CLDERA: Developing a Novel Foundational Approach for Attributing Localized Source Forcings in the Climate

Principal Investigators: Diana Bull, Kara Peterson

Thrust Leads: Irina Tezaur, Lyndsay Shand, Laura Swiler

Sandia National Laboratories

22nd IACM Computational Fluids Conference (CFC) 2023

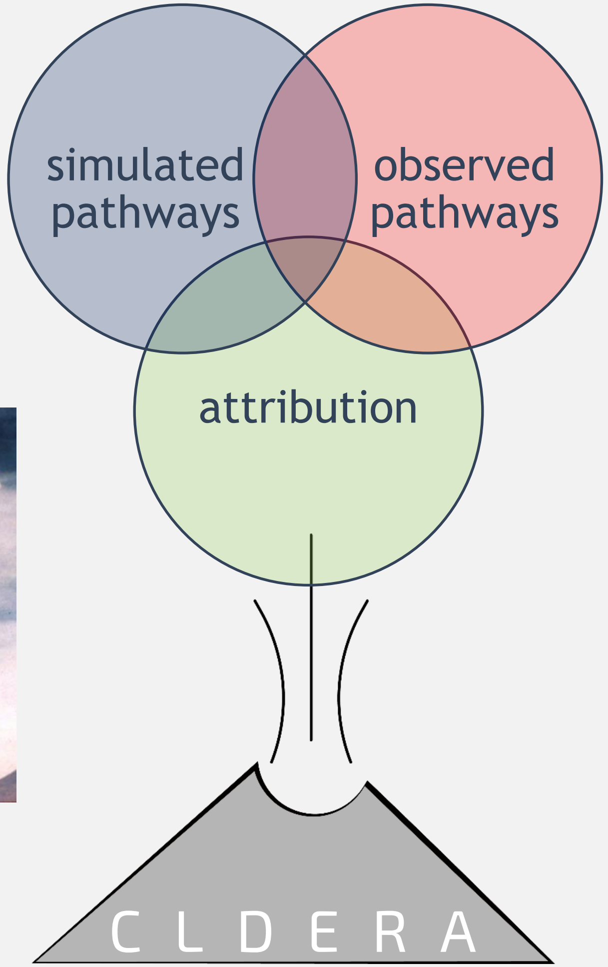
Cannes, France. April 25-28, 2023.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SAND2023-02095C

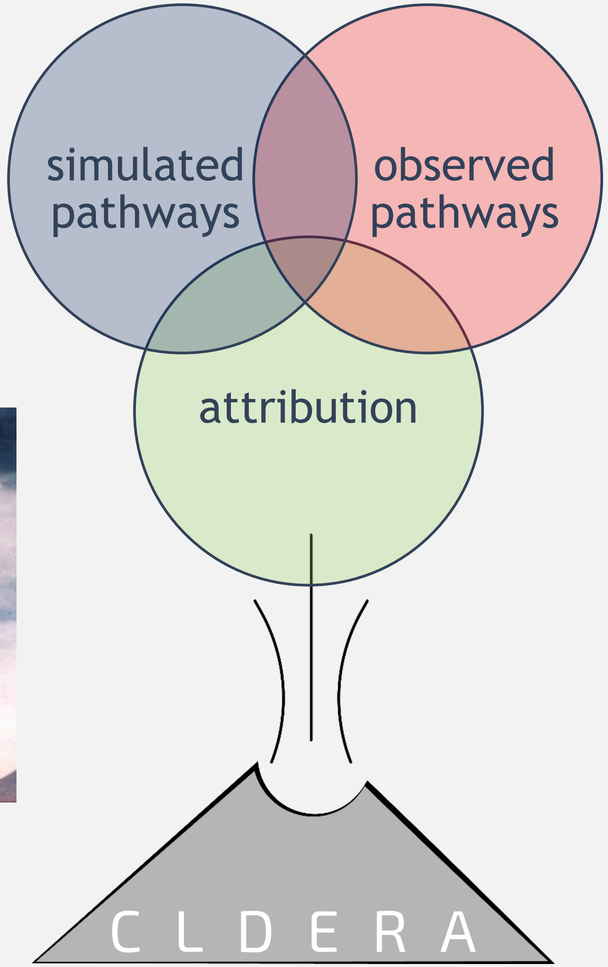
Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- CLDERA Research Composition
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- Summary



Outline

- **Background**
  - **Motivation**
  - The CLDERA Project
  - Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- CLDERA Research Composition
  - Simulations
  - Simulated Pathways Thrust
  - Observed Pathways Thrust
  - Attribution Thrust
- Verification & Validation
- Summary



Motivation

Climate Change is a Growing Global Security Concern!

- Governments are interested in **climate risk assessments** toward informing **decision making** (policies, treaties, security posture, etc.)
  ⇒ requires identifying **impacts** from climate change **sources:**
  - Anthropogenic climate change (natural or human-caused)
  - Climate interventions (a.k.a., geoengineering*)

Currently, **confident scientific attribution** of a source (e.g., Sky River) to a physical impact (e.g., regional drought over Southeast Asia) is at **best onerous** and at **worst impossible!**

China is seeding clouds to replenish its shrinking Yangtze River

By Wayne Chang, Simone McCarthy and Shawn Deng, CNN and Reuters

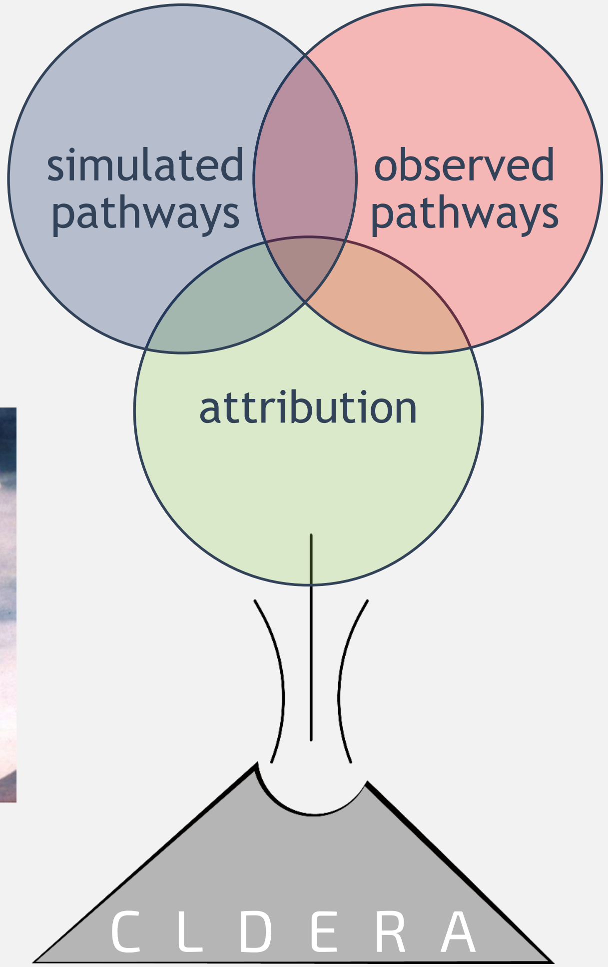
Aug 17, 2022

- **Challenges in tackling climate attribution problem:**
  - High **internal variability** in the Earth system
  - **Complex coupling** of processes in Earth System Models (ESMs), which obscures the connective relationships between sources and impacts
  - **Limited ESM ensembles**
  - Historically limited **observational data**
  - **Multiple sources** contributing to an impact

* Deliberate manipulation of the Earth system to try to counteract effects of climate change.

Outline

- **Background**
  - ➢ Motivation
  - ➢ **The CLDERA Project**
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- CLDERA Research Composition
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- Summary



The CLDERA Grand Challenge LDRD Project

A Novel Foundational Approach to Understanding the Causation of Impacts

CLDERA: CLimate impact – Determining Etiology thRough pAthways

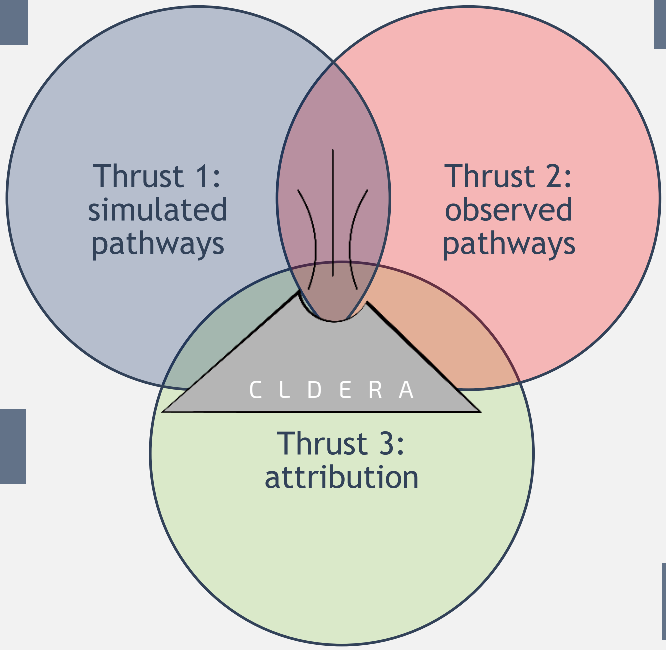
LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Need

Determine how a **geographically** and **temporally localized source** drives the climate system to respond with particular **impacts** to enable **downstream impact attribution.**

Technical Approach

- Build upon **key strengths of Sandia** (modeling & simulation, detection & attribution, data science)
- Develop novel methods and tools in **three cross-validating thrusts**
- Use the 1991 eruption of **Mt. Pinatubo** as exemplar



Duration: FY22-FY24
Budget: \$5M-\$6M/year
Staffing: ~45 Sandians, 4 Academic Partners

Hypothesis

Tracing **pathways** between **source and impacts** will **increase certainty** of **attribution** and deepen understanding of dependent causal-like relationships.

Pathways *represent the* ***spatio-temporally*** *evolving* ***chain of physical processes*** *that connects a source to impacts.*

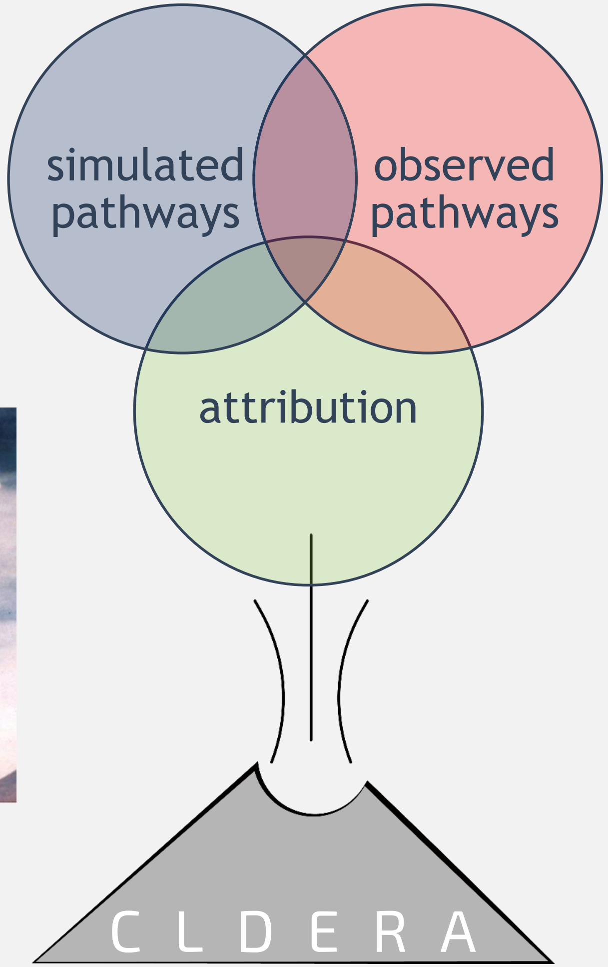
Outcome

Advance climate attribution science by identifying impacts from localized sources.

M | ATM | I | COLUMBIA UNIVERSITY | Sandia National Laboratories

Outline

- **Background**
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ **Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)**
- CLDERA Research Composition
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- Summary



Mt. Pinatubo Eruption

Stratospheric Aerosol Injection (SAI)

CLDERA R&D is be driven using an exemplar of **Stratospheric Aerosol Injection (SAI)**: the 1991 eruption of Mt. Pinatubo.

- June 15, 1991: largest eruption of the satellite era
  - ➢ Released ~18-19 Tg SO_2 gas (1 Tg = 1 Mt = 10^{12} g)
  - ➢ "Fast" reactions and ice/ash fallout reduced the "climatically-relevant" SO_2 injection to 10 Tg SO_2 gas.
- SO_2 gas released by Mt. Pinatubo converted to SO_4 , H_2SO_4, H_2O and aerosols via oxidation, nucleation and chemical reactions

Mt. Pinatubo before eruption

Large Eruption (June 12, 1991)

Main Eruption (June 15, 1991)

Mt. Pinatubo Eruption
Stratospheric Aerosol Injection (SAI)

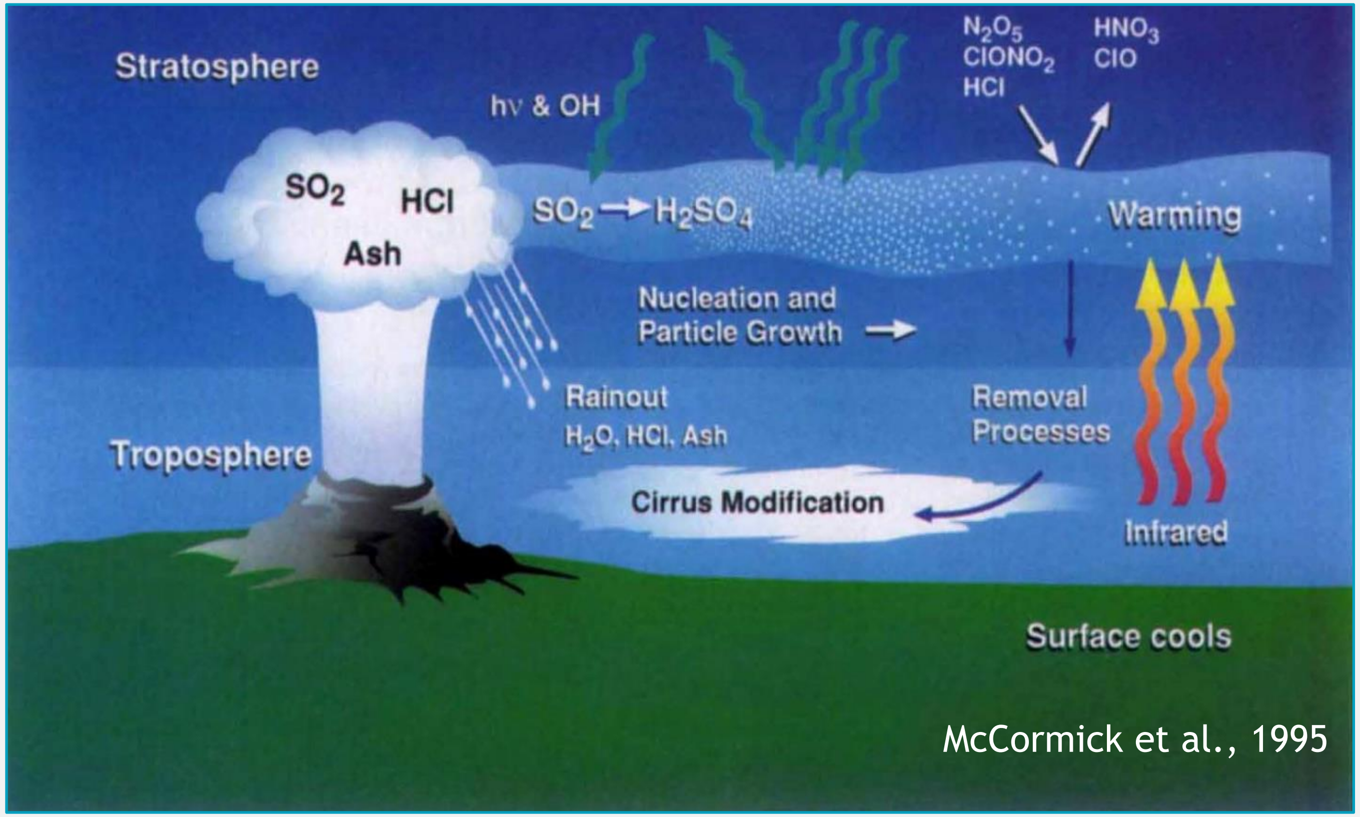
Effects of sulfate aerosols:

- **Scatter incoming solar** (long-wave) **radiation**: increases planetary albedo, cools the climate system (less energy in)
- **Absorb infrared** (short-wave) **radiation** emitted at surface: heats the stratosphere

Net results:

- 0.4-0.6°C **global cooling at Earth's surface** that lasted through 1993.
- **Warming of the stratosphere** up to ~3°C.

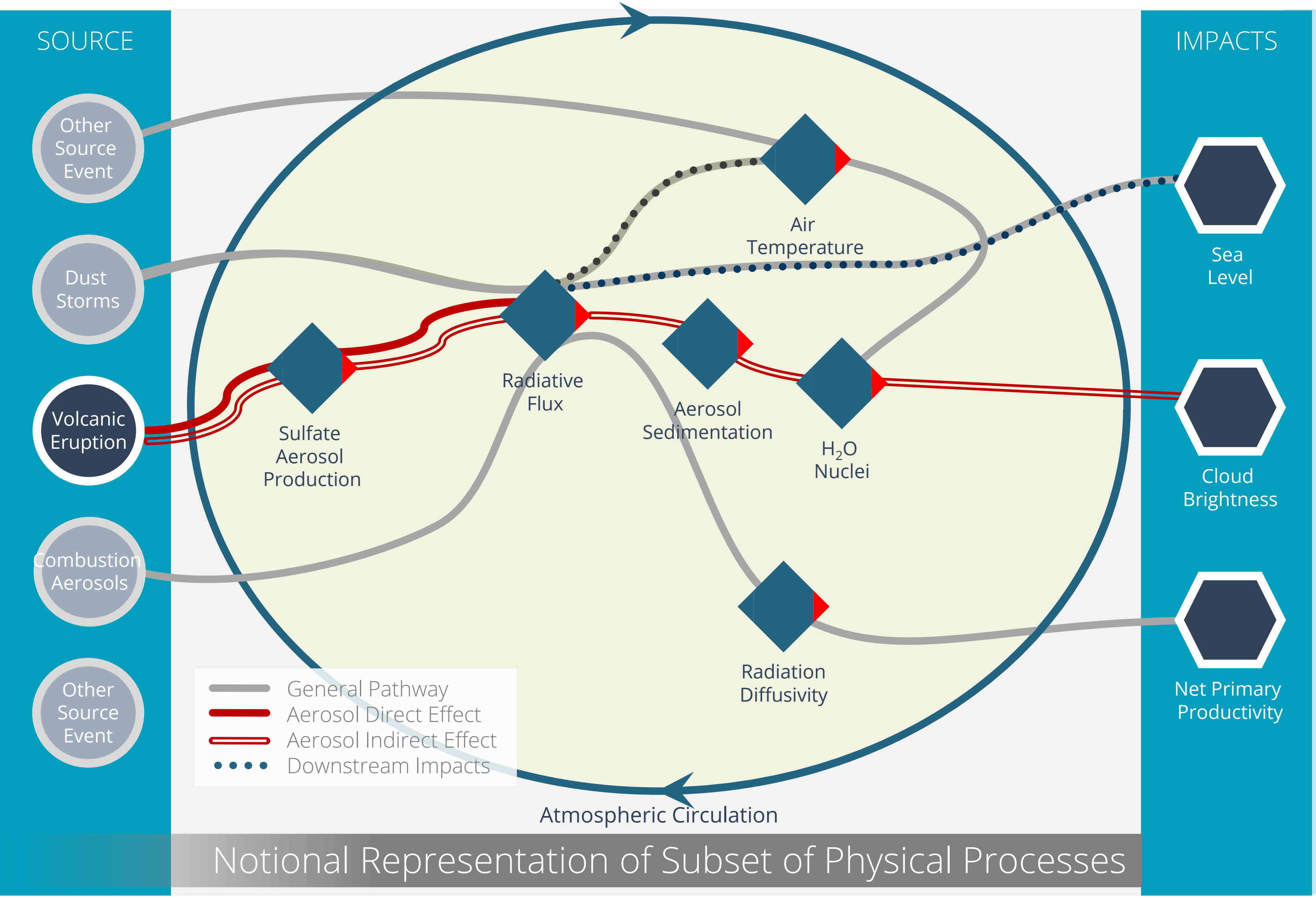
Schematic of Immediate Effects post SAI



***Important nodes in pathway**: SAI → secondary aerosols (sulfate) → radiation effects → temperature*

Mt. Pinatubo Eruption

Impact Space & Notional Representation of Pathways



"Known" pathways/impacts:

