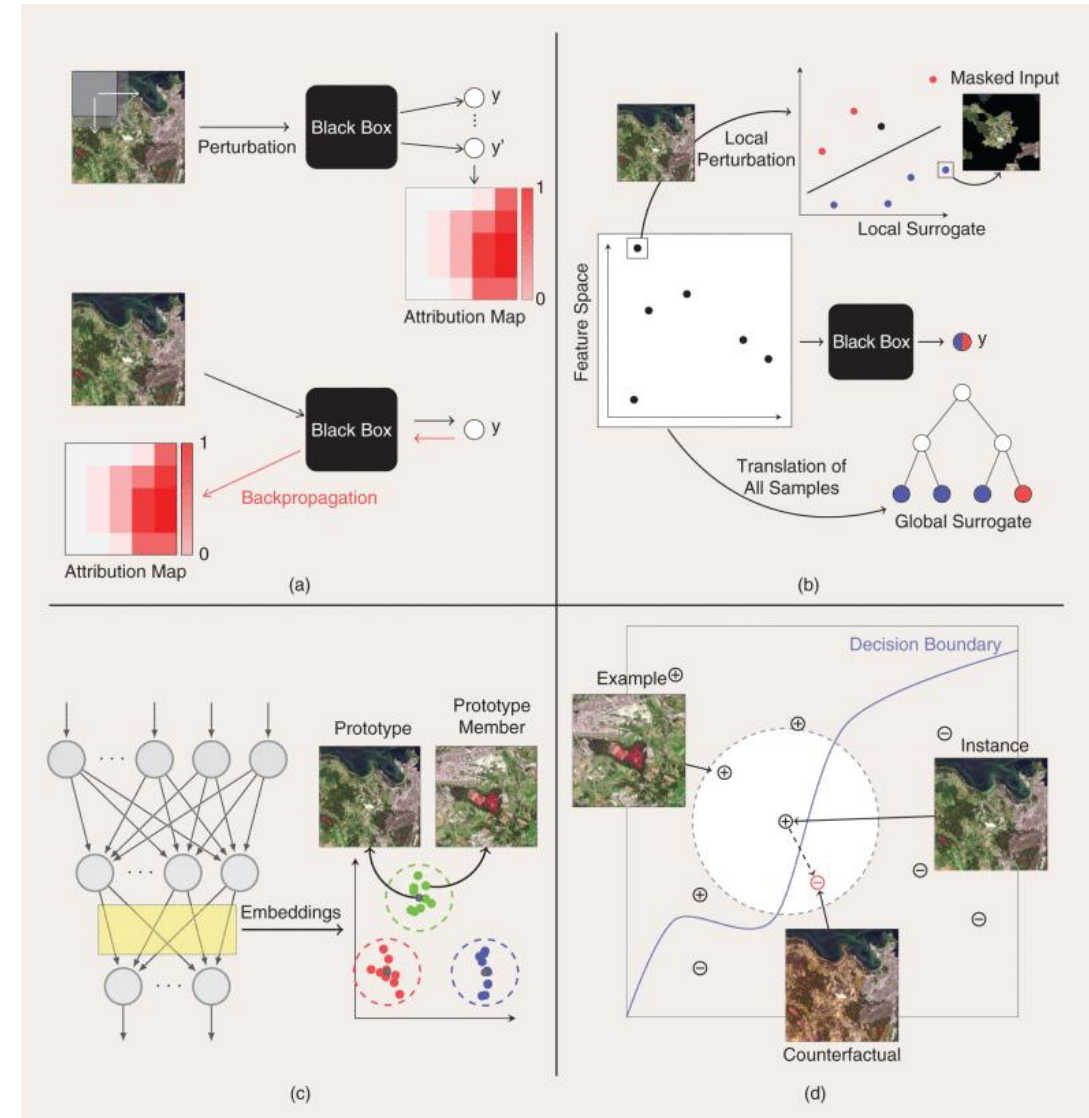
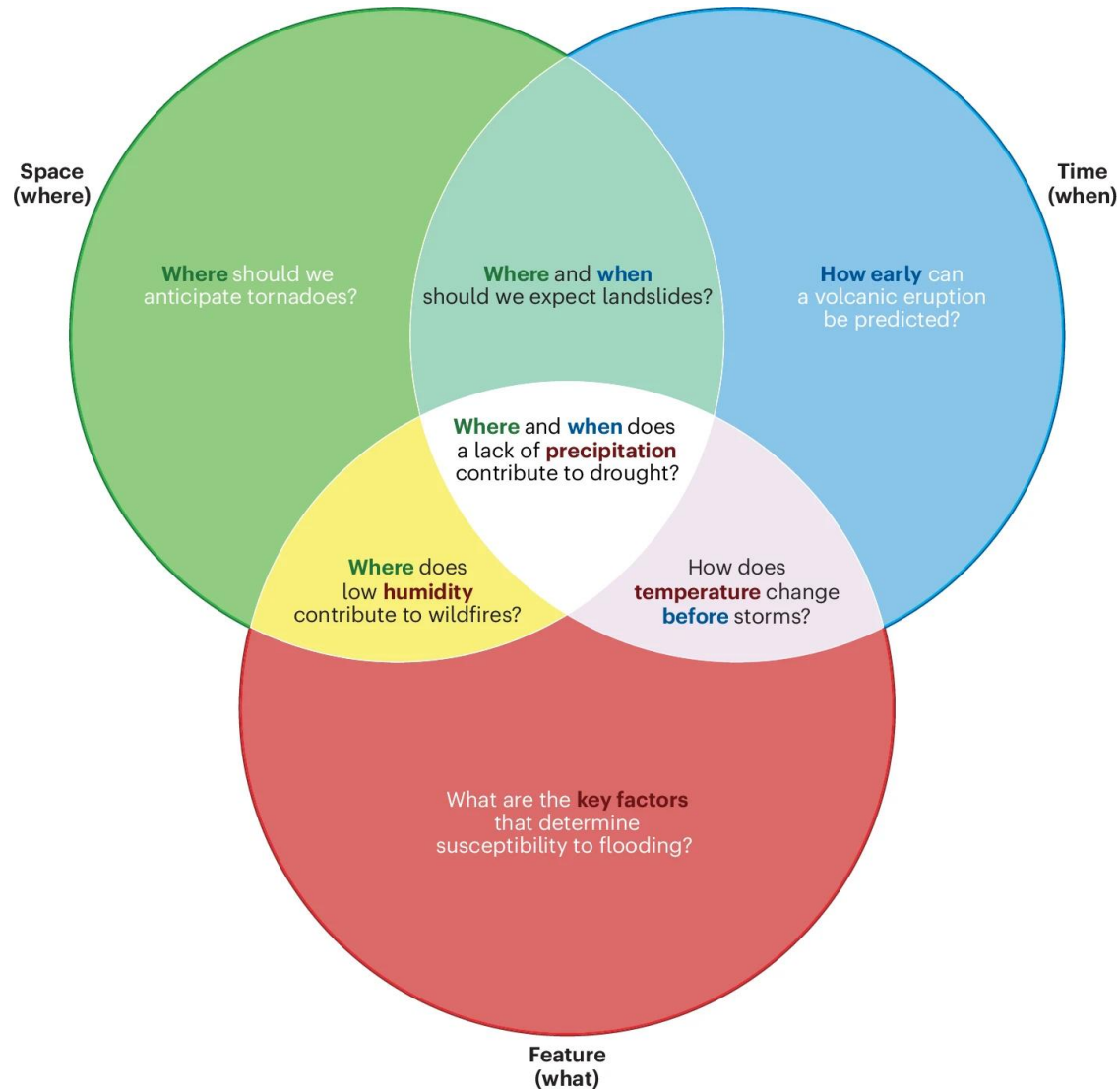


