Machine Learning Enhancement for Global Weather and Climate Simulation

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ICAMS Workshop
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Timeline of ML Integration with NWP and Evolution to ESDTs

!960s-1970s: advent of Numerical Weather Prediction (NWP)

First calculation of NWP on a computer: Charney, J. G., Fjoertoft, R. & Neumann, J. v. Numerical integration of the barotropic vorticity equation. Tellus 2, 237–254 (1950).

1980s: Use of statistical methods and improved numerical schemes in weather forecasting

Robert, A. J. A semi-Lagrangian and semi-implicit numerical integration scheme for the primitive meteorological equations. J. Meteorol. Soc. Jpn 60, 319–324 (1982).

1990s: Emergence of neural networks, sophisticated data assimilation

Daley, R. Atmospheric Data Analysis (Cambridge Univ. Press, 1991).

Rumelhart, D. E., Hinton, G. E. & Williams, R. J. Learning representations by back-propagating errors. Nature 323, 533–536 (1986).

2000s: ML enhancements to data assimilation and advanced data assimilation algorithms

Grell, Georg A., and Dezső Dévényi. "A generalized approach to parameterizing convection combining ensemble and data assimilation techniques." *Geophysical Research Letters* 29.14 (2002): 38-1.

2010s: Deep learning applications in weather forecasting, hybridization of NWP and ML models

O'Gorman, Paul A., and John G. Dwyer. "Using machine learning to parameterize moist convection: Potential for modeling of climate, climate change, and extreme events." *Journal of Advances in Modeling Earth Systems* 10.10 (2018): 2548-2563.

2020s: Real-time forecasting and generative models, rise of explainable AI, early development of Earth System Digital Twins (ESDTs) and Foundation Models for weather and climate

Bauer, Peter, Bjorn Stevens, and Wilco Hazeleger. "A digital twin of Earth for the green transition." *Nature Climate Change* 11.2 (2021): 80-83.

Schmude, Johannes, et al. "Prithvi WxC: Foundation Model for Weather and Climate." ***arXiv preprint arXiv:2409.13598*** **(2024).**

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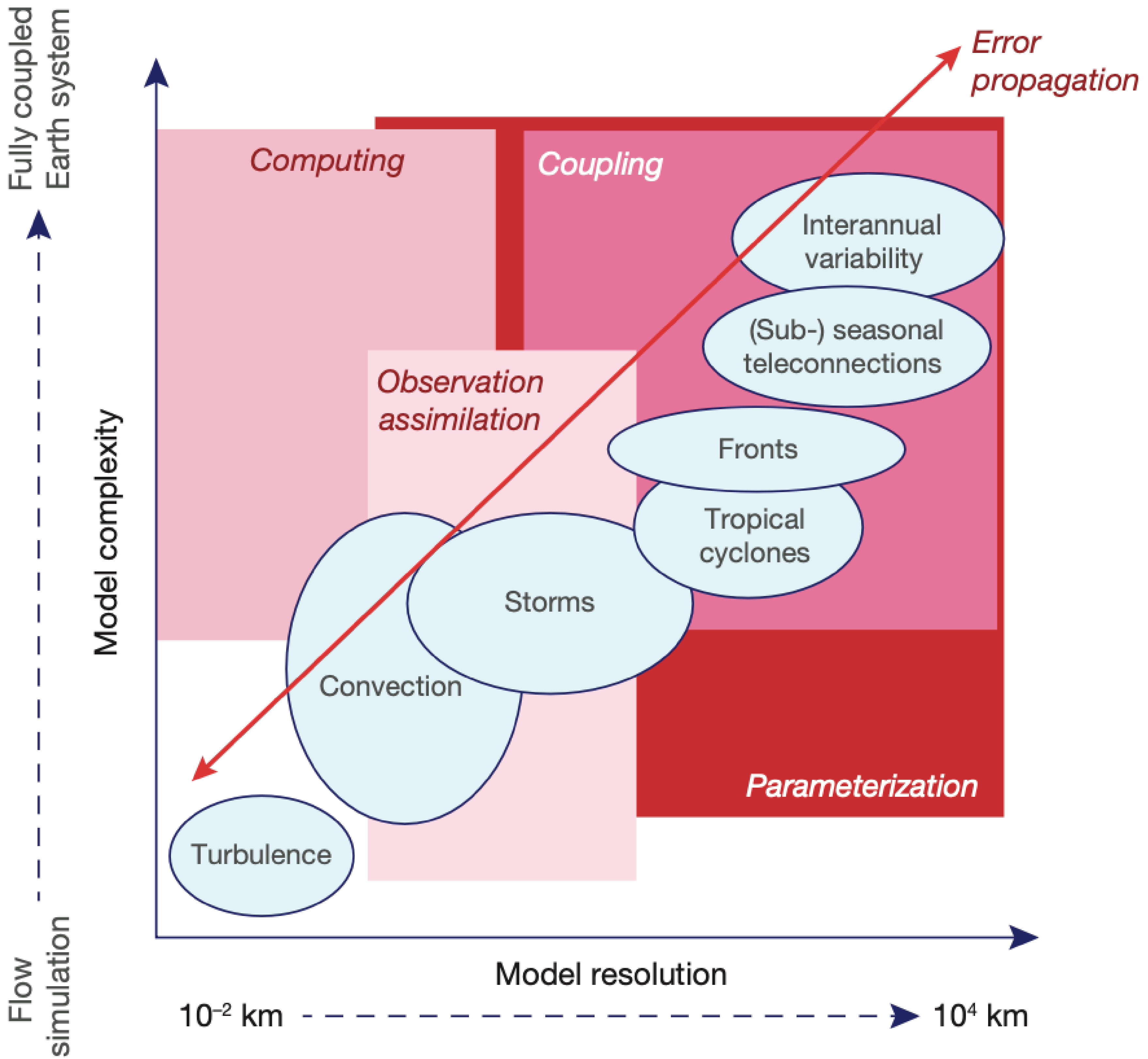
Complexity vs. Scale in ML Applications

Parameterizations: Early applications of ML in NWP often focused on simplifying complex processes (like cloud formation and turbulence) through ML-based parameterizations. These models aimed to capture intricate atmospheric phenomena with reduced computational complexity, making them suitable for large-scale models that require efficiency without sacrificing significant accuracy.

Hybrid Models: The integration of ML into existing NWP frameworks has led to the development of hybrid models, which combine traditional numerical approaches with machine learning. This synergy allows for improved performance at various scales, balancing complexity with computational feasibility.

Digital Twins: The concept of digital twins represents a holistic approach to simulating the Earth's systems, integrating atmospheric, oceanic, and terrestrial models into a unified framework. This requires managing substantial complexity due to the interactions between different components of the Earth system.



Bauer, Peter, Alan Thorpe, and Gilbert Brunet. "The quiet revolution of numerical weather prediction." *Nature* 525.7567 (2015): 47-55.

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NWP at Goddard: GCMs for Weather and Climate

General Circulation Models (GCMs) are complex computer models used to simulate the Earth's climate and weather systems. They are essential tools for understanding atmospheric processes and predicting future climate changes.

The Goddard Earth Observing System version 5 (GEOS-5) atmospheric model is a weather and climate numerical model developed for analyses and weather forecasts of Earth's atmosphere, climate simulations and predictions, and chemistry-resolving simulations.