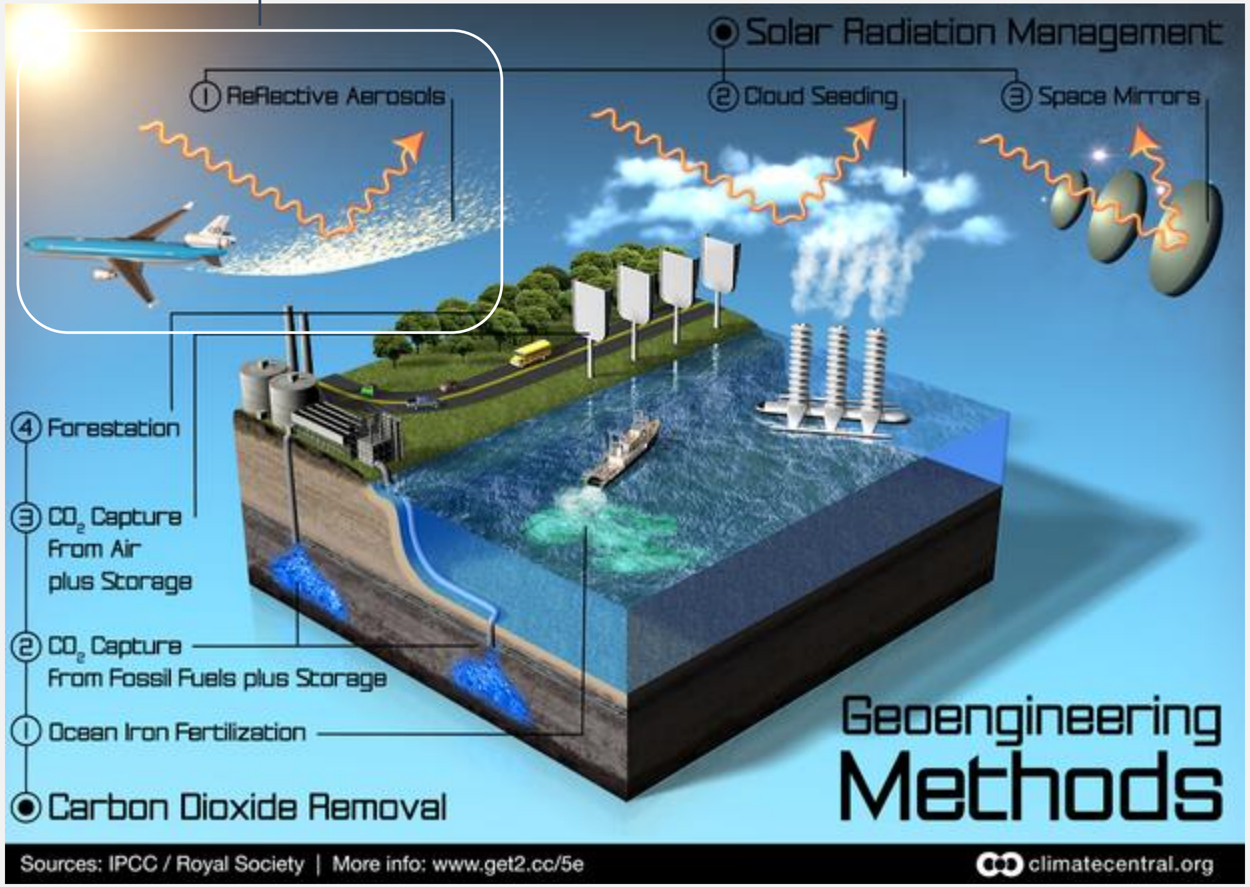
- Tropospheric cooling; stratospheric warming; northern-hemisphere winter warming
- Increase in planetary albedo
- Effects on soil, agriculture, vegetation
- Global reduction in precipitation, evaporation, water vapor
- Interactions with atmospheric modes of variability (e.g., NAO)
- Interactions with coupled modes of variability (e.g., ENSO, AMOC)
- Interactions with Asian monsoon
- Stratospheric chemistry (e.g., ozone depletion)
- Aerosol indirect effects (e.g., cirrus clouds)
- Sea level decrease

Mt. Pinatubo Eruption
Stratospheric Aerosol Injection (SAI)

Exemplar Strengths:

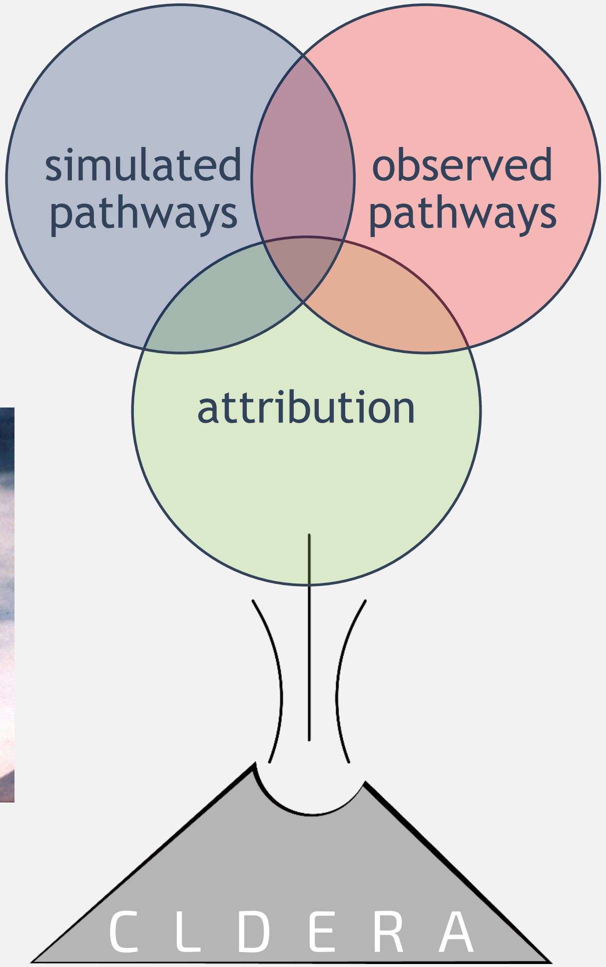
- The source is **external** to climate feedbacks
- Its impacts are **large enough** to rise above internal variability of climate system
- It provides ample **observational data** demonstrating the event's direct and indirect effects for **validation** of pathways
- It possesses a **climate intervention** analog (1 Tg SO_2/yr may produce ~0.1℃ cooling)

SAI as climate intervention



Outline

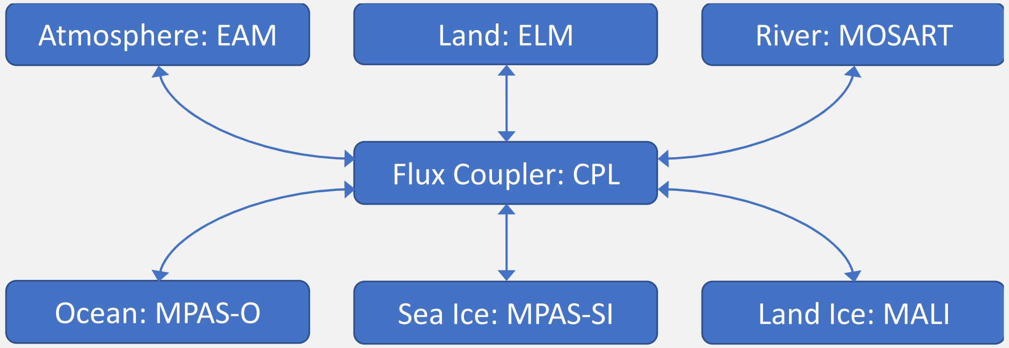
- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- **CLDERA Research Composition**
  - ➢ **Simulations**
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- Summary



Energy Exascale Earth System Model (E3SM)*
For Simulating Mt. Pinatubo & SAI

Simulation Lead:
Kara Peterson

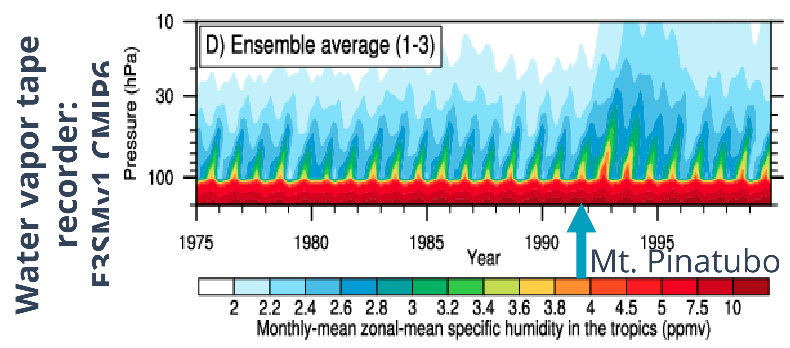
- **E3SM:** U.S. DOE-funded Earth system model
- Collaboration among **8 national labs** and **12 academic institutions**
- Designed to run on DOE's **advanced computing platforms** and address **energy-relevant science questions**
- CLDERA uses E3SM version 2 (v2), obtained in late 2021 through **collaboration agreement** with the E3SM project
- **Capabilities** to model Mt. Pinatubo eruption and impacts
  - ➢ **Resolves stratosphere:** 72 vertical levels with 0.1 hPa (64 km) model top
  - ➢ Includes **key process models** for clouds, ozone and aerosols [Golaz et al., 2019]
- **Key limitation before CLDERA:** no prognostic volcanic aerosols in E3SM (radiative forcing due to aerosols from volcanic eruptions was prescribed)

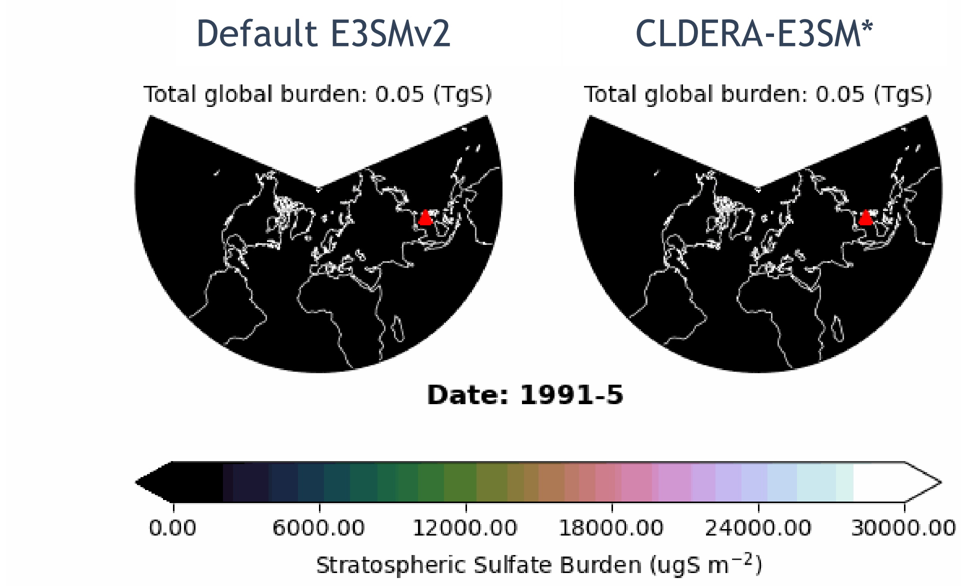


* www.e3sm.org, https://github.com/E3SM-Project/E3SM

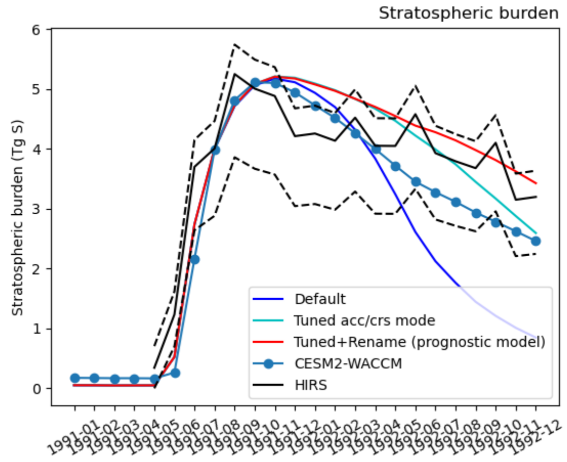
Simulating Mt. Pinatubo in E3SM

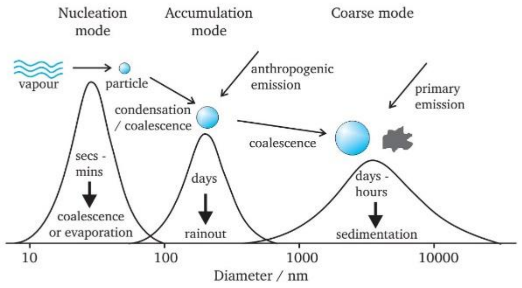
- Implemented **prognostic volcanic aerosols** in E3SMv2 MAM4 aerosol model
  - ➢ **Changed aerosol coarse** and **accumulation mode properties** to match stratospheric size distributions
  - ➢ **Validated** against High resolution Infrared Radiation Sounder (HIRS) data and CESM2/WACCM
- **Evaluated** E3SM simulation capabilities
  - ➢ Assessed **Quasi-Biennial Oscillation (QBO):** QBO in E3SMv2 has slightly short period
  - ➢ Evaluated E3SM's **Brewer-Dobson circulation** via Age-of-Air tracers and water vapor tape recorder: E3SMv2 underestimates upward transport of water





* https://github.com/sandialabs/CLDERA-E3SM

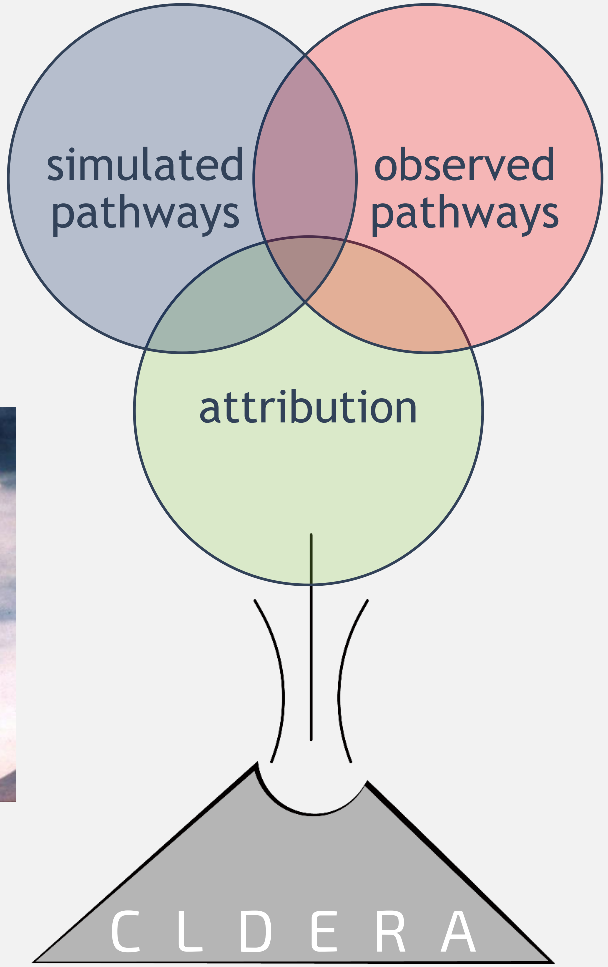




Team: B. Wagman, H. Brown, X. Liu [TAMU], A. Hu [TAMU], C. Jablonowski [U Michigan], J. Hollowed [U Michigan]

Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- **CLDERA Research Composition**
  - ➢ Simulations
  - ➢ **Simulated Pathways Thrust**
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- Summary



Simulated Pathways Thrust
Finding Impacts from a Source

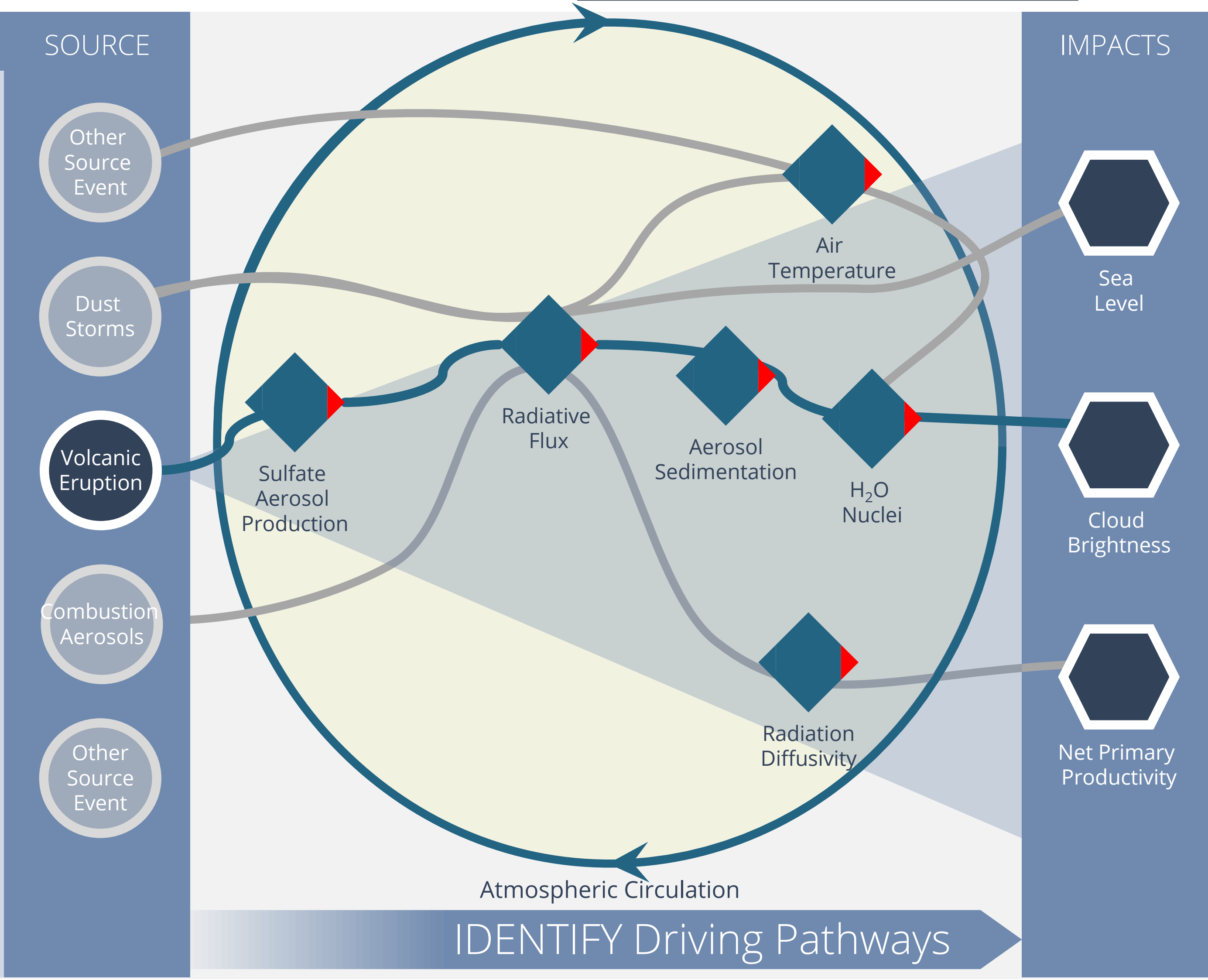
Thrust Lead:
Irina Tezaur

Research Composition:

1. Statistical Approaches: use and extend Random Forest Regression and sensitivity analysis to identify and rank physical pathways while establishing susceptibility to initial conditions and E3SM representations

2. Computational Monitoring: instrument E3SM with tracers and profiling capabilities to enable pathway detection.

3. Signature-based Clustering: find and track non-stationary variable clusters for use as features in pathways identification

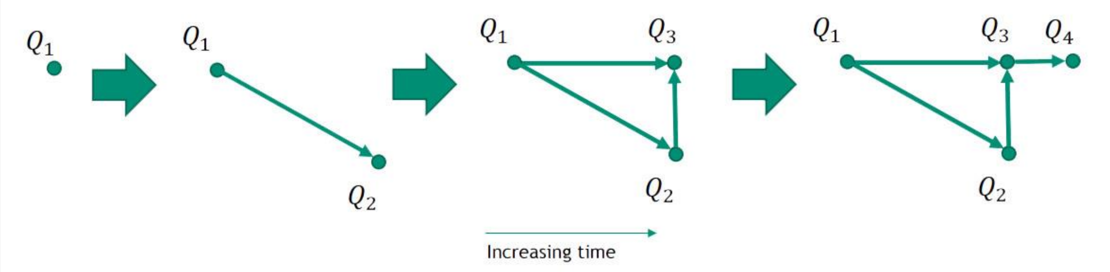


Simulated Pathways Thrust
What is a Simulated Pathway?

Heuristic definition: a *pathway* is the chain of physical processes from a source to impacts and their evolution in space and time.