Contents

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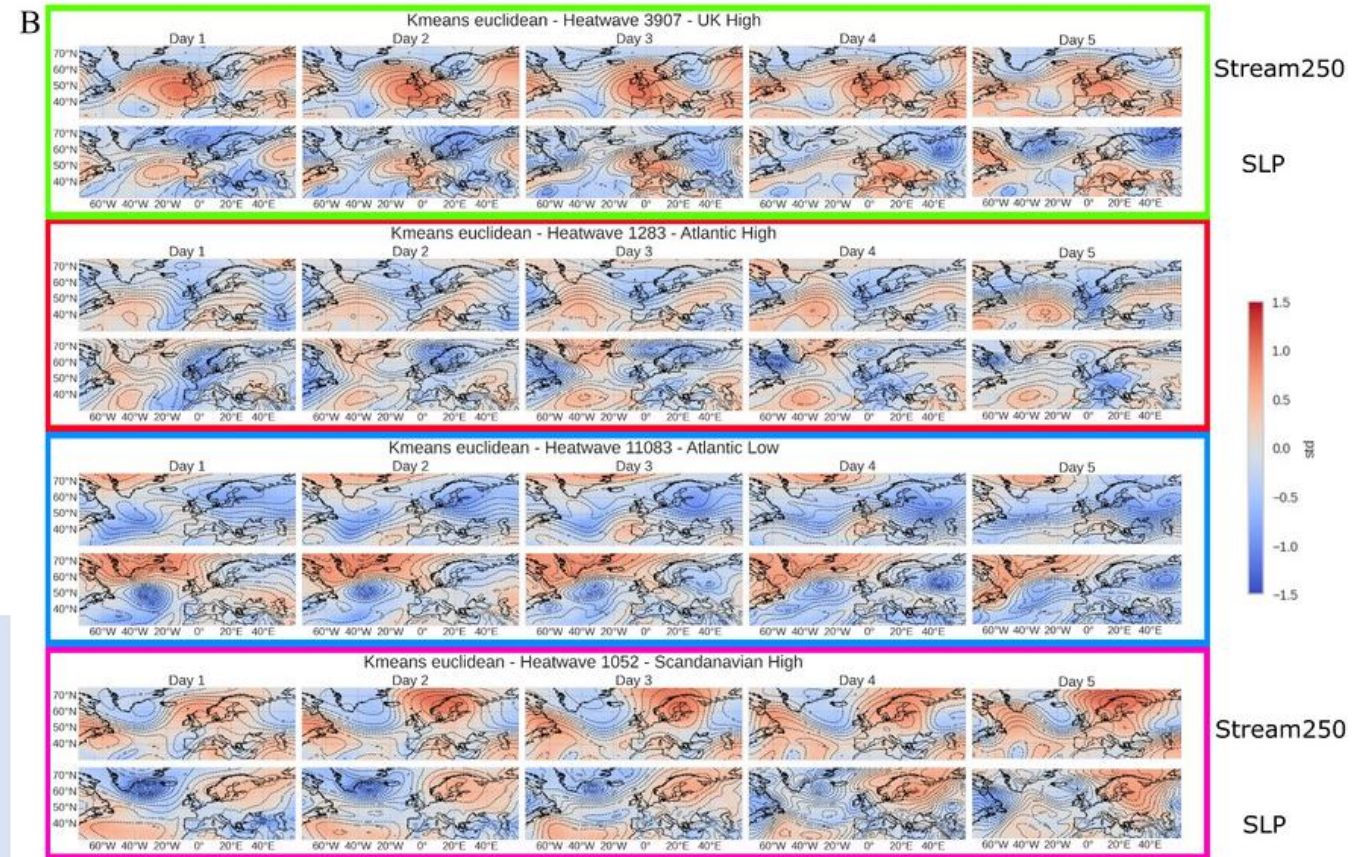
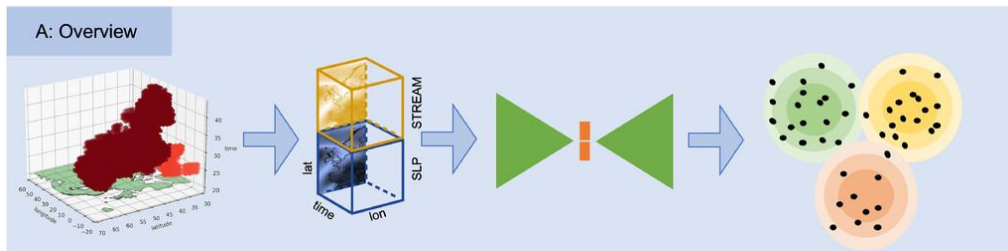
4 The Interpretability Triad: What, Where, When