All versions of GEOS are developed and maintained by the **Global Modeling and Assimilation Office (GMAO) at NASA Goddard Space Flight Center (GSFC)**

The Goddard Institute for Space Studies (GISS) develops a framework of coupled atmosphere-ocean modules for climate simulation and prediction called **ModelE**.

The E3.x series of model configurations has progressed structurally from the E2.1/E2.2 generations in the pursuit of two primary goals: fidelity of cloud processes, and increased resolution in all components.

ML at Goddard – Published work

Atmospheric science
Foley et. al. 2024, *EGUsphere*
Barahona et. al. 2024, *AIES*
Gao et. al. 2023, *AMT*
Caraballo-Vega et. al. 2023, *RSE*
Anderson et. al. 2023, *ACP*
Anderson et. al. 2022, *GMD*
Gao et. al., 2022, *AMT*
Li et. al. 2022, *AMT*
Andela et. al., 2022, *Sci. Adv.*
Sayeed et. al. 2022, *AMT*
Fedkin et. al. 2021, *AMT*
Gao et. al., 2021, *AMT*
Lee et. al., 2021, *Rem. Sens.*
Yorks et. al. 2021, *Atmosphere*
Chen et. al., 2020, *JAMES*
Chen et. al. 2014, *N. Geo.*

Foundation model development for weather and climate
Schmude et. al., 2024, *arXiv*
Mukkavilli et. al. 2023, *arXiv*

Radiative-transfer/satellite emulators
Kalb et. al. 2023, *Earth and Space Sci.*
Stegmann et. al. 2022, *JQSRT*
Vasilkov et. al., 2022, *Rem. Sens.*

Planetary observation and exploration
Valizadegan et. al. 2022, *TAJ*
DaPoian et. al. 2021, *Computer*
Adriani et. al. 2023, *PRL*
Brill 2023, *arXiv*
Olmschenk et. al., 2021, *TAJ*
Mengwall & Guzewich 2023, *Icarus*
Kalb et. al. 2023, *ESS*

Hydrology and land processes
Li & Rodell 2023, *AMS*
Clyvihk et. al. 2023, *WRR*
Yatheendradas et. al. 2023, *AMS*
Biswas et. al 2022, *Front. Earth Sci.*
Elders et. al. 2022, *RSA*
Amatya et. al. 2021, *Eng. Geo.*
Stanley et. al., 2021, *Front. Earth Sci.*
Rodriguez-Fernandez et. al. 2015, *IEEE*

Simulation of biogeochemical processes and oceanography
O'Shea et. al. 2023, *R.S. Env.*
Fasnacht et. al., 2022, *Rem. Sens.*
Pahlevan et. al. 2022, *Rem. Sens. Env.*
Craig & Karaköylü, 2019, *EarthArXiv*

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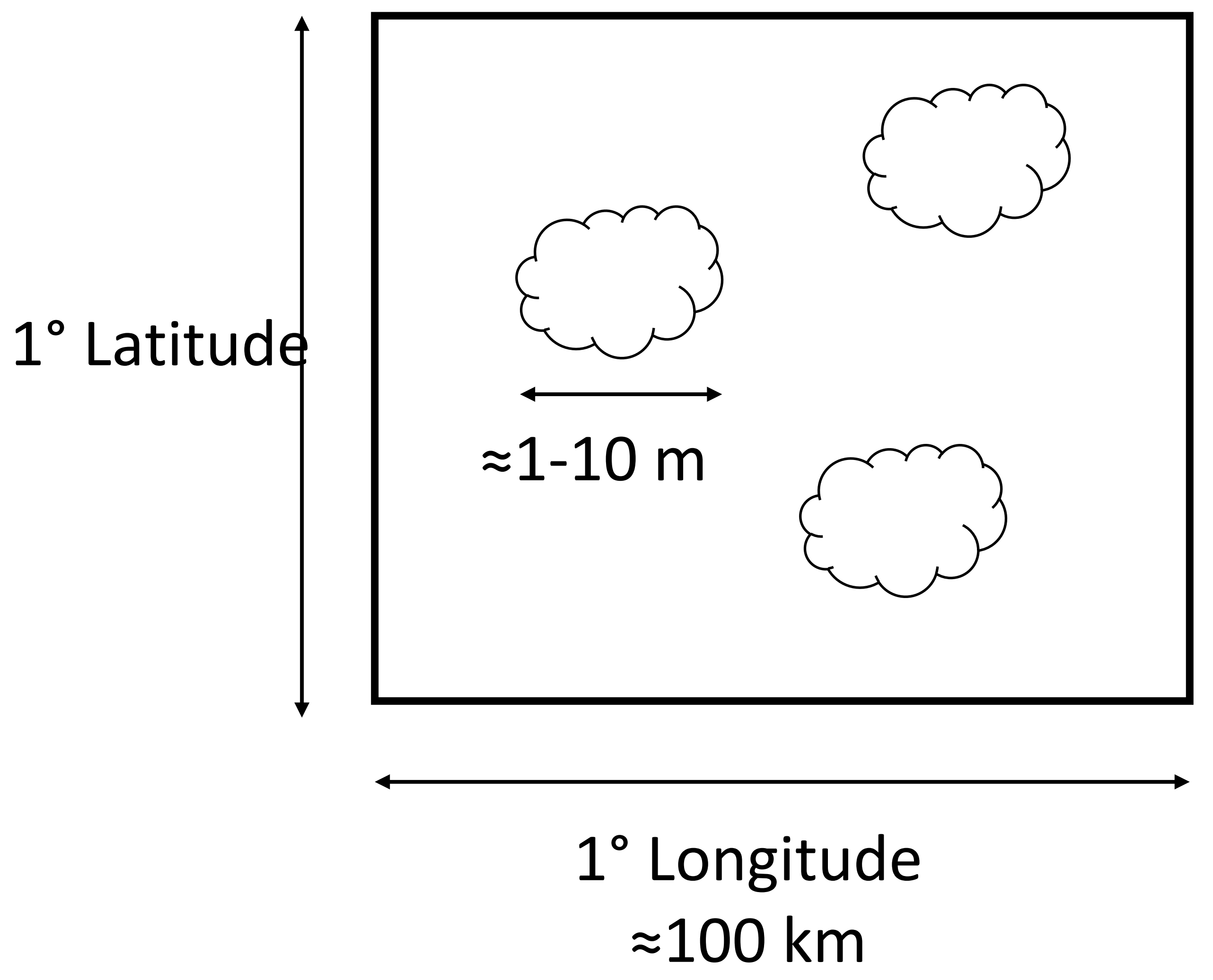
Subgrid-scale Dynamics are Highly Uncertain in GCMs



- **Problem: Physics occurring on micro/subgrid scales cannot be fully-resolved at typical GCM resolutions**
- We need accurate parameterizations for subgrid-scale dynamics!
- **Numerical Solution: Best available theory + data assimilation**
  - Numerical methods can be computationally expensive
  - Lack of fundamental scientific knowledge at relevant scales

Deep Learning (DL) Solution: Leverage patterns inherent in data (simulated+observed)

- Unless otherwise constrained, off-manifold (physically inconsistent) predictions are common

