Sandia National Laboratories

An Overview of the CLDERA Grand Challenge LDRD Project:

Developing a Novel Foundational Approach for Attributing Climate Impacts

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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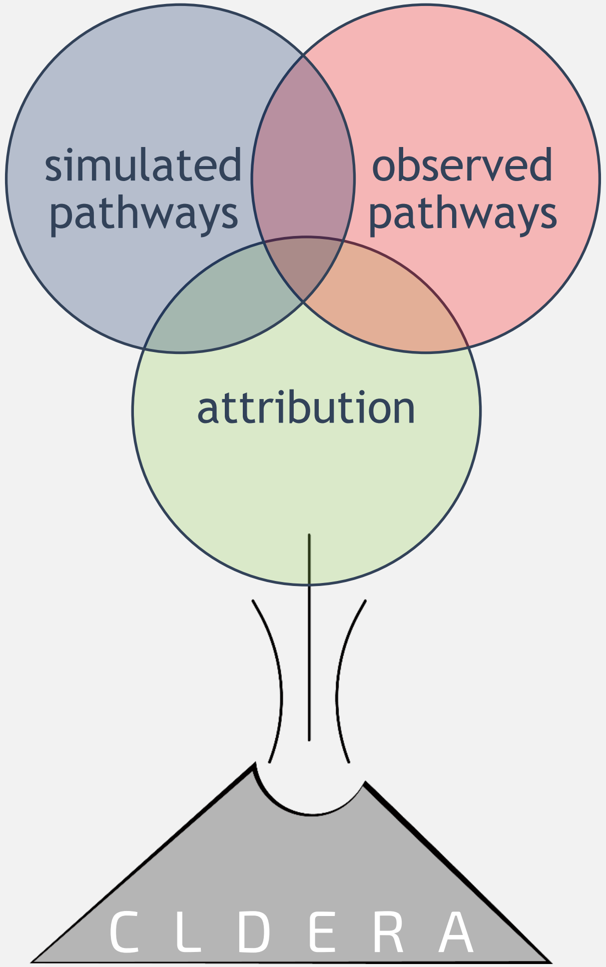
Outline

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



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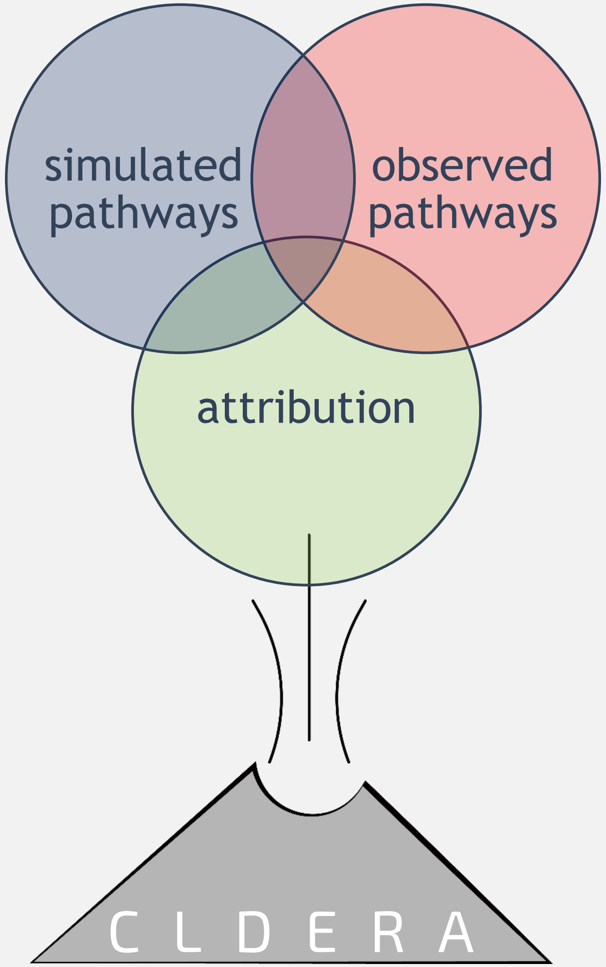


Motivation

Climate Change is a Growing National & Global Security Concern!

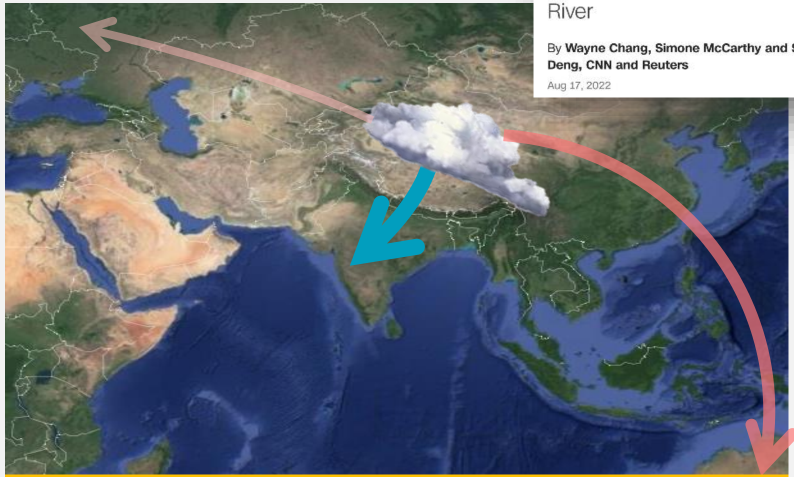
- **Sources of climate change:** natural forcings, policy choices, climate interventions (geo-engineering*).

- Federal agencies (DHS, DoD, DOS, DOE) have articulated an interest in **risk assessments** of **climate impacts** due to both **natural climate change events** and **climate interventions**.
  - ➢ The ability to **distinguish** the impacts of **intervention**, **anthropogenic climate change**, and **natural variability** will become increasingly important as the effects of climate change compound.

- **Decisions** will need to be made on policy, legislation, treaties and national security posture.
  - ➢ As an FFRDC and National Security Lab, we must be prepared to **inform these decisions**.

Timely example: China's Sky River Project

- **Unilaterally** launched form of climate intervention to **control rainfall** over the **Tibetan Plateau.**
- 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!**


'Sky River' cloud seeding impacts

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

Motivation
Tools to Identify Source-Impact Relationships are Lacking

Attribution: the process of ***evaluating the relative contributions of multiple causal factors to a change or impact*** with an assignment of statistical confidence.

Technical Challenges/Limitations:

- High **internal variability** of the Earth system **obscures** the **connective relationships** between **sources** and **impacts.**
  - ➢ Earth system is like a tangled ball of yarn!
  - ➢ Exacerbated by complex coupling of processes in Earth System Models (ESMs)
- **Limited** simulation **data** and limited observation data until recently.
- Wealth of **recent high-resolution measurements** have been historically **under-utilized** to improve our knowledge of the Earth system.

Modified from: http://www.thesourgrapevine.com/2019/11/the-ball-of-string-theory-for-learning.html

- **Attribution techniques** capable of identifying a dominant source are **infeasible** with current approaches due to **ill-posedness** of the **attribution inverse problem** (many possible sources lead to similar impacts).

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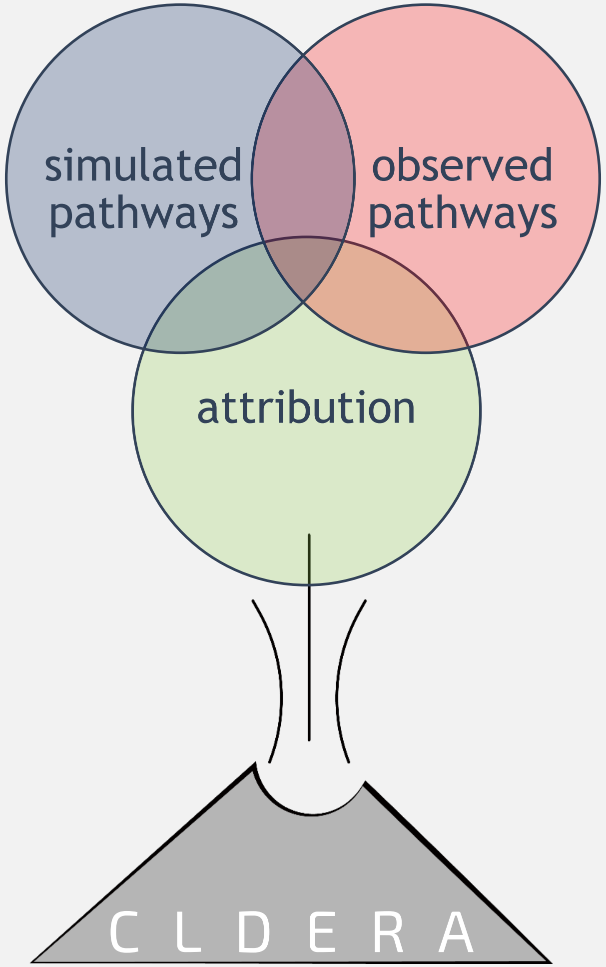


The CLDERA Grand Challenge LDRD Project

A Novel Foundational Approach to Understanding the Causation of Impacts

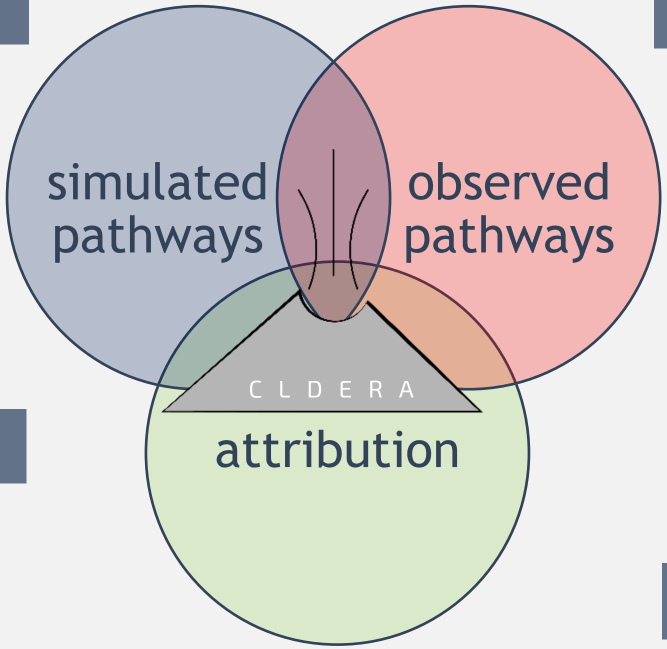
CLDERA: CLimate impact – Determining Etiology thRough pAthways

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, risk analysis)
- Develop novel methods and tools in **three cross-validating thrusts**
- Use the 1991 eruption of **Mt. Pinatubo** as exemplar



Duration: FY22-FY24
Budget: $5M/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.*

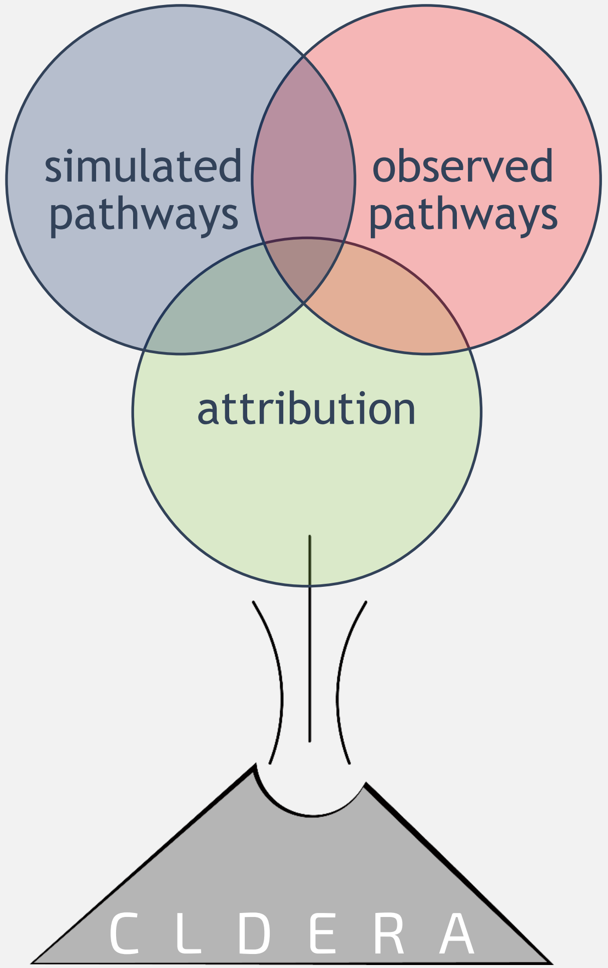
Outcome

Advance climate attribution science by identifying impacts from localized sources.

COLUMBIA UNIVERSITY

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.**

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.

What is a Grand Challenge LDRD Project?

LDRD: Laboratory Directed Research & Development

- "Transformational research inspired by & enabling the mission"
- Funding program at the national labs that focuses on high-risk/high-reward ideas
- Extremely competitive!
- 1-3 year projects, \$200K-\$600K/year.
- Structured into Research Foundations, Mission Foundations and Strategic Initiatives

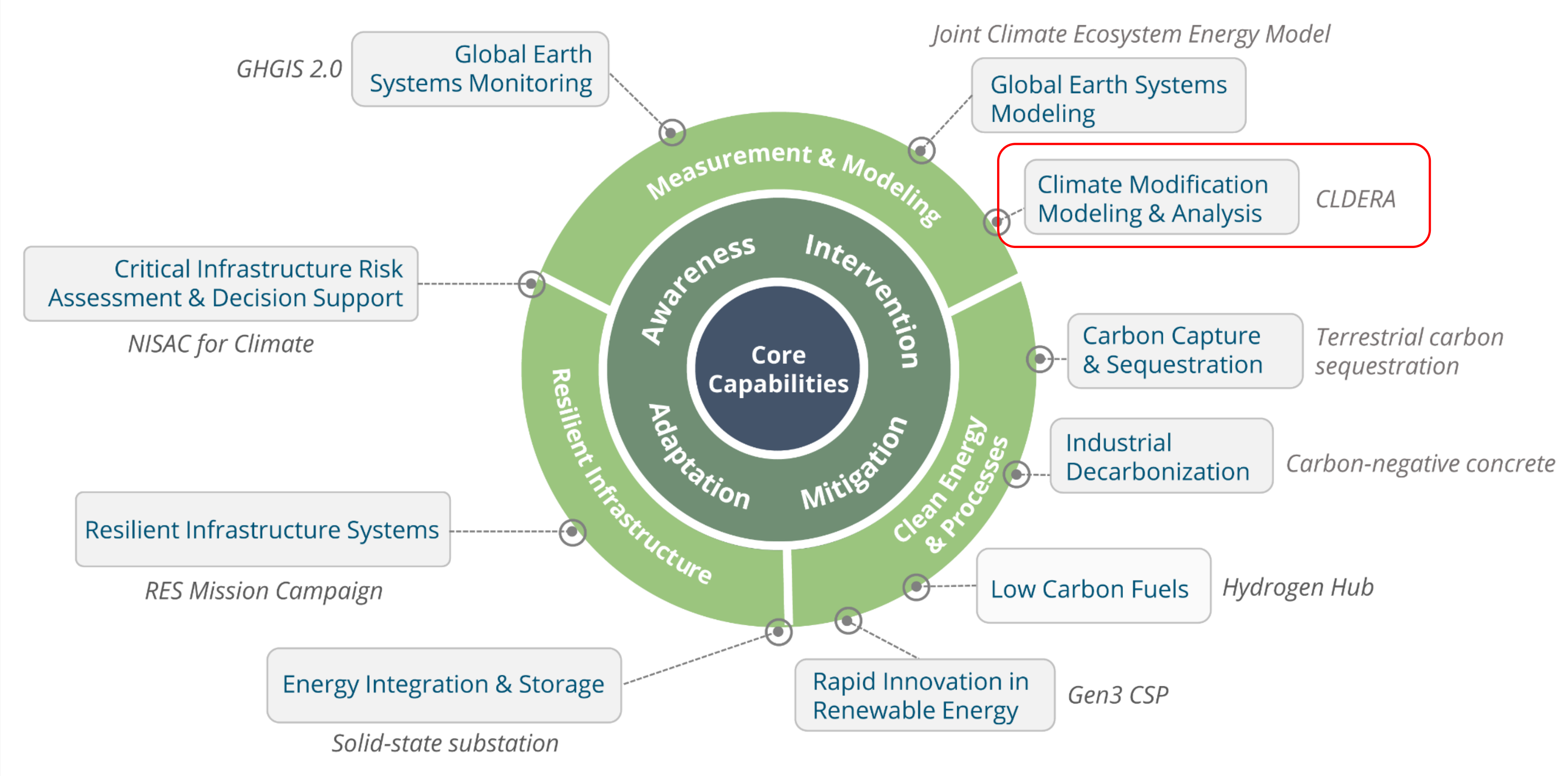
Grand Challenge (GC) LDRD: LDRD++

- One of the Strategic Initiatives in the LDRD program
- Even more competitive than regular LDRD!
- 3-year projects with maximum \$5M/year budget
- Focused on building differentiating capability relevant to critical national security problems
- Focused on building talent pipeline and fostering critical skills
- Projects must have a targeted roadmap for maturing results to achieve mission impact
- Projects aimed at making strides towards tackling recognized "Grand Challenge" problems

CLDERA is one of 4 currently-funded GC LDRDs at Sandia and the 1st one focused on climate.