4

XAI and Process Understanding (I): Heatwave Latent Representations

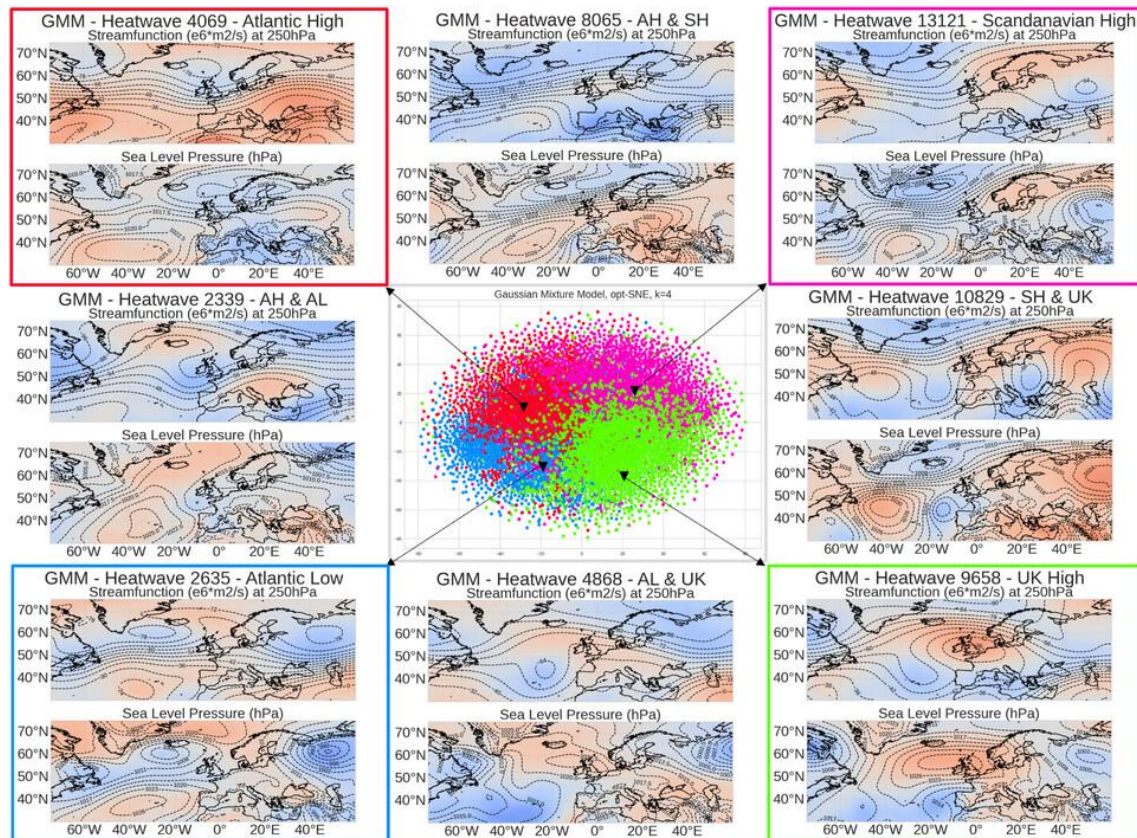
- GDBSCAN detects ~14,000 summer heatwaves (July-August) across 1,600 years of KNMI-LENTIS climate simulations, extracting 5-day windows of sea level pressure and 250-hPa streamfunction for surface and upper-level dynamics
- 3D VAE compresses high-dimensional atmospheric circulation into a 128-dimensional latent space
- 4 synoptic regimes: Unsupervised clustering (K-means, GMM) isolated four distinct heatwave circulation patterns: U.K. High, Scandinavian High, Atlantic High, and Atlantic Low