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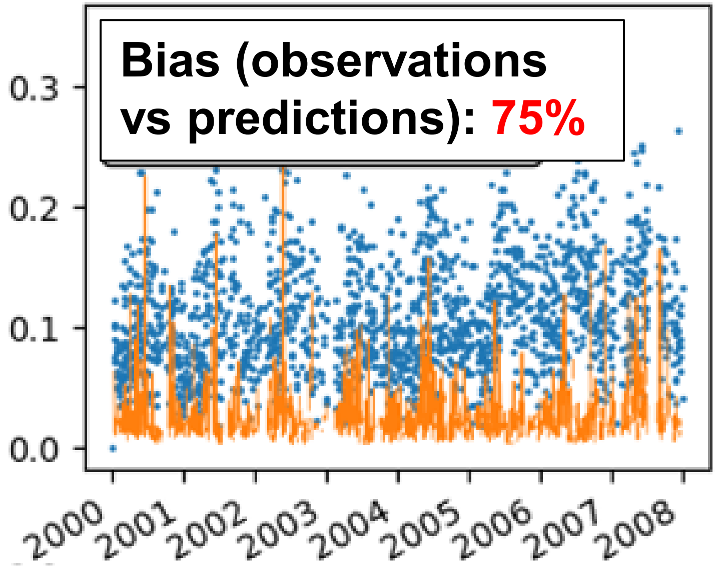
Example application: Wnet (PI: Donifan Barahona)

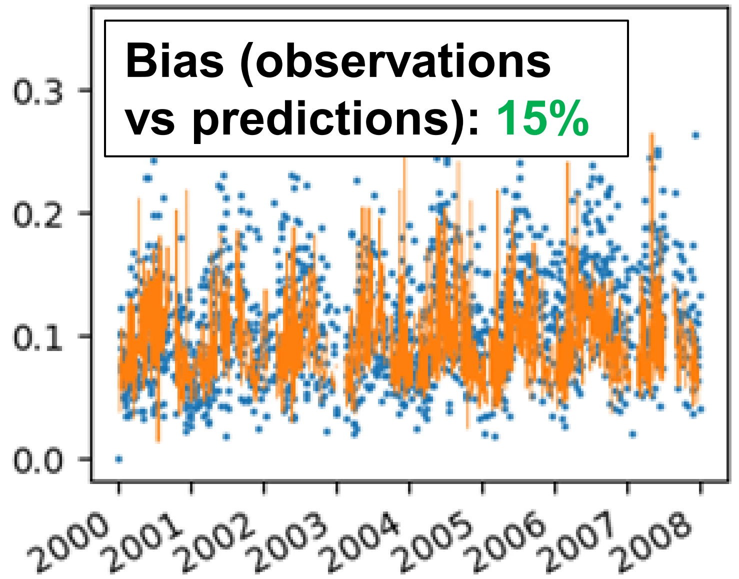
Wnet prediction (G5NR, unconstrained)



Probabilistic learning of sub-grid physics

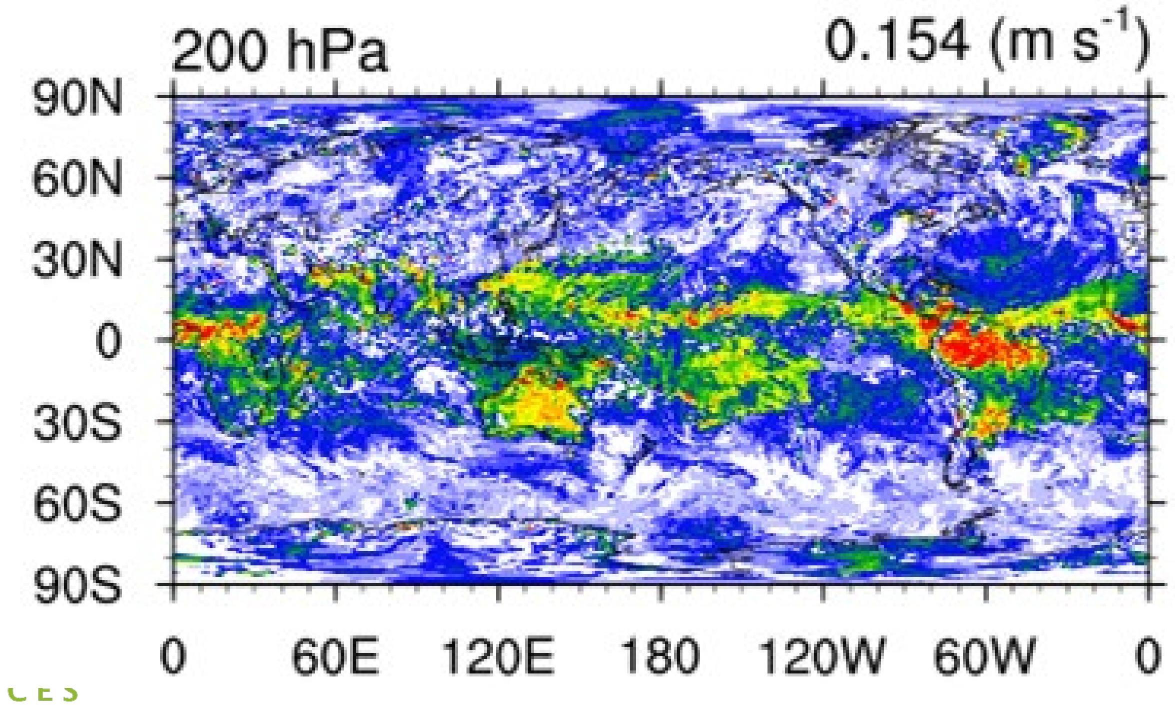
Daily mean σ_w (m/s). Obs vs. – Prediction