Connection to Sandia Missions & Strategies

CLDERA is aligned with Sandia's recently-launched ***climate security strategy****, which aims to* ***advance*** *the* ***state-of-the-art*** *in the following key climate capabilities.*



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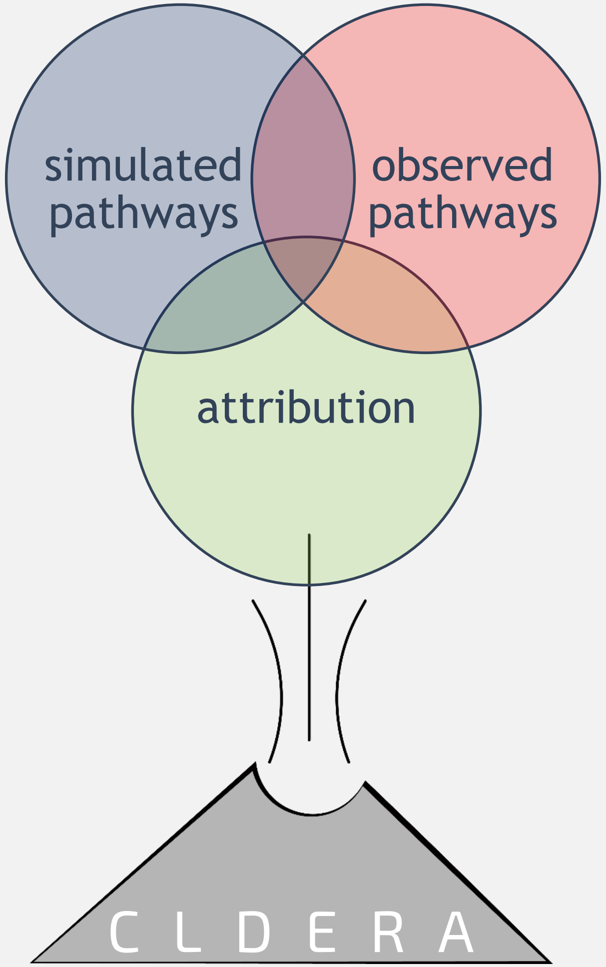


Mt. Pinatubo Eruption

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 H_2SO_4, H_2O and aerosols via oxidation, nucleation and chemical reactions

Mt. Pinatubo before eruption

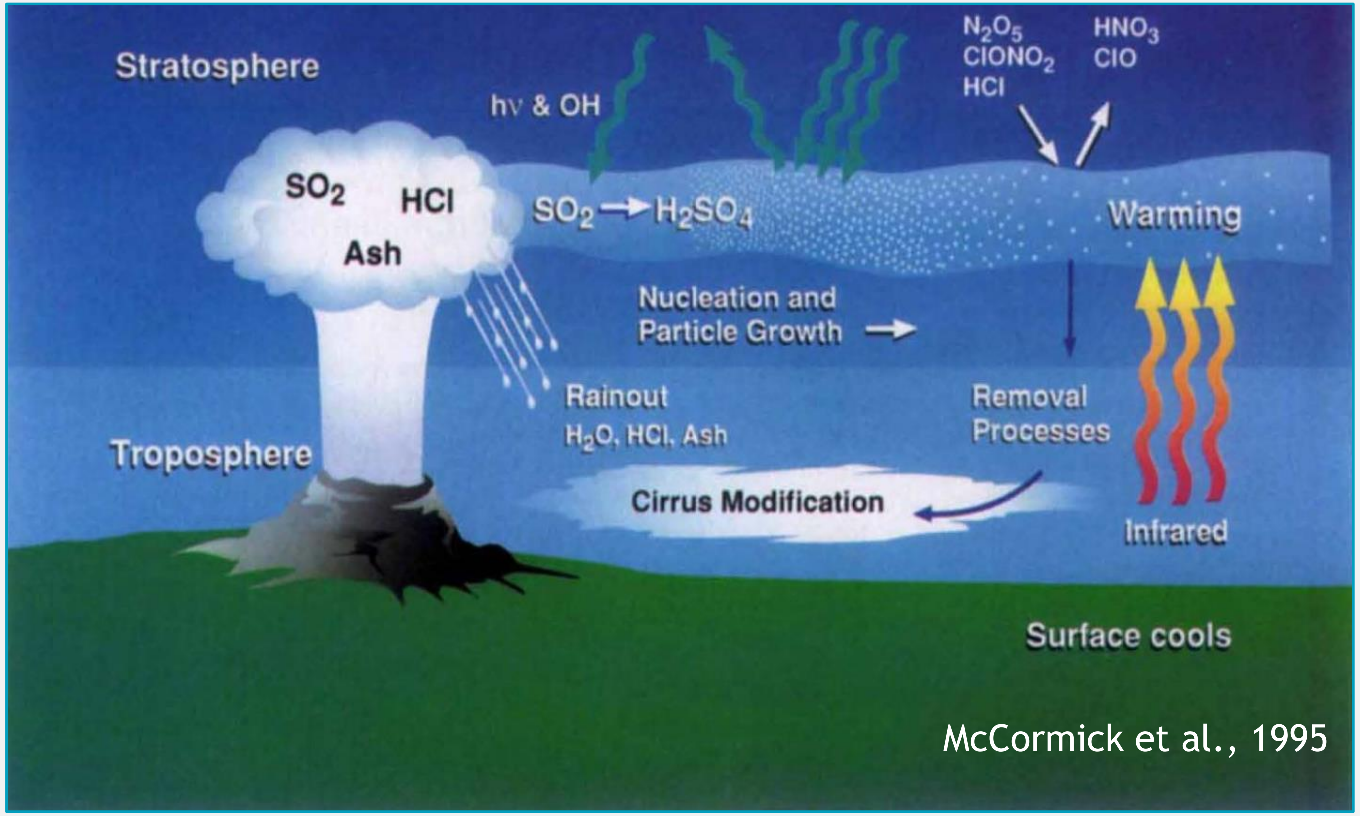
Large Eruption (June 12, 1991)

Main Eruption (June 15, 1991)

Mt. Pinatubo Eruption

Stratospheric Aerosol Injection (SAI)

Schematic of Immediate Effects post 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

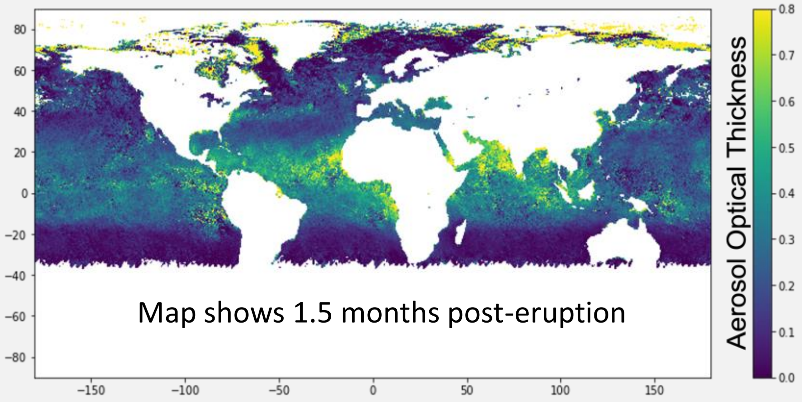
Net results:

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

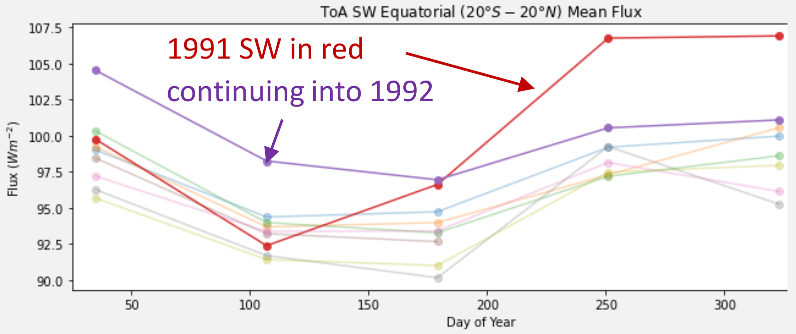
***Important nodes in pathway**: SAI → secondary aerosols (sulfate) → radiation effects → temperature*

Mt. Pinatubo Eruption
Temperature Impacts

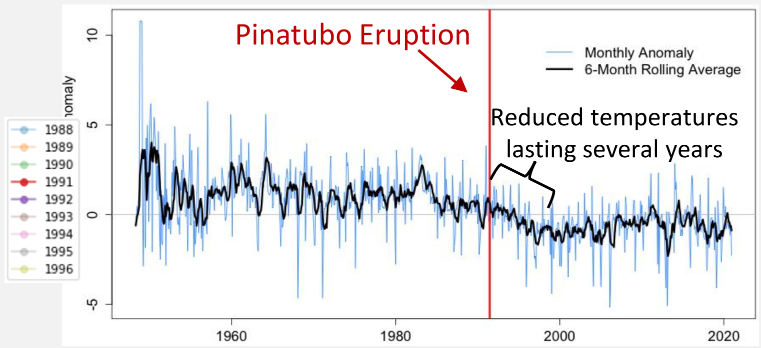
Emission/Aerosol Formation
Aerosol Optical Depth (AOD)*



Change in Radiation Flux
Net shortwave & longwave



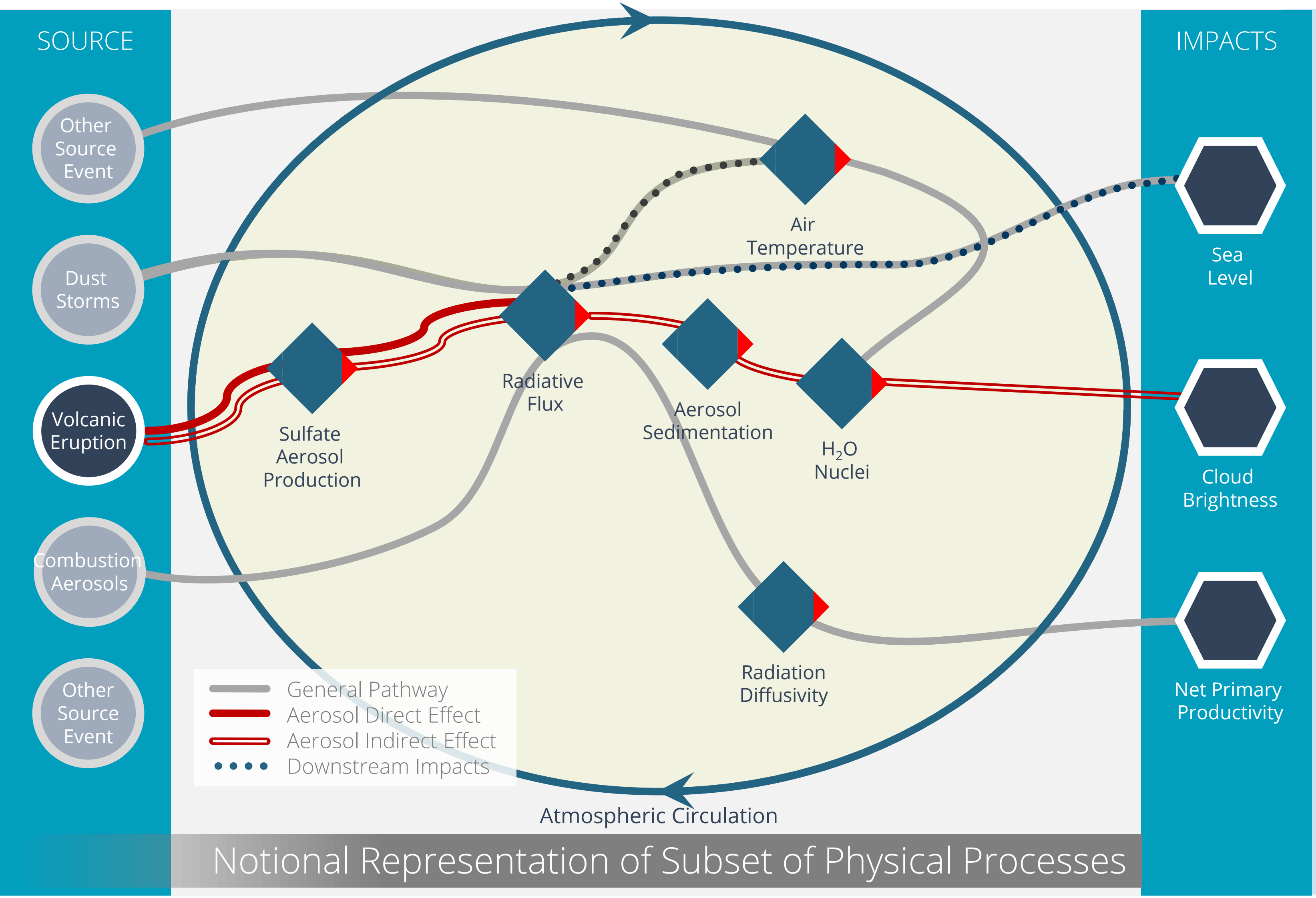
Temperature Change
2m and 50hPa



	Stratosphere	Troposphere	Northern Hemisphere (NH) Winter Warming
MECHANISM	• Absorption of terrestrial longwave (LW) and incident solar near-IR radiation by sulfate aerosols • Confounding factors: ozone changes	• Reduction in solar radiation at surface due to scattering by sulfate aerosols • Water vapor feedback [Soden et al., 2002] • Confounding factors: ENSO, LW radiation, aerosol indirect effects, climate dynamics	• Tropical stratospheric warming intensifies polar vortex and induces a strong positive phase in the NAO • Disputed: natural variability or forced by eruption
IMPACT	• Observed ~3°C warming at 50-hPa, [Angell 1997]	• Observed 0.4-0.6°C global mean cooling [McCormick et al., 1995]	• Warming in NH first winter after tropical eruption [Robock & Mao, 1992]

* Measure of extinction of solar beam by dust/haze (how much direct sunlight prevented from reaching ground by aerosols)

Mt. Pinatubo Eruption
Impact Space & Notional Representation of Pathways



Broader Impact Space

- 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

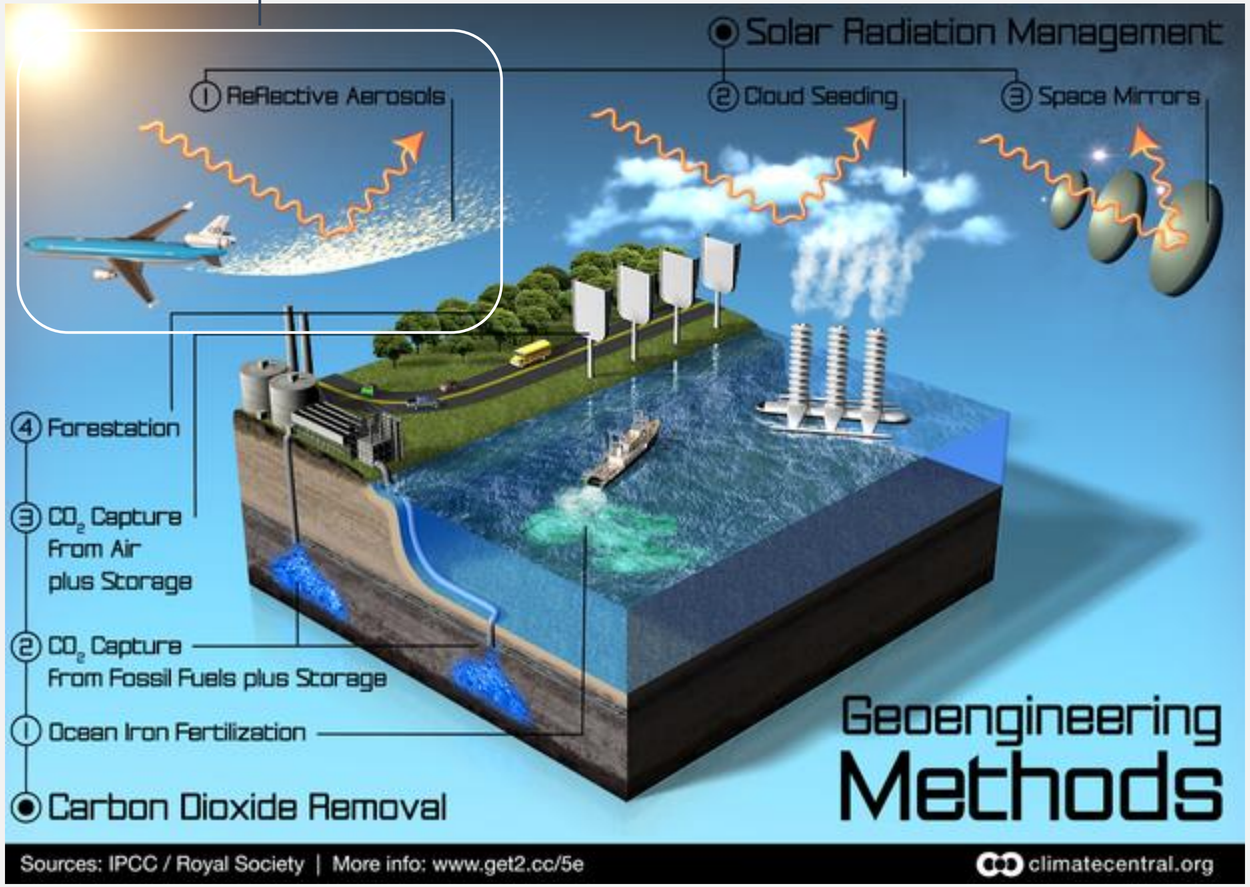
Mt. Pinatubo Eruption
Stratospheric Aerosol Injection (SAI)