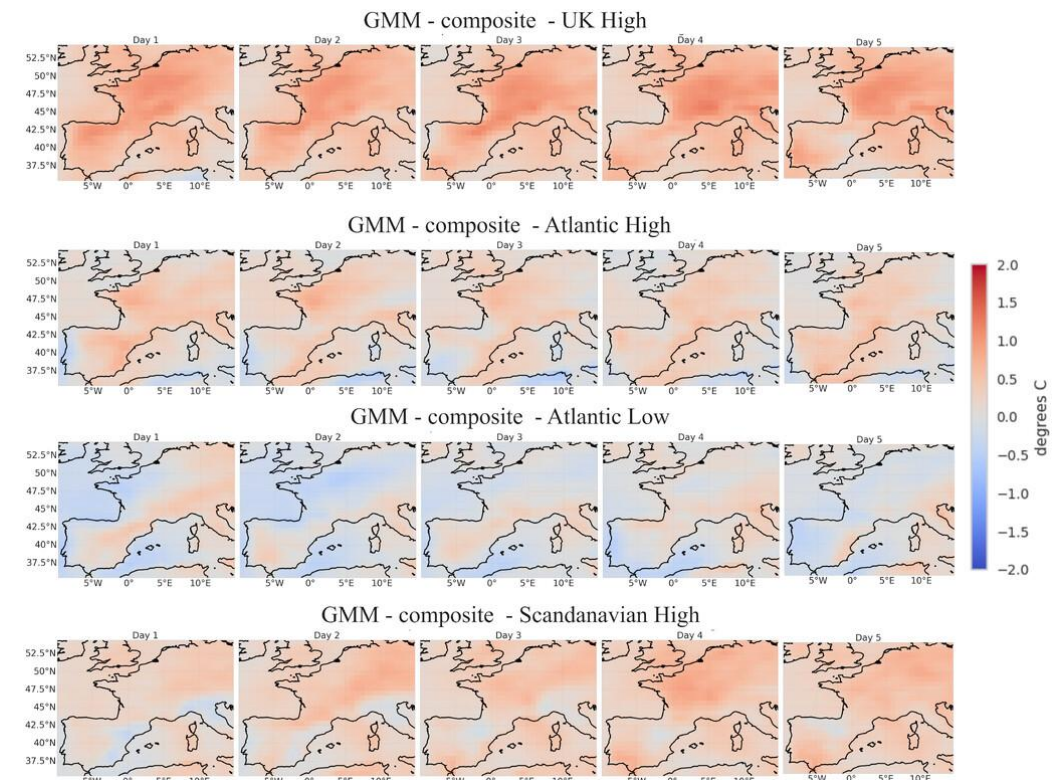
4

XAI and Process Understanding (I): Heatwave Latent Representations

- **Continuous phase space**: Discovered latent manifold displays continuous transitions without rigid borders, reflecting the synoptic life cycle and atmospheric evolution of European heatwaves
- **Probabilistic classification**: **Gaussian Mixture Models** provide soft classification probabilities to model transitional heatwaves



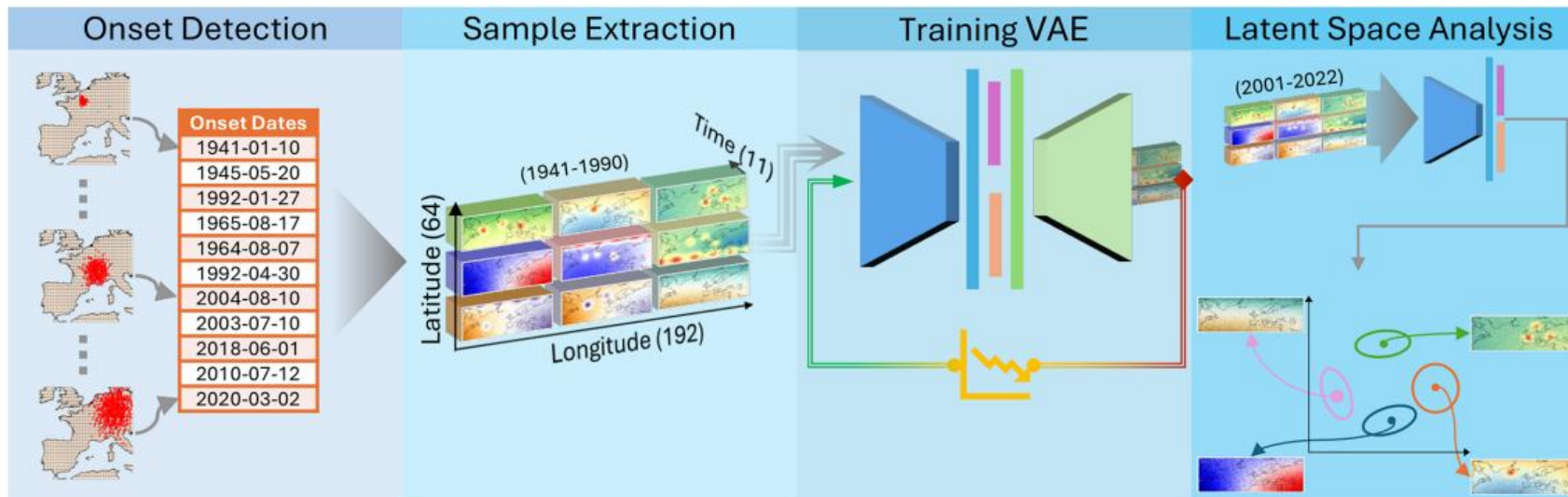
Temperature anomalies of the 4 central heatwaves for GMM