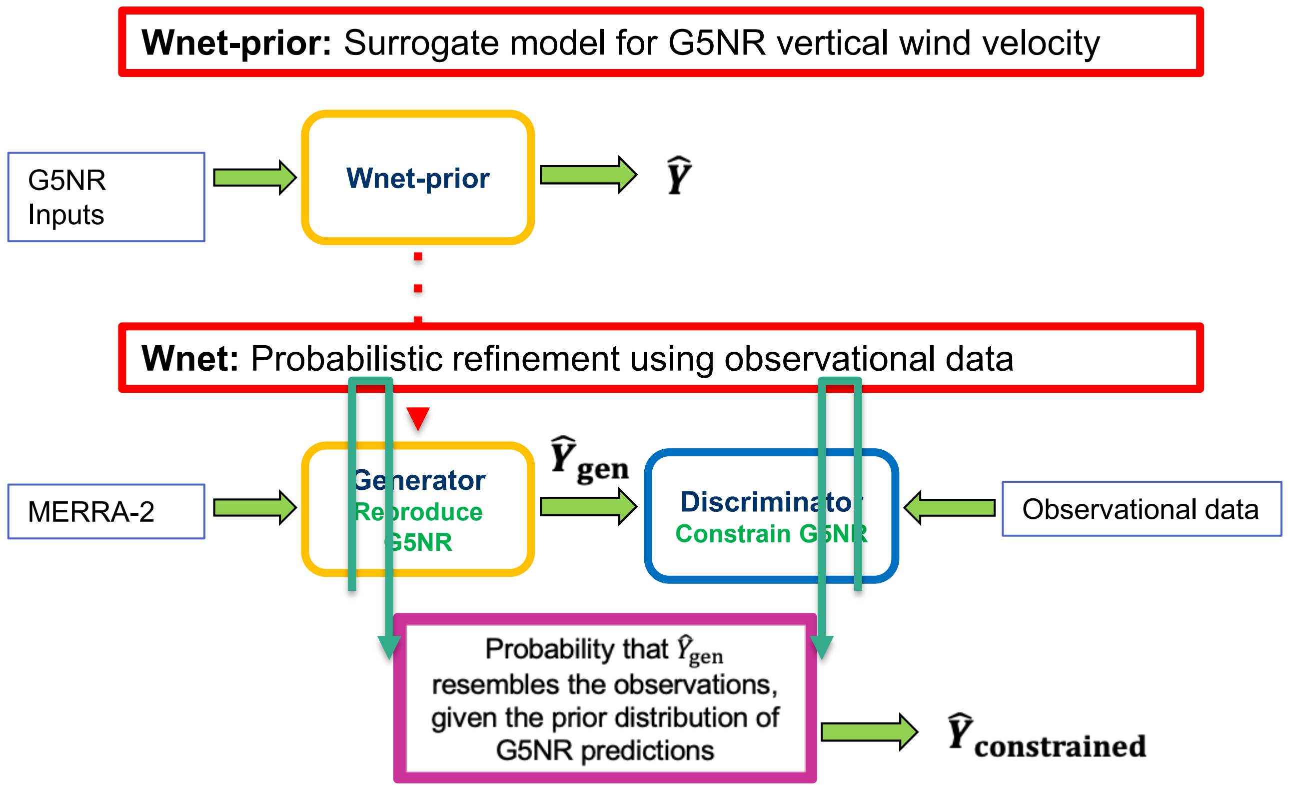
Wnet prediction constrained by obs



Constrained Wnet prediction of σ_W driven by MERRA-2

sigmaW (m/s) 01-Jan 2019 (01H)





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Barahona, Breen et. al. (2024) Deep Learning Parameterization of Vertical Wind Velocity Variability via Constrained Adversarial Training, *AIES*

Limitations in Traditional Deep Learning Parameterizations

Challenges:

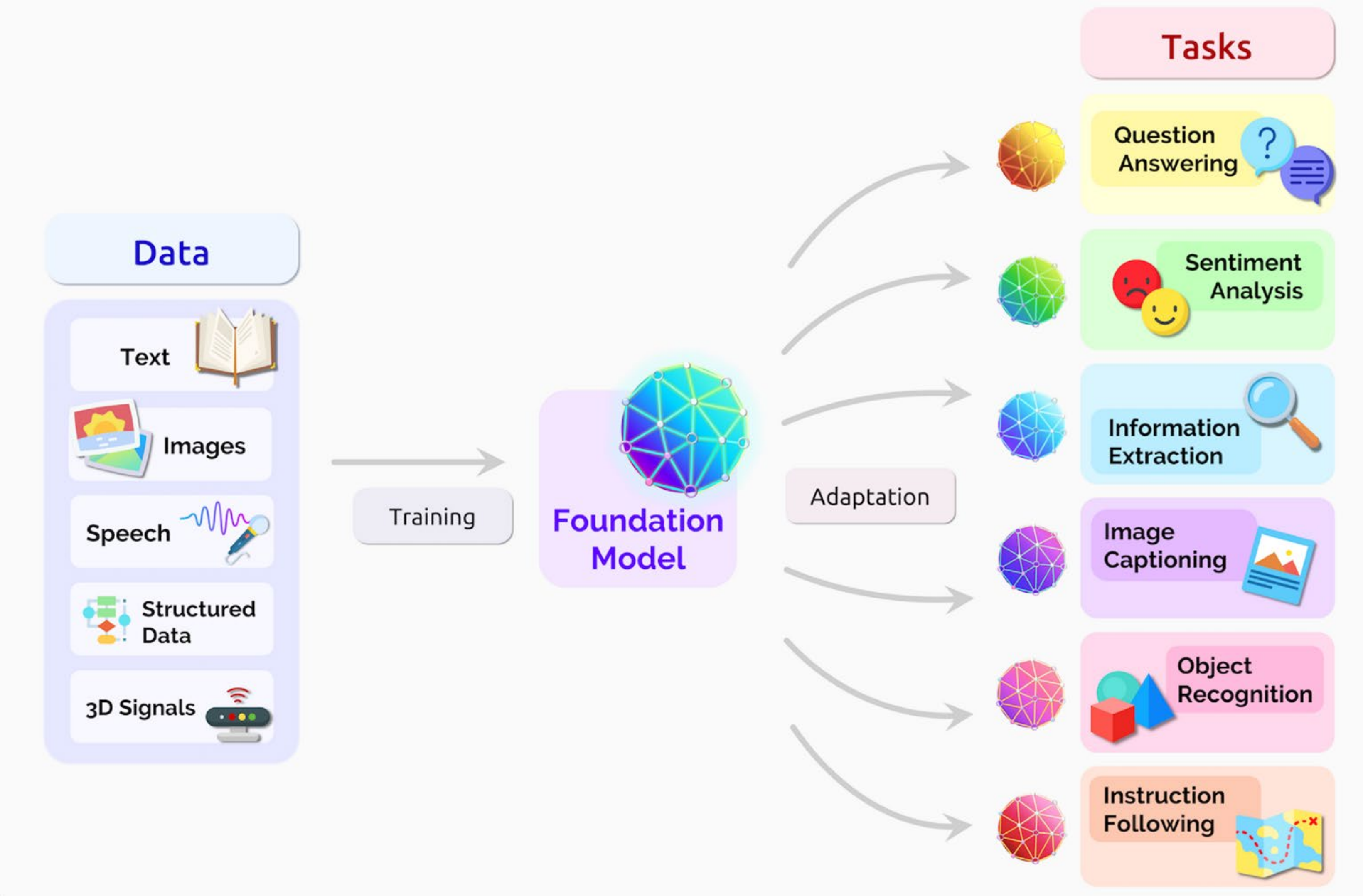
- NNs do not generalize well to new data when the state is outside the variability of the training data set (EX: extreme events, changing climate)
- Without constraints, physically implausible predictions are possible (EX: negative precipitation)
- Model-observation biases present in the GCM are inherited by the emulator – requires correction/constraints/post-processing

Computing:

- Software:
  - Integration of Python ML models with legacy code bases – dependent on developing software
  - Development of pure-Python GCMs – in process but not operational
- Hardware:
  - Increasing complexity of ML model configurations necessitates hardware acceleration and increases in wall time relative to numerical models

Foundation Models

Seminal Stanford CRFM white paper, 2021



- Stanford introduced the concept of **foundation models** in 2021 to tackle some of the limitations in traditional deep learning.
- Defined as models trained on broad data (generally using **self-supervision** at scale) that can be adapted to a wide range of downstream tasks.
- The “**pretrained model**” description was not enough because it suggested that the noteworthy action all happened **after** **“pretraining”**.

