Building AI-based Earth Systems Models and the TERRAHydro Terrestrial Digital Twin

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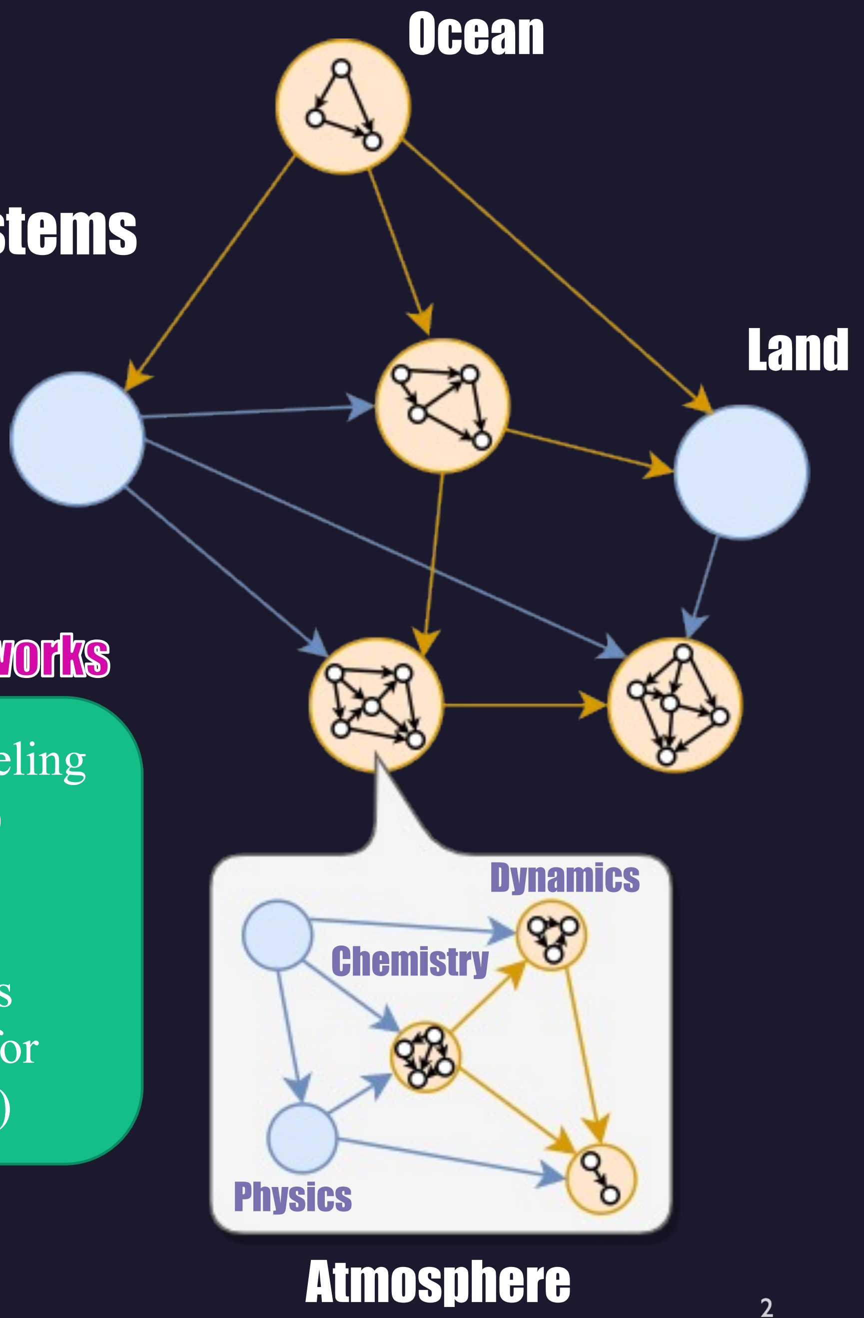
The Structure of Earth Systems Models

- Composed of a coupled set of sub-systems or models of physical processes.
- Organizable into a hierarchal graph with components developed and maintained by domain experts across multiple organizations (e.g., government, academia, industry).
- Frameworks for coupling, organization, and operation of large ESMs/climate models are essential to developing and maintaining large open-source open-science systems.
- Existing frameworks mostly written in/for Fortran and parallelized with MPI for scalability on large CPU-based clusters and not designed for integrating AI technogies.

Some existing frameworks

- Earth Systems Modeling Framework (GEOS)
- MAPL (GEOS)
- NASA's Land Information Systems (operational driver for land surface models)

A Diagram of a Hierarchal Systems Model



Adoption of AI-based Technology

- Data-Driven models have emerged across many Earth Science domains and have been shown to be a powerful alternative to traditional modeling.
- Very few operational AI-based Earth Systems models exists today (one counter example is Google's flood forecasting system).
- Integration into existing modeling frameworks is a significant challenge to the adoption AI-based technologies.

This is relevant today. AI technologies already exist that offer improved capabilities.