4

Process Understanding (II): Tracking Climate Shifts in Latent Space

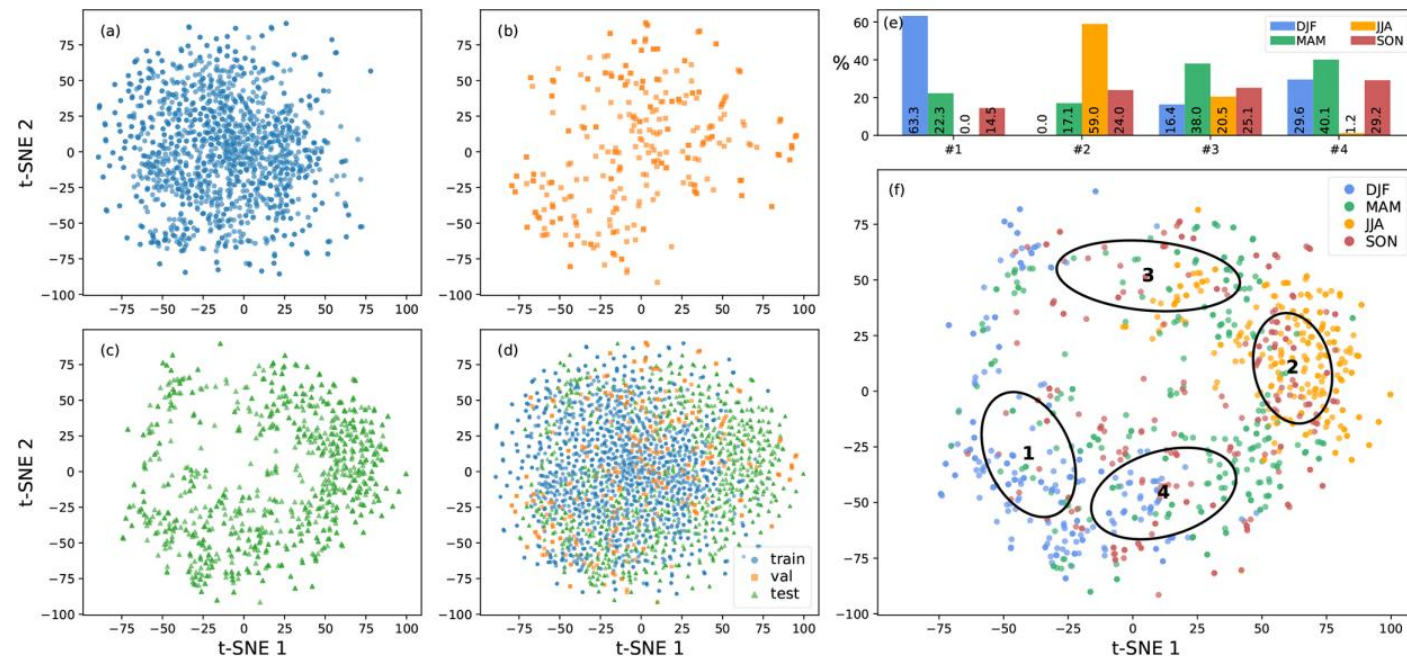
- **9 atmospheric variables from ERA5 reanalysis**: geopotential height, sea level pressure, air temperature 2m, stream function, wind vectors u/v, cloud coverage, relative humidity, and solar radiation
- **11 days**, longer period to capture early build-up dynamics and decay phases
- Daily standardized anomalies across the **entire year**: **winter blocking/warm spells, summer extreme heat, and two contrasting transition-season circulation modes**
- Trained **3D VAE** on 1941–1990 and evaluated on 2001–2022 to **track non-stationary climate shifts**