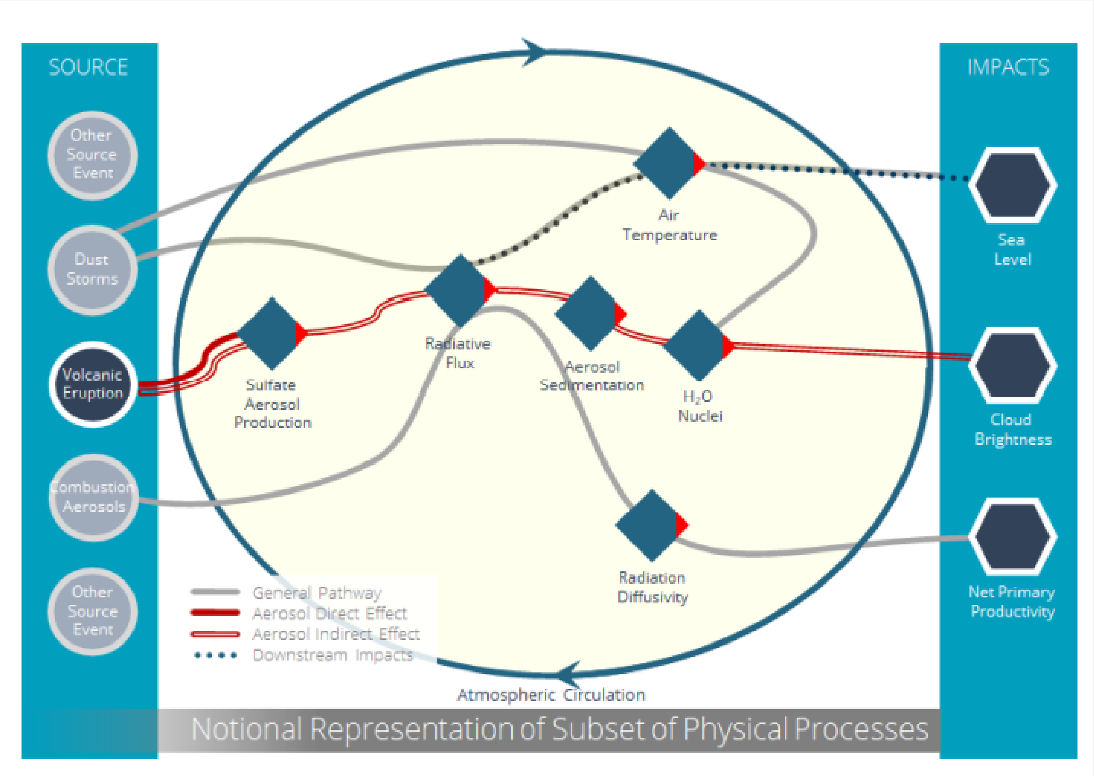
- *Example*: Mt. Pinatubo eruption → sulfate aerosol production → sedimentation → transport of aerosols into the troposphere → modification of cloud optical properties → increased cloud brightness/decreased rainfall.

Mathematical definition: a *pathway* is a time-dependent directed acyclic graph (DAG) representing the dynamics of a physical system.



Q_i = impacts = “nodes” on pathway graph

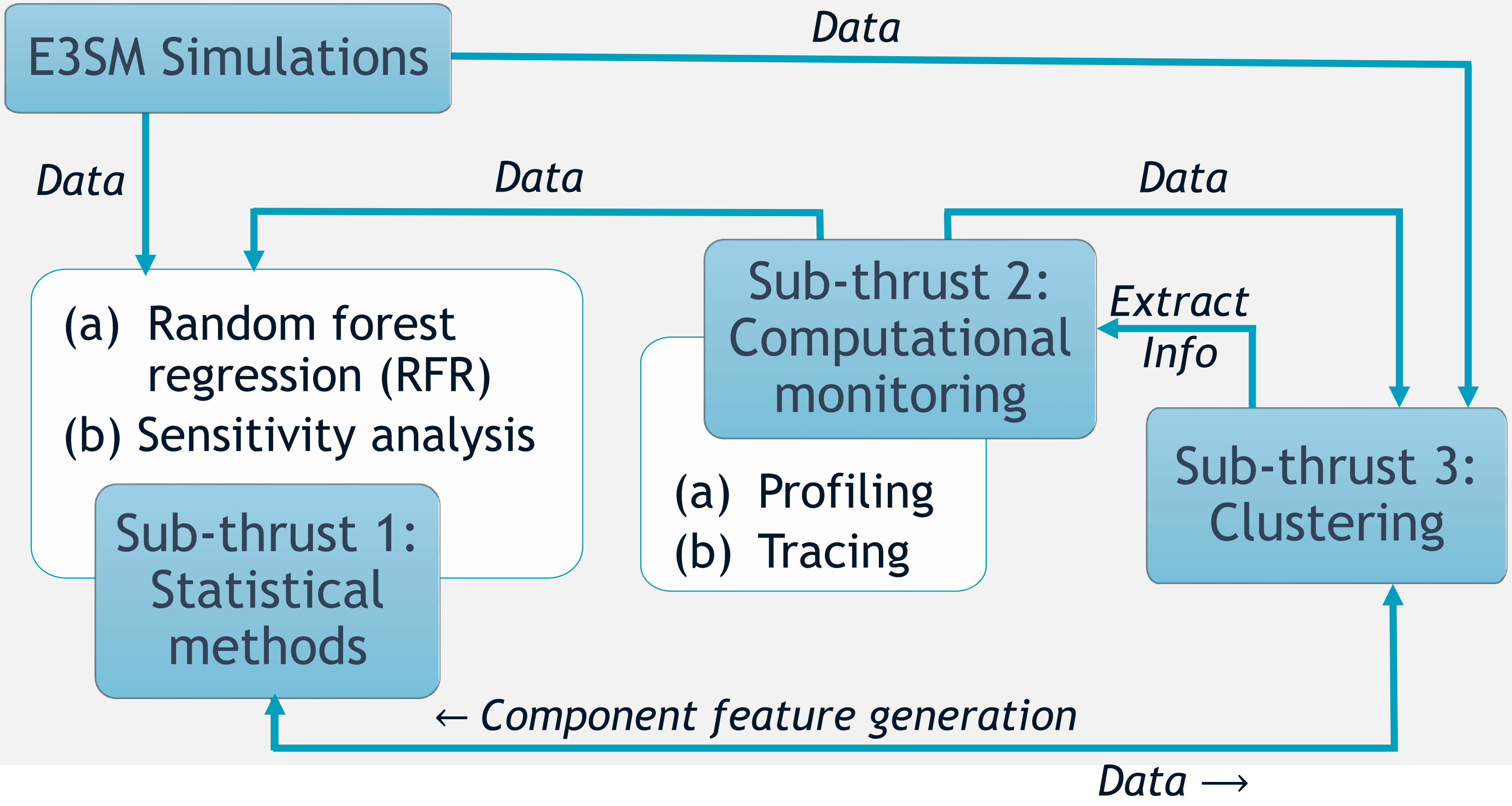
Edge from Q_i to Q_j ⇒ Q_j is impacted by Q_i at time t



Simulated Pathways Thrust

Sub-thrusts

Development of the proposed framework for identifying & ranking pathways will be pursued using **three complementary research sub-thrusts** that **fuse** Sandia's strengths in **data analytics**, **computational modeling** and **E3SM/climate science**.

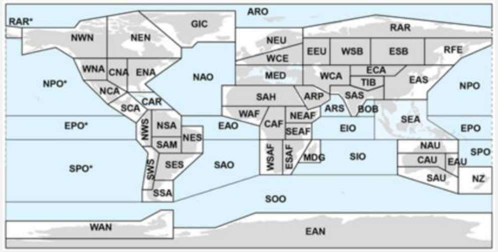


- Simulated pathways thrust will generate **simulation data** for CLDERA.
- Methods developed in one sub-thrust will **feed into** the others.
- Multiple sub-thrusts **minimize risk.**
- Identifying same pathway with different methods will provide **confidence**.

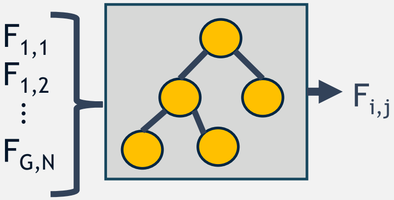
Simulated Pathways Thrust
Statistical Methods

Random forest regression (RFR): use feature importances from Random Forests (RFs) to **identify weighted pathways** from one variable to another and determine **pathways strengths**

Spatially-partitioned time series data/features



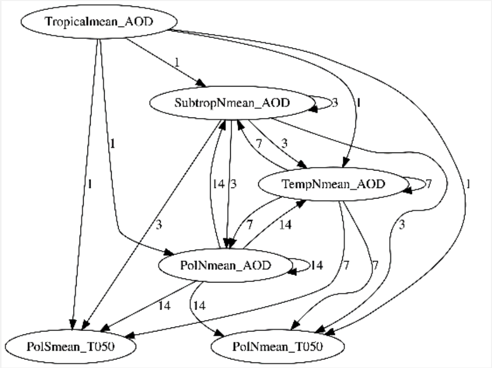
Train RF Regressors



Calculate Pairwise Feature Importances

	$F_{1,1}$	…	$F_{G,N}$
$F_{1,1}$	0.1	…	0.5
⋮	…	…	…
$F_{G,N}$	0.99	…	0.1

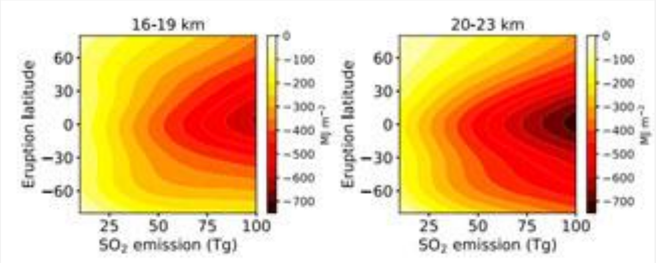
Convert to Pathway Graph



Team: M. Peterson, M. Brown, J. Nichol, W. Davis, I. Tezaur

Sensitivity analyses (SA): vary **eruption elements**, e.g., mass, time, height, location

- **Generate data** for RFR, Signature-based Clustering and Attribution thrust
- Provide **insight** into how Mt. Pinatubo **could have been**
- Determine **robustness of pathways** to changes in SAI-related inputs
- Answer **"how low can you go?"** question in terms of attribution



Sensitivity study perturbing various characteristics of Pinatubo-like volcanic eruption [Marshall et al. 2019]

Team: I. Tezaur, K. Peterson, H. Brown, B. Wagman

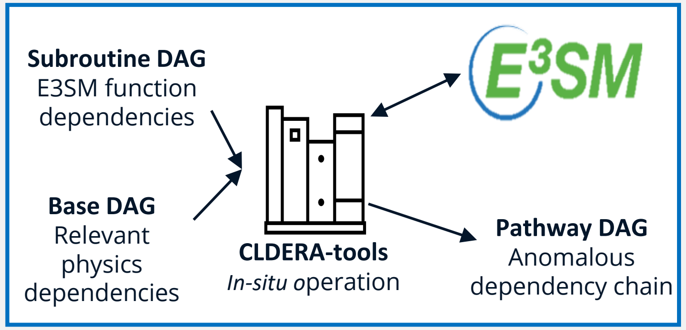
Simulated Pathways Thrust
Computational Monitoring

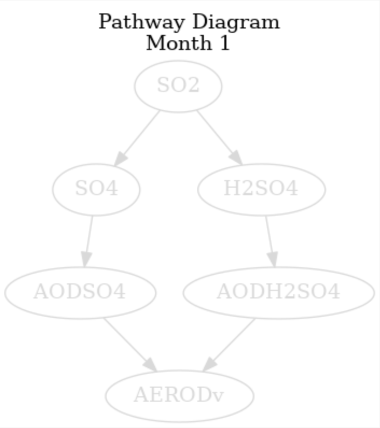
*See talk by **E. Wenzel** for more on analyses using Lagrangian Coherent Structures*

Profiling: finding pathways ***in-situ*** while running E3SM

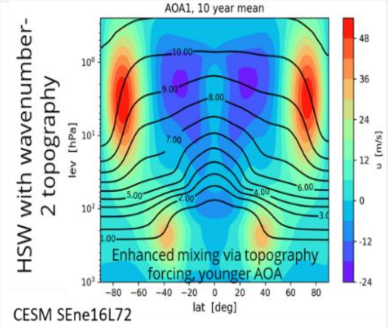
- **Instrument E3SM** and develop DAGs of process interactions executed ***in situ*** within code
- CLDERA-tools performs **statistical analysis** by comparing QOIs inside code with baseline and tracking **propagation of "anomalies" in real time.**

Small overhead (<1% for idealized HSW++ E3SM test)!

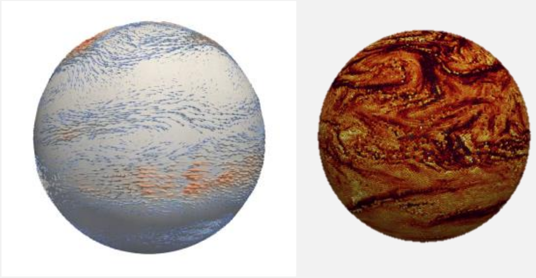




Team: A. Steyer, J. Watkins, L. Bertagna, G. Harper, I. Tezaur



Age-of-Air clock tracer from HSW idealized-climate test



(a) (b)

(a) LCS traced out by velocity field in E3SM simulation. (b) Finite Time Lyapunov Exponent (FTLE) for E3SM simulation.

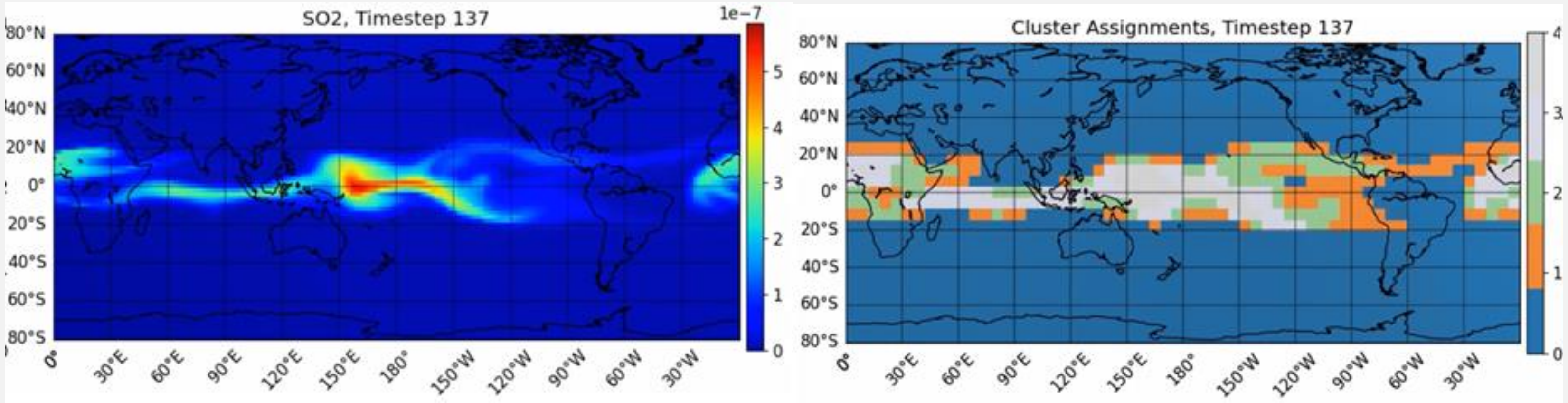
Tracers: add tracers to E3SM, use them to **evaluate E3SM &** explore ways to repurpose them to **identify source-impact pathways**

- ***Passive tracers***: evaluate climatological dynamics (e.g., "Age-of-Air", Brewer-Dobson circulation) and changes to those dynamics
  - ***Lagrangian coherent structures (LCS):*** surfaces of trajectories that exponentially attract/repel tracers, anomalies in which may represent elements in pathway
- ***Active (source-tagged) tracers***: enable partitioning of impacts due to different aerosol sources, towards tracking of relative contributions along nodes in a pathway

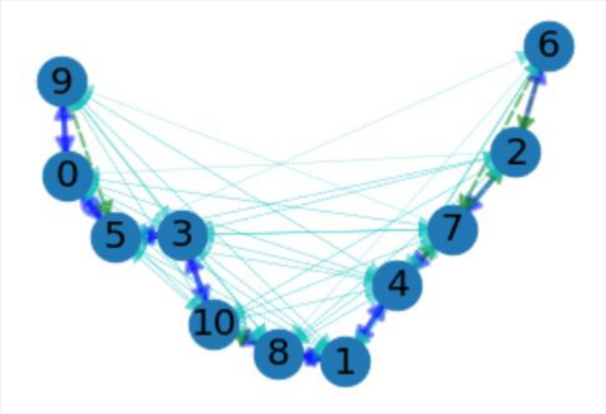
Team: B. Hillman, E. Wenzel, B. Wagman, C. Jablonowski [U Michigan], J. Hollowed [U. Michigan], I. Tezaur

Simulated Pathways Thrust
Signature-based Clustering

- **Goal:** find & track non-stationary variable clusters for use as features in pathway identification
- **Approach:** combine existing anomaly (event) detection algorithms [Davis et al. 2021] with clustering to enable **spatio-temporal anomaly progression**, defining pathways
  - ➢ Use **signatures** (compressed representation of data) for clustering
  - ➢ User **clusters** to inform pathway analyses



Space-time varying cluster identification in response to Mt. Pinatubo source

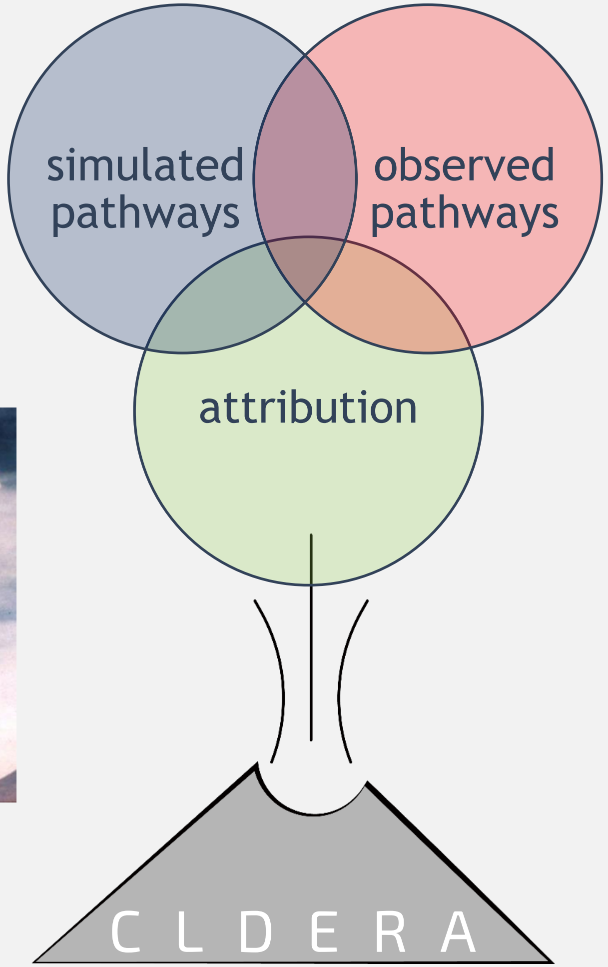


Force-directed graph of cluster transition probabilities over Mt. Pinatubo simulation

Team: W. Davis, M. Carlson, I. Tezaur

Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- **CLDERA Research Composition**
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ **Observed Pathways Thrust**
  - ➢ Attribution Thrust
- Verification & Validation
- Summary

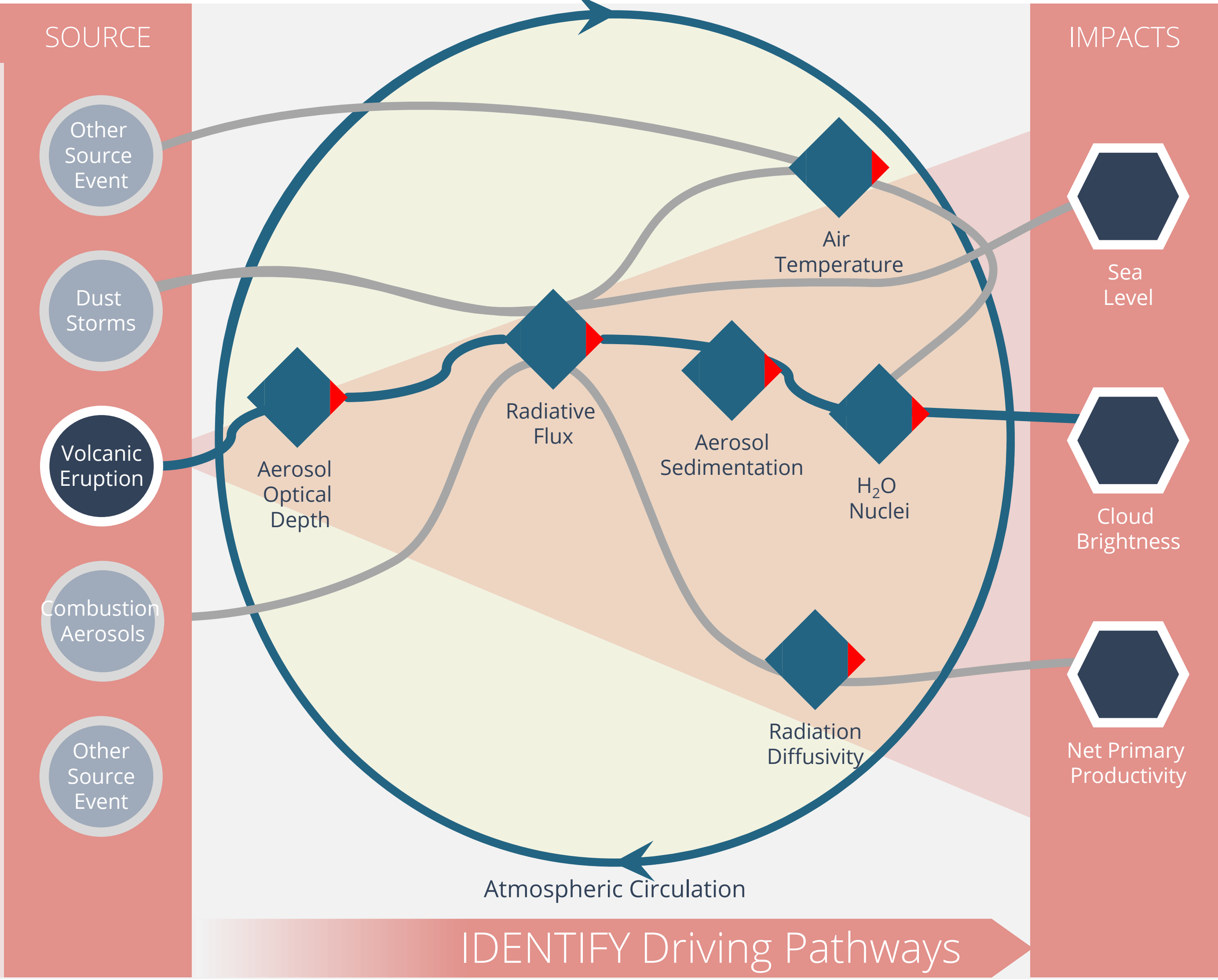


Observed Pathways Thrust
Finding Impacts from a Source

Thrust Lead:
Lyndsay Shand

Research Composition:

1. **Data Fusion:** strategically source and fuse relevant data of varying resolutions and fidelities to create a “near-global” picture of the relevant processes
2. **Changepoint Detection:** identify the underlying fundamental shifts in climate processes
3. **Dynamic space-time models:** adapt Bayesian hierarchical approaches to incorporate multiple nodes and establish correlations between nodes
4. **Explainable Echo State Networks (ESNs):** develop explainable and interpretable methods to quantify relationships between pathway nodes as modeled by recurrent neural networks



Observed Pathways Thrust

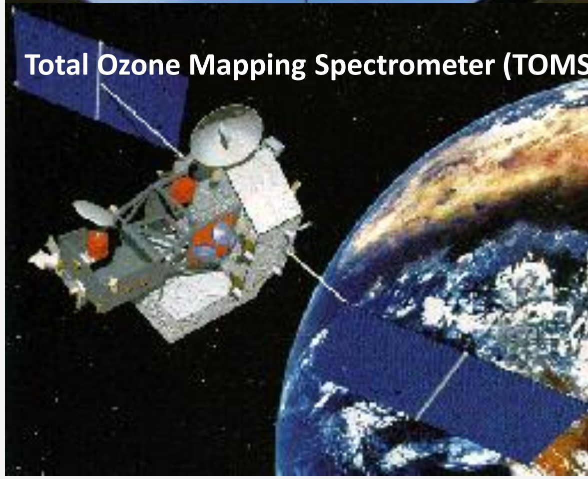
What is an Observed Pathway?