Some Barriers to Adoption

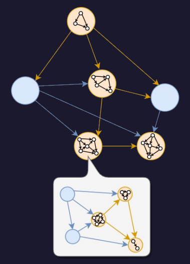
- Existing frameworks do not provide gradients to train fully integrated AI technologies.
- The AI community leverages powerful (Python) tensor-based software which is not easily integrated within existing Fortran frameworks.
- AI-models use differently structured data (sequence-to-one sequence-to-sequence, image stacks/series)
- Assimilation techniques in AI can use tensor gradients techniques.

A Coupled Reusable Earth System Tensor (CREST) Framework

An AI-First Python framework for building coupled open-science Earth Systems Models

Combines the idea of ESM hierarchal graphs with Tensor Network graphs.

Tensor Network Backend



Earth Systems Model Hierarchal Graph

CREST Hierarchal Tensor Graph/Model

- Provides a specification/map between a Tensor Network graph and ESM graph.
- Standardizes how data is passed between sub-systems.
- Internally handles different types of AI-models: Keras, Pytorch, Jax, Black-box models.
- Creates a layer between the tensor backend to enable flexible, extensible, agnostic infrastructure to be built.

CREST Operational Infrastructure

Infrastructure to build, maintain, and operate ESMs.

- **Data Management** for loading large geo-spatial-temporal data.
- **Data Asssimilation** for ingestion of near real-time data and adaptability.
- **Easy-to-use GUI-based driver** for operation and analysis.
- **Training, inference, and scenario analysis workflows** to perform operational simulations.

Traditional Modeling In CREST

- It is easier to express physical processes in Tensor Networks than integrate tensor networks in physical-based model.
- Any physical-based or process-based parameterized model can be written using tensor-based software.
- Some work on incorporating physical constraints within AI models.
- Some approaches to estimate gradients of black-box models which would allow wrapping of Fortran-based models into python for inclusion in CREST.
- Some efforts towards Fortran auto-diff.

Integrating traditional models in CREST is targeted for future development.

NEED GRADIENTS

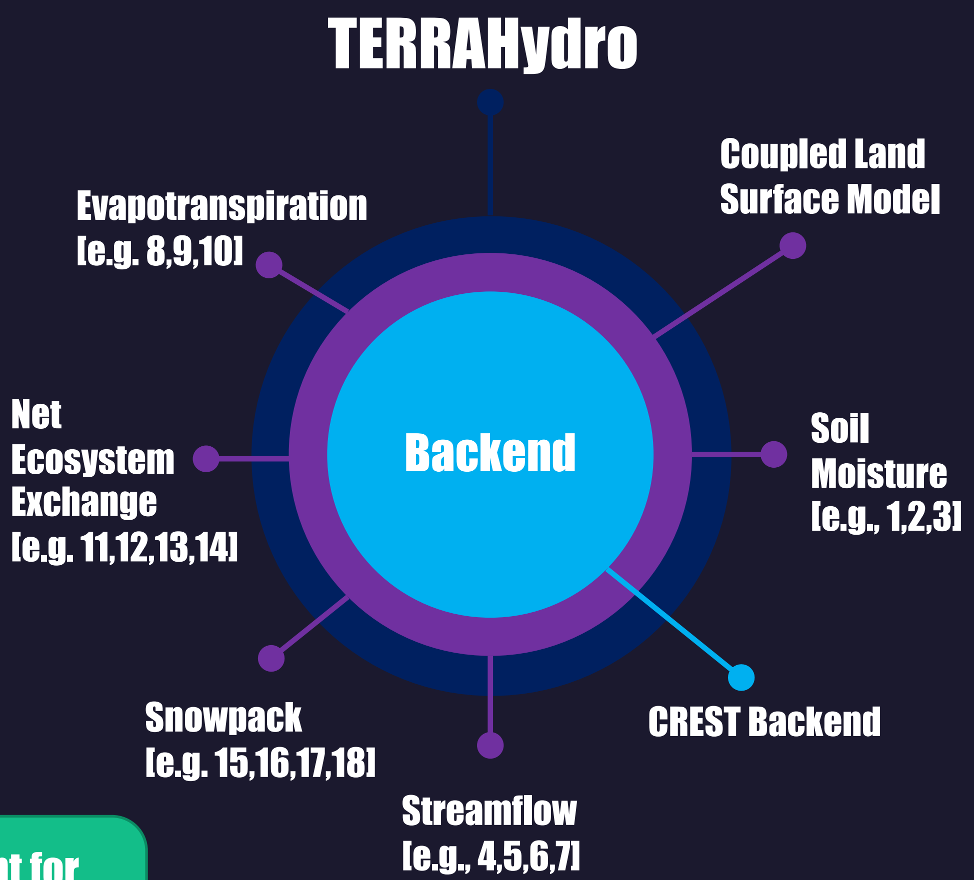
Potential Approaches

- **Rewrite (Fortran) models in a tensor language.**
- **Leverage black-box gradient estimates.**
- **Development of a reliable auto-differentiator for Fortran.**
- **Apply physical constraints on AI models.**

Emerging packages like JAX offer the use of numpy-like numerical packages that make this easier.