4

Process Understanding (II): Tracking Climate Shifts in Latent Space

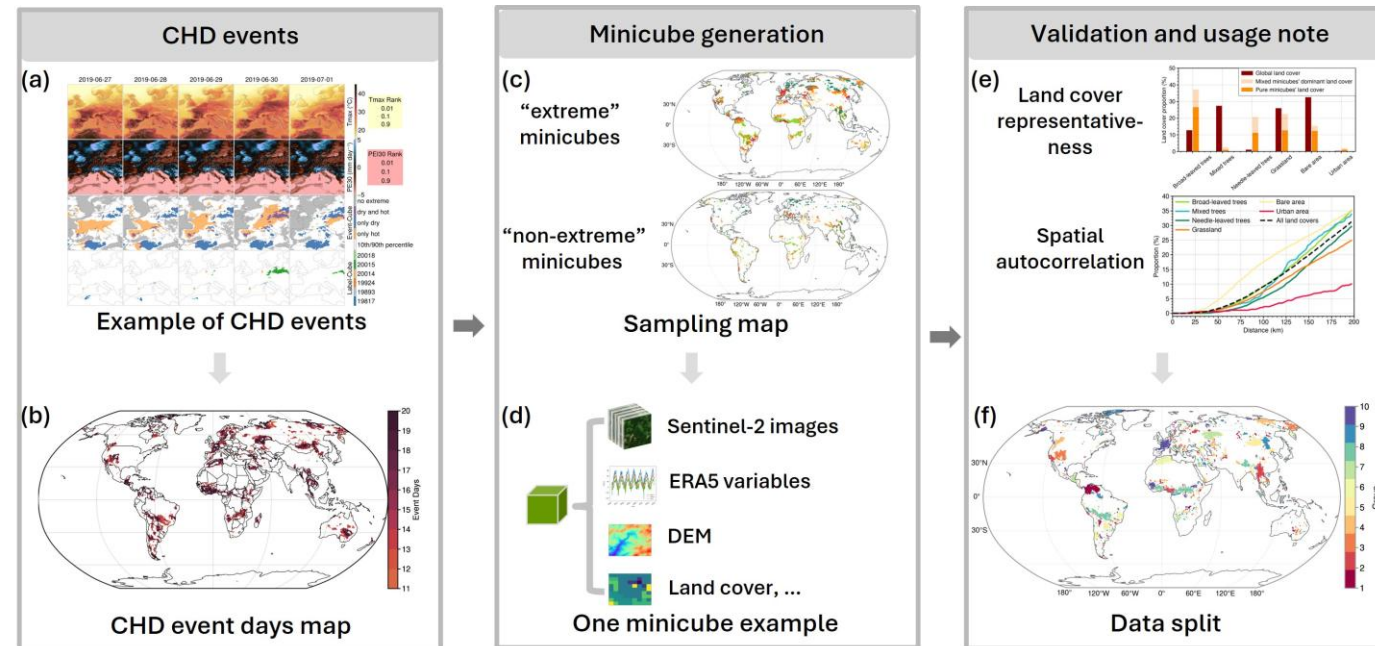
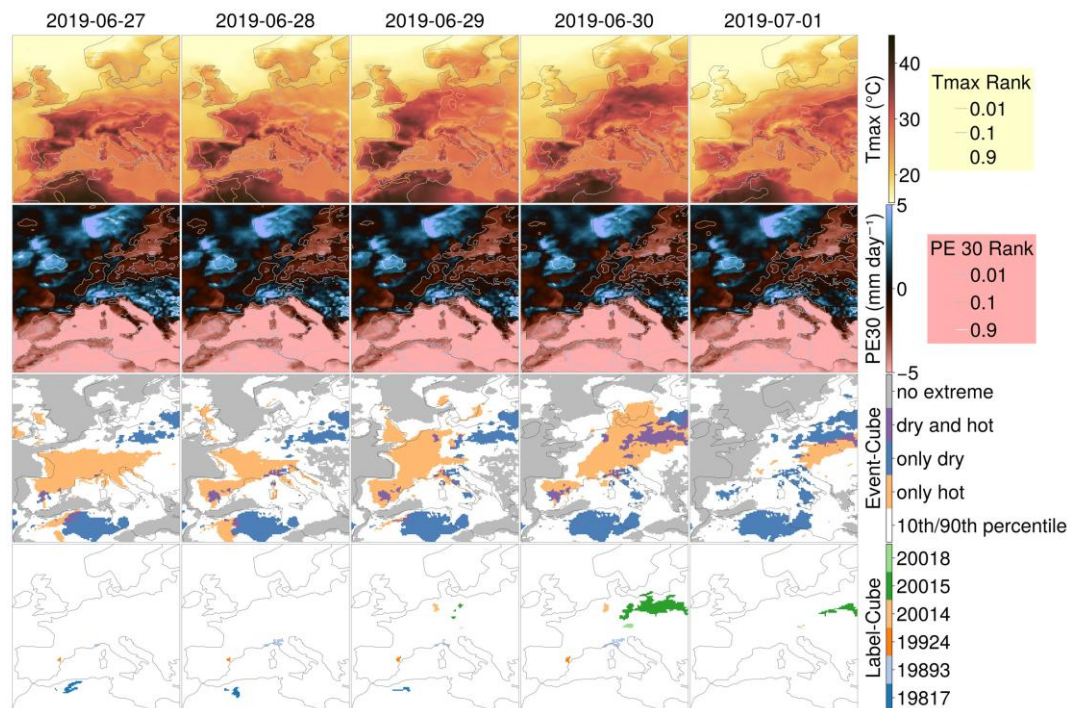
- Winter blocking/warm spells, summer extreme heat, and two contrasting transition-season circulation modes
- **Latent space climate drift**: Recent heatwaves (2001–2022) drift into unpopulated regions of the latent space relative to historical training samples (1941–1990), signaling evolving extreme event behavior
- **Thermodynamic vs. structural drivers**: Summer latent shifts are strongly governed by thermodynamic mean warming, while winter/transition seasons maintain statistically significant structural/dynamical shifts
- **Precursor process identification**: Composite trajectories reveal clear precursor signals up to 5 days prior to onset, such as North Atlantic troughing, blocking highs, and cloud-radiation feedback loops.