Definition: *observed pathways* are interpreted as **relationships** (or *correlations*) between **dependent climate processes** (*pathway nodes*).

Objective: rather than finding pathways that have not been postulated, **validate proposed pathways** and **quantify changes** in the **relationship between pathway nodes.**

Approach: develop **statistical methods** that can account for the **dynamic evolution** of aerosols over space and time, **multiple complementary sources of data** and **uncertainty**.

SO_2 → H_2SO_4 → Net Radiative Flux → Temperature Changes



Observed Pathways Thrust

Available Satellite Data for Mt. Pinatubo

+ Reanalysis data, e.g., ERA-5, MERRA (observations filled in with model run data)

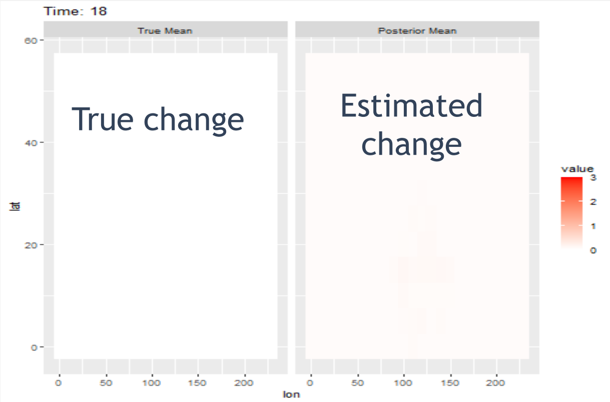
Instrument	Satellite	Measurements	Satellite Orbit	Data Collected
Total Ozone Mapping Spectrometer (**TOMS**)	Nimbus-7	UV albedo (nadir)	Polar, sun-synchronous	SO_2 mass and ozone [Bluth et al. 1992; McPeters et al. 1992]
Solar Backscatter Ultraviolet Spectral Radiometer (**SBUV**)	NOAA-11	UV albedo (nadir)	Polar, sun-synchronous	SO_2 mass and ozone [McPeters et al.1992]
NOAA Advanced Very High Resolution Radiometer (**AVHRR**)	NOAA-10, -11, -12	4 Vis-IR channels (nadir)	Polar, sun-synchronous	Aerosol optical depth [Stowe et al. 1992; Long and Stowe 1994], plume height [Lynch and Stephens 1996], cloud cover [Stowe et al. 1999]
High Resolution Radiation Sounder (**HIRS**)	NOAA 6-17	19 IR channels (nadir)	Polar, sun-synchronous	SO_2 mass and cloud-top height [Miles et al. 2017]
Stratospheric Aerosol and Gas Experiment (**SAGE II**)	Earth Radiation Budget Satellite (ERBS)	5 channels, Vis—IR (limb scanning)	Polar	Aerosol optical depth/extinction, aerosol max heights, Ozone [McCormick and Veiga 1992]
Microwave Sounding Unit (**MSU**)	NOAA-10,-11,-12	4 MW channels (nadir)	Polar, sun-synchronous	Surface-Upper Stratospheric temperature anomalies [Spencer et al. 1990; Dutton and Christy 1992]
Improved Stratospheric and Mesospheric Sounder (**ISAMS**)	Upper Atmosphere Research Satellite (UARS)	8 IR channels (limb scanning)	Near-Polar	Aerosol extinction, mass, and height [Lamberte et al. 1993]
Microwave Limb Sounder (**MLS**)	UARS	4 MW channels (limb scanning)	Near-Polar	SO_2 mass and temperature profiles [Read et al. 1993]

Observed Pathways Thrust
Changepoint Detection

Goal: inform pathways by finding significant changes/shifts in climate processes, towards accounting for them in statistical models

- **Space-time Changepoint Detection:** establish dependence between local climate shifts & distance from source using "epidemic" changepoint model

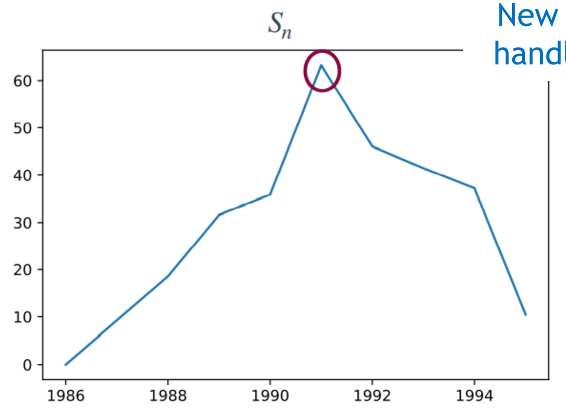
$$Y_k(\boldsymbol{s}_i, u) = \mu(\boldsymbol{s}_i, u) + \boxed{\mathbb{I}(\tau_1(\boldsymbol{s}_i) < k \leq \tau_2(\boldsymbol{s}_i))}\delta(\boldsymbol{s}_i, u) + \epsilon_k(\boldsymbol{s}_i, u)$$



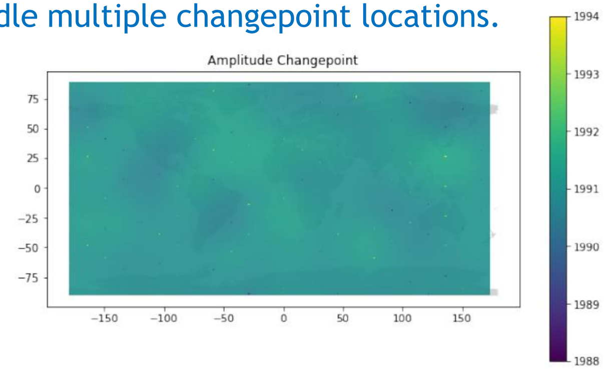
Model allows for and finds multiple changepoint times τ_i using test statistic, unlike traditional "at most one change" changepoint model.

Model can reconstruct spatial pattern and magnitude of changepoints in synthetic dataset with known changepoints

- **Elastic Functional Changepoint Detection:** identify climate shift using functional time series methodologies, elastic distance & diffeomorphisms, to account for phase variability



New approach [Tucker at al. 2023] can handle multiple changepoint locations.



Phase shift (left) and amplitude (right) changepoints identified in ERA-5 Reanalysis Data (1986-1995). Phase shift changepoint and majority of amplitude changepoints are in 1991.

Team: D. Tucker, L. Shand, B. Li [UIUC], S. Jun [UIUC]

Observed Pathways Thrust
Dynamic Space-Time Models

Goal: adopt space-time dynamic models to detect pathway changes following the Mt. Pinatubo eruption.

Approach: develop a multivariate evolution-based *space-time dynamic model* for variables on a pathway

n locations, k bases, n_t time points

$$\boldsymbol{Y}_t = \boldsymbol{U}_t + \boldsymbol{\epsilon}_t, \quad \boldsymbol{\epsilon}_t \sim N(0, \sigma_t^2 \boldsymbol{I}_n)$$

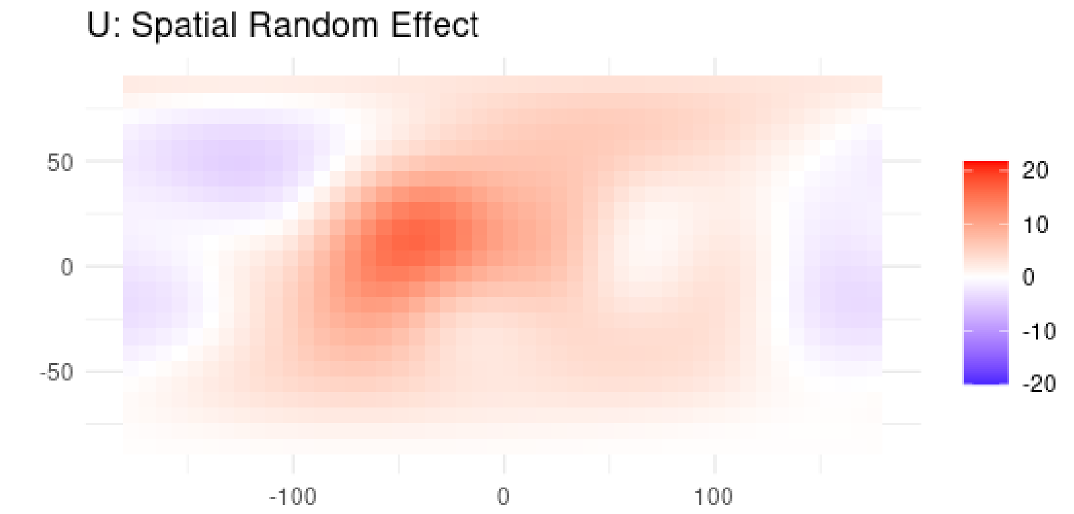
$$\boldsymbol{U}_t = \boldsymbol{\Phi}\boldsymbol{\alpha}_t$$

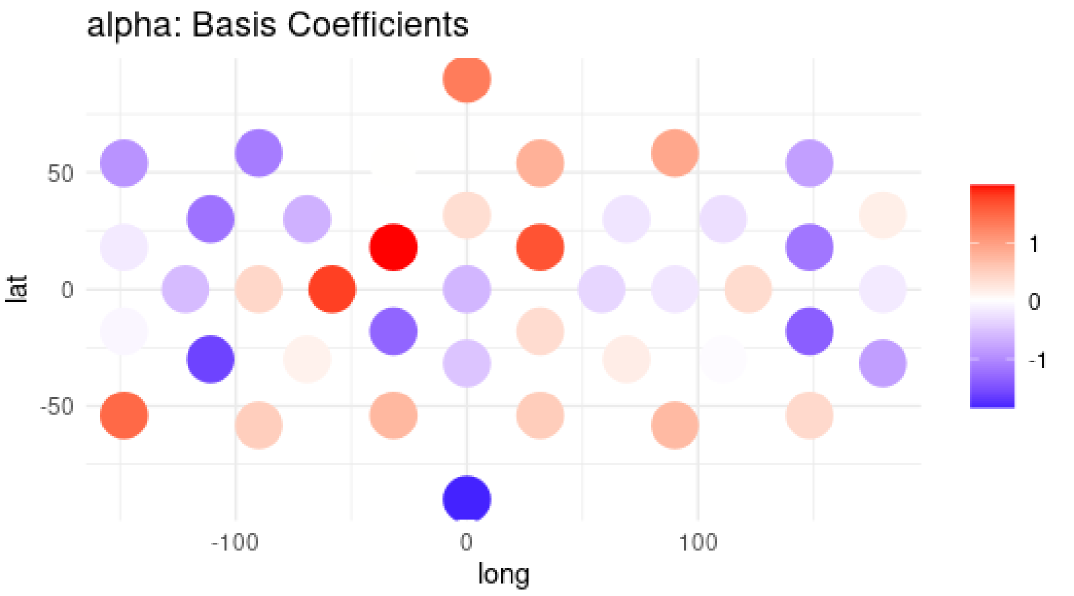
$$\boldsymbol{\alpha}_t = \boldsymbol{A}\boldsymbol{\alpha}_{t-1} + \boldsymbol{\nu}_t, \quad \boldsymbol{\nu}_t \sim N(0, \tau^2 \boldsymbol{\Sigma}_\alpha)$$

$$\boldsymbol{A} = diag(a_1, a_2, ..., a_k)$$

Linear temporal dynamics model with multivariate inputs/outputs.

- Estimate $\boldsymbol{U}_t$ with **Multiresolution Basis** Functions [Nychka et al. 2017] to represent the complex spatial patterns
- **Kalman filtering** used to sample from posteriors of time-varying basis functions
- Basis function coefficients are **space-** and **time-varying,** borrowing information from space-time neighbors
- $\boldsymbol{A}$ matrix represents **correlation** between basis coefficients and captures dependence across variables





Team: R. Garrett, G. Huerta, L. Shand

Observed Pathways Thrust
Explainable Echo State Networks (ESNs)

Goal: characterize (quantify) relationships between pathway variables in observed data using machine learning

"Black-Box" Echo-State Networks (ESNs)

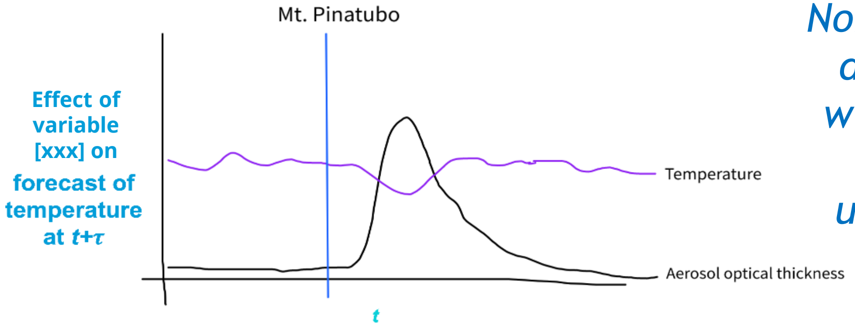
- Use reservoir computing to efficiently estimate recurrent neural networks (RNNs), which can capture short-term/long-term spatio-temporal dependence
- All params learned from data, very fast since few params

Data stage	$Z_t \approx \Phi\alpha_t + \delta_t(s),\ \delta_t(s) =$ spatio-temporal residual	
Output stage	$\alpha_t = V_1 h_t + V_2 h_t^2 + \eta_t,\ \eta_t \sim N(0, \sigma_\eta^2 I)$	RNN
Hidden stage	$h_t = g_h\left(\frac{v}{\lvert\lambda_W\rvert} W h_{t-1} + U\tilde{x}_t\right)$	

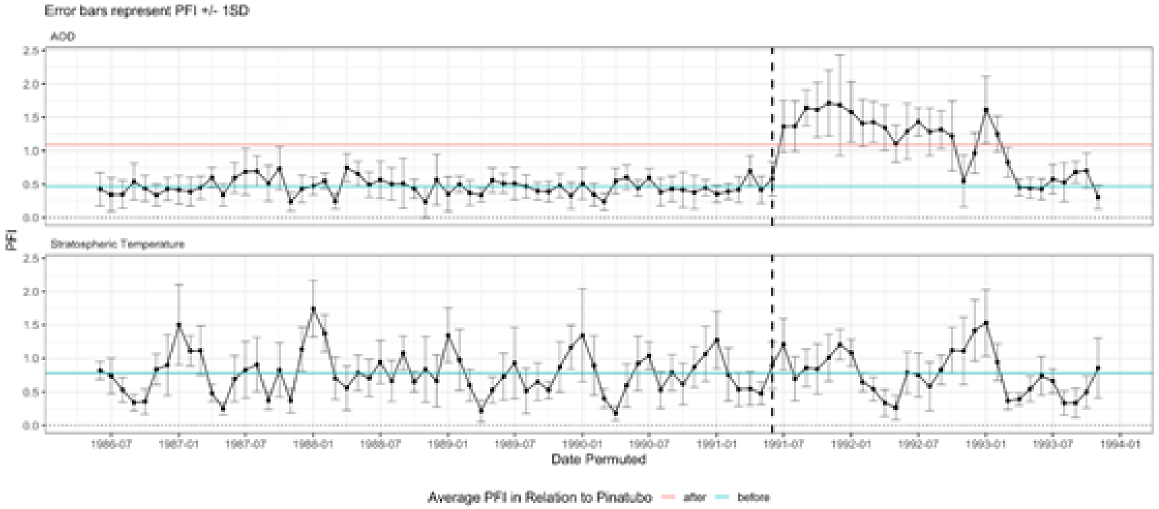
Zero Feature Importance (ZFI) – *new approach!*

- Determines which variables at which times are important for forecasting.
- Based on permutation feature importance (PFI)
- Increases explainability of ESNs

Team: D. Ries, K. Goode, K. McClernon, L. Shand



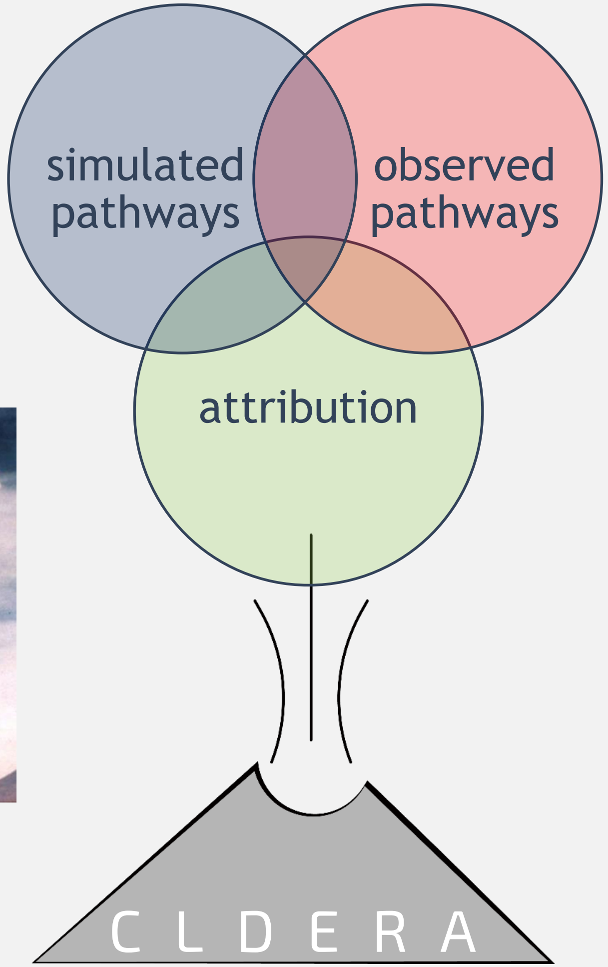
Nonlinear temporal dynamics model with multivariate (EOF) inputs, univariate (EOF) outputs.



ZFI of lagged AOD and lagged temperature: importance of AOD increases dramatically after Pinatubo eruption while importance of temperature corresponds to seasons.

Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- **CLDERA Research Composition**
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ **Attribution Thrust**
- Verification & Validation
- Summary



Attribution

Finding Predominant Source Driving Impact

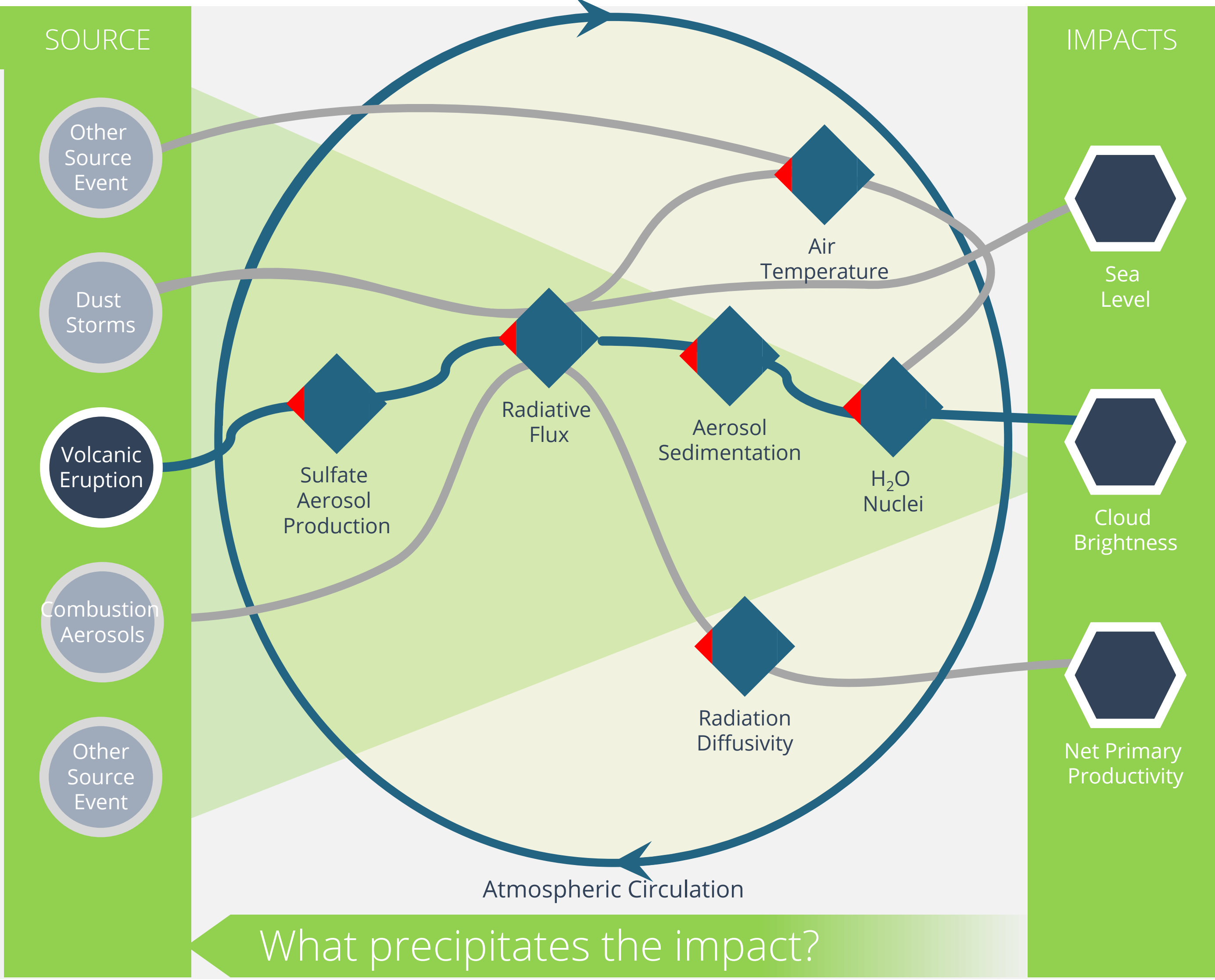
Thrust Lead: Laura Swiler

Research Composition

1. **Enhanced Fingerprinting:** use pathway information to expand multi-variate analyses, sharpening the signal-to-noise ratios and enabling significant correlations between source-impact

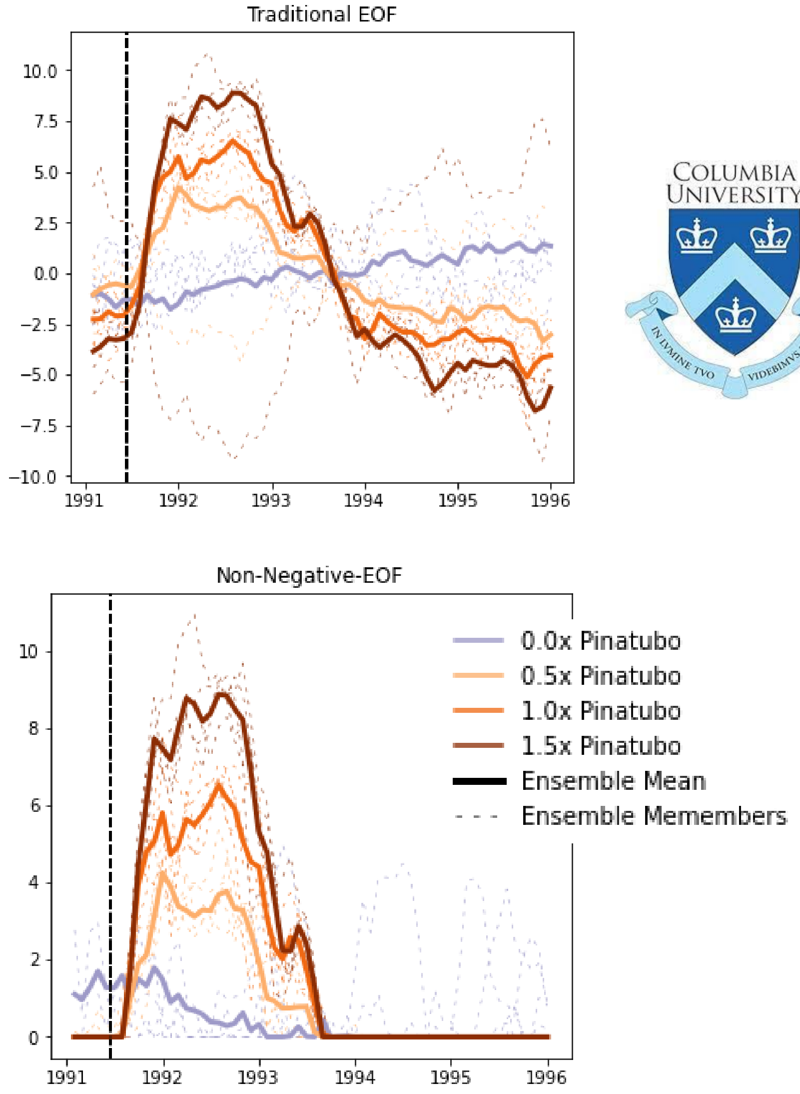
2. **Causal Modeling:** identify causal relationships and dominant pathways by developing causal networks through iterative independence tests and the resulting directed acyclic graphs

3. **Inverse Optimization:** develop deep operator neural networks (DONNs) to model parts of E3SM to enable PDE-constrained optimization without intrusion into the E3SM code directly; pathways will act as penalty terms or constraints



Attribution
Enhanced Fingerprinting

- **“Fingerprint”** = a spatial and/or temporal pattern that highlights an impact
  - ➢ Commonly the first principal component or empirical orthogonal function (EOF) from an SVD of a data matrix
- **Detection** involves identifying if the signal projected back onto the EOF goes out of 2σ limits.
- **Attribution** involves examining the magnitude of the fingerprint in a regression formulation and checking its significance (signal-to-noise ratio).
- **Enhanced Fingerprinting Approach:**
  - ➢ Investigate **advanced PCA** (tensor-based, non-negative, Joint & Individual Fingerprints or JIF, etc.)
  - ➢ Employ **multiple variables** along a **pathway** to sharpen signal-to-noise ratios & enable downstream attribution
  - ➢ Use pathway info to refine fingerprints for use within a **short-term SAI event** with a more **regional impact**

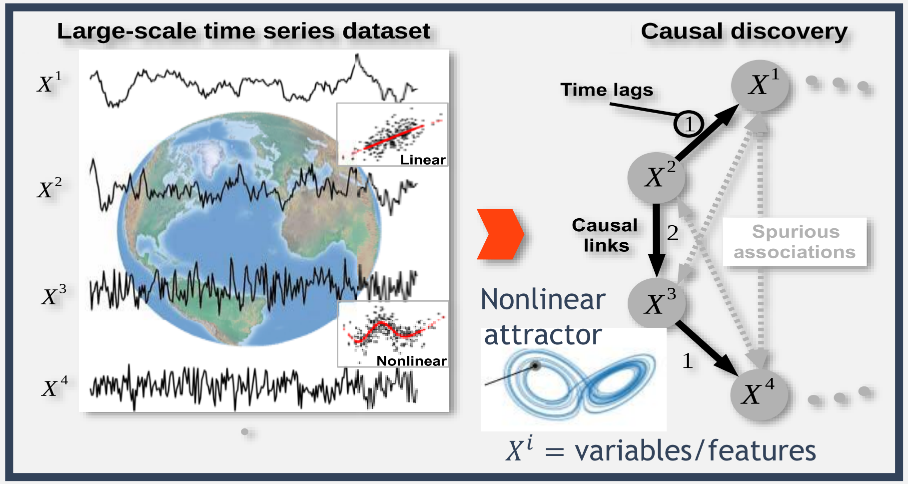


Fingerprints from varying volcanic forcings: non-negative PCA strengthens Pinatubo effect on temperature [Weyland et al 2023 (in prep)].

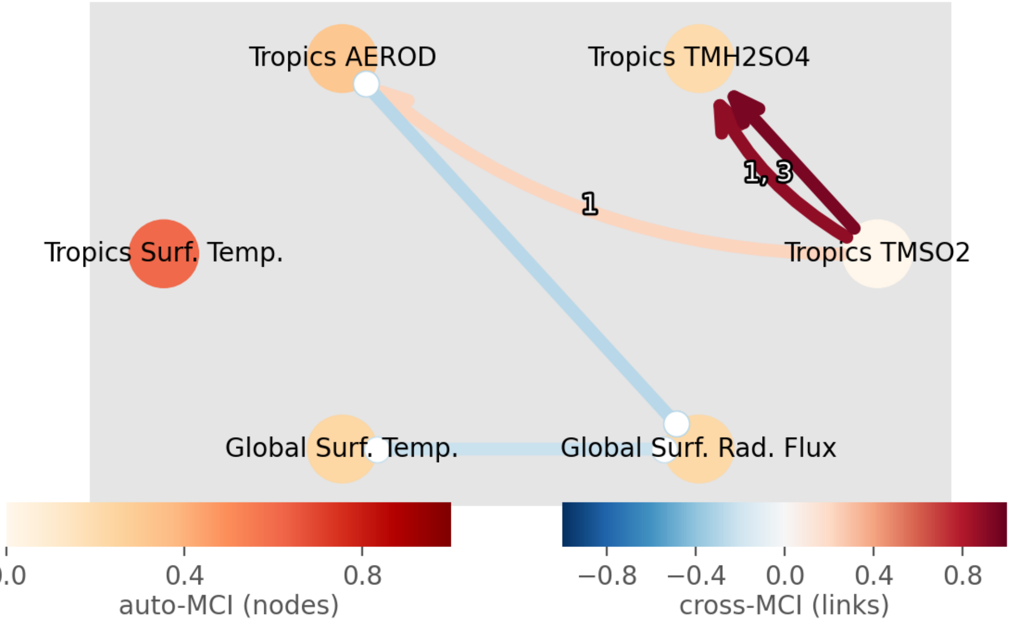
Team: B. Wagman, L. Swiler, K. Tsigaridis [Columbia]

Attribution
Causal Modeling

- **Goal:** establish relationships between a set of variables to discover or confirm a causal relationship
- **Causal Network Learning Approach:**
  - Fit a **graphical model** of covariates by iterative **conditional independence tests.**
  - **PCMCI algorithm:** Peter Clark Momentary Conditional Independence [Runge, 2019]
  - Allows for and detects **contemporaneous dependencies**, removes spurious associations



Preliminary Causal Network Results on Mt. Pinatubo Simulation Data with Prognostic Aerosols



- Tropical SO_2 causes Tropical H_2SO_4 (over a 1 and 3 month lag)
- Tropical SO_2 causes a change in aerosol optical depth (AEROD)
- Tropical AEROD shows a negative contemporaneous dependence with global surface radiation flux.

Team: J. Nichol, M. Smith, L. Swiler, C. Wentland, M. Weylandt

Attribution
Inverse Optimization

*See next talk by **M. Gulian** for more details on inverse optimization using DONNs.*

Goal: identify magnitude, height and location of the source is a **large-scale, PDE constrained inverse problem**

Find source parameters θ that minimize the difference between simulated and observed aerosol concentration s.t. atmosphere PDEs as constraints:

$$\min_\theta J(\theta) = \sum_{i=1}^{n} \int_\Omega \left[c_{\text{obs}}(x,t_i) - c_{\text{sim}}(x,t_i,\theta)\right]^2 dx$$

$$\text{s.t.} \quad \left.\begin{aligned} \frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \boldsymbol{v}) \\ \frac{\partial \boldsymbol{v}}{\partial t} &= -\frac{1}{\rho}\nabla p - \boldsymbol{g} + \boldsymbol{F} - 2\boldsymbol{C}\boldsymbol{v} \\ &\vdots \end{aligned}\right\}$$

Approximated by DONNs ~~E3SM Energy Exascale Earth System Model~~

Approach:

- Develop **deep operator neural networks (DONNs)** to enable PDE-constrained optimization
- **Bayesian approach** to deal with ill-posedness & incorporate UQ
- Add **pathway information** as penalty terms in the objective and/or additional constraints

Team: J. Hart, M. Gulian, I. Manickam, L. Swiler

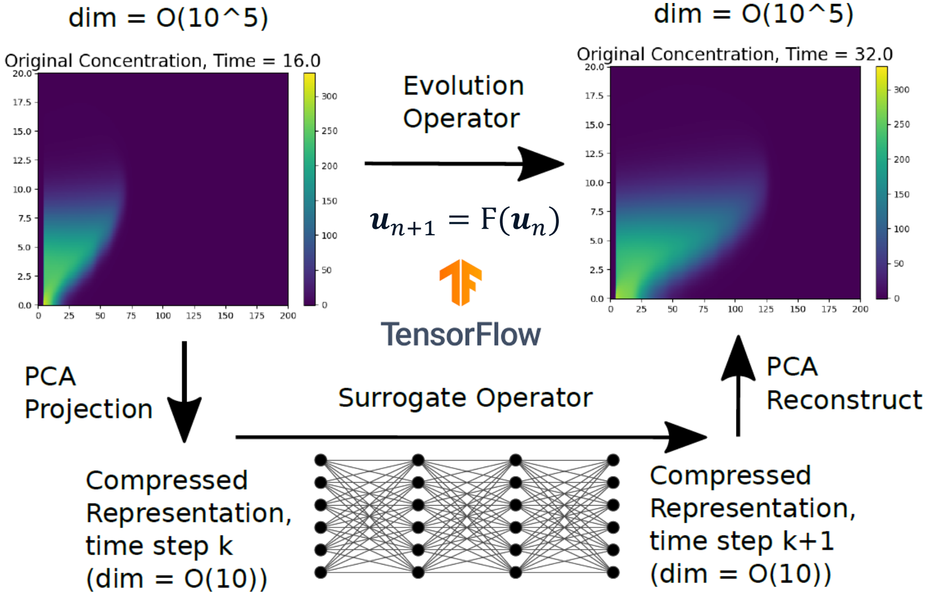
Gaussian Plume+: Advection-Diffusion-Reaction with Gaussian Plume Source

(test case for initial prototyping)

$$\min_\theta J(\theta) = \sum_{i=1}^{n}\sum_{j=1}^{m} \left[c_{\text{obs}}(x_j,t_i) - c_{\text{sim}}(x_j,t_i,\theta)\right]^2 + R(\theta)$$

$$\begin{aligned} &\frac{\partial c}{\partial t} - \kappa \nabla^2 c + \boldsymbol{v}\cdot\nabla c - S\boldsymbol{e}_y \cdot \nabla c = R(c) + f && \text{on } \Omega \times [0,T] \\ &\nabla c \cdot \boldsymbol{n} = 0 && \text{on } \partial\Omega \times [0,T] \\ &c = 0 && \text{on } \Omega \times \{0\} \end{aligned}$$

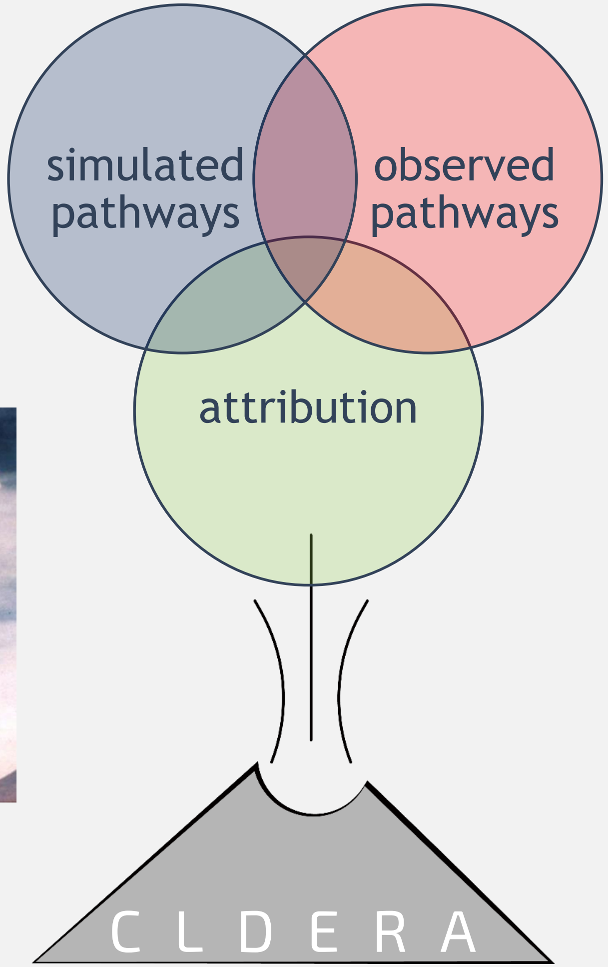
RAPID OPTIMIZATION LIBRARY



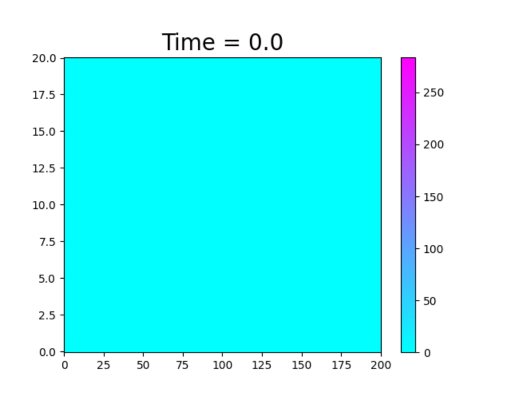
[Hart et al. 2023]

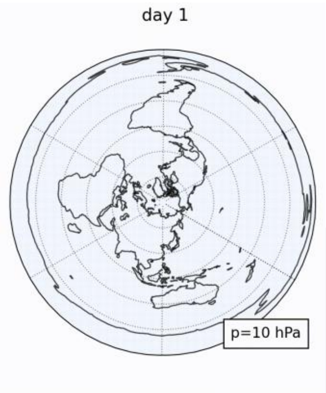
Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- CLDERA Research Composition
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- **Verification & Validation**
- Summary



Tiered Verification Approach





Test Sensitivity of Method FY22

Method form informed by Real Data

Refine Method Formulation

Apply to **Synthetic Cases**

Establish Viability of Method FY23

Apply to idealized cases

Refine Method Formulation

Prove Usefulness of Method FY23/FY24

Apply to Mt. Pinatubo

Sensitivity Analyses

Refine Method Formulation

Synthetic ✔

Coupled ODEs devoid of governing physics that enable exploration of tool/method sensitivities

$$Y_{1,t} = 0.5Y_{1,t-1} + 2I[t > 250] + \epsilon_{Y_{1,t}}$$
$$Y_{2,t} = 0.2Y_{1,t-1} + 0.6Y_{2,t-1} + \epsilon_{Y_{2,t}}$$

Idealized ✔

Gaussian Plume+

Basic physics (advection-diffusion-reaction), reduced dimensionality, reduced coupling

HSW++

Realistic Earth circulation, idealized forcings/ topography/chemistry, controllable relationships

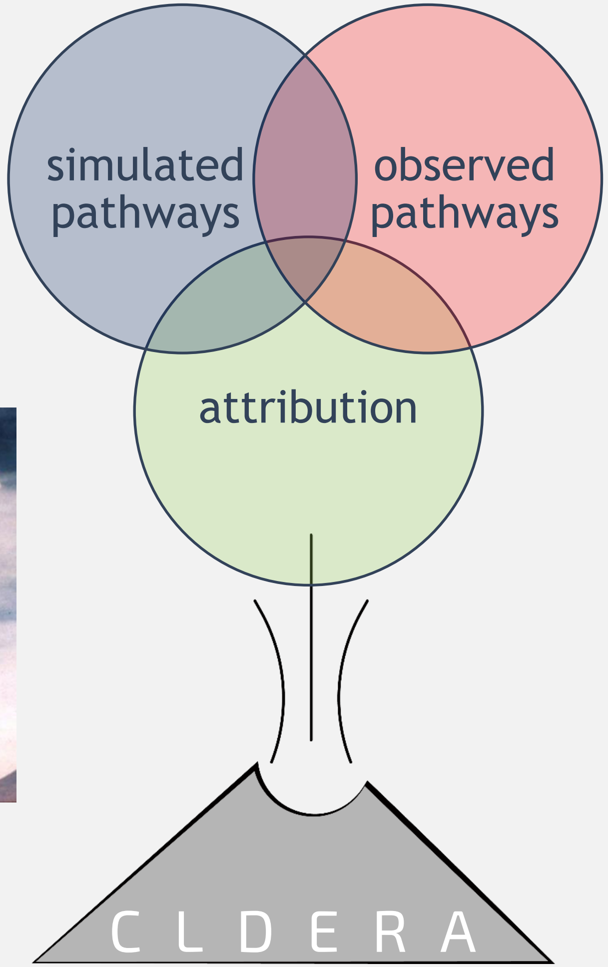
Pinatubo Pathways (WIP)

Full complexity of Earth's climate – verify method solution against known pathways