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)

*While impacts of Mt. Pinatubo are well-characterized, **no publications** have demonstrated concrete pathways connecting >2 processes.*

SAI as climate intervention



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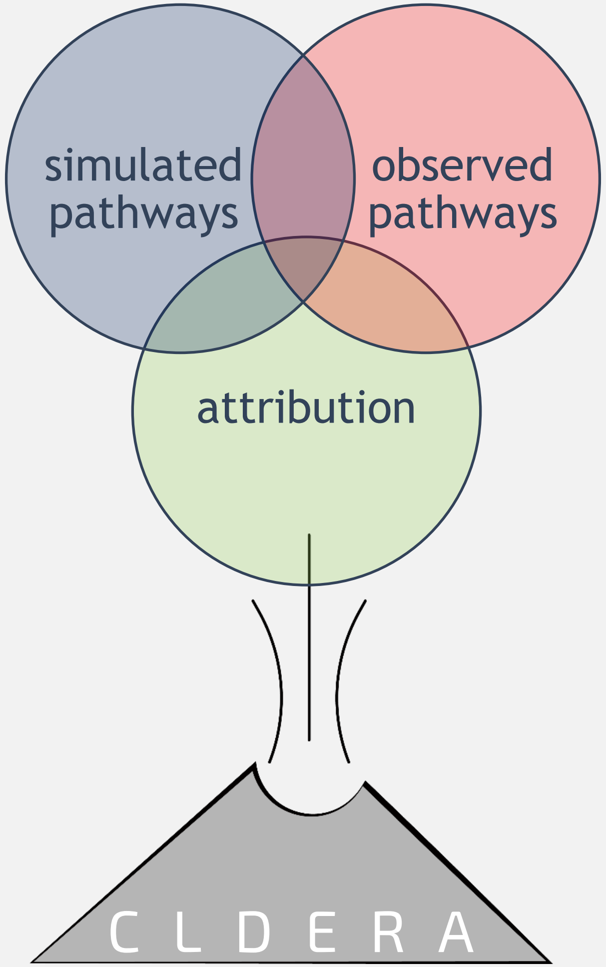
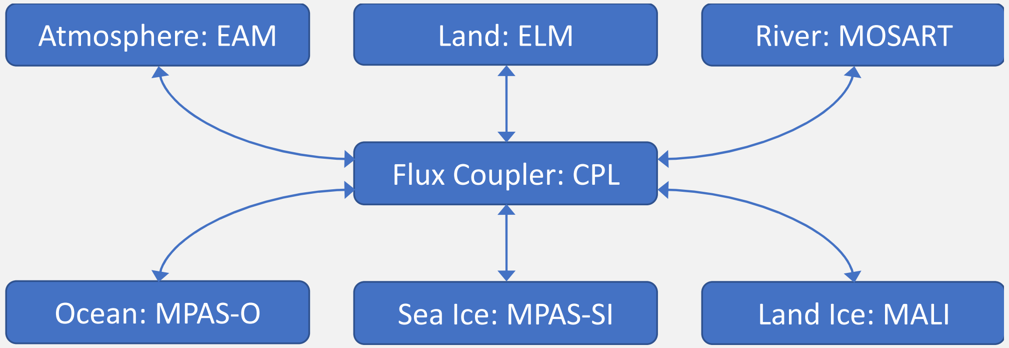


Energy Exascale Earth System Model (E3SM)

Earth System Models (ESMs) are the **primary testbed** for understanding future climate impacts.

- **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.
- Development driven by **DOE Office of Science mission interests**: energy/water issues looking out 40 years.
- CLDERA used E3SM version 2 (v2) obtained through **collaboration agreement** with the E3SM project to facilitate data and code sharing.



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

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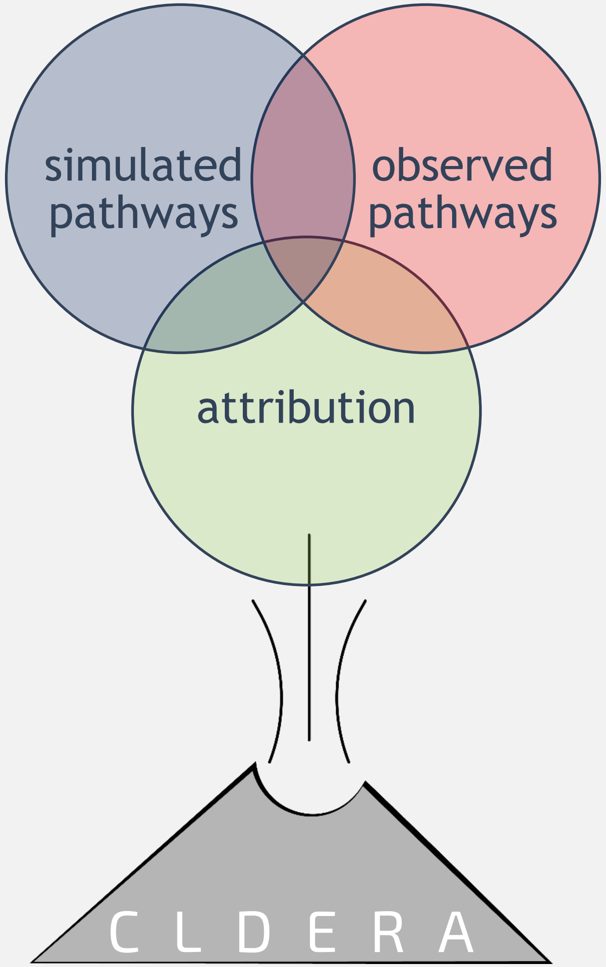
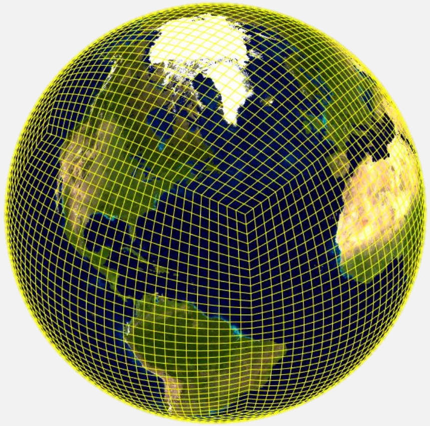


Simulating Mt. Pinatubo in E3SM

Simulation Lead Lead:
Kara Peterson
(Org. 1442)

Simulating the effects of **stratospheric aerosol injection (SAI)** is **challenging** for most climate models and is an active area of research.



E3SMv2 Capabilities:

- E3SM atmosphere model (EAM) includes stratosphere.
  - 72 vertical levels with 0.1hPa (64 km) model top.
  - Most runs will be with 1° resolution horizontal grid.
- E3SM also includes key process models for clouds, ozone and aerosols [Golaz, et al. 2019].
  - Turbulence closure: Cloud Layers Unified By Binormals (CLUBB) [Larson & Golaz 2005].
  - Cloud Microphysics: Morrison and Gettleman version 2 (MG2) [Gettleman, et al. 2015].
  - Linearized ozone photochemistry: Linoz v2 [Hsu & Prather 2009].
  - Aerosols: Modal Aerosol Model (MAM4) [Liu, et al. 2016].

Key Limitation:

- Before CLDERA, there were no prognostic volcanic aerosols in E3SM (radiative forcing due to aerosols from volcanic eruptions was prescribed).

Simulating Mt. Pinatubo in E3SM

- **Initial modifications** made to run E3SM with stratospheric SO_2 injection demonstrated that SO_2 evolves into H_2SO_4 but **aerosols sediment out too quickly**.
- **Improved implementation** of **prognostic volcanic aerosols** in E3SMv2 (MAM4)
  - ➢ **Changed aerosol coarse** and **accumulation mode properties** to match stratospheric size distributions
  - ➢ **Validated** against High resolution Infrared Radiation Sounder (HIRS) data and CESM/WACCM
- **Evaluating E3SM simulation capabilities**
  - ➢ Assess **Quasi-Biennial Oscillation (QBO)** and realism of E3SM's **stratospheric circulation**
  - ➢ Evaluate E3SM's **Brewer Dobson circulation** via age-of-air tracers and water vapor tape recorder

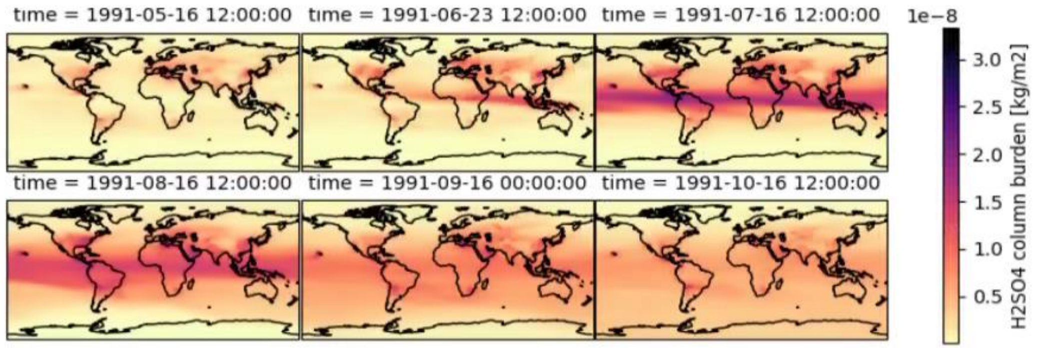
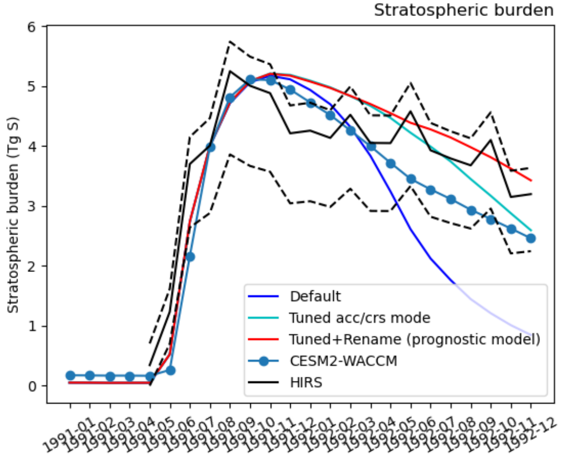
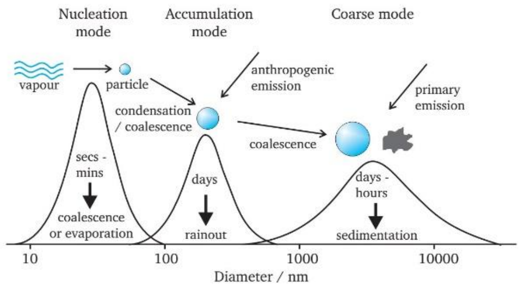
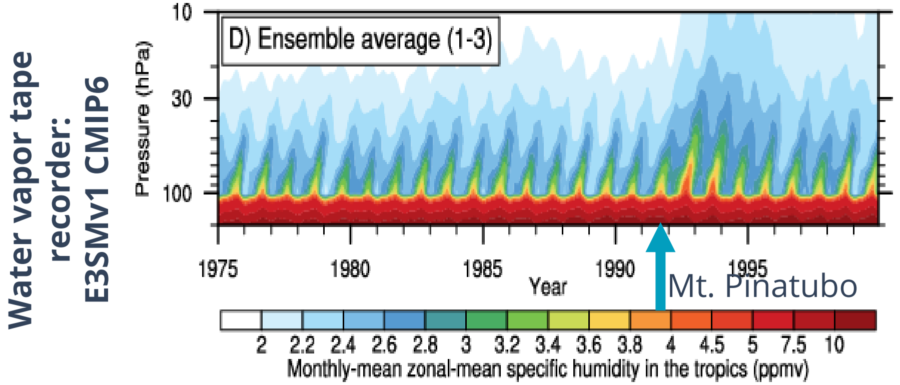


Fig. 5. H_2SO_4 mass per m² in the E3SMv2 experimental "SO_2" prognostic volcanic aerosol simulation.

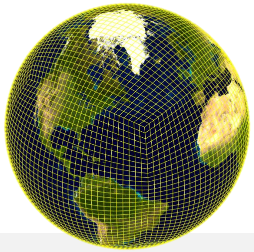






Team: B. Wagman, H. Brown, X. Liu [TAMU], A. Hu [TAMU], C. Jablonowski [U Michigan], J. Hollowed [U Michigan]

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) and Sandia HPC (Skybridge, Boca)
- 1° resolution E3SM can achieve:
  - 24 simulated years per day (SYPD) on 6 nodes of Skybridge
  - 10 SYPD per 285 nodes on Cori at NERSC
- May supplement 1° resolution with cheaper 7.5° resolution runs

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

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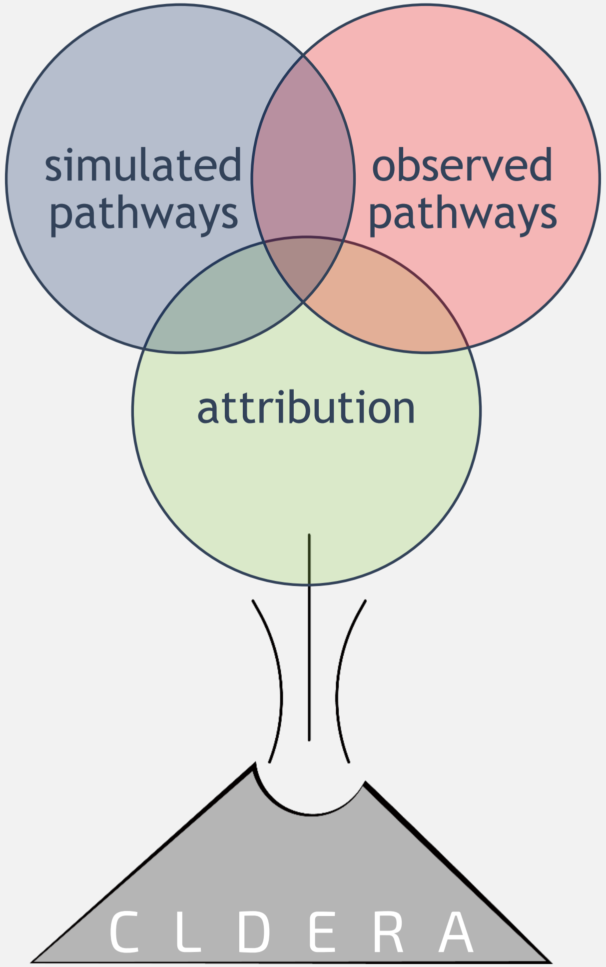