4

Process Understanding (III): Gradient-Based Attribution in RS

- DeepExtremeCubes database**: ~40000 minicubes of size 128 x 128 x 495 (pixels x pixels x timesteps) (20 m spatial resolution, 5-daily temporal resolution)



● Broad-leaved trees ● Mixed trees ● Needle-leaved trees ● Grassland ● Bare area ● Urban area

Ji, C., Fincke, T., Benson, V., Camps-Valls, G., Fernández-Torres, M. Á., Gans, F., ... & Mahecha, M. D. (2025).
 DeepExtremeCubes: Earth system spatio-temporal data for assessing compound heatwave and drought impacts. *Scientific Data*, 12(1), 149.

4

Process Understanding (III): Gradient-Based Attribution in RS

- ConvLSTM for vegetation impact (kNDVI) 5-day forecasting
- Integrated Gradients applied to high-dimensional data to extract **local (single input) attributions per minicube**
- Global attribution (aggregation of minicube attributions) for the analysis of the **October 2020 central South America heatwave**

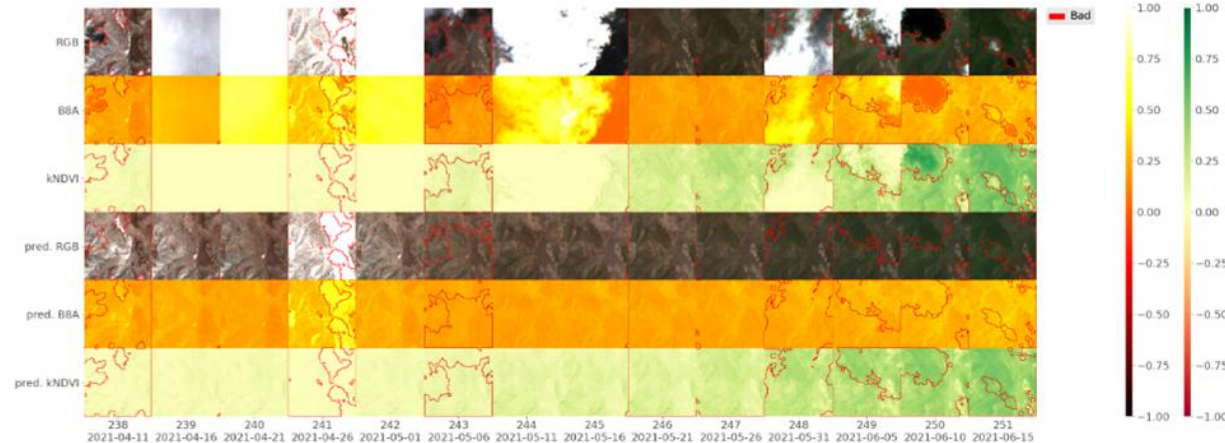
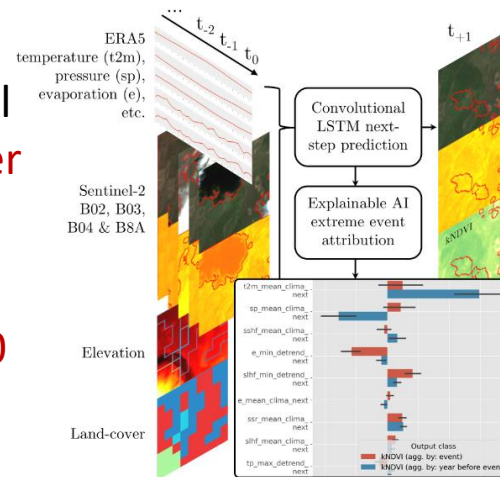
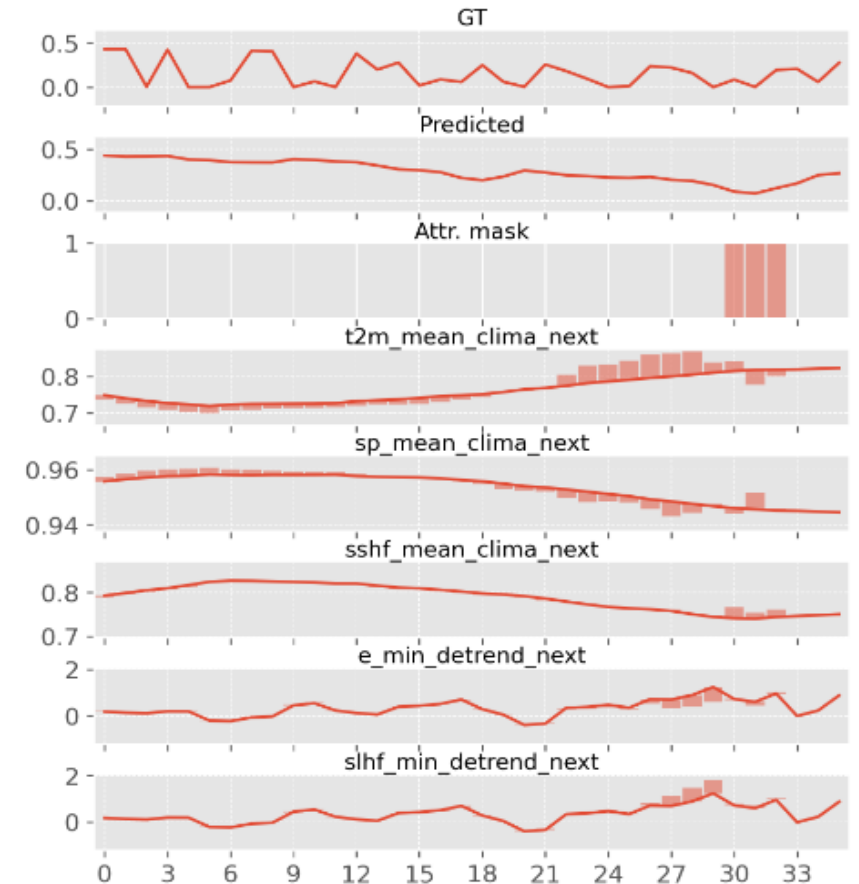