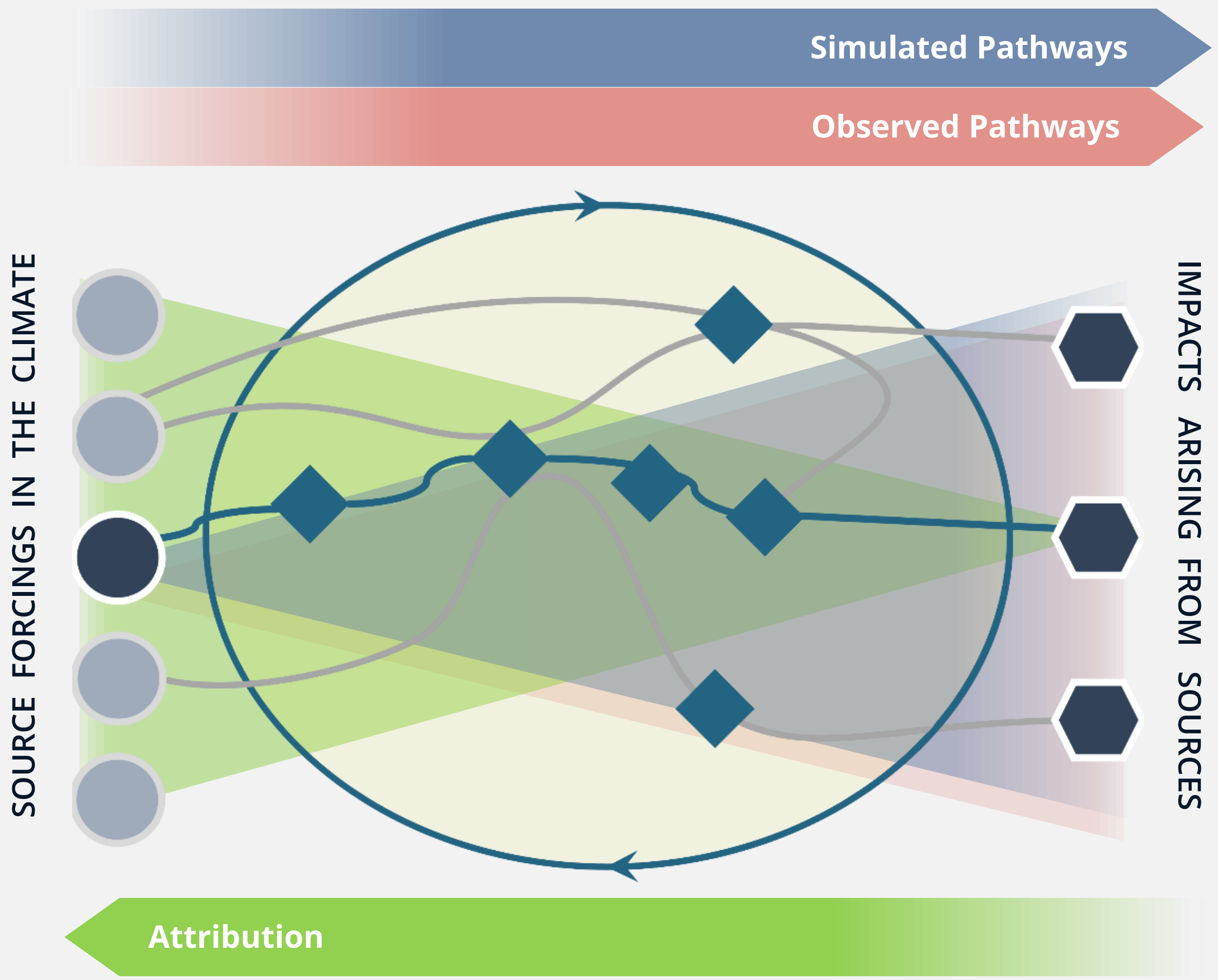
HSW = Held-Suarez-Williamson [Williamson et al., 1998]

Outline

- Background
  - ➢ Motivation
  - ➢ The CLDERA Project
  - ➢ Driving Exemplar: Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- CLDERA Research Composition
  - ➢ Simulations
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- **Summary**



Summary of CLDERA



OUTCOMES

Tools to discover and represent pathways, and analyses to establish pathway robustness to changing conditions.
Cross-validation using simulated and observed pathways will inform areas for model improvement and new measurements.

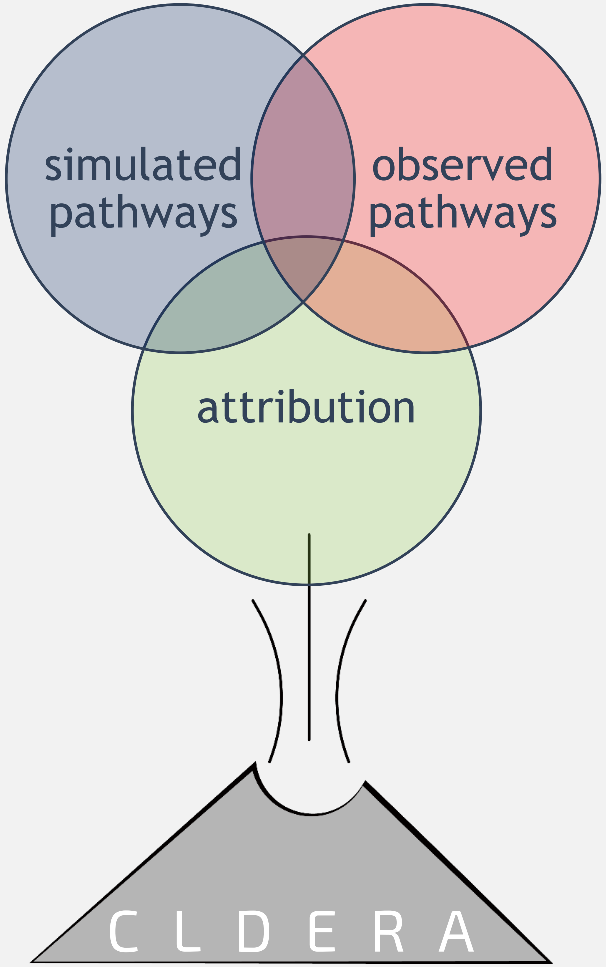
Contributory ranking of sources to specific impacts using pathways.
Capability enables robust risk analysis and offers the potential to guide future climate actions.

Attribution of source characteristics using inverse optimization methods.
Will provide credible methodology to deter unilateral implementation of climate interventions.

Beginning-to-end attribution in the climate system
Tracing evolving chains of physical processes to enable attribution of climate impacts from a localized source.

Outline

- Motivation
- The CLDERA Grand Challenge LDRD Project
- Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
- Energy Exascale Earth System Model (E3SM) & Simulating Mt. Pinatubo in E3SM
- The Three CLDERA Thrusts
  - ➢ Simulated Pathways Thrust
  - ➢ Observed Pathways Thrust
  - ➢ Attribution Thrust
- Verification & Validation
- **Summary**



CLDERA Team

L. Bertagna
H. Brown
M. Carlson
W. Davis
G. Harper
B. Houchens
J. Lien
D. Krofchek
J. Nichol
M. Peterson
A. Steyer
J. Watkins
E. Wenzel
C. Jablonowski (U Michigan)
J. Hollowed (U Michigan)
X. Liu (TAMU)
A. Hu (TAMU)

K. Goode
R. Garrett
J. Hickey
B. Hillman
G. Huerta
J. Li
K. McClernon
D. Ries
D. Tucker
A. McCombs
B. Li (UIUC)
S. Jun (UIUC)

M. Gulian
M. Brown
J. Hart
I. Manickam
K. Maupin
M. Smith
B. Wagman
C. Wentland
M. Weylandt
K. Tsigaridis (Columbia U)

CLDERA Leadership Team

CLDERA PI: D. Bull
CLDERA Deputy PI: K. Peterson
Simulated Pathways Lead: I. Tezaur
Observed Pathways Lead: L. Shand
Attribution Lead: L. Swiler

Thank you for your attention!





References

- Caldwell, P., et al., *Statistical significance of climate sensitivity predictors obtained by data mining*. Geophysical Research Letters, 2014. **41**.
- Finley, Andrew, Banerjee, Sudipto,Gelfand, Alan. (2012). Bayesian Dynamic Modeling for Large Space-Time Datasets Using Gaussian Predictive Processes. Journal of Geographical Systems. 14. 29-47.
- Golaz, J.-C., et al., The DOE E3SM Coupled Model Version 1: Overview and Evaluation at Standard Resolution. Journal of Advances in Modeling Earth Systems, 2019. 11(7): p. 2089-2129.
- Goode, K., Ries, D., and Zollweg, J. "Explaining Neural Networks with Functional Data Using PCA and Feature Importance". AAAI 2020 Fall Symposium on AI in the Government and Public Sector. November 13-14, 2020. https://arxiv.org/abs/2010.12063.
- Hall, A. et al., *Progressing emergent constraints on future climate change*. Nature Climate Change, 2019. **9,** p 269-278.
- Hasselmann, K., *Multi-pattern fingerprint method for detection and attribution of climate change*. Climate Dynamics, 1997. **13**(9): p. 601-611.
- Hegerl, G.C. and G.R. North, *Comparison of Statistically Optimal Approaches to Detecting Anthropogenic Climate Change*. Journal of Climate, 1997. **10**(5): p. 1125-1133.
- Kravitz, B., et al., *First Simulations of Designing Stratospheric Sulfate Aerosol Geoengineering to Meet Multiple Simultaneous Climate Objectives*. Journal of Geophysical Research: Atmospheres, 2017. **122**(23): p. 12,616-12,634.
- Marvel, K., M. Biasutti, and C. Bonfils, *Fingerprints of external forcings on Sahel rainfall: aerosols, greenhouse gases, and model-observation discrepancies*. Environmental Research Letters, 2020: p. Medium: ED; Size: Article No. 084023.
- McDermott, Patrick & Wikle, Christopher. (2018). Deep echo state networks with uncertainty quantification for spatio-temporal forecasting. Environmetrics. 30. 10.1002/env.2553.
- National Academies of Sciences Engineering Medicine (NASEM), *Reflecting Sunlight: Recommendations for Solar Geoengineering Research and Research Governance*. 2021, Washington, DC: The National Academies Press. 328.
- Nowack, P., et al., *Causal networks for climate model evaluation and constrained projections*. Nature Communications, 2020. **11**(1): p. 1415.
- Runge, J., et al., *Inferring causation from time series in Earth system sciences*. Nature Communications 2019. **10**(1).
- Tezaur, I., et al., Global sensitivity analysis of ultra-low resolution E3SM. Submitted to JAMES, 2022.
- Wagman, B. M., L. P. Swiler, K. Chowdhary, B. Hillman. "The Fingerprints of Stratospheric Aerosol Injection in E3SM." LDRD project 224535 final report, Sept. 2021.
- Williamson, MS et al., *Emergent constraints on climate sensitivities*. Reviews of Modern Physics, 2021. **93** (2) 2021.

References (cont'd)

- J. Hart, M. Gulian, I. Manickam, L. Swiler. Solving High-Dimensional Inverse Problems with Auxiliary Uncertainty via Operator Learning with Limited Data, ArXiv pre-print: https://arxiv.org/abs/2303.11379.
- D. Tucker, D. Yarger. Elastic Functional Changepoint Detection. ArXiv pre-print: https://arxiv.org/abs/2211.12687.
- M. Weylandt, L. Swiler. Beyond PCA: Additional Dimension Reduction Techniques to Consider for Climate Data. J. Climate, 2023 (in prep).

Start of Backup Slides

Current State-of-the-Art

In Establishing Connective Relationships in Earth's Climate

Confounding characteristics of the climate attribution* problem:

- High internal variability in the Earth system
- Limited ESM ensembles
- Historically limited observational data
- Multiple sources contributing to an impact

Techniques currently applied to climate attribution:

- Fingerprinting (e.g., Hasselmann, 1997; Hegerl & North, 1997; Marvel et al., 2020)
- Structural Causal Modeling (e.g., Runge et al., 2019; Nowack et al., 2020)
- Emergent Constraints (e.g., Hall et al., 2019; Williamson et al., 2021)

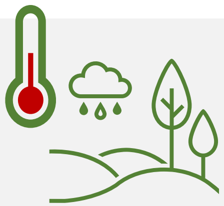
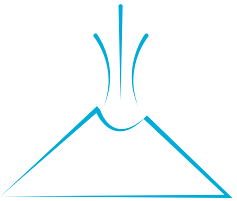

"Pecking Order", Edgar Hunt

"Connective relationships are often **unbounded from etiological relationships** allowing **physically meaningless** source-impact correlations." [Caldwell et al., 2014]

Under CLDERA, we are moving beyond a correlative approach – establishing connective relationships.

* Process of evaluating relative contributions of multiple causal factors to a change/impact with an assignment of statistical confidence

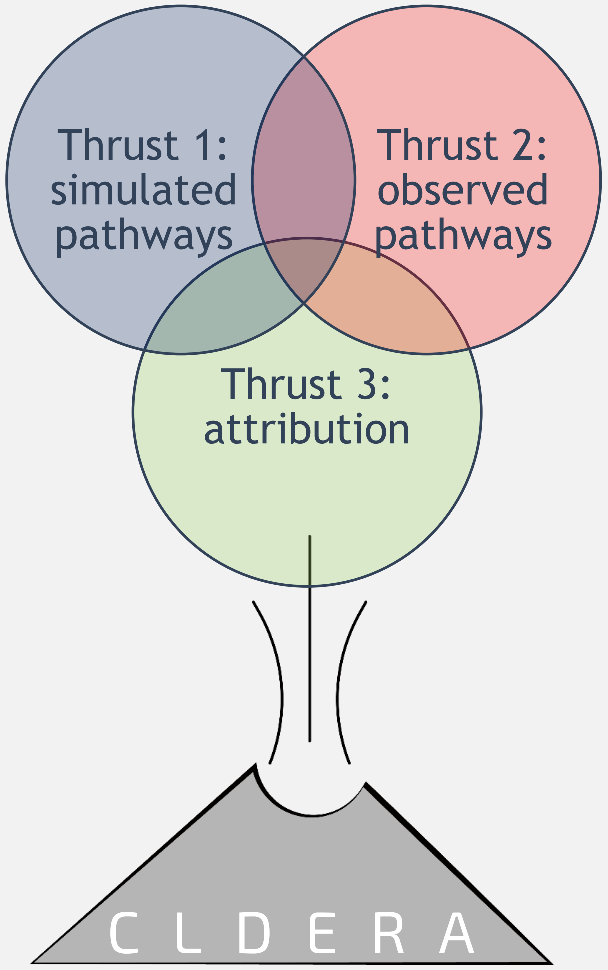
Attribution in Climate

				**CLDERA** 
What is the question?	How do rising concentrations of GHGs in the atmosphere affect climate state variables?	What are the relative contributions of different sectors, activities, and entities to concentrations of GHGs in the atmosphere?	How do changes in the global climate system affect the relative frequency and severity of extreme events?	What are the downstream impacts from large, spatio-temporally localized sources within the climate?
What is the source?	Long-term, slowly accumulating GHG emissions	Sector-specific emissions	Changes to global climate system	Geographically and temporally localized source forcings in the climate
Examples	WG1 and WG2 IPCC reports	Cement industry, transportation	Likelihood of Hurricane Katrina	Volcanic eruptions, wildfires
Is the attribution direct/ quantitative?	WG1- yes (temp/precip/…) WG2 – normally no, notional linkage	yes	no, notional connection	yes, linked through multiple process-nodes

The goal of CLDERA is to develop new tools to enable *downstream impact attribution* from geographically and temporally localized source forcings in the climate.

The CLDERA Grand Challenge LDRD Project

A Novel Foundational Approach to Understanding the Causation of Impacts



Motivating Research Questions:

- ***Can pathways be discovered*** within simulation and observation datasets that reveal the connective relationships between source and impacts?
- ***Can pathways*** inform contributory ***rank***ing of sources to an impact?
- ***Can pathways*** cull the included space while preserving complex climate features to more confidently ***enable attribution***?

Hypothesis: tracing **pathways** between sources and impacts will increase **certainty** of **attribution.**

Connection to Sandia Capabilities & Other Applications

Multi-component Sensor Systems

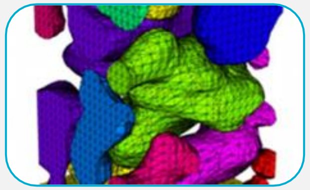
RAPID OPTIMIZATION LIBRARY

Inverse Optimization

Information Sciences

Bio-Security

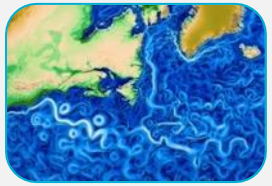
Cyber-Security



Multi-Physics Modeling

DAKOTA

Uncertainty Quantification



Computational Science

Regulatory Frameworks

Analysis of Extremes

"Always/ Never" Ethos

Modeling & Simulation

Detection & Attribution

Risk Analysis & High-Reliability Engineering

Dual-Nature National Security Issues

CLDERA-Critical Capabilities

Bioscience

Materials Science

Engineering Science

Earth Science

Nanodevices & Microsystems

Computing & Information Science

Radiation, Electrical, & High Energy Density Science

Foundational Research that Enables Climate Work

Exemplar: June 1991 Mt. Pinatubo Eruption

Stratospheric Aerosol Injection (SAI) Exemplar

Why this exemplar?

Largest eruption of the satellite era, releasing ~18-19 Tg SO_2 gas

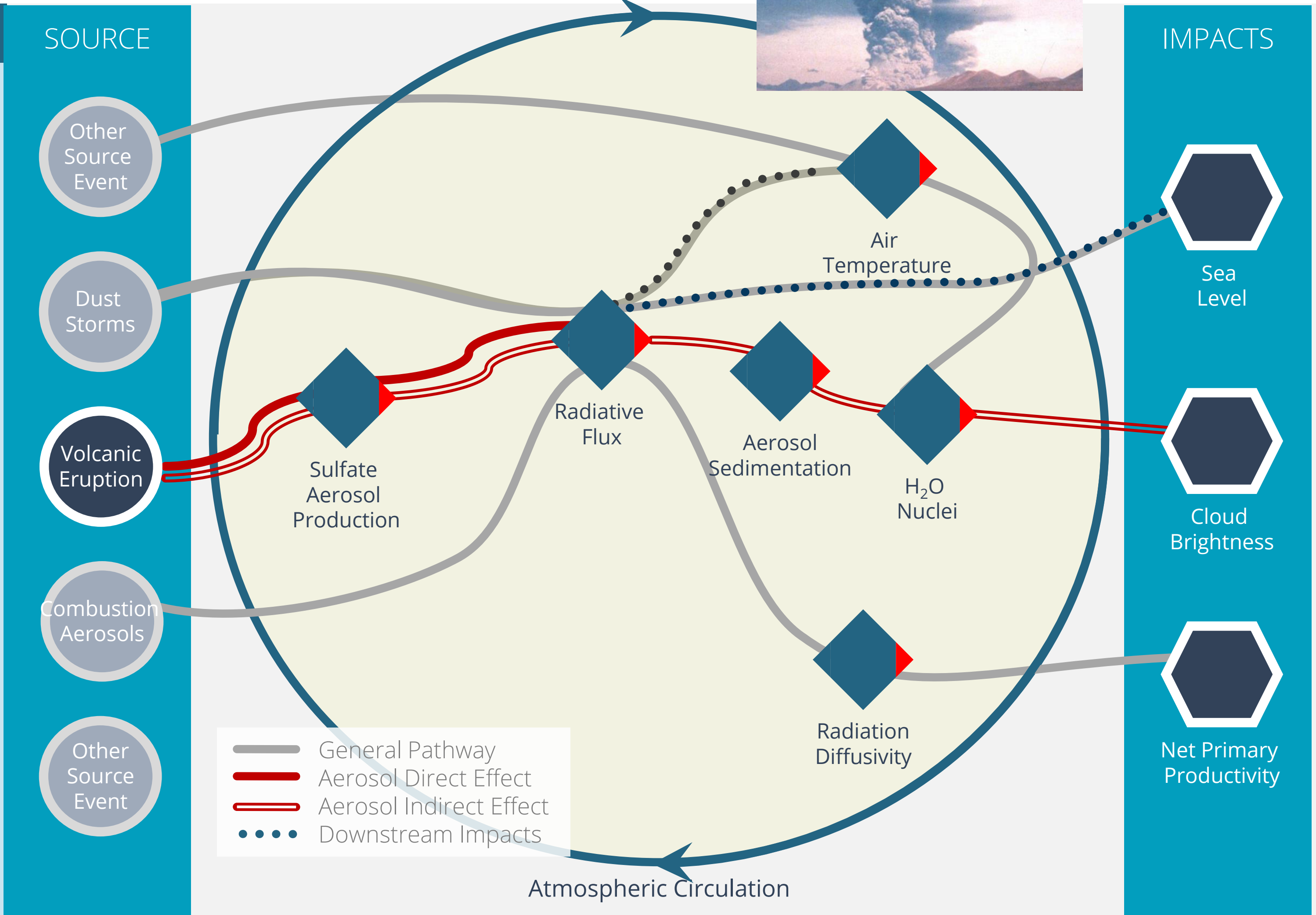
- Impacts large enough to rise above **internal variability** of climate system
- Led to 0.4-0.6°C **global cooling** → 1993.