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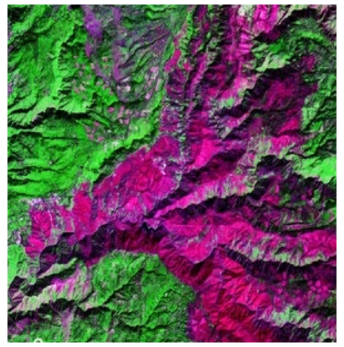
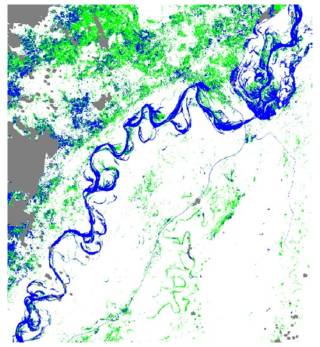
Foundation Models for Science

- Adopting foundation models for science requires some additional **quality assurance** to establish trust and set applicability expectations.
- Our approach to foundation models follows these key areas:
  - **adaptability** (e.g. multiple sensors, multiple tasks)
  - **accessibility** (e.g. computational efficiency, software availability)
  - **trust** (e.g. latent space representation, science output)
  - **validation** (e.g. experimentation, produce better science)
- We want to understand foundation models **strengths** and **weaknesses** to establish when does it make sense to use them, but also how to select the most appropriate models for better science.
- And lastly when do we need to build a new one rather than fine tuning an existing one.

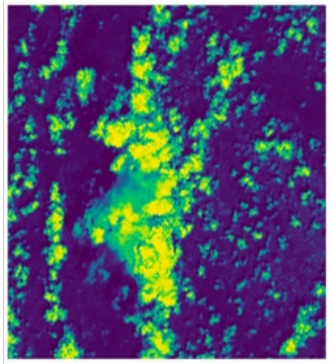
Earth Science Applications of Foundation Models (Large overlap with classic-ML applications)



LU/LC



Surface Water Extent

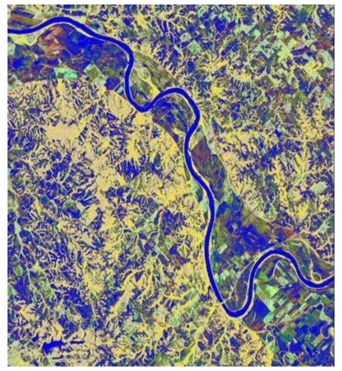


Cloud Masks

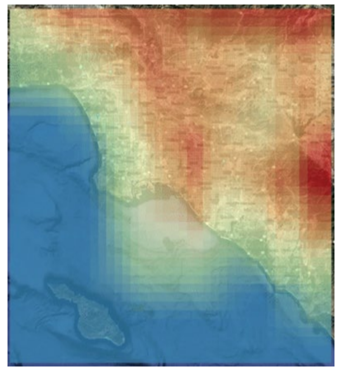
Spectral Unmixing

Recognition and Classification

On the ground and onboard



Hydrology



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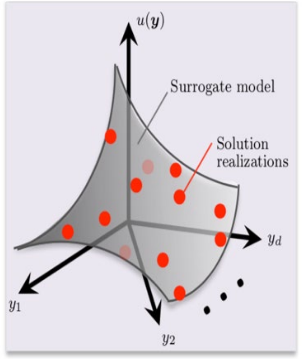
Forecasting and Nowcasting



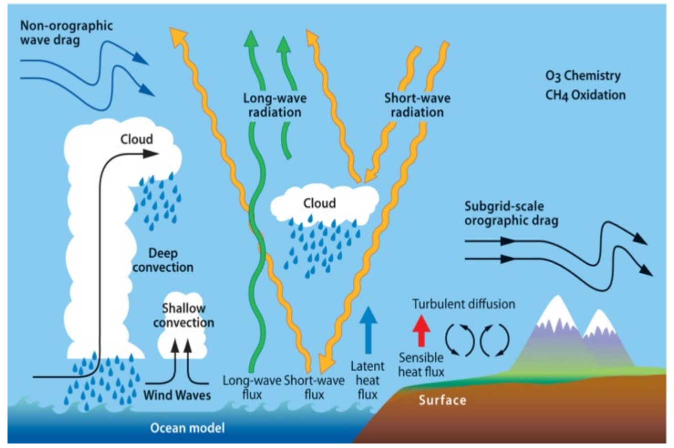
Fast Inversions

Four Cast Net

Fast Models

Surrogate Models

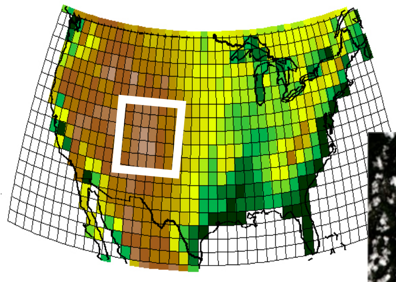
Boundary Conditions



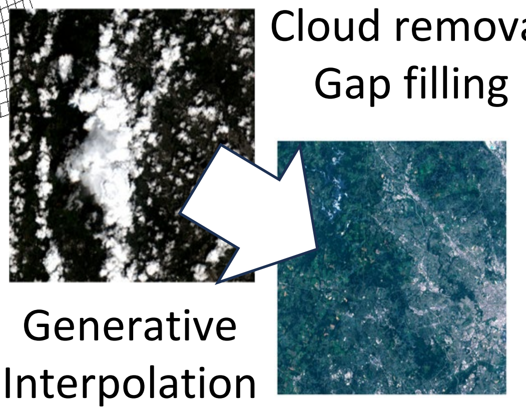
Governing Equations

Parameterizations

Model Understanding and Physics-Inspired ML



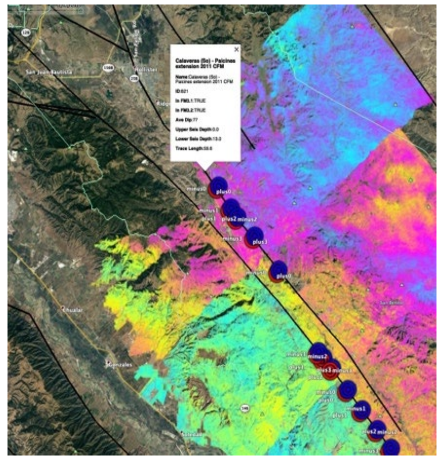
Downscaling



Cloud removal
Gap filling

Generative Interpolation

Interpolation and Reconstruction



Data Fusion

Show me the relationship between SST and algae blooms over the last decade.

Bespoke NLP interfaces

Domain-specific Language Models

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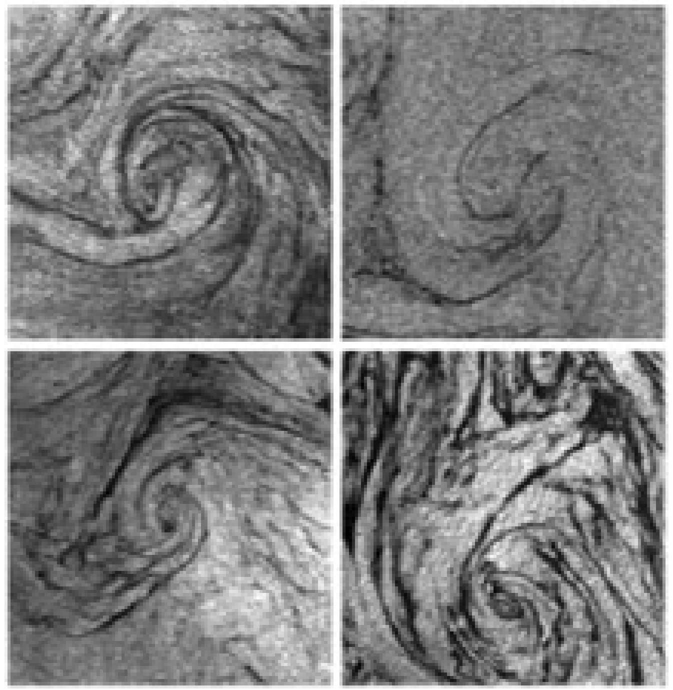
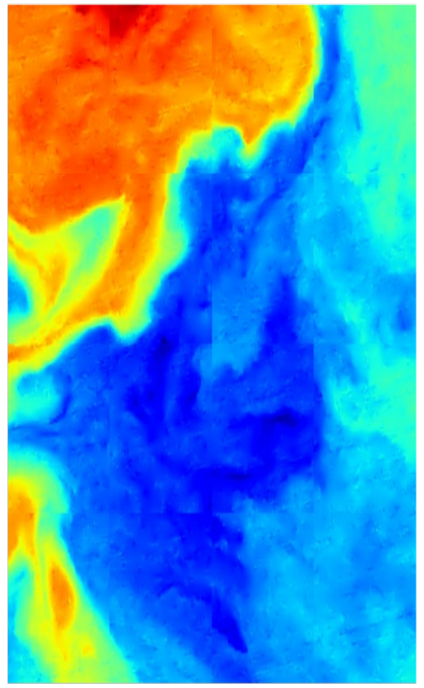
AIST R&D in Foundation Models