Simulated Pathways Thrust
Finding Impacts from a Source

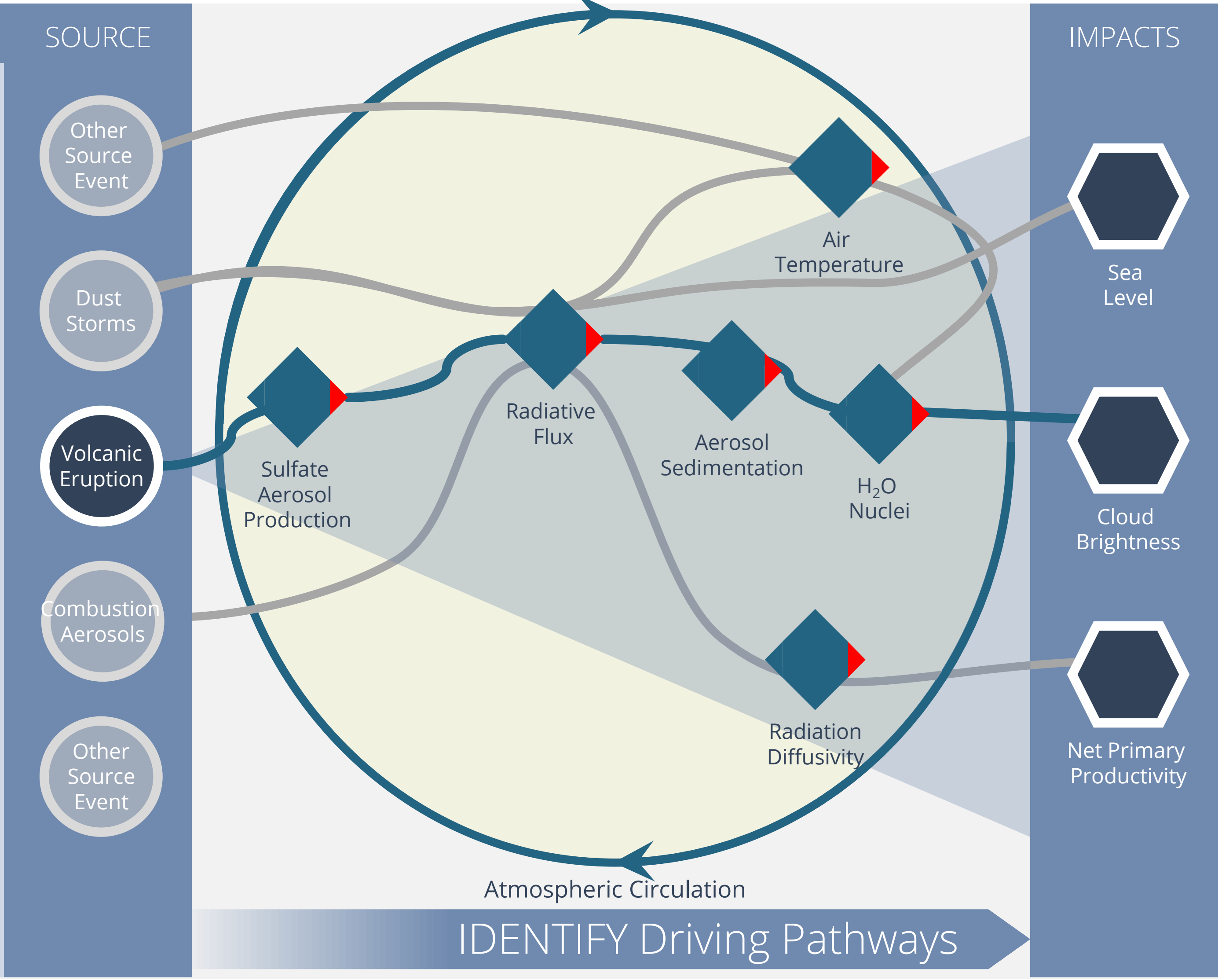
Thrust Lead:
Irina Tezaur
(Org. 8734)

Research Composition:

1. Statistical Approaches: use and extend **sensitivity analyses** and **Random Forest Regression** 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; additionally deploy **novel simulation strategies** to elucidate Mt. Pinatubo impacts on climate

3. Anomaly Detection: define pathways through extensions to existing anomaly detection algorithms in order to **spatio-temporally** trace **anomaly** progression

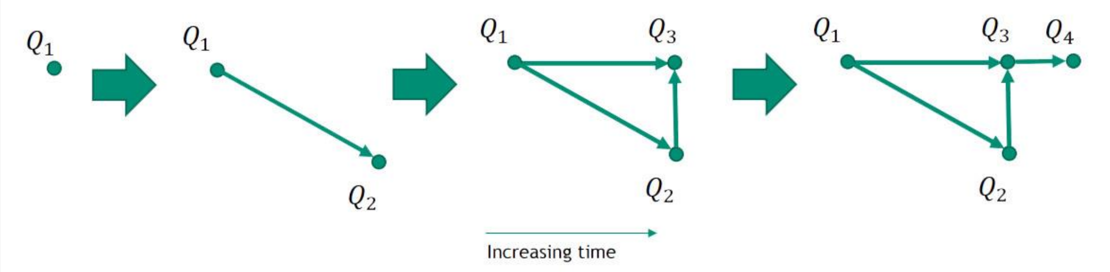


Simulated Pathways Thrust
What is a Simulated Pathway?

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

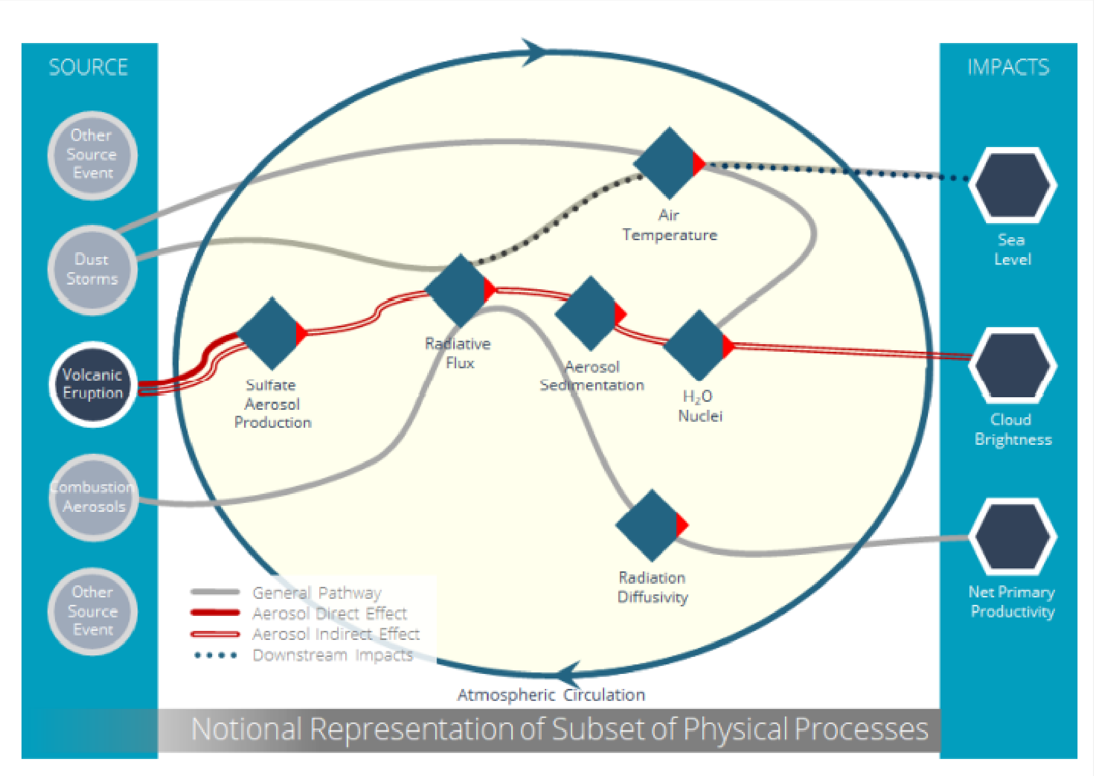
- *Example*: Mt. Pinatubo eruption → sulfate aerosol production → sedimentation → transport of aerosols into the troposphere → modification of cloud optical properties → increased cloud brightness/decreased rainfall.

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

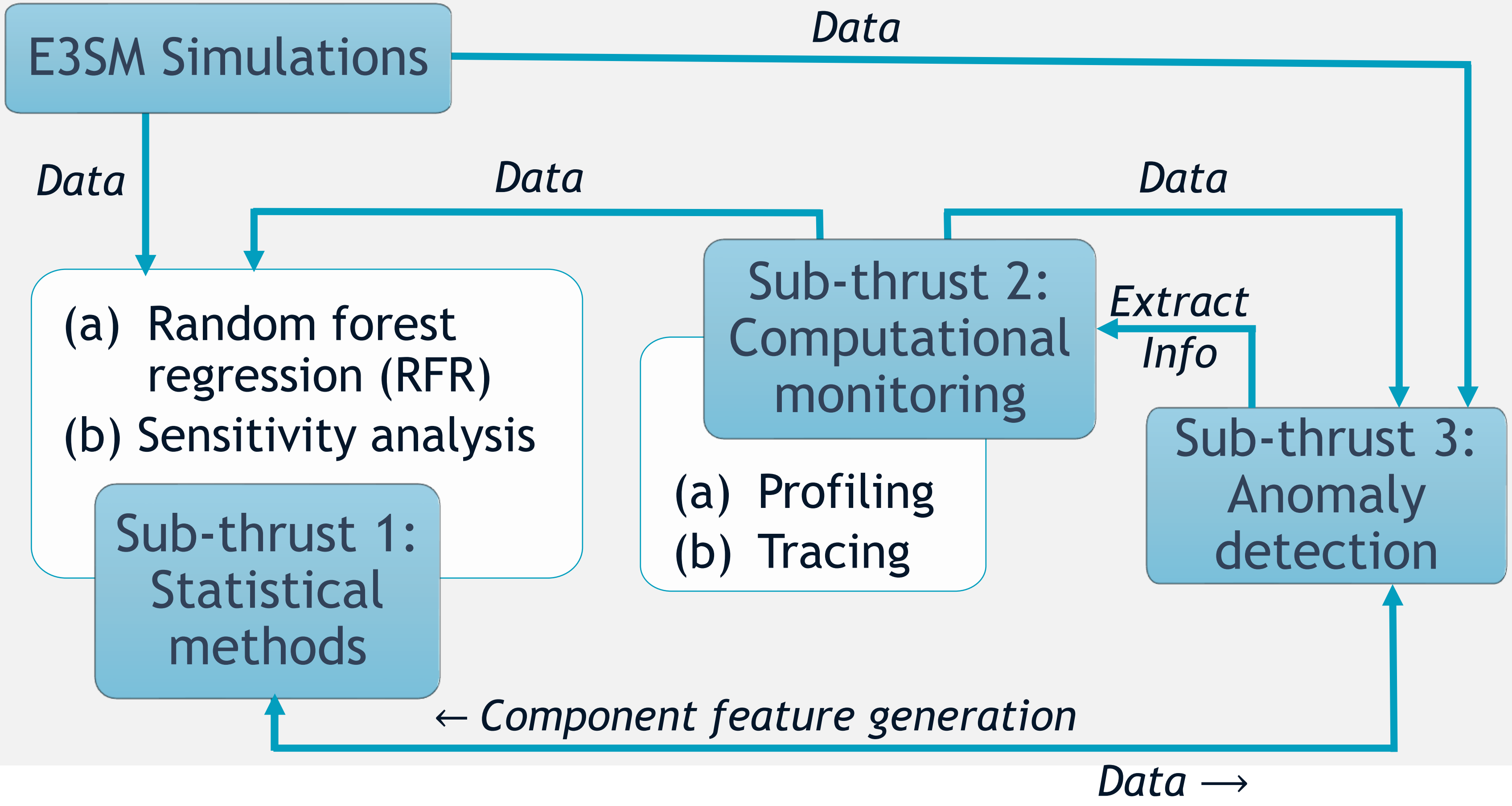
Edge from Q_i to Q_j ⇒ Q_j is impacted by Q_i at time t



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**.



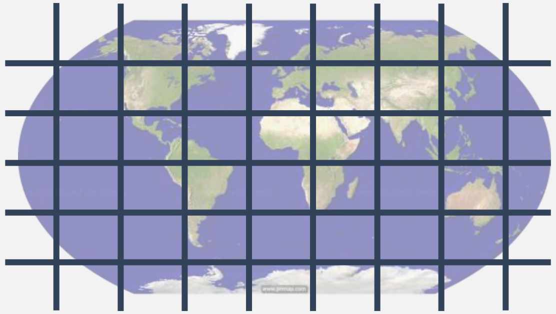
- Simulated pathways thrust will generate **simulation data** for CLDERA.
- Methods developed in one sub-thrust will **feed into** the others.
- Multiple sub-thrusts **minimize risk.**
- Identifying same pathway with different methods will provide **confidence**.

Simulated Pathways Thrust
Statistical Methods

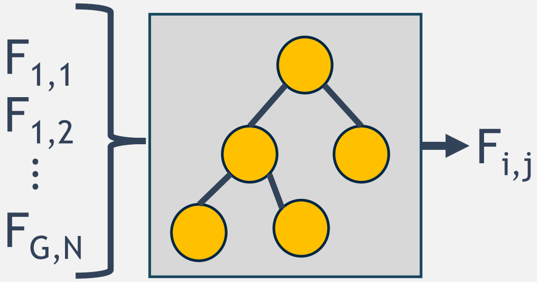
(a) Random forest regression (RFR):

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

Raw data



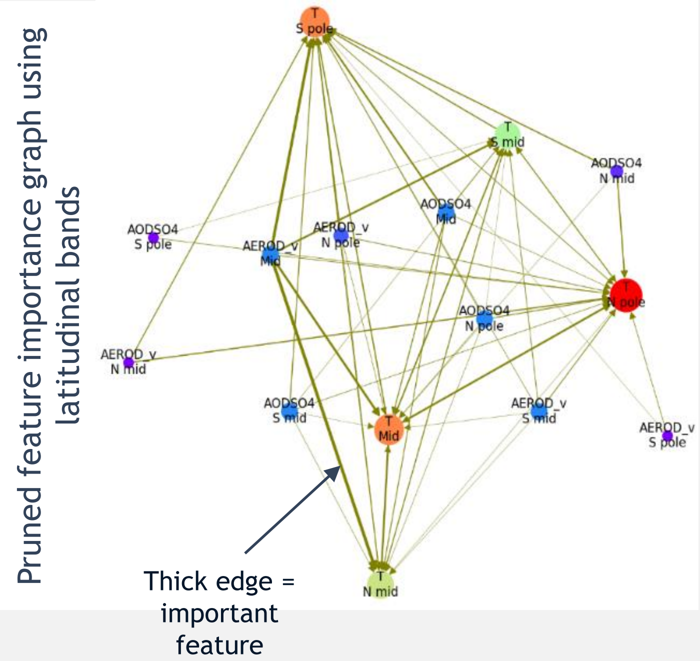
Train RF Regressors



Calculate Feature Importances

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

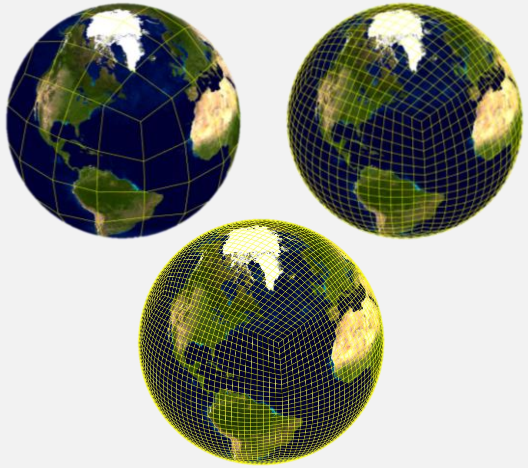
Team: M. Peterson, J. Nichol, W. Davis, I. Tezaur