The source is an **analog for a climate intervention technique**

- 1 Tg SO_2 per yr may produce on the order of 0.1°C cooling [Kravitz et al., 2017]

The source **forcing is external to the feedbacks** within the Earth's climate

It provides **ample observational data** and, because the impacts and pathways are relatively well characterized it **offers validation of our analysis techniques within the approach**



Notional Representation of Subset of Processes

Simulation Plan

Simulation Set	Number of runs per year 1-deg resolution			Number of runs per year 7.5-deg resolution			Total processor hours
	FY22	**FY23**	**FY24**	**FY22**	**FY23**	**FY24**	
Mt. Pinatubo with prognostic aerosols	40	30	20				5M
Mt. Pinatubo with double radiation call	40	30					4M
Control simulation with prognostic aeosols and no Mt. Pinatubo	40	30	20				5M
Control simulation prescribed 1990, no aerosol forcing	20	30					3M
Control simulation with fields nudged towards Mt. Pinatubo aerosol forcing		20	30				3M
Mt. Pinatubo with branching (initiate new simulations periodically from original no aerosol forcing)		20	30				3M
Sensitivity study on Mt. Pinatubo eruption characteristics (magnitude, height, location, & timing of injected material)	40	50	30	300	150		7M
Sensitivity study on select E3SM aerosol (MAM4) and cloud microphsyics (MG2) parameters		50	50		150	300	6M
Total processor hours	**10M**	**14M**	**10M**	**144K**	**144K**	**144K**	**34M**

- Simulations will be performed for ~5 simulated years.
- Runs are being performed on NERSC (Cori, Perlmutter) and Sandia HPC (Skybridge, Boca)
- 1° resolution E3SM can achieve:
  - 18 SYPD per 58 AMD CPU nodes on Perlmutter at NERSC
- May supplement 1° resolution with cheaper 7.5° resolution runs

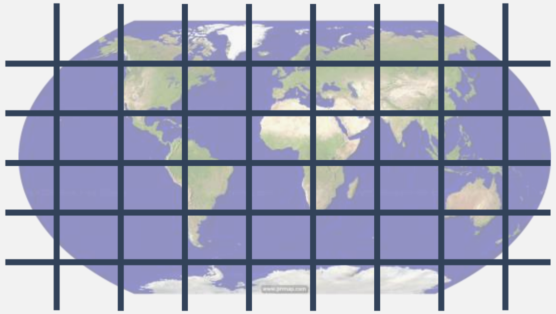
Planned simulations expected to require ~O(10^7) CPU-hours!

Simulated Pathways Thrust
Statistical Methods

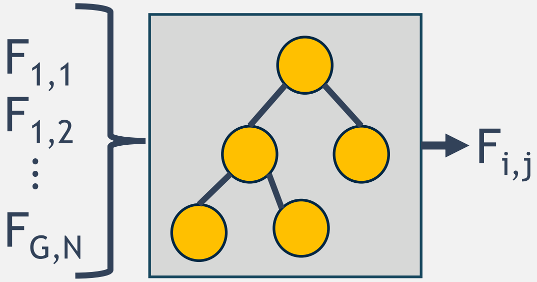
(a) Random forest regression (RFR):

- **Goal:** use feature importances from Random Forests (RFs) to **identify weighted pathways** from one variable to another

Raw data



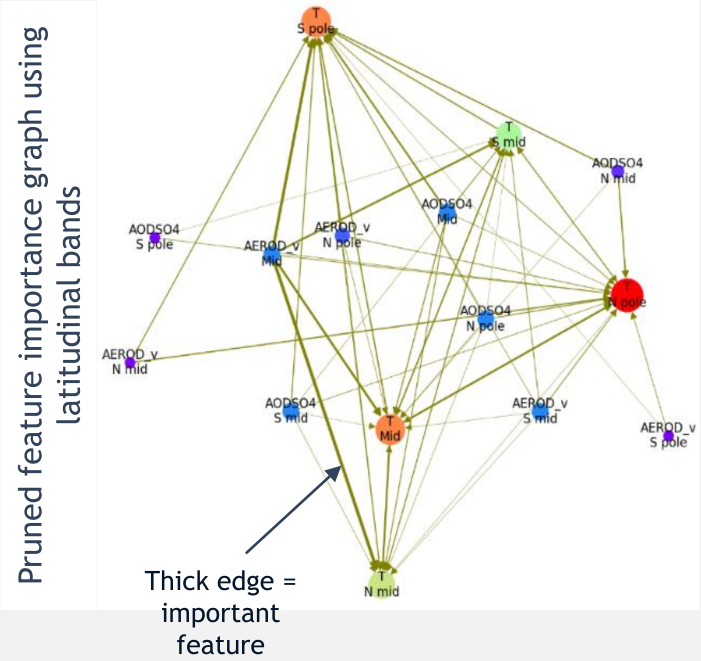
Train RF Regressors



Calculate Feature Importances

	$F_{1,1}$	…	$F_{G,N}$
$F_{1,1}$	0.1	…	0.5
$\vdots$	…	…	…
$F_{G,N}$	0.99	…	0.1

Create Pathway Graph



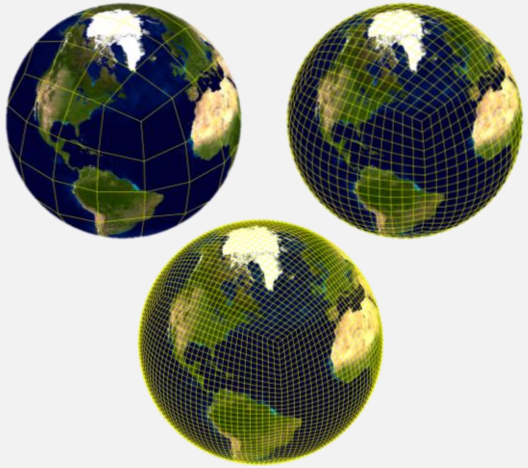
- **Inputs:** time-series of various features or variables of interest (simulated or observed data)
- **Output:** a list of “single-hop” paths that form a network/graph
  - ➢ Graph can be queried to see what kinds of paths exist between features and their relative strengths

Team: M. Peterson, M. Brown, J. Nichol, W. Davis, I. Tezaur

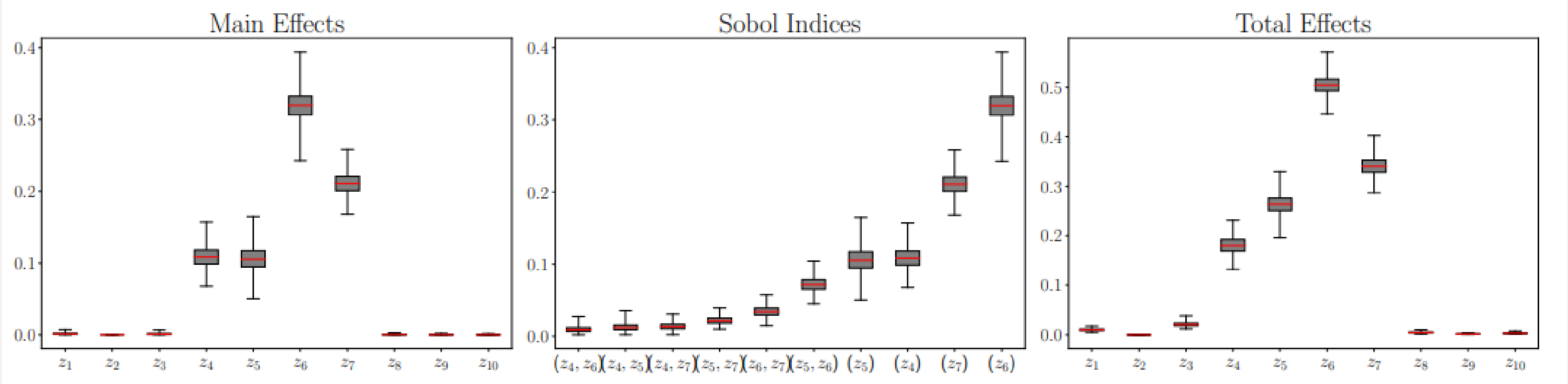
Simulated Pathways Thrust
Statistical Methods

(b) Sensitivity analyses (SA)

- **Generate data** for RFR, anomaly detection and Attribution thrust
- Determine **robustness of pathways** to changes in SAI-/model-related inputs
- **Two kinds** of sensitivity studies using **different resolutions** of E3SM:
  - (i) Vary **eruption elements**, e.g., mass, time, height, location (how Mt. Pinatubo could have been – "how low can you go?")
  - (ii) Vary MAM4 aerosol and MG2 cloud microphysics **model parameters**



Above: ultra-low (ULR), medium-low (MLR) and standard 1° resolution E3SM grids



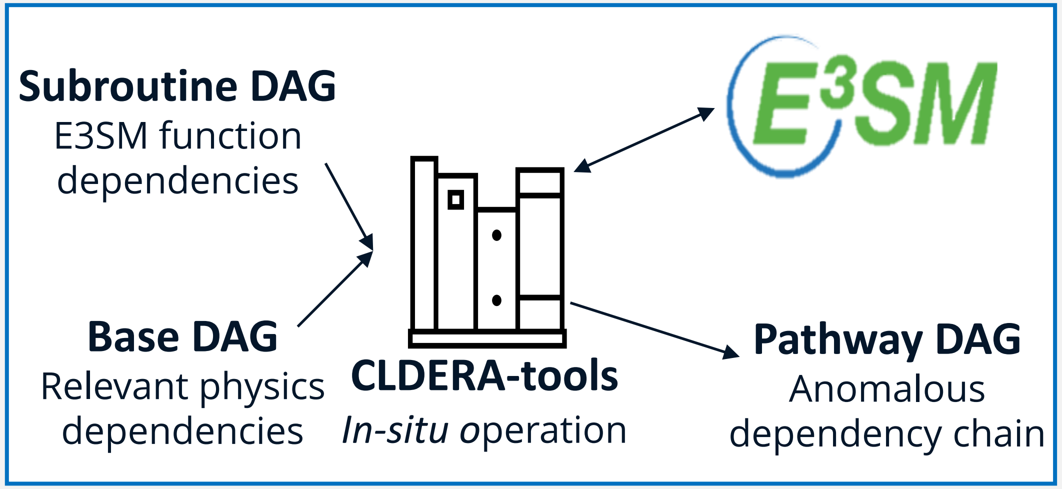
Right: global sensitivity analysis (GSA) results for surface temperature QOI using ULR E3SMv1 [Tezaur et al., 2022]

Team: I. Tezaur, K. Peterson, B. Wagman, H. Brown

Simulated Pathways Thrust
Computational Monitoring

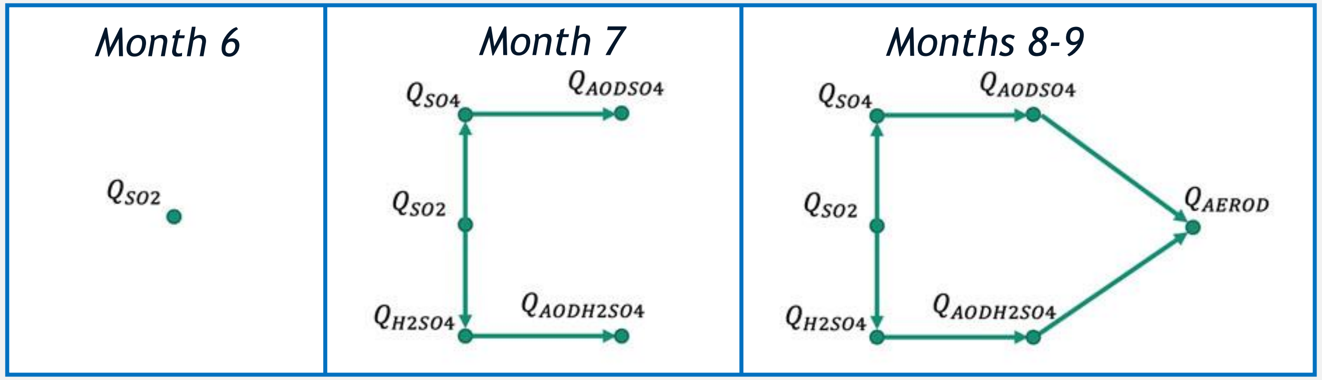
(a) Profiling: finding pathways *in-situ* while running E3SM

- **Goal:** instrument E3SM and develop Directed Acyclic Graphs (DAGs) of process interactions executed within code
- Control runs (e.g., no Mt. Pinatubo eruption run) generate baseline.
- CLDERA-tools performs statistical analysis by comparing QOIs inside code with baseline and tracking propagation of "anomalies" in real time.



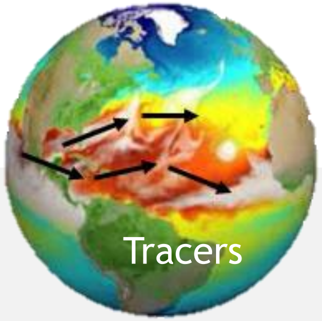
Inputs: baseline, "base DAG" (tells E3SM what to track)

Outputs: Time-evolving pathway DAG



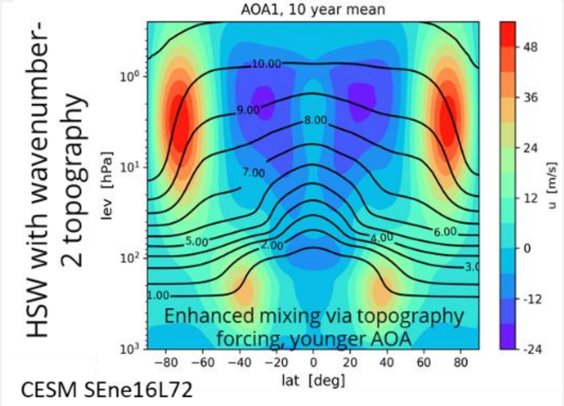
Simulated Pathways Thrust

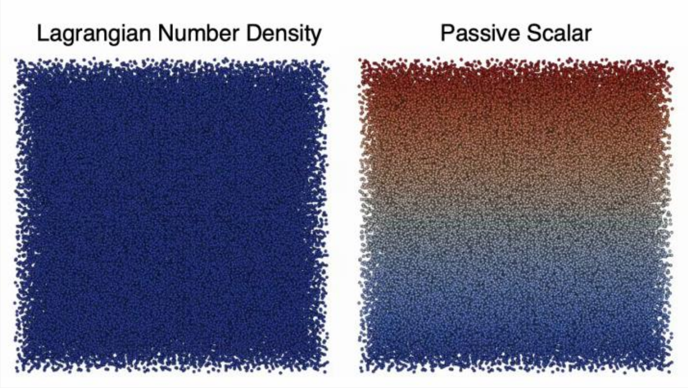
Computational Monitoring



(b) Tracing: add tracers to E3SM, use them to **evaluate E3SM** and explore ways to repurpose them to **identify source-impact pathways**

- **Passive tracers:** do not feedback to the atmosphere, but can track source evolution
  - ➢ **Evaluate climatological dynamics** (like "Age of Air") and changes to those dynamics.
  - ➢ **Infer pathways/pathway changes** by detecting tracer flow patterns/evolution using **Lagrangian Coherent Structures (LCS):** surface trajectories which exponentially attract or repel tracers.



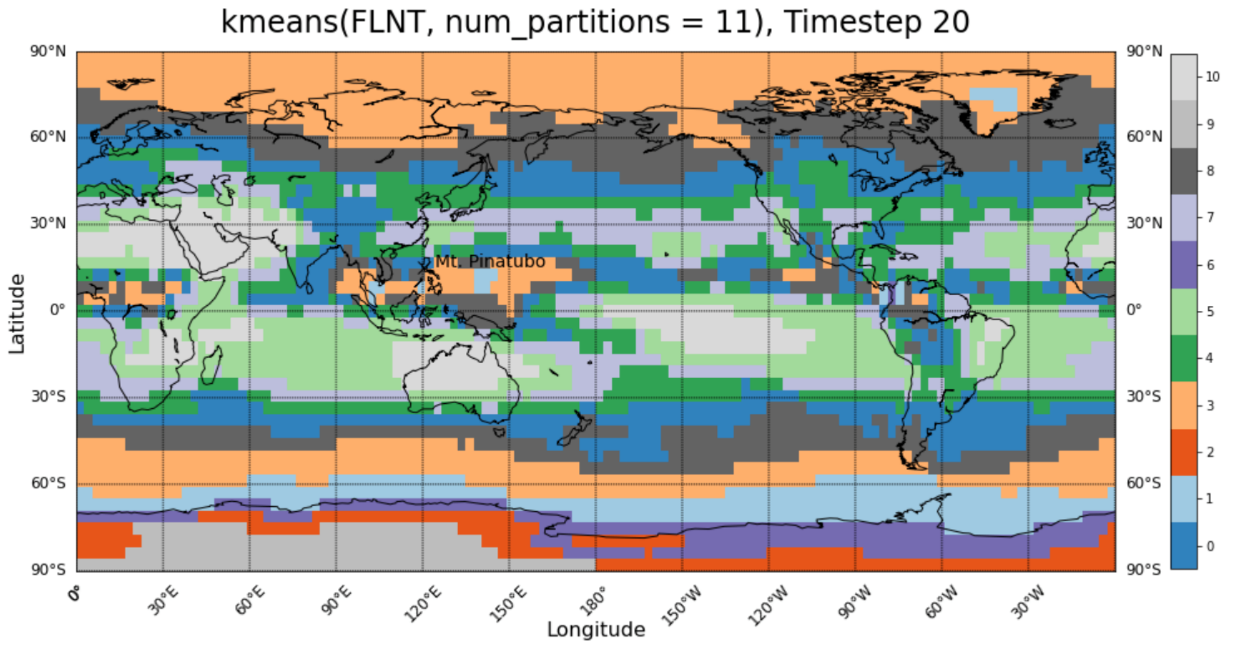


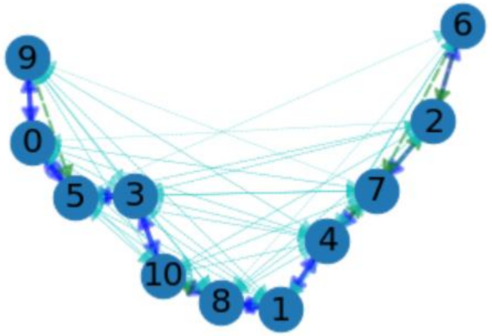
- **Active ("tagged") tracers:** feedback into atmosphere through physics processes
  - ➢ Enable tracking of **relative contributions** along nodes in pathway.

Simulated Pathways Thrust

*Anomaly Detection**

- **Goal:** produce clusterings over climate simulations that can serve as foundations of pathway discovery
- **Approach:** combine existing anomaly (event) detection algorithms [Davis et al., 2021] with clustering to enable spatio-temporal anomaly progression, defining pathways
- **Leverages** "In-Situ Machine Learning for Intelligent Data Capture on Exascale Platforms" (ISML) project (PI: W. Davis)
- Compressed ISML **signatures** used for clustering
- Clusters used to **inform pathway analysis**






```
{'1, 8, 1, 4, 1': [534, 0.19553277187843282],
 '1, 8, 1, 4, 2': [1472, 0.5389967045038447],
 '1, 8, 1, 4, 3': [3, 0.0010984987184181618],
 '1, 8, 1, 4, 5': [4, 0.0014646649578908824],
 '1, 8, 1, 4, 6': [14, 0.005126327352618088],
 '1, 8, 1, 4, 7': [660, 0.2416697180519956],
 '1, 8, 1, 4, 8': [41, 0.015012815818381545],
 '1, 8, 1, 4, 10': [3, 0.0010984987184181618]}
```


Team: W. Davis, M. Carlson, I. Tezaur

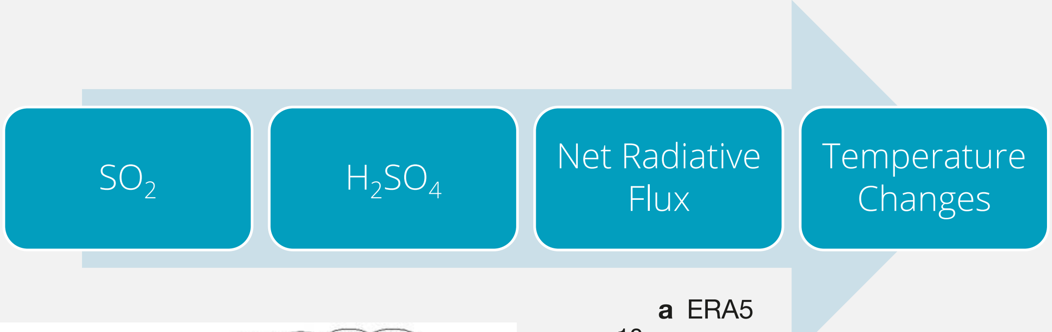
*Finds "interesting" (localized in space or time) events or outliers

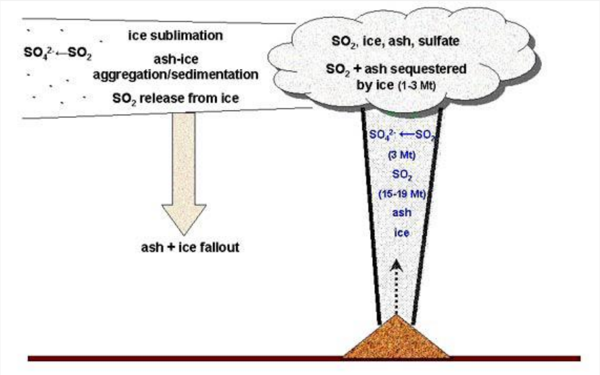
Observed Pathways Thrust
What is an Observed Pathway?