SLICE: Semi-supervised Learning from Images of a Changing Earth

Wilson, JPL; AIST-21-0025



Eddy Detection from SAR imagery

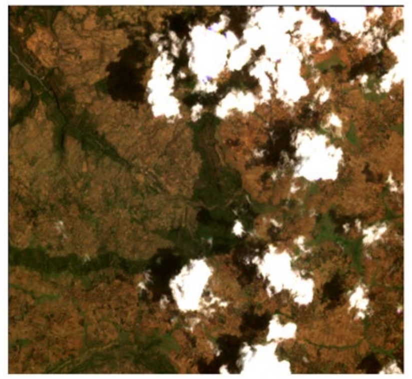


SST reconstruction under clouds

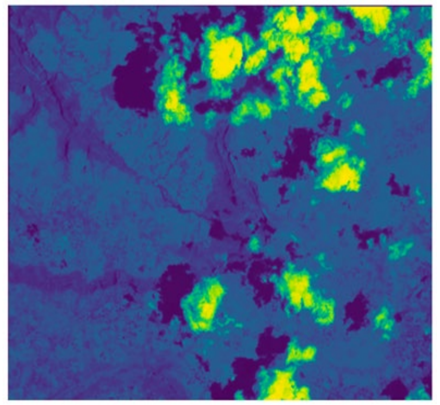
Applications of Vision Transformers and **semi-supervised ML** to enable hard remote sensing problems and increase performance despite scarce labeled data.

Coupled Statistics-Physics Guided Learning

Xie, UMD; AIST-21-0068



original



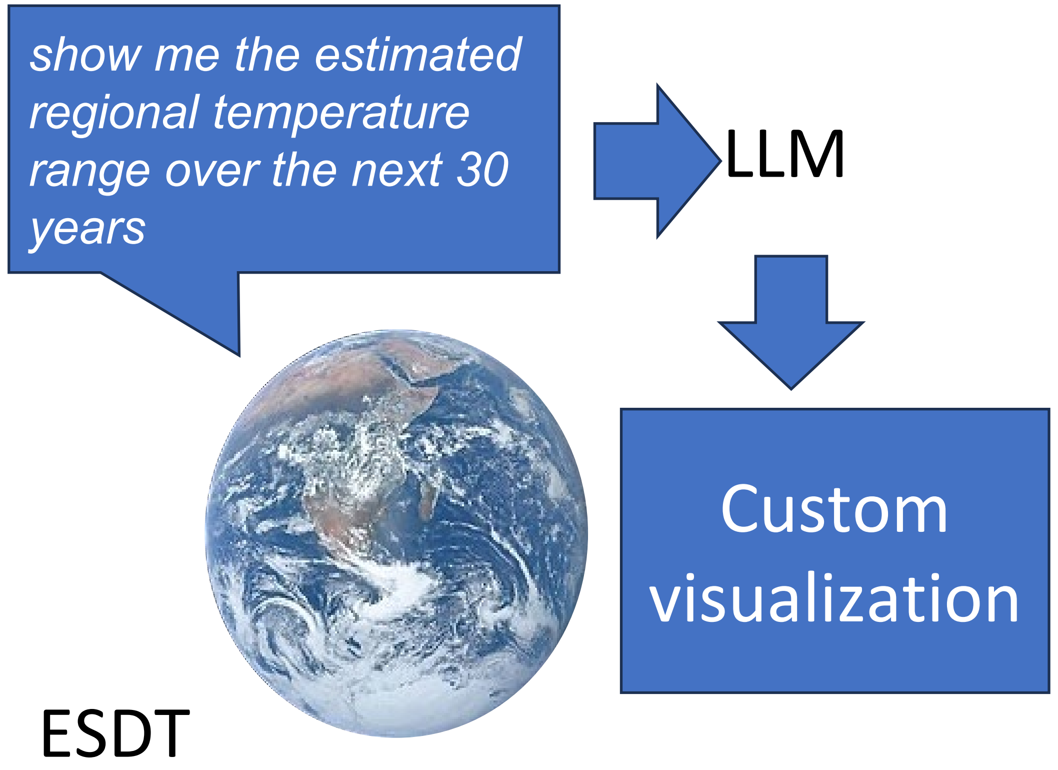
Cloud masks

reconstruction

Semi-supervised learning; physics-guided; and heterogeneity-aware learning.