Simulated Pathways Thrust

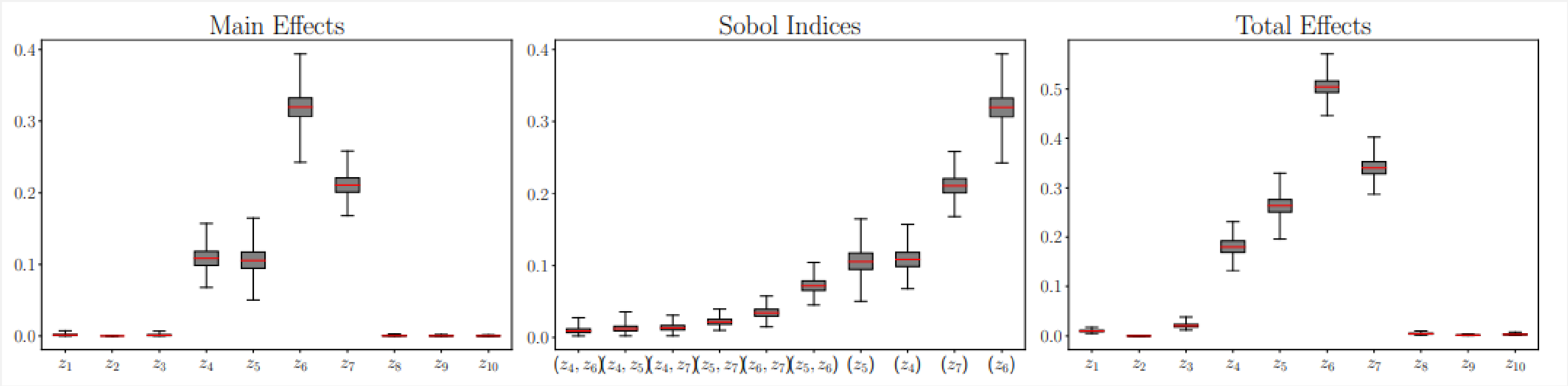
Statistical Methods

(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



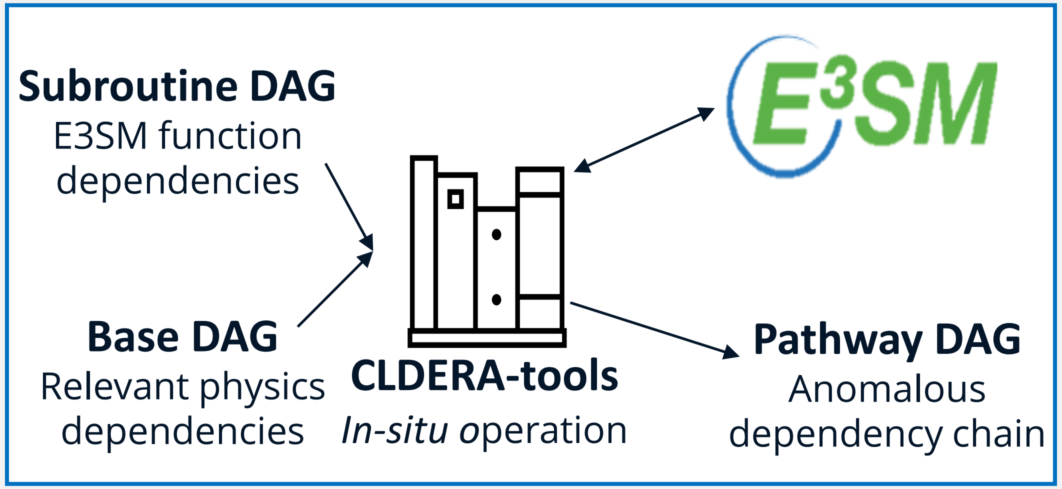
Right: global sensitivity analysis (GSA) results for surface temperature QOI using ULR E3SMv1 [Tezaur et al., 2022]

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

Simulated Pathways Thrust
Computational Monitoring

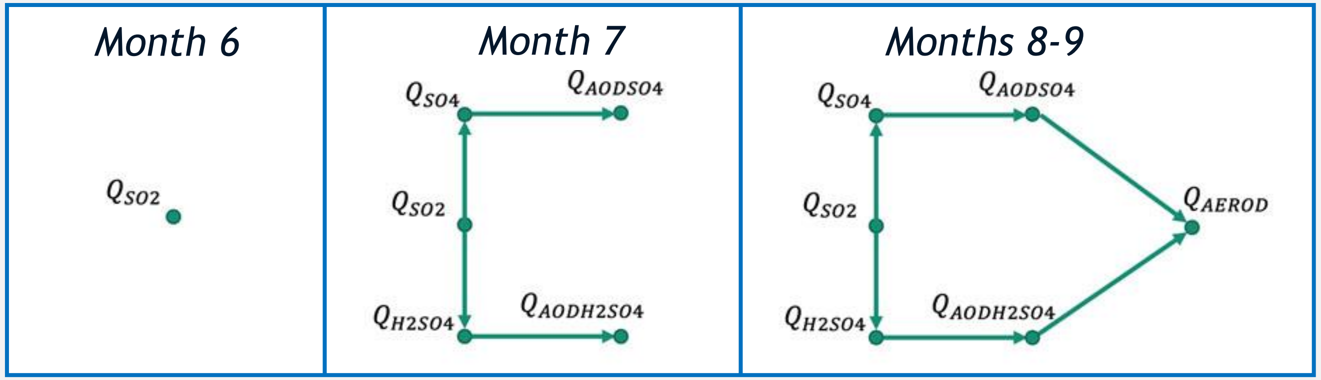
(a) Profiling: finding pathways *in-situ* while running E3SM

- **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)

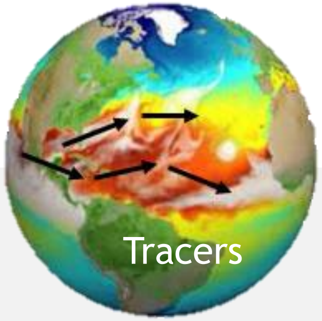
Outputs: Time-evolving pathway DAG



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

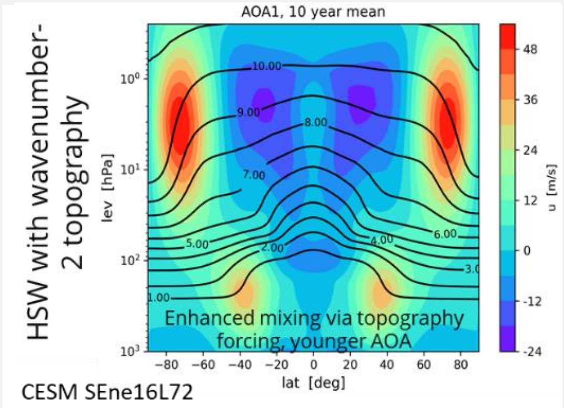
Simulated Pathways Thrust

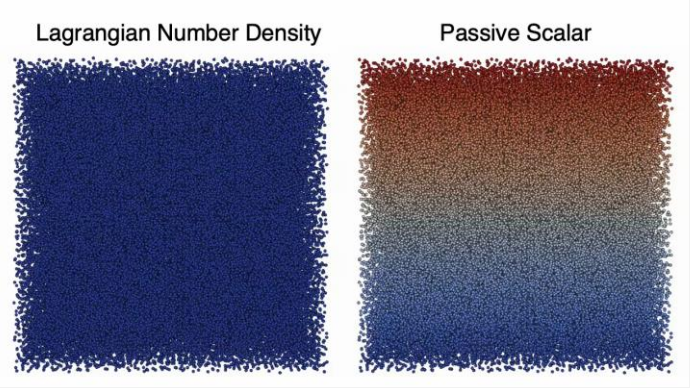
Computational Monitoring



(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.

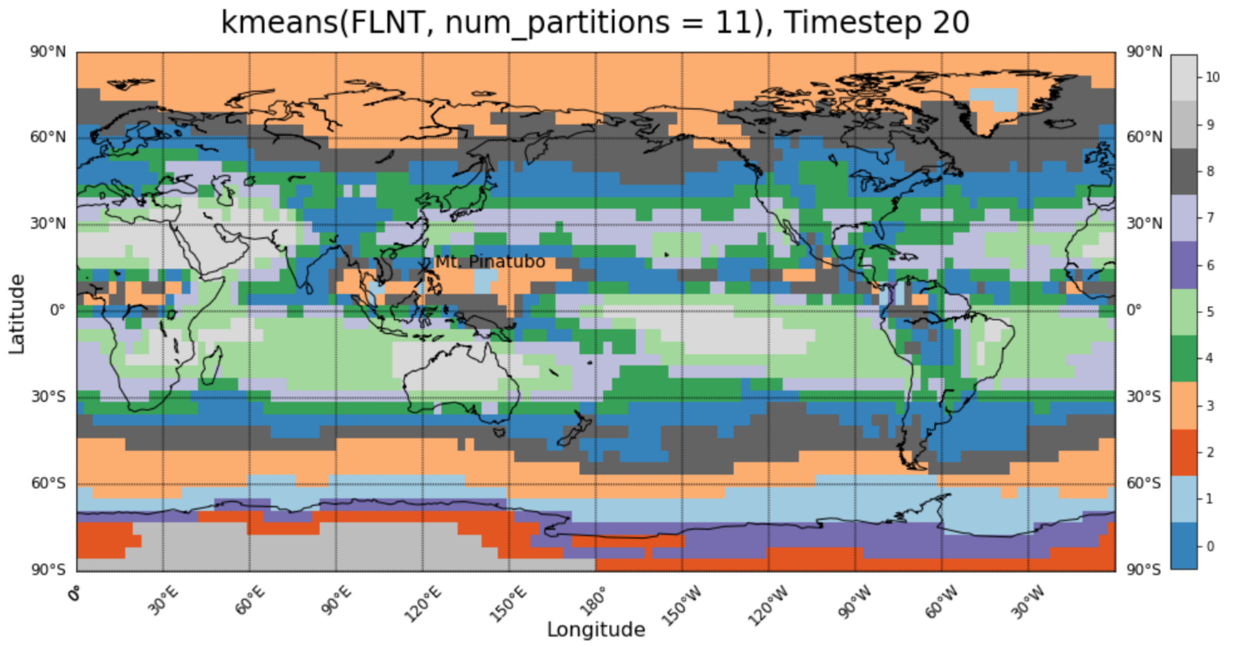


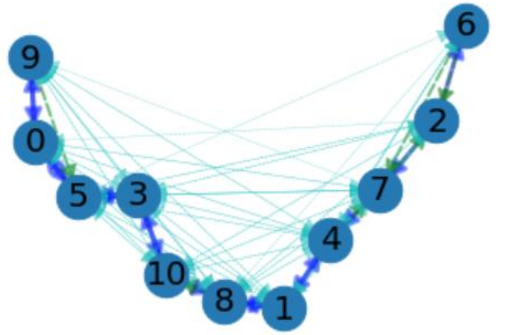


- **Active ("tagged") tracers:** feedback into atmosphere through physics processes
  - ➢ Enable tracking of **relative contributions** along nodes in pathway.

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**





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'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

Outline

- Motivation
- The CLDERA Grand Challenge LDRD Project
- Mt. Pinatubo & Stratospheric Aerosol Injection (SAI)
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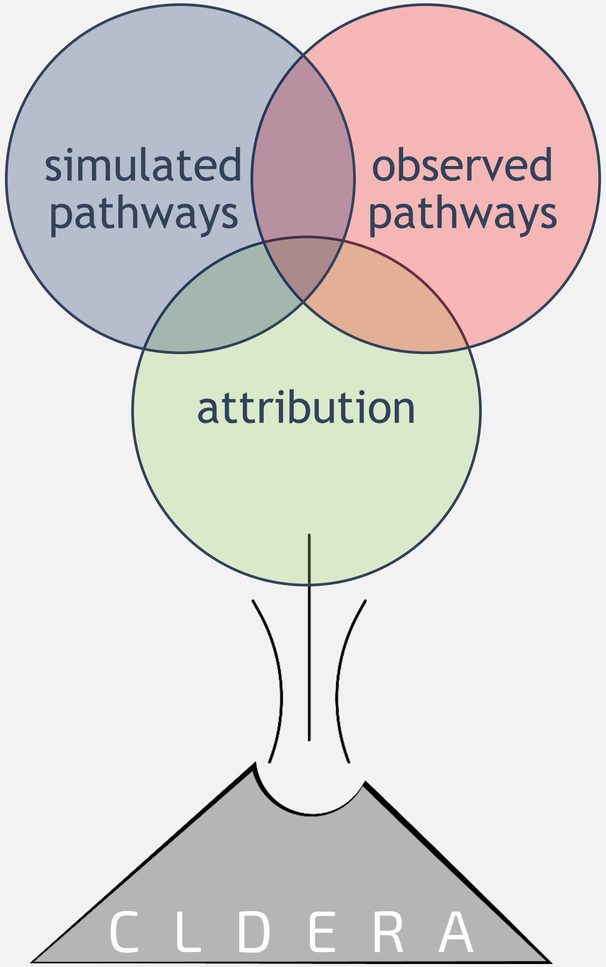
- Simulating Mt. Pinatubo using E3SM
- **The Three CLDERA Thrusts**
  - ➢ Simulated Pathways Thrust
  - ➢ **Observed Pathways Thrust**
  - ➢ Attribution Thrust
- Verification & Validation
- Some Early Simulation Results
- Summary



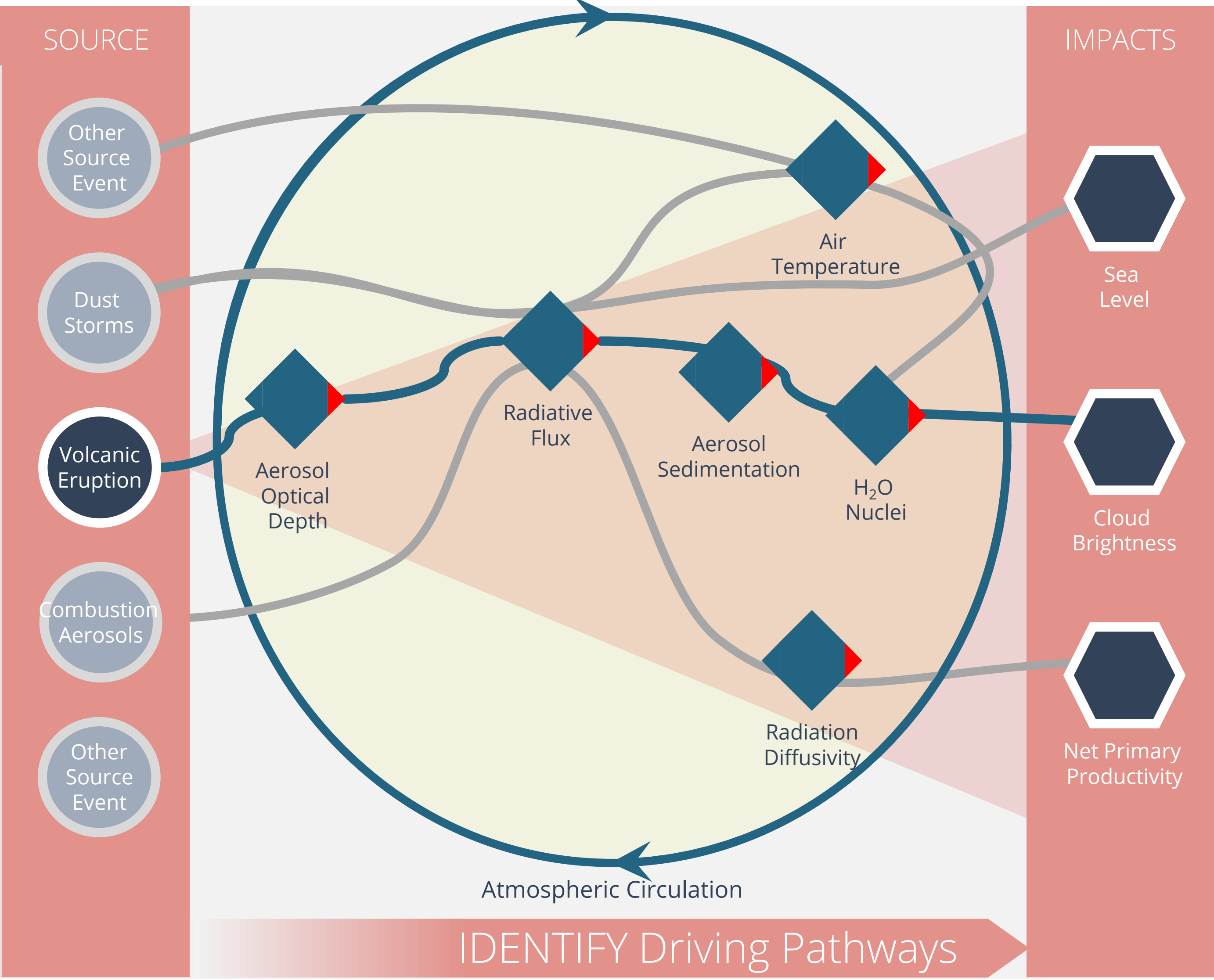
Observed Pathways Thrust

Finding Impacts from a Source

Thrust Lead:
Lyndsay Shand
(Org. 5573)

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. **Change Point:** identify the underlying fundamental shifts in climate processes
3. **Space-Time Statistical Methods:** adapt **Bayesian hierarchical approaches** to represent process dependencies and their dynamic spatio-temporal evolution over the first 3-4months post eruption
4. **Hybrid Statistical & Deep Learning (DL) Methods:** develop hierarchical statistical approaches **embed**ded with **DL** techniques to trace secondary and tertiary temporally-lagged effects



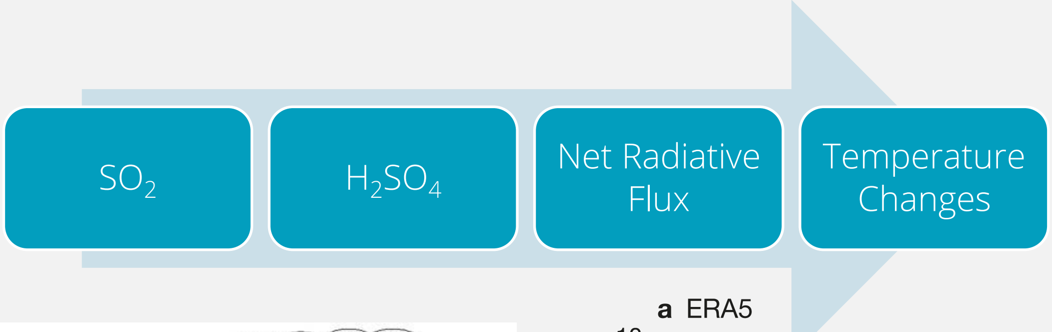
Observed Pathways Thrust

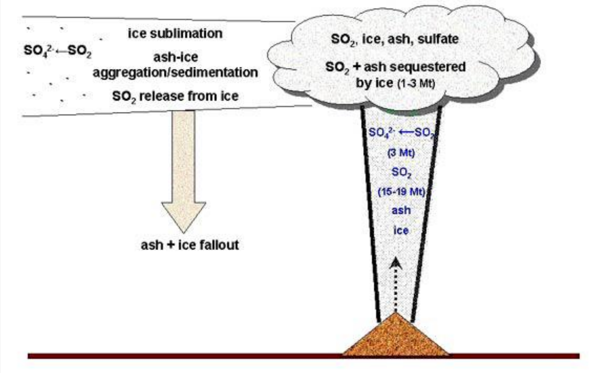
What is an Observed Pathway?