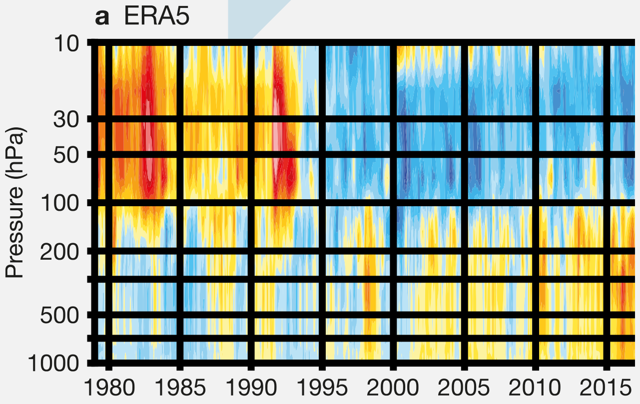
Definition: *observed pathways* are interpreted as **relationships** (or correlations) between **dependent climate processes** (*pathway nodes*).

Objective: rather than finding pathways that have not been postulated, **validate proposed pathways** and **quantify changes** in the **relationship between pathway nodes.**

Approach: develop **statistical methods** that can account for the **dynamic evolution** of aerosols over space and time, **multiple complementary sources of data** and **uncertainty**.







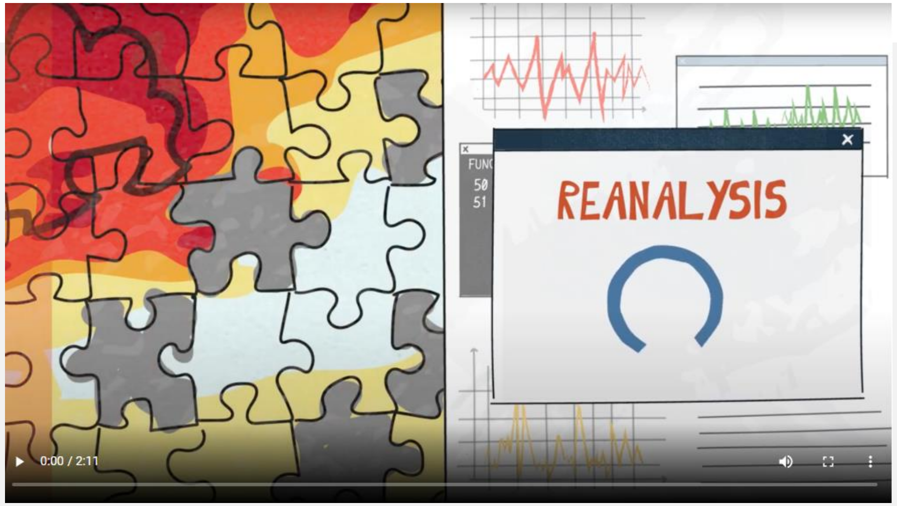
Driving Science Questions:

- What are the spatio-temporal signatures of the temp. change due to Mt. Pinatubo?
- For how long after can we link sulfates created by Mt Pinatubo to climate effects? When does signal become too noisy or convoluted?
- When and where do we first see changes due to the event? How precise can we get with uncertainties?

Observed Pathways Thrust
Available Satellite Data for Mt. Pinatubo

Instrument	Satellite	Measurements	Satellite Orbit	Data Collected
Total Ozone Mapping Spectrometer (**TOMS**)	Nimbus-7	UV albedo (nadir)	Polar, sun-synchronous	SO_2 mass and ozone (Bluth et al., 1992; McPeters et al., 1992)
Solar Backscatter Ultraviolet Spectral Radiometer (**SBUV**)	NOAA-11	UV albedo (nadir)	Polar, sun-synchronous	SO_2 mass and ozone (McPeters et al., 1992)
NOAA Advanced Very High Resolution Radiometer (**AVHRR**)	NOAA-10, -11, -12	4 Vis-IR channels (nadir)	Polar, sun-synchronous	Aerosol optical depth (Stowe et al., 1992; Long and Stowe, 1994), plume height (Lynch and Stephens, 1996), cloud cover (Stowe et al., 1999)
High Resolution Radiation Sounder (**HIRS**)	NOAA 6-17	19 IR channels (nadir)	Polar, sun-synchronous	SO_2 mass and cloud-top height (Miles et al., 2017)
Stratospheric Aerosol and Gas Experiment (**SAGE II**)	Earth Radiation Budget Satellite (ERBS)	5 channels, Vis—IR (limb scanning)	Polar	Aerosol optical depth/extinction, aerosol max heights, Ozone (McCormick and Veiga, 1992)
Microwave Sounding Unit (**MSU**)	NOAA-10,-11,-12	4 MW channels (nadir)	Polar, sun-synchronous	Surface-Upper Stratospheric temperature anomalies (Spencer et al., 1990; Dutton and Christy, 1992)
Improved Stratospheric and Mesospheric Sounder (**ISAMS**)	Upper Atmosphere Research Satellite (UARS)	8 IR channels (limb scanning)	Near-Polar	Aerosol extinction, mass, and height (Lamberte et al., 1993)
Microwave Limb Sounder (**MLS**)	UARS	4 MW channels (limb scanning)	Near-Polar	SO_2 mass and temperature profiles (Read et al., 1993)

Observed Pathways Thrust
Available Reanalysis Data for Mt. Pinatubo



https://climate.copernicus.eu/climate-reanalysis

What is reanalysis data?

- **Blend** of **observations** with past short-range weather/climate **forecasts** rerun with modern weather/climate forecasting models.
- Generated using **data assimilation** techniques.
- Provides the **most complete picture** of past weather and climate.

Available reanalysis data for Mt. Pinatubo eruption:

- ***ERA-5 reanalysis***
  - 1979-present
  - Observations from various satellites, radiosonde data and surface observations
  - Model input is from ECMWF (European Centre for Medium-Range Weather Forecasts) forecast model, which takes into account forcing from total solar irradiance, GHGs, ozone and some aerosols.
- ***MERRA-2 reanalysis***
  - 1979-present
  - Uses similar observations to ERA-5
  - Model input is from NASA Goddard Earth Observing System (GEOS) model

Observed Pathways Thrust

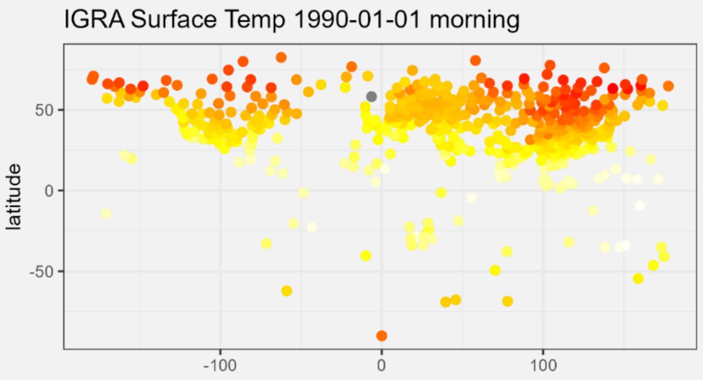
Data Fusion

- **Challenge:** observational data sets are incongruent, coming from different instruments and possessing different scales and different spatial and temporal ranges

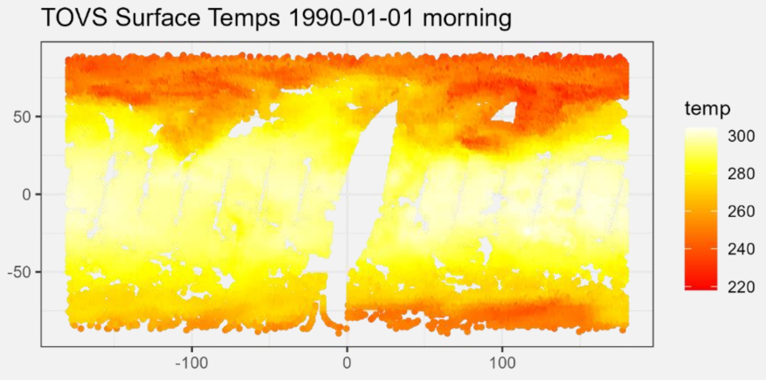
- **Goal:** fuse observational datasets to obtain near-real time measurements and produce a spatio-temporally complete observational dataset with UQ

  ⇒ simple Kriging does not propagate uncertainty from different sources

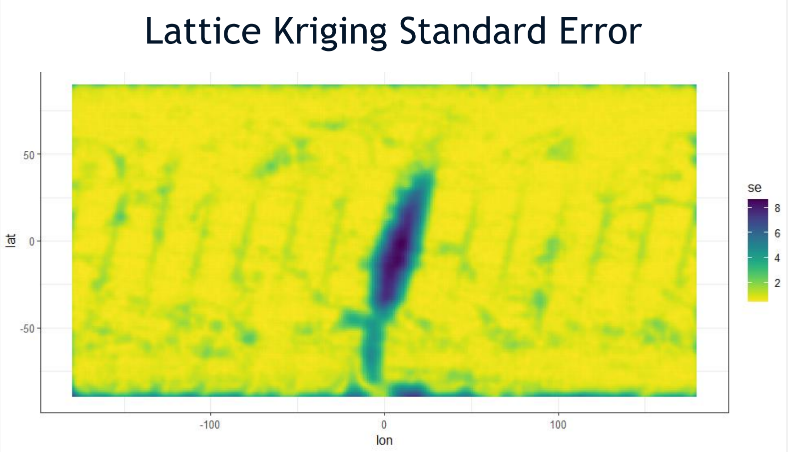
  - **Lattice Kriging:** nonparametric approach with multi-resolution basis function representations and Gaussian error structure [Nychka et al. 2017]
  - **Spatial Random Effects Model** [Nguyen et al. 2012, 2013, 2017, 2018]
  - **Bayesian Hierarchical Framework** using **Integrated Nested Laplacian Approximation (INLA)** [Campos et al. 2023]

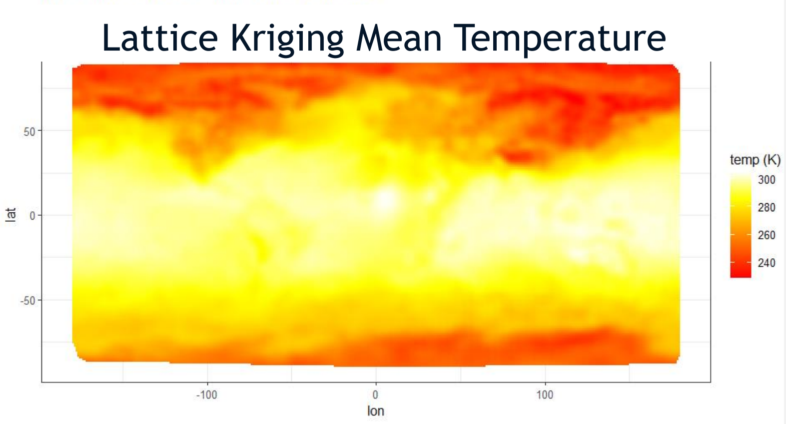


Observational data



Observational data





Fused data

Team: J. Li, A. McCombs, L. Shand

Synthetic Test Case Formulation

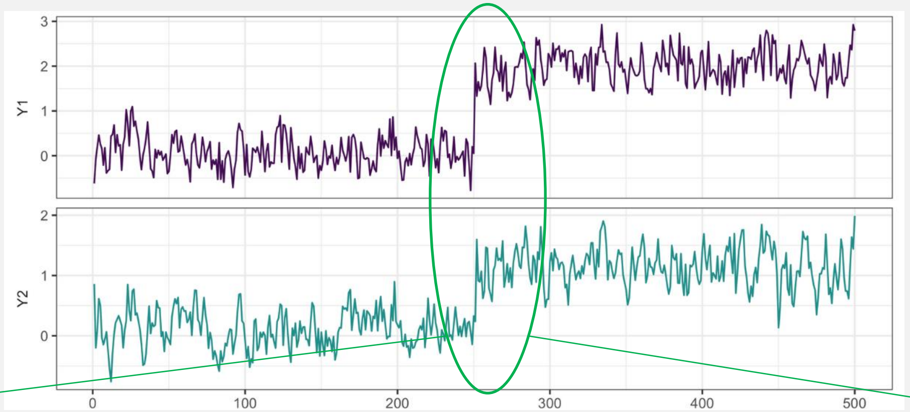
- **Tiered Datasets, four formulations across**
  - ➢ Temporal trends
  - ➢ Temporal trends on spatial grid
  - ➢ Temporal trend on linearly-trended spatial grid
- **Characteristics**
  - ➢ Distinct numbers of couplings with both linear and nonlinear relationships
  - ➢ Distinct lags
  - ➢ Quasi-periodicity
  - ➢ Noise degree
  - ➢ Change in mean value

Two Variable Changepoint Exemplar

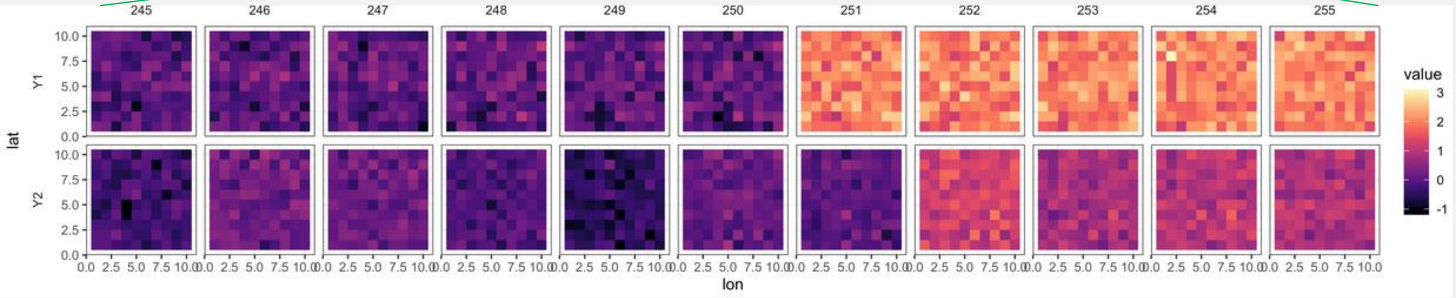
$$Y_{1,t} = 0.5Y_{1,t-1} + 2I[t > 250] + \epsilon_{Y_{1,t}}$$
$$Y_{2,t} = 0.2Y_{1,t-1} + 0.6Y_{2,t-1} + \epsilon_{Y_{2,t}}$$

$$\epsilon_{Y_{1,t}} \sim N(0, 0.1)$$
$$\epsilon_{Y_{2,t}} \sim N(0, 1)$$

Temporal Trend

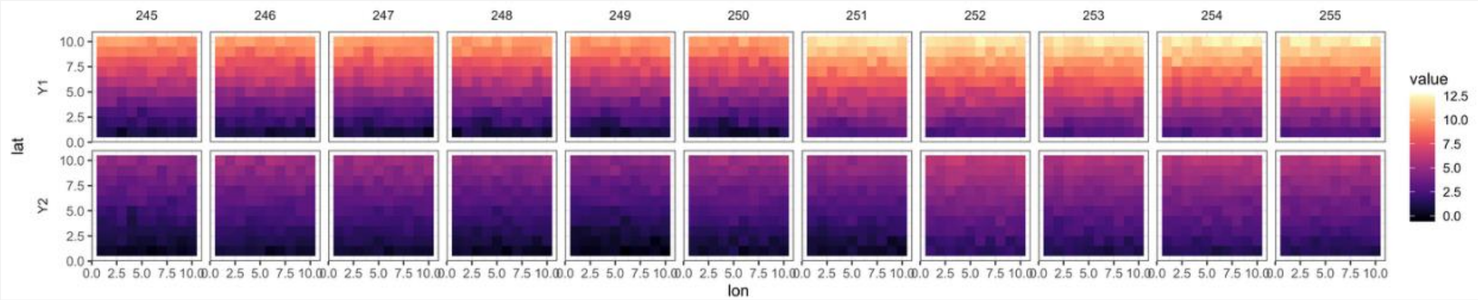


Temporal Trend in Space



Spatio-Temporal Trend

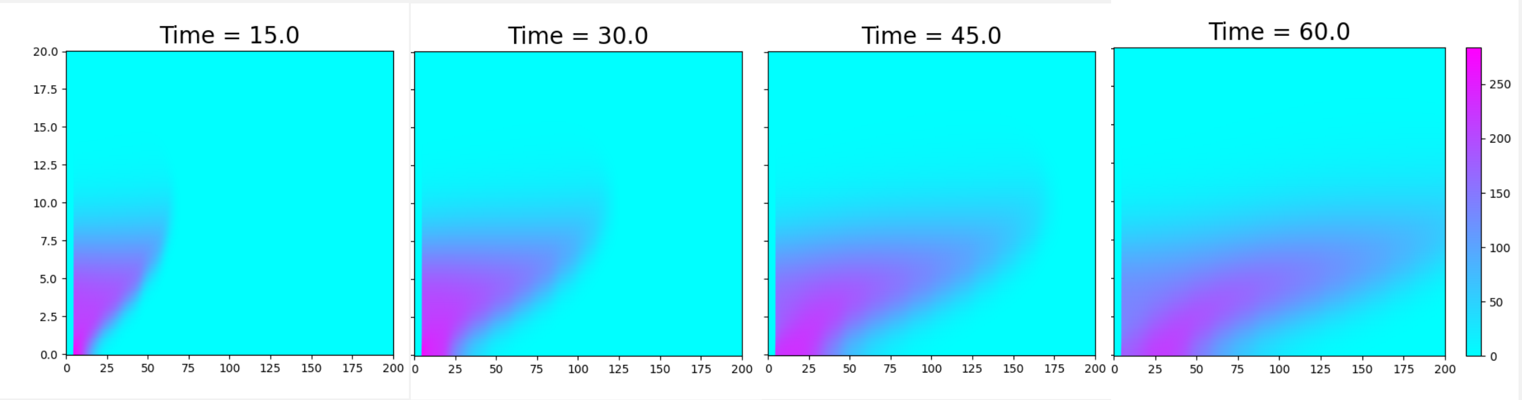
Linearly-trended Spatial Grid



Idealized Test Case Formulations

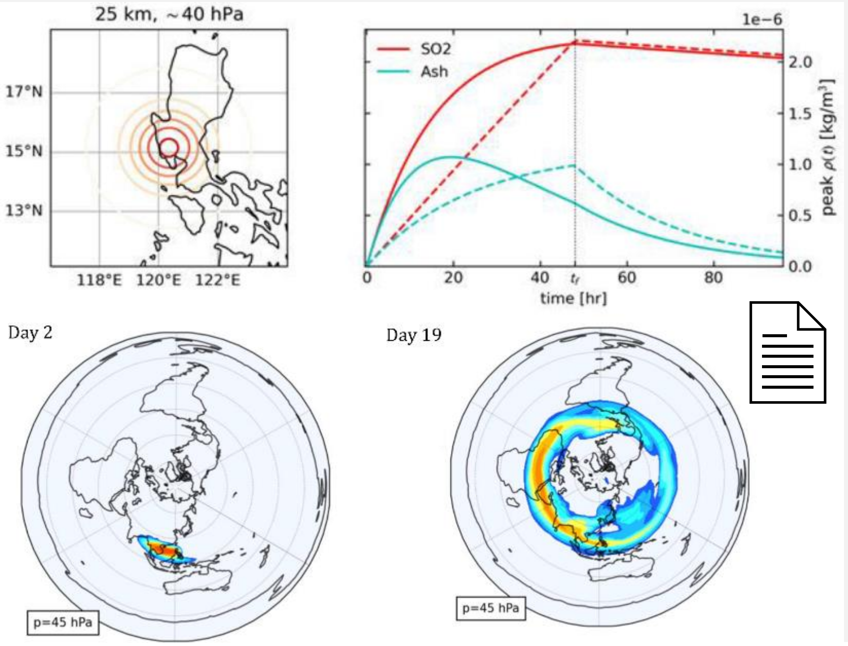
Gaussian Plume Plus

- PDE solution: based on transient convection-diffusion-reaction PDE in 2D.
- **Input:** variable winds, reaction functions for chemistry, realistic lifetimes, and variable source magnitudes/durations



Held-Suarez Williamson ++

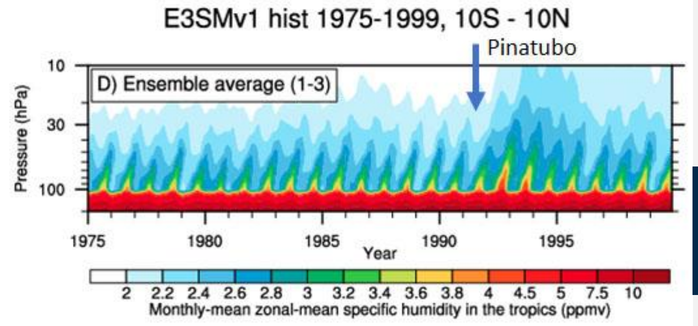
- Create realistic circulation with E3SM's dynamic solver using idealizations for process physics/forcings
  - ➢ Radiation: Newtonian temperature relaxation towards T_{eq}
  - ➢ Planetary boundary layer: Rayleigh friction & optional topography
- Mimic Mt. Pinatubo eruption via a prescribed, time-limited injection of an SO_2 and ash Gaussian plume
- Develop series of correlated tracers for 'toy' chemistry, develop temperature/radiation feedbacks in plume, …



Mt. Pinatubo Validation

An identified **pathway** will be considered "correct" if it contains as "nodes" most of the known **aerosol direct, indirect** and **downstream effects** from Mt. Pinatubo eruption

- Validation requires **assessments** of SAI-related processes in E3SM ✔
  - ➢ Conservation checks
  - ➢ STE processes in E3SM (figure below)
  - ➢ E3SM's climatic response to Pinatubo
  - ➢ Compare E3SM's circulation to reanalysis products (ERA-5)
  - ➢ Idealized tracer transport experiments



Above: enhanced H_20 vapor in 1992-93 ("tropical tape recorder", CMIP6 E3SMv1 coupled historical simulations)