Digital twin technologies for climate projections

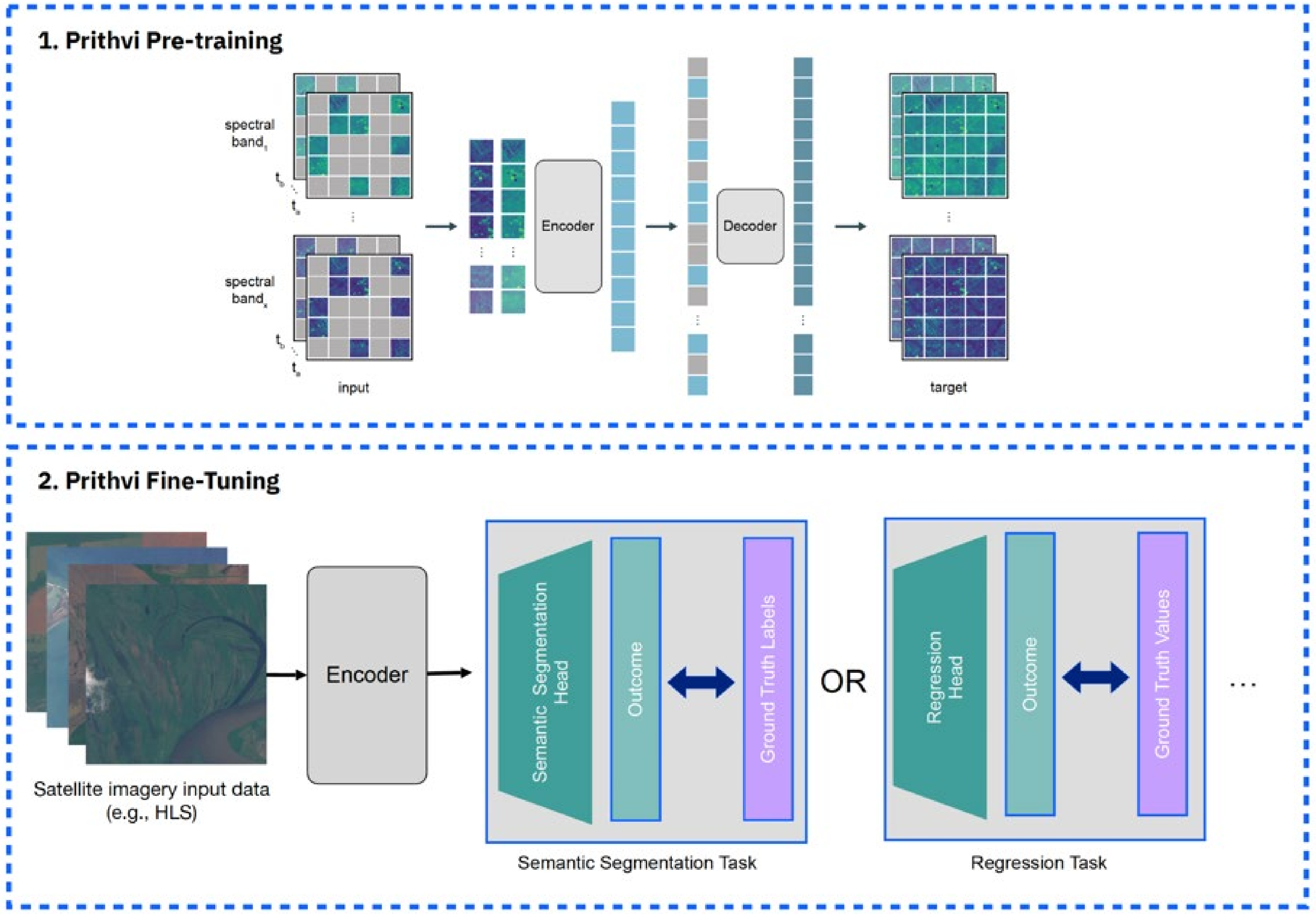
Schmidt, GISS; AIST-QRS-23-0005

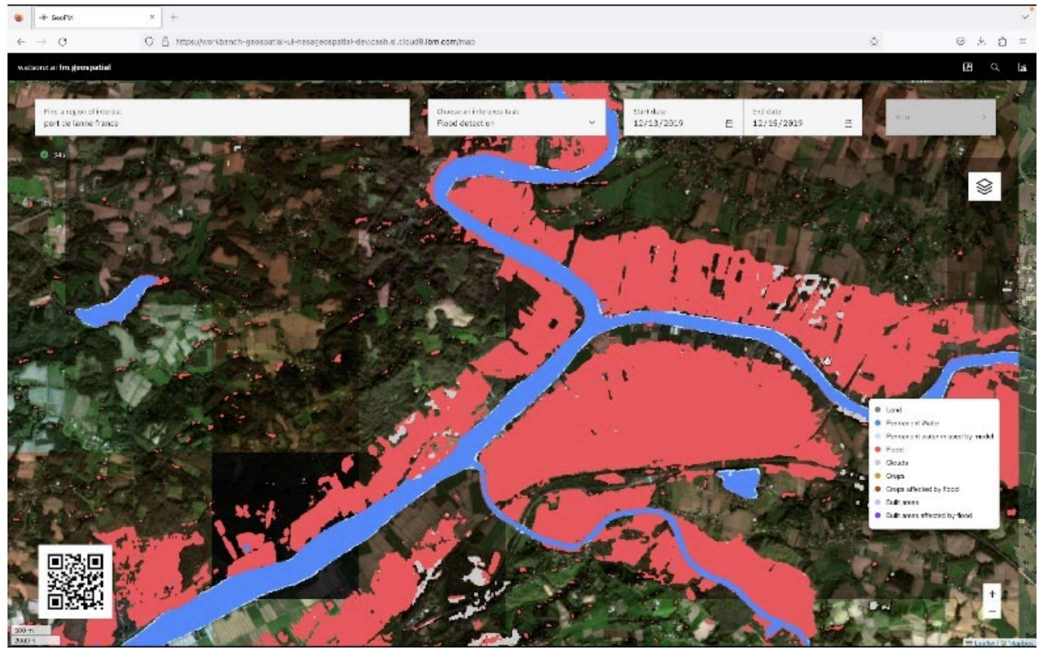


Large Language Models (LLM) to generate bespoke data visualizations for user queries

CSDO, HEC & ESDS R&D in Foundation Models with Collaboration with IBM Research

- **LLM for NASA's Science Mission Directorate**
  - Base Encoder Model - encoder-only transformer model, tailored for SMD applications
  - Sentence Transformer - Generates embeddings for queries and sentences, enhancing information retrieval
  - Passage Reranker - fine-tuned model that takes a search query, and a passage, and calculates the relevancy score of the passage w.r.t the query
- **Prithvi-HLS** - Geospatial FM based on HLS data to support Land Surface Processes and Application
  - Initial version
  - *Working on updated global version*
- **Prithvi-Weather and Climate (WxC) FM** - the focus is not just on Forecasting/Prediction but also on different categories of downstream applications
  - *First version May 2024*
- **Helio/Space Weather FM** - based on SDO data for space weather applications (just started)





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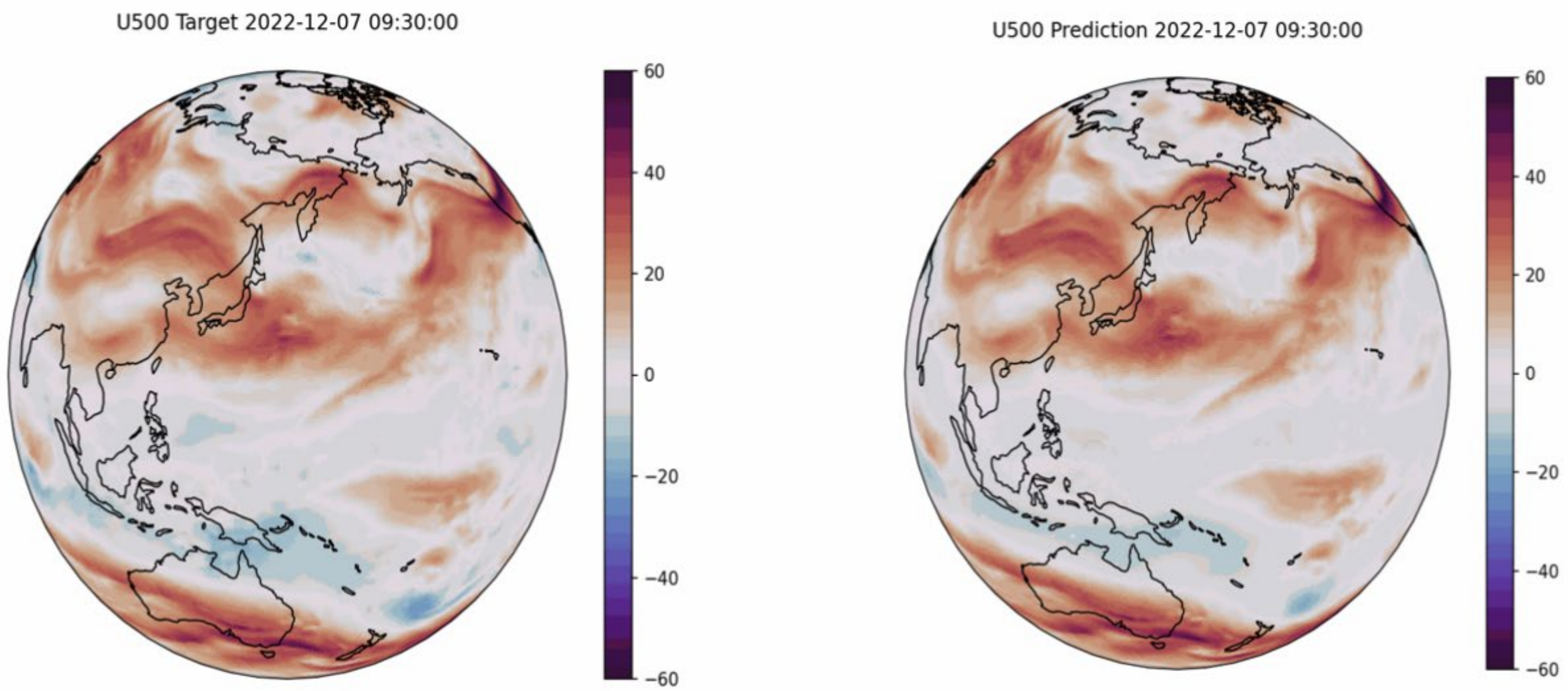
HEC & ESDS R&D in Foundation Model
Prithvi-WxC (Weather & Climate) Foundation Model