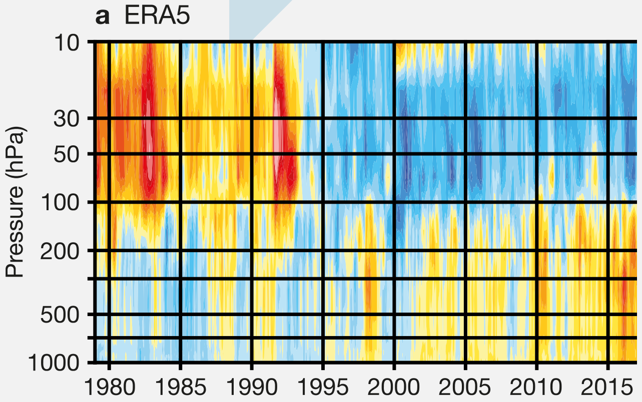
Definition: *observed pathways* are interpreted as **relationships** (or correlations) between **dependent climate processes** (*pathway nodes*).

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?

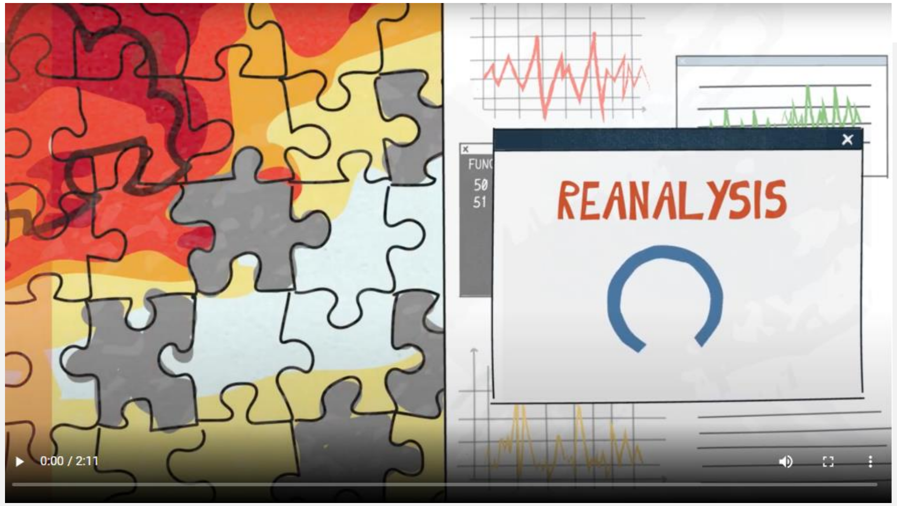
Observed Pathways Thrust

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

ECMWF

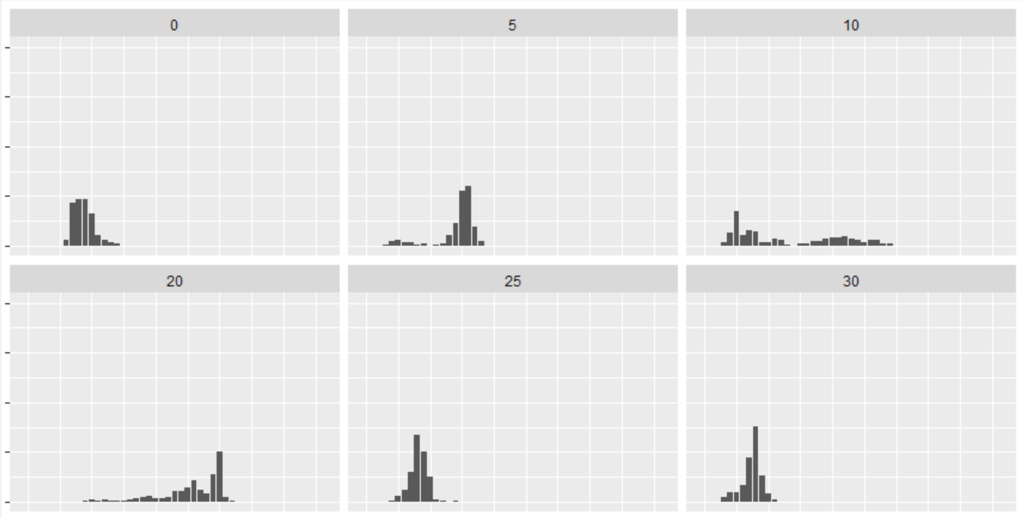
Observed Pathways Thrust

*Changepoint Detection**

* Significant persistent shift in underlying mean or variance of a process (not just an outlier)

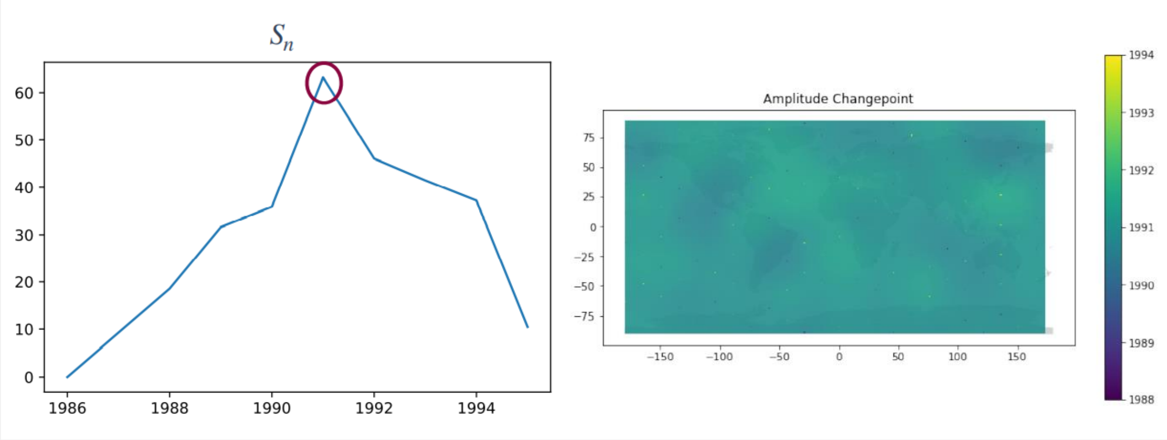
Goal: inform pathways by finding significant changes/shifts in climate processes, towards accounting for them in statistical models.

- **Space-time methods:** can detect when and where climate shifts have occurred w.r.t. source.



Posterior distribution of estimated spatially-varying changepoints for 6 different locations (using synthetic data)

- **Elastic Functional Warping Methods** [Tucker et al., 2019]**:** use diffeomorphisms/elastic distance to isolate amplitude and phase shifts not due to expected weather patterns.



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

Space-Time Statistical Methods

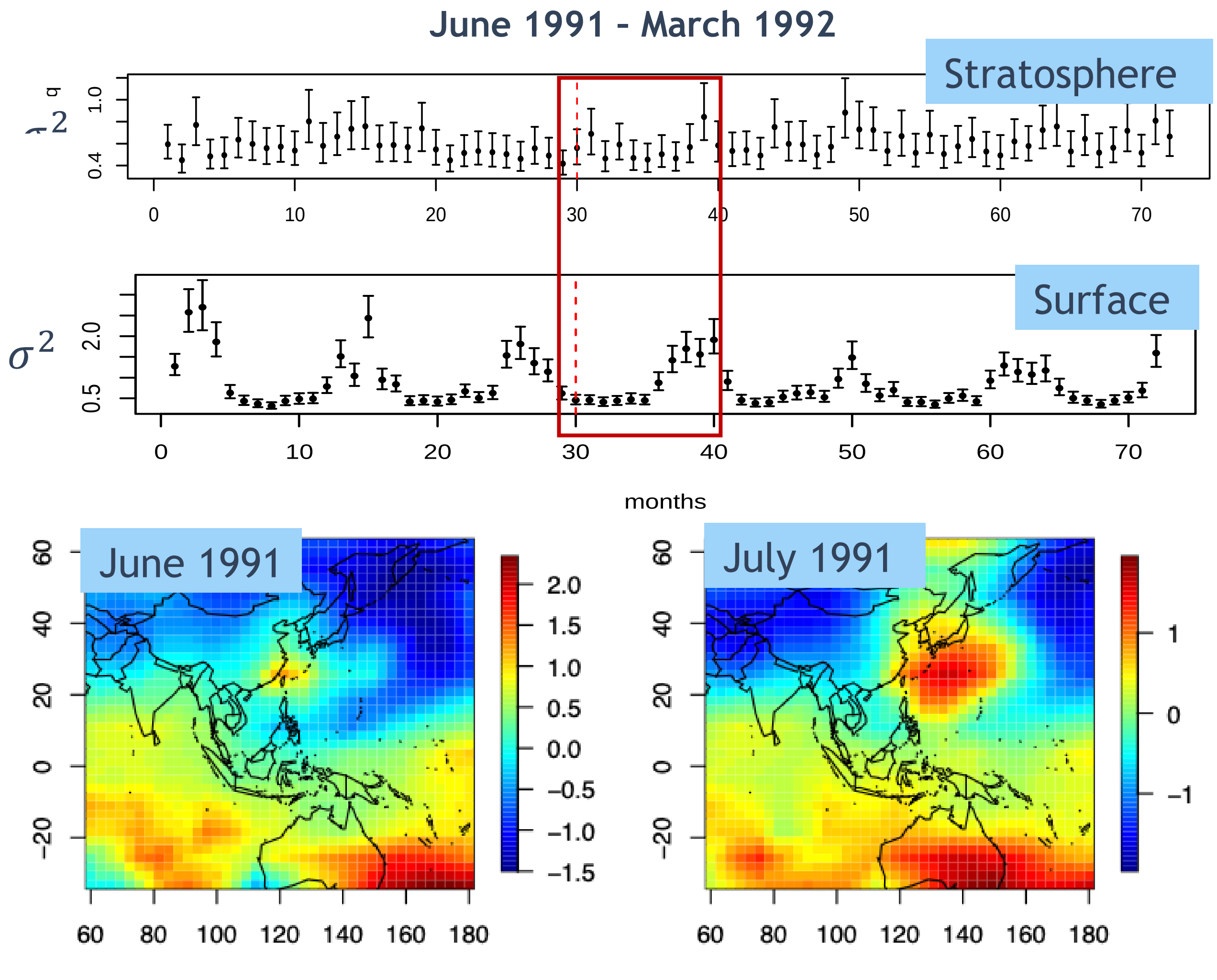
- **Goal:** quantify the spatio-temporal evolution of aerosols and climate impacts with interpretable approaches.
- **Dynamic spatio-temporal models:** intuitive and interpretable ways to represent complex, dependent physical processes that change across space and time simultaneously.

$$\mathbf{y}_t(\mathbf{s}) = \mathbf{X}_t(\mathbf{s})'\boldsymbol{\beta}_t + \mathbf{u}_t(\mathbf{s}) + \boldsymbol{\epsilon}_t(\mathbf{s}),\ \boldsymbol{\epsilon}_t(\mathbf{s}) \overset{iid}{\sim} N(0, D)$$

$$\boldsymbol{\beta}_t = \boldsymbol{\beta}_{t-1} + \boldsymbol{\eta}_t,\ \boldsymbol{\eta}_t \overset{iid}{\sim} N(0, \boldsymbol{\Sigma}_\eta),\ \boldsymbol{\beta}_0 \sim N(\mathbf{m}_0, \boldsymbol{\Sigma}_0)$$

$$\mathbf{u}_t(\mathbf{s}) = \mathbf{u}_{t-1}(\mathbf{s}) + \mathbf{w}_t(\mathbf{s}),\ \mathbf{w}_t(\mathbf{s}) \overset{ind}{\sim} NNGP(\mathbf{0}, \tilde{\mathbf{C}}(\cdot,\cdot\,|\,\boldsymbol{\theta}_t))\ .$$

- **New idea:** quantifying pathways via **multivariate** covariance matrix D
  - ➢ Allows modeling of relationships between variables while quantifying their dependencies



Time-varying variance parameter estimates with red line representing time of event (top) and estimated spatial dynamic components (bottom) of the dynamic model applied to stratospheric temps.

Observed Pathways Thrust
Hybrid Statistical and Deep Learning (DL) Methods

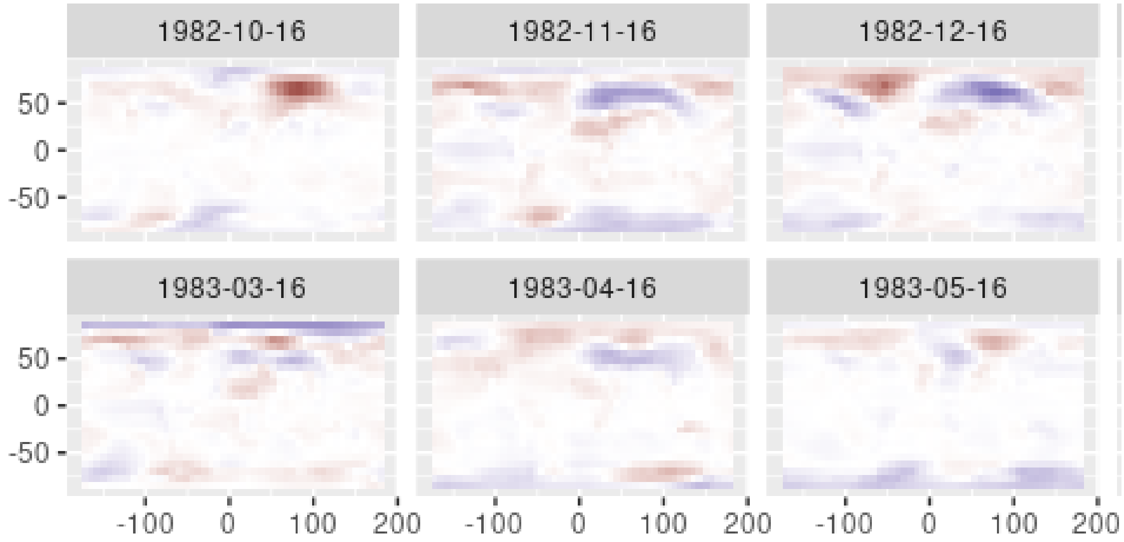
Goals:
- Understand trends in observation data using interpretable/explainable methods
- Test if data supports postulated pathways

Echo-State Networks (ESNs)
- Use reservoir computing to efficiently estimate recurrent neural networks (RNNs), which can capture short-term/long-term spatio-temporal dependence

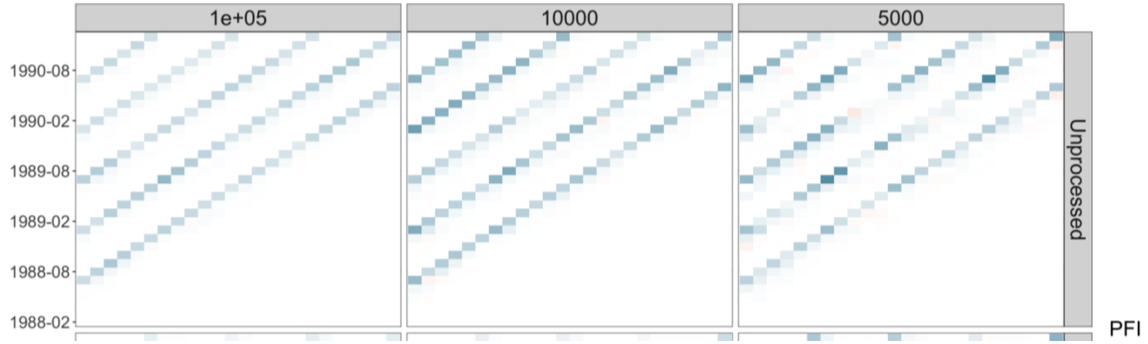
Data stage	$Z_t \approx \Phi\alpha_t + \delta_t(s)$, $\delta_t(s) =$ spatio-temporal residual	
Output stage	$\alpha_t = V_1 h_t + V_2 h_t^2 + \eta_t,\ \eta_t \sim N(0, \sigma_\eta^2 I)$	RNN
Hidden stage	$h_t = g_h\left(\frac{v}{\lvert\lambda_W\rvert} W h_{t-1} + U\tilde{x}_t\right)$	

Permutation Feature Importance (PFI)
- Determines which variables at which times are important for forecasting.
- Novel method to increase explainability of ESNs.

Quadratic ESN Residuals: need for increased spatial fidelity to correctly account for high latitude temperatures



PFI: identifying how ESNs make use of historical temperatures by investigating influence of lagged temperature on forecast temperatures



Team: K. Goode, B. Hillman, G. Huerta, J. Li, L. Shand

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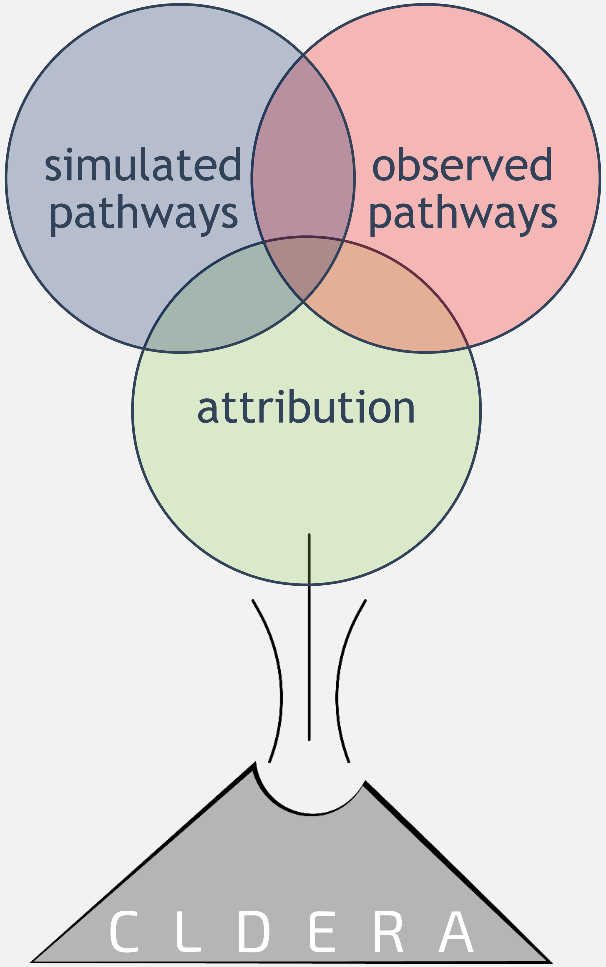


Attribution

Finding Predominant Source Driving Impact

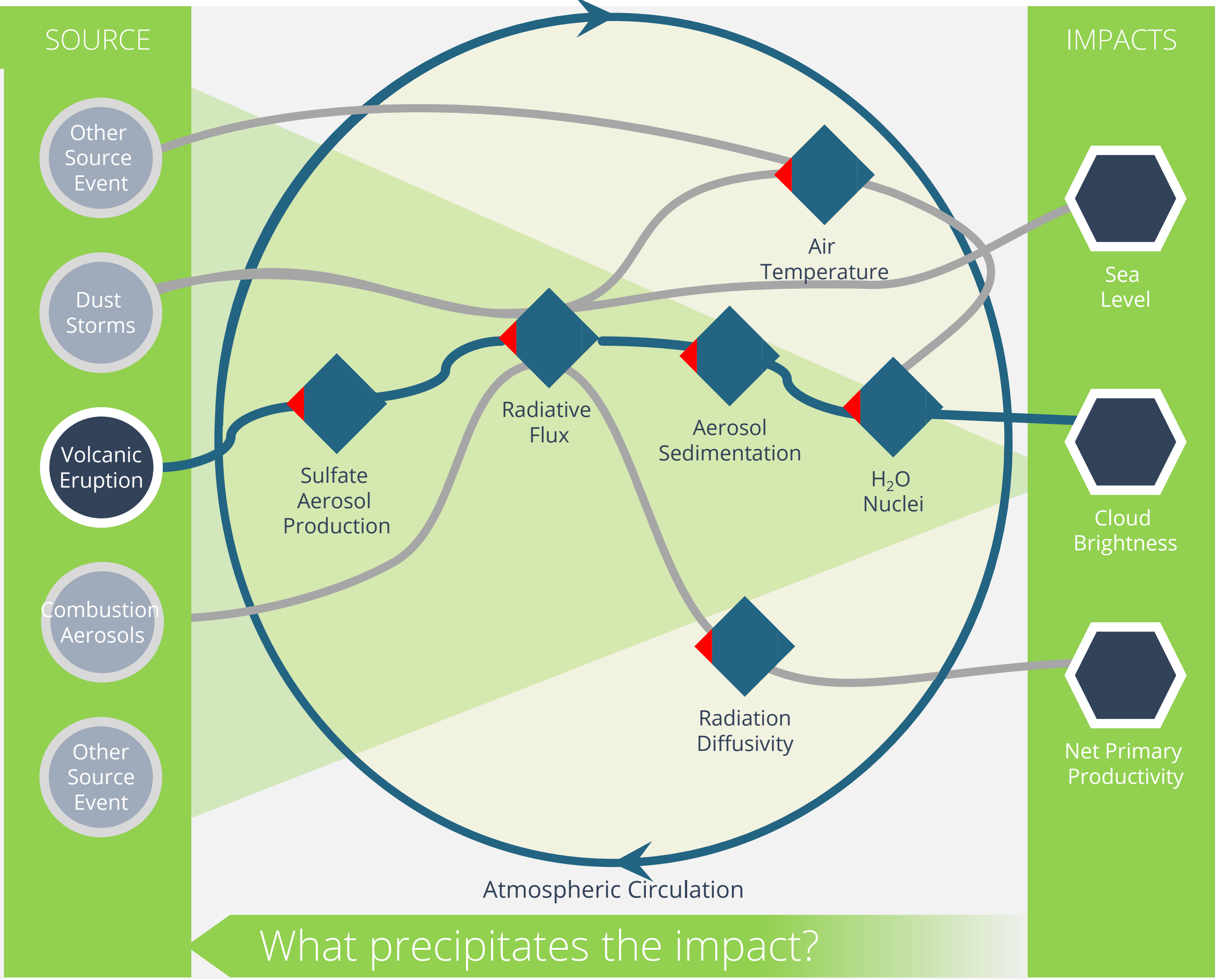
Thrust Lead:
Laura Swiler
(Org. 1400)

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. **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

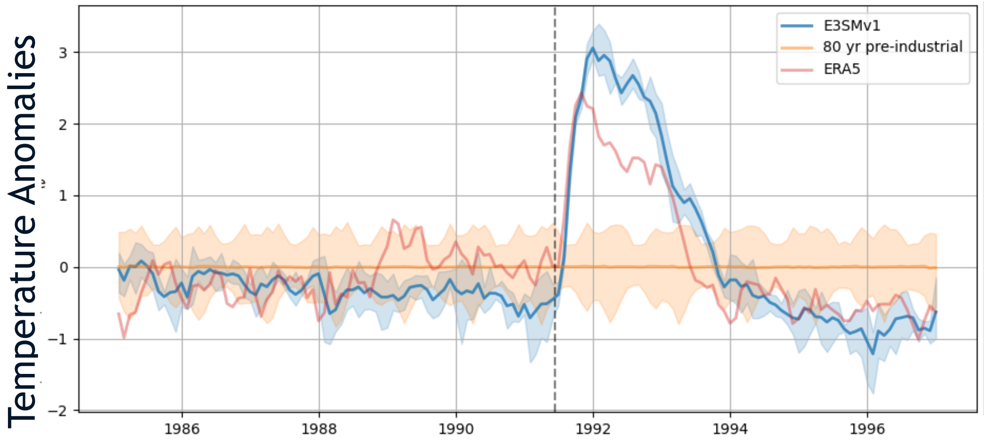
3. **Causal Modeling:** ID causal relationships and dominant pathways by developing **causal networks** through iterative independence tests and the resulting directed acyclic graphs



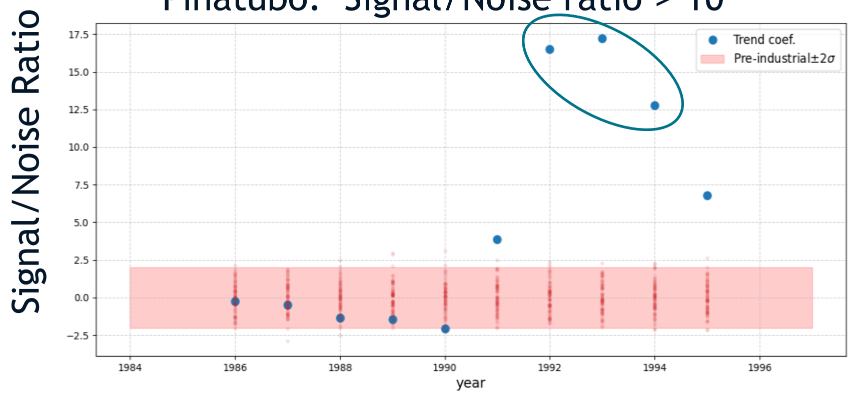
Attribution
Enhanced Fingerprinting

- **“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/Noise ratio).
- **Enhanced Fingerprinting Approach:**
  - ➢ **Multivariate** fingerprints
  - ➢ Use **multiple variables** along a **pathway** in the fingerprint
  - ➢ Use pathway info to refine fingerprints for use within a **short-term SAI event** with a more **regional impact** (fingerprints typically used over long-time period data to detect changes decadal means).

Traditional Fingerprint – Detection of Pinatubo



Attribution of Temperature Anomaly to Pinatubo. Signal/Noise ratio > 10



Leverages [Wagman et al. 2021]

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

Attribution
Inverse Optimization

- **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:

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

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

Approximated by DONNs

- **Core idea:** develop **deep operator neural networks (DONNs)** to model parts of E3SM to enable PDE-constrained optimization without intrusion into the E3SM code directly.
- Add **pathway information** as penalty terms in the objective and/or additional constraints.

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

(test case for initial prototyping)

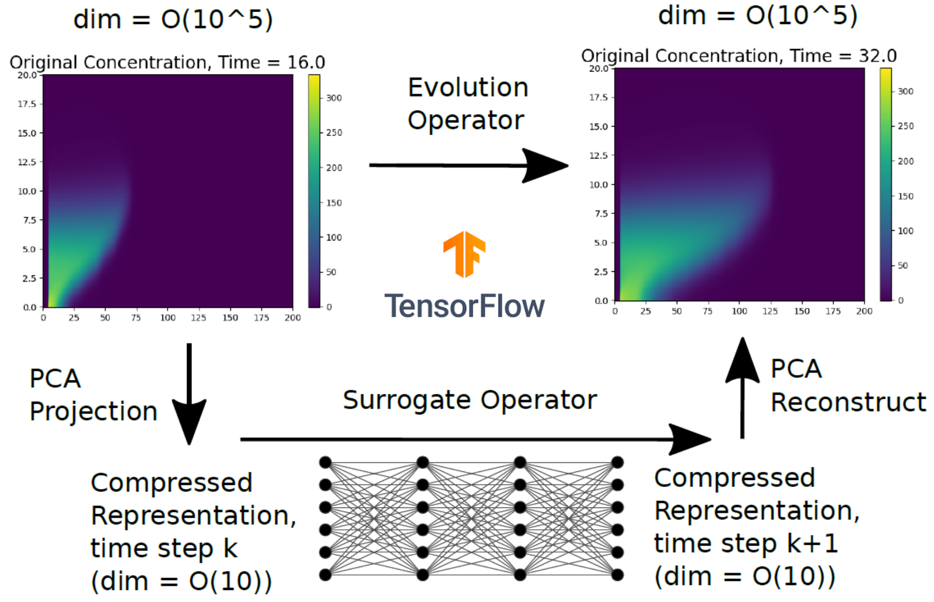
$$\min_{\theta} J(\theta) = \sum_{i=1}^{n}\sum_{j=1}^{m} [c_{\text{obs}}(x_j,t_i) - c_{\text{sim}}(x_j,t_i,\theta)]^2 + R(\theta)$$

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

$$\nabla c \cdot \boldsymbol{n} = 0 \quad \text{on } \partial\Omega \times [0,T]$$

$$c = 0 \quad \text{on } \Omega \times \{0\}$$

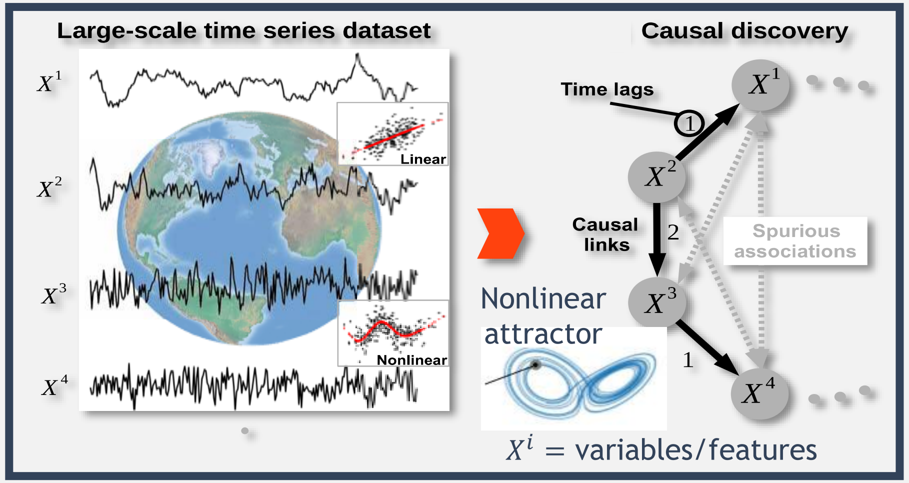
RAPID OPTIMIZATION LIBRARY



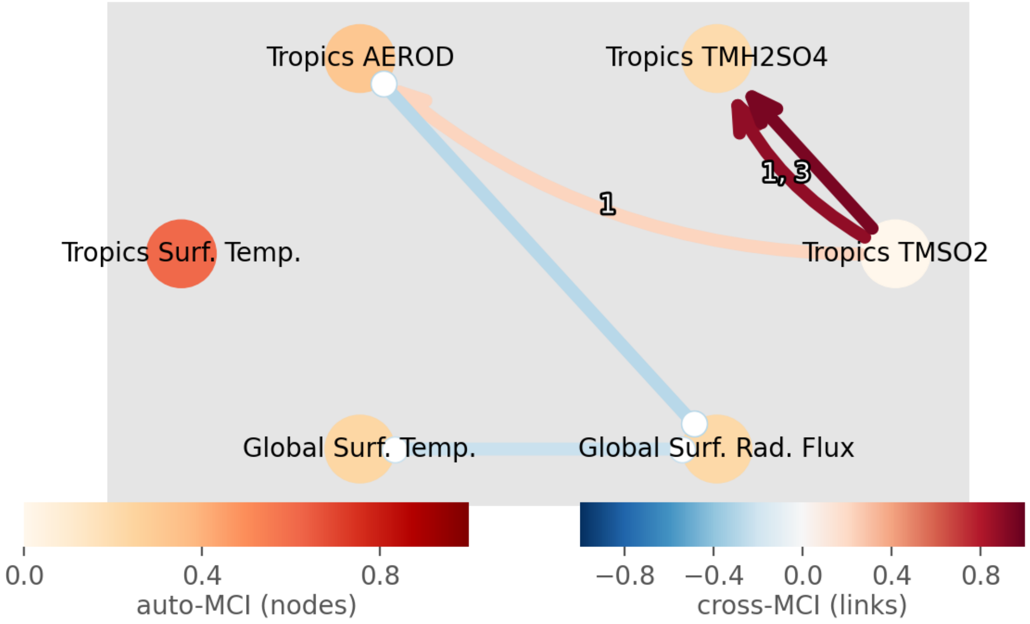
Team: J. Hart, M. Gulian, I. Manickam, L. Swiler