Fig. 4. A Minicube at location 101.95°E, 46.97°N (Mongolia), from 2021-04-11 to 2021-06-15. Top three rows: ground truth RGB_{next} , $B8A_{next}$, and $kNDVI_{next}$. Bottom three rows: model predictions. Red outline: $cloud_mask$ (labeled as "bad"). Minicube L_1 : 0.0351, L_2 : 0.0587, R^2 : 0.9288, NNSE: 0.9335, bias: 0.0095



e (evaporation), slhf (surface latent heat flux), sp (surface pressure), sshf (surface sensible heat flux), t2m (temperature at 2m).

Pellicer-Valero, O. J., Fernández-Torres, M. A., Ji, C., Mahecha, M. D., & Camps-Valls, G. (2025). Explainable Earth Surface Forecasting under Extreme Events. *Earth's Future*

Bridge C: Advances and Horizons in Explainable AI

- **Advances:**

- **Latent Space Dynamics and Synoptic Regimes:** 3D VAEs and unsupervised clustering to extract physically distinct synoptic heatwave regimes across multi-century climate simulations
- **Tracking Non-Stationary Climate Drift:** VAEs separate thermodynamic mean warming from structural dynamical shifts, identifying atmospheric precursor signals 5 days prior to event onset
- **Gradient-based Earth Surface Feature Attribution:** Applying Integrated Gradients reveals shifting driver mechanisms during extremes

- **Horizons:**

- **Physics-Informed and Intrinsically Interpretable AI:** Inherently enforce thermodynamic conservation laws and physical balance equations, use concepts/prototypes
- **Causal Discovery for Compound Events:** Feedback loops, land-atmosphere interactions, and multi-hazard cascading pathways
- **XAI Storylines and Contextual Aggregation:** Bridge fine-grained pixel attribution maps with macro-level ecosystem process understanding



Contents

1. Introduction: AI for Weather and Climate Extremes
2. AI Methodologies for Detection and Forecasting
3. Model Calibration and Uncertainty Quantification
4. Explainable Artificial Intelligence and Process Understanding
5. Conclusion: Bridging Advances with Horizons

References

5 Conclusion: Bridging Advances with Horizons

- **Advances:**

- **Domain Knowledge-Driven AI Pipelines:** Priors and spatio-temporal label self-correction into DL architectures, reducing false alarm rates and generalizing better for unseen locations
- **Model Calibration and Uncertainty Quantification:** Improve model performance and enable rejection strategies that improve decision reliability during extreme events
- **Process Understanding via Latent Spaces and Attribution:** Employed 3D VAEs and gradient-based attribution to extract synoptic regimes, trace non-stationary climate drift, and uncover drivers

- **Horizons:**

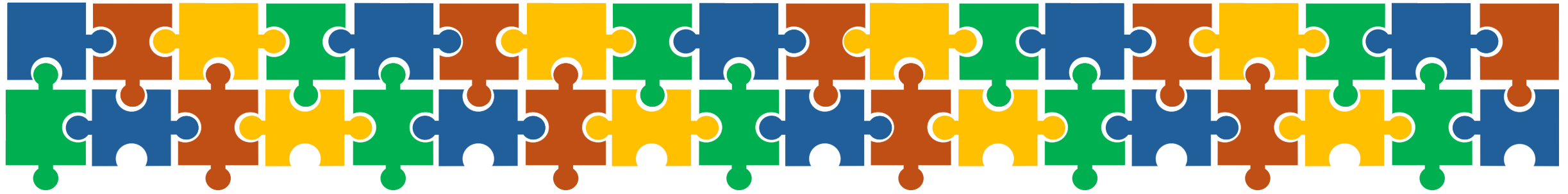
- **From Single-Hazard to Compound/Cascade Events:** Using probabilistic and/or foundation models; e.g., *soil moisture deficit* → *extreme heat* → *wildfires*
- **Overcoming Tail-Risk and Rapid-Onset Limits:** Resolving onset detection bottlenecks and rectifying skill deficits in models for extreme tail-risk events
- **Physics-Informed and Intrinsically Interpretable AI:** From post-hoc attribution toward inherently interpretable models (prototypes, concepts) that enforce thermodynamic laws and causal structures
- **Operational and Expert Integration Early Warning Systems:** Integrating UQ and XAI into operational, human-in-the-loop warning systems for compound events

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Bridging Advances with Horizons in Uncertainty Quantification and Explainable Artificial Intelligence for Weather and Climate Extremes

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