- **Goals**

- AI FM for Weather and Climate not focused on Forecasting/Prediction but for different categories of downstream applications
- Model will multiresolution both spatial and temporal to be able to use different types of data such as MEERA, ERA and HRRR
- Quickly establish the credibility of the WxC model and move on to develop multimodal climate applications for ES2A



- **Approach**

- Core architectures under consideration: SWIN, Hiera
- Extensions/modifications include:
  - Multi-level and multi-resolution approaches to accommodate data at different spatial and temporal scales.
  - Diffusion-based architectures to incorporate additional information and enhance model predictions.
- Evaluation using seven different types of use cases

- **Team**

- Broader participation for Science experts to ensure right direction, evaluation and future adoption of the model in their workflows
- [NASA, DOE ORNL, IBM Research, NVIDIA, Academia - University of Colorado, University of Alabama in Huntsville, Stanford]

AIST Earth System Digital Twins

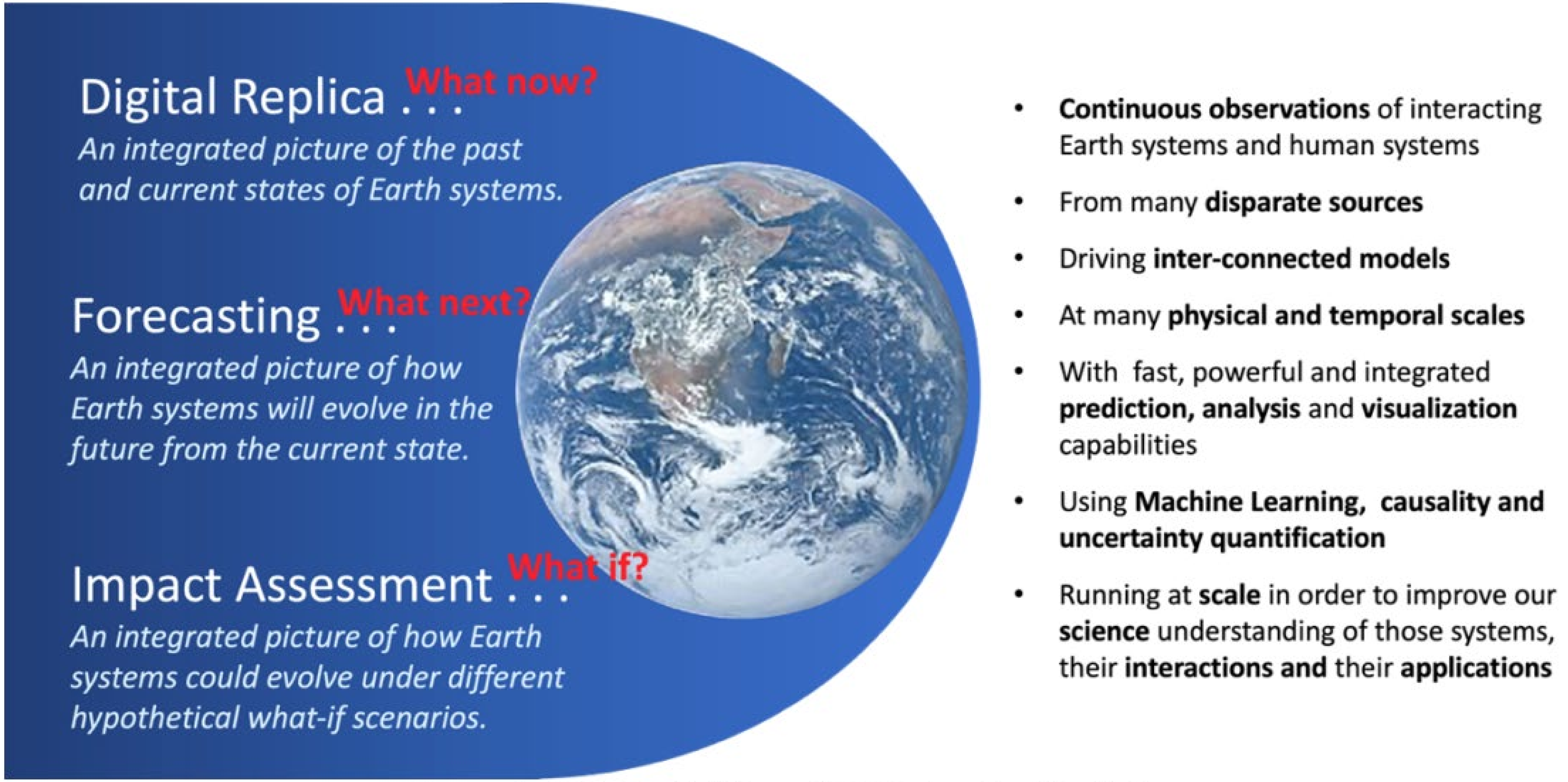


Figure 1. ***AIST Definition of ESDT for the Workshop***

NASA ESDT Workshop Report, 2022

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AIST ESDT cont.

Earth Systems Digital Twins (ESDTs) are an emerging capability for understanding, forecasting, and conjecturing the complex interconnections among Earth systems, including anthropomorphic forcings and impacts to humanity.

- ESDTs will play a critical role in NASA's new Earth Science to Action initiative.
- AIST-21 Solicitation, first US government Solicitation requesting Digital Twins Technology for Earth Science ESTO AIST Earth System Digital Twins (ESDT)
- As of 2023, 16 current ESDT technology development projects funded under the Advanced Information Systems Technology (AIST) program focusing on developing:
  - Underlying analytic capabilities to build Digital Replicas
  - Novel ESDT infrastructure technologies
  - Surrogate modeling and ML emulators
  - Preliminary prototypes including interconnected modeling.

Visit the dedicated ESDT webpage at: https://esto.nasa.gov/earth-system-digital-twin/

Thank You

Questions?