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.**



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

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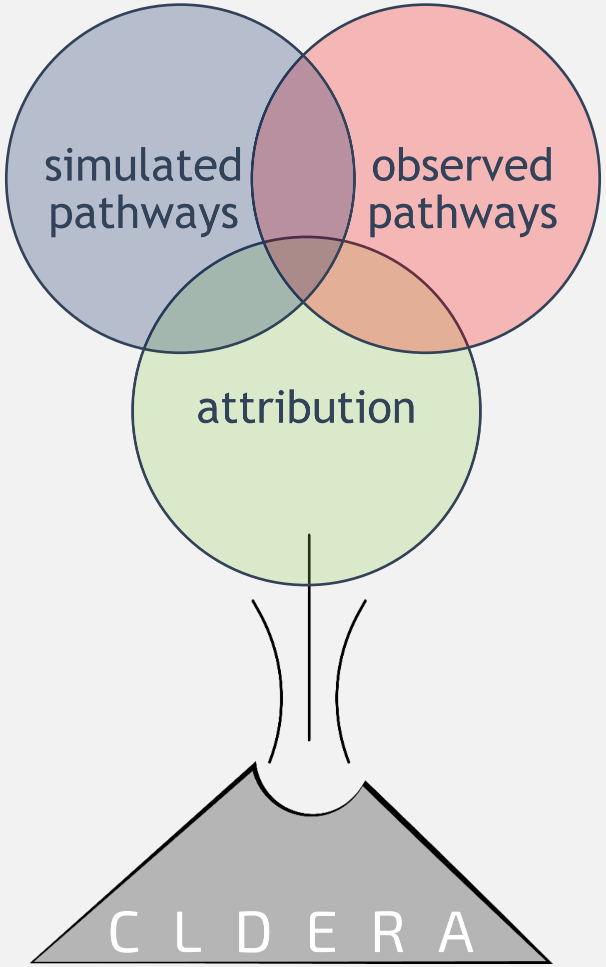
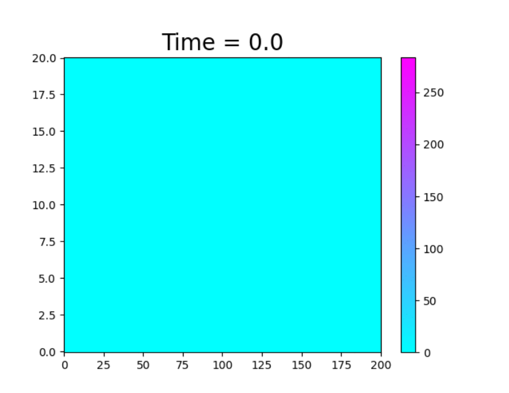
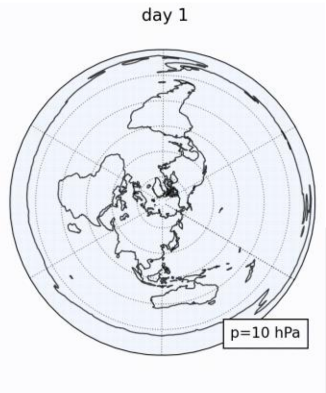
- The Three CLDERA Thrusts
    - ➢ Simulated Pathways Thrust
    - ➢ Observed Pathways Thrust
    - ➢ Attribution Thrust
- **Verification & Validation**
- Some Early Simulation Results
- Summary



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

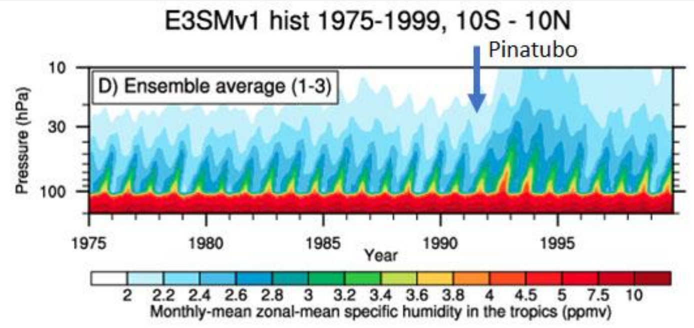
Full complexity of Earth's climate – verify method solution against known pathways

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

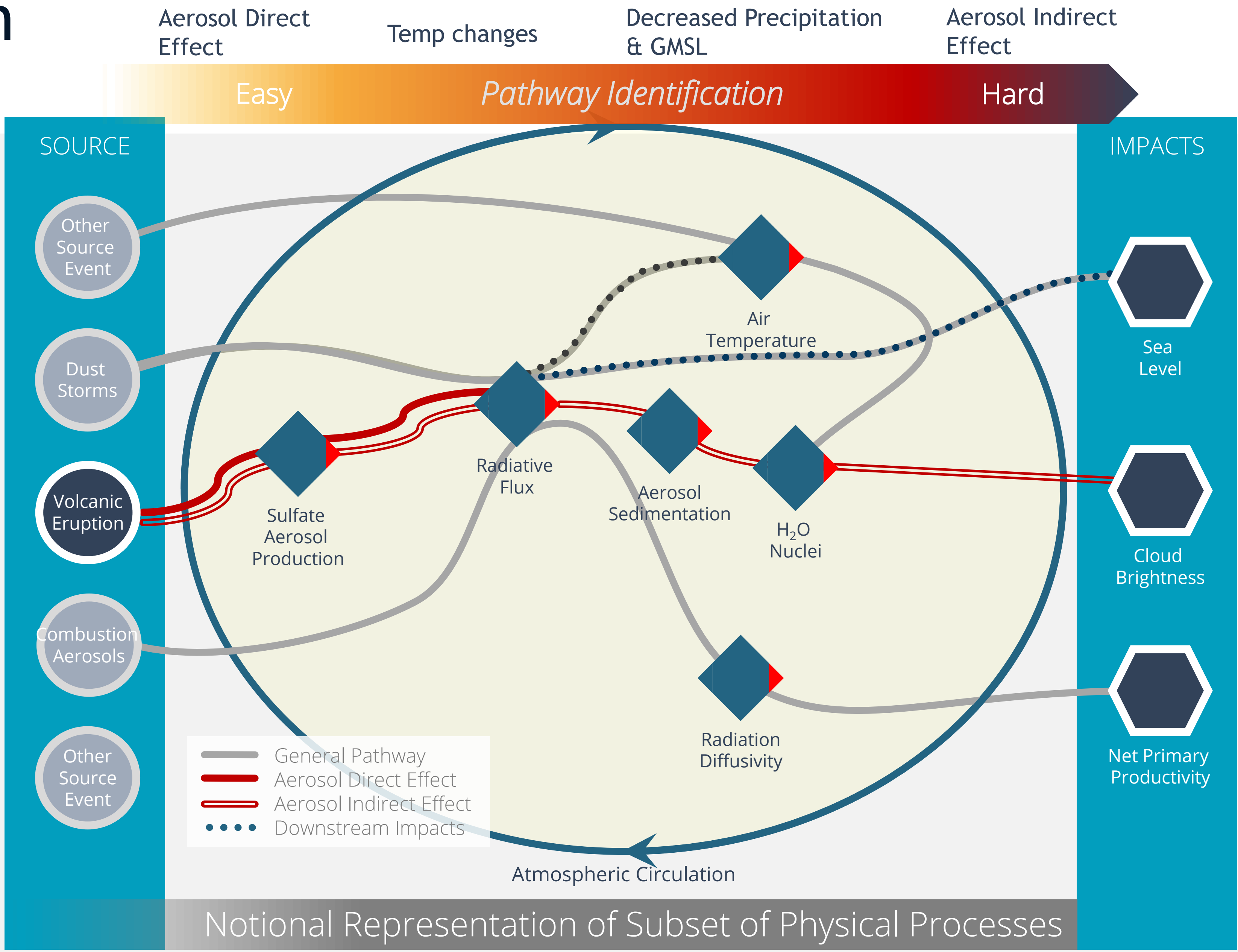
Mt. Pinatubo Validation

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)



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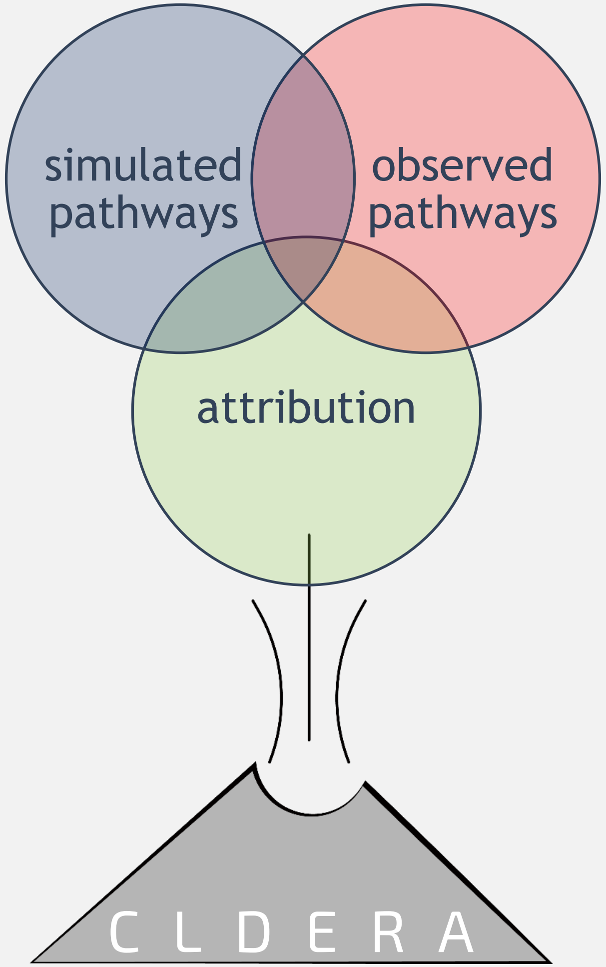
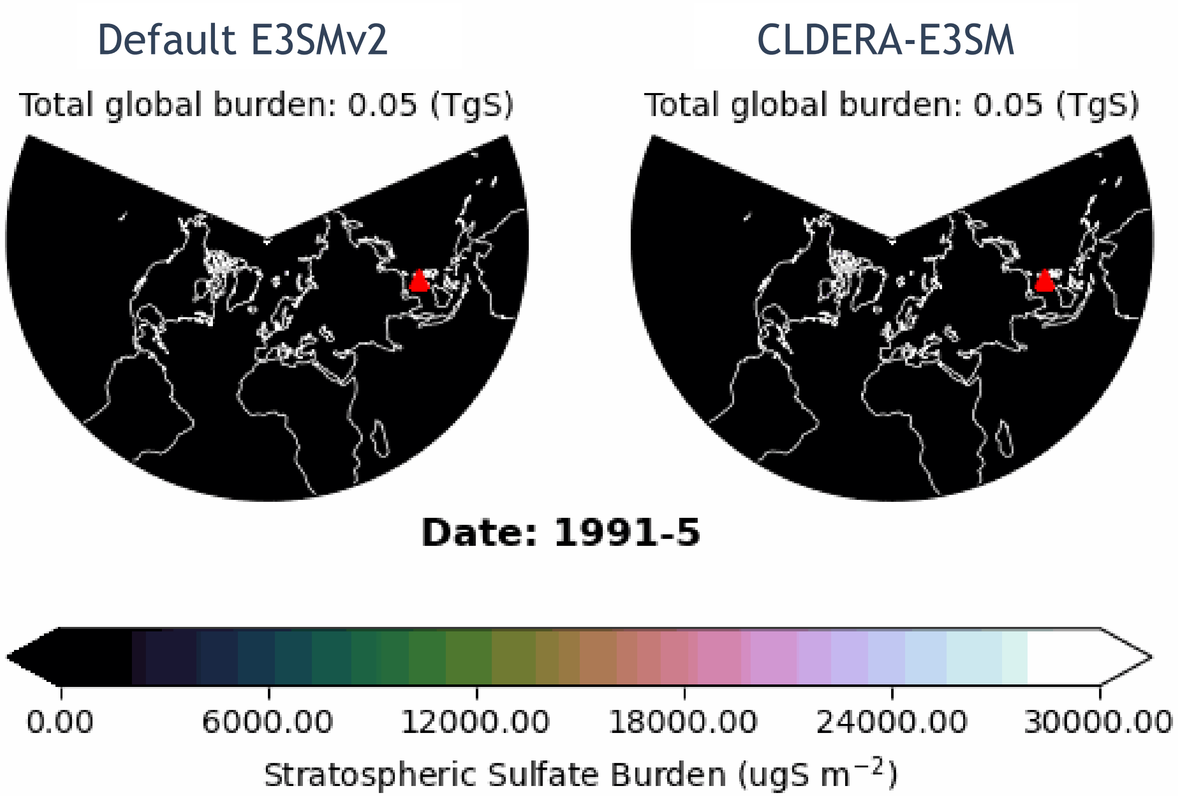
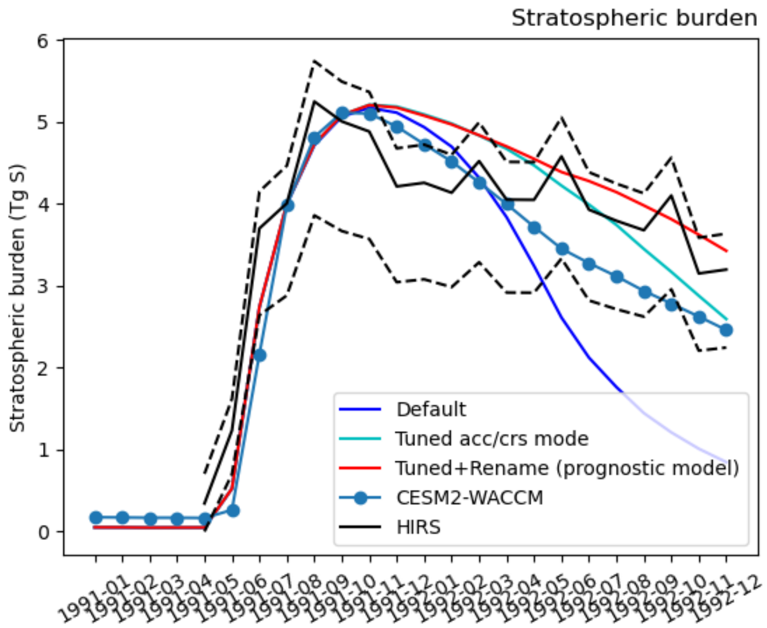


Some Early Simulation Results



Movie above: **stratospheric sulfate burden** from Mt. Pinatubo eruption for **default E3SMv2** (left) and **CLDERA-E3SM** simulation with tuned aerosols (right) 1 month before → 30 months after Mt. Pinatubo eruption.



CLDERA-E3SM prognostic model tuned to **better represent stratospheric aerosol lifetime** and **evolution**, and agrees better with observations (red curve in figure above).

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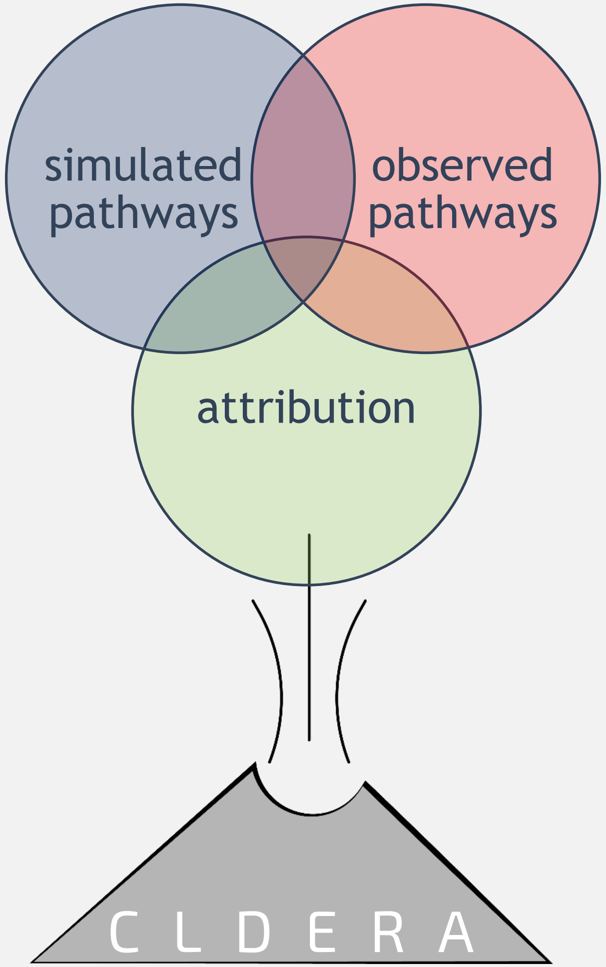