TERRAHydro

- Takes the next step in data-driven hydrology by coupling together 5 existing AI-based land surface components to assemble a land surface digital twin.
- Demonstrates an application of the CREST framework for assembling coupled AI-based Earth Systems Models --- guides the development.
- Enables new tensor-gradient-based data assimilation techniques in addition to traditional Bayesian approaches for near-real time ingestion of data.
- Computational efficiency and use of hardware accelerators enables rapid adaptability and scenario analysis beyond current capabilities.
- Potential for improved accuracy. References can be found on the last slide.



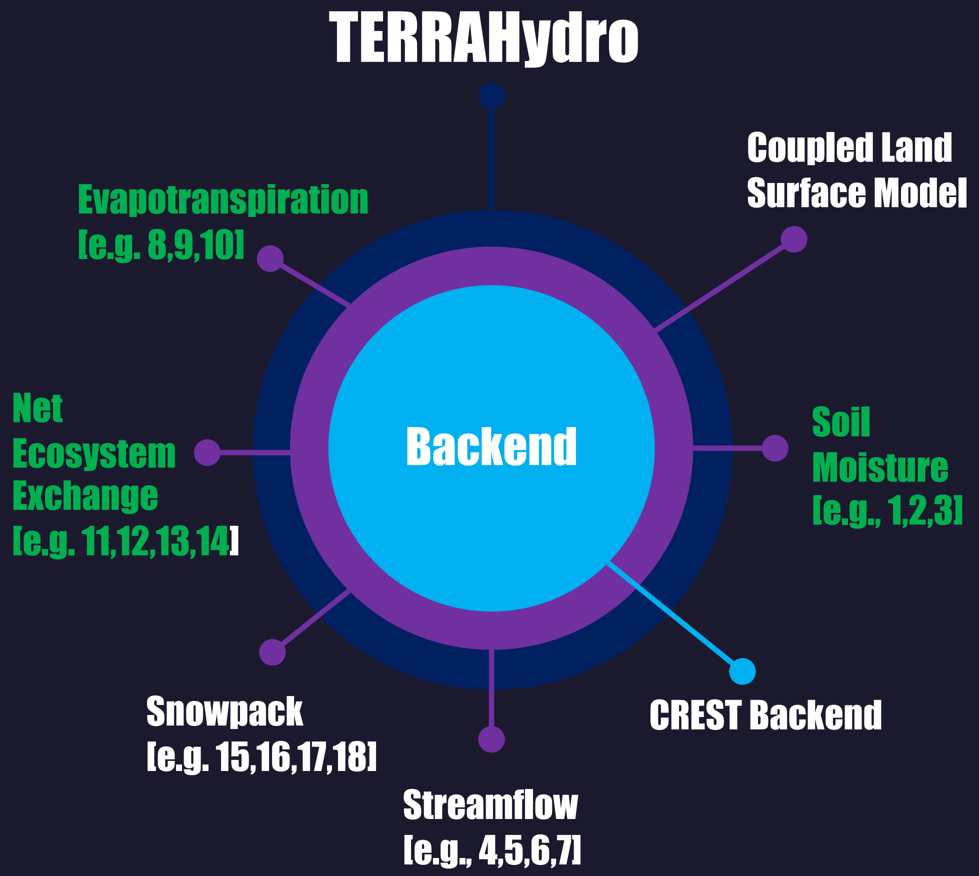
Important for Digital Twin capabilities

CREST Progress

Data Loading	Model Specification	Training and Validation	Inference
crest.Dataset crest.StructuredDataset	crest.HierarchalTensorGraph	crest.Batcher crest.Model	TBD
Efficiently loads large heterogeneous gridded geospatial-temporal data	Currently restricted to TensorFlow (Keras) AI-based models.	Builds Keras models and efficiently batches data contained in Dataset.	Inference can be performed but software design still being conceptualized

TERRAHydro Progress

- Soil Moisture, Evapotranspiration, Net Ecosystem Exchange (3 of 5) land surface components have been implemented and moderately validated.
- ESMWF (ERA5), Soil Moisture Active Passive (SMAP), and FluxNet data has been ingested for training.
- Large scale validation to reproduce paper results underway.
- A coupled Soil Moisture + Evapotranspiration model is underway with a target demonstration of coupled Soil Moisture + Evapotranspiration + Net Ecosystem Exchange model for an 18-month demo.



Timeline

September, 2022	1st year milestone	18 month demo	2nd year milestone	3rd year
Project kick-off.	End-to-end capabilities in CREST and a simplified coupled model with SM+ET.	TERRAHydro retrospective demonstration of a coupled land surface (SM+ET+NEE) model for a hydrological event.	TERRAHydro coupled land surface model and assimilation completed along with all relevant CREST features for the third-year demo.	Full scale retrospective demonstration including data assimilation and scenario analysis on relevant hydrological events.

Thank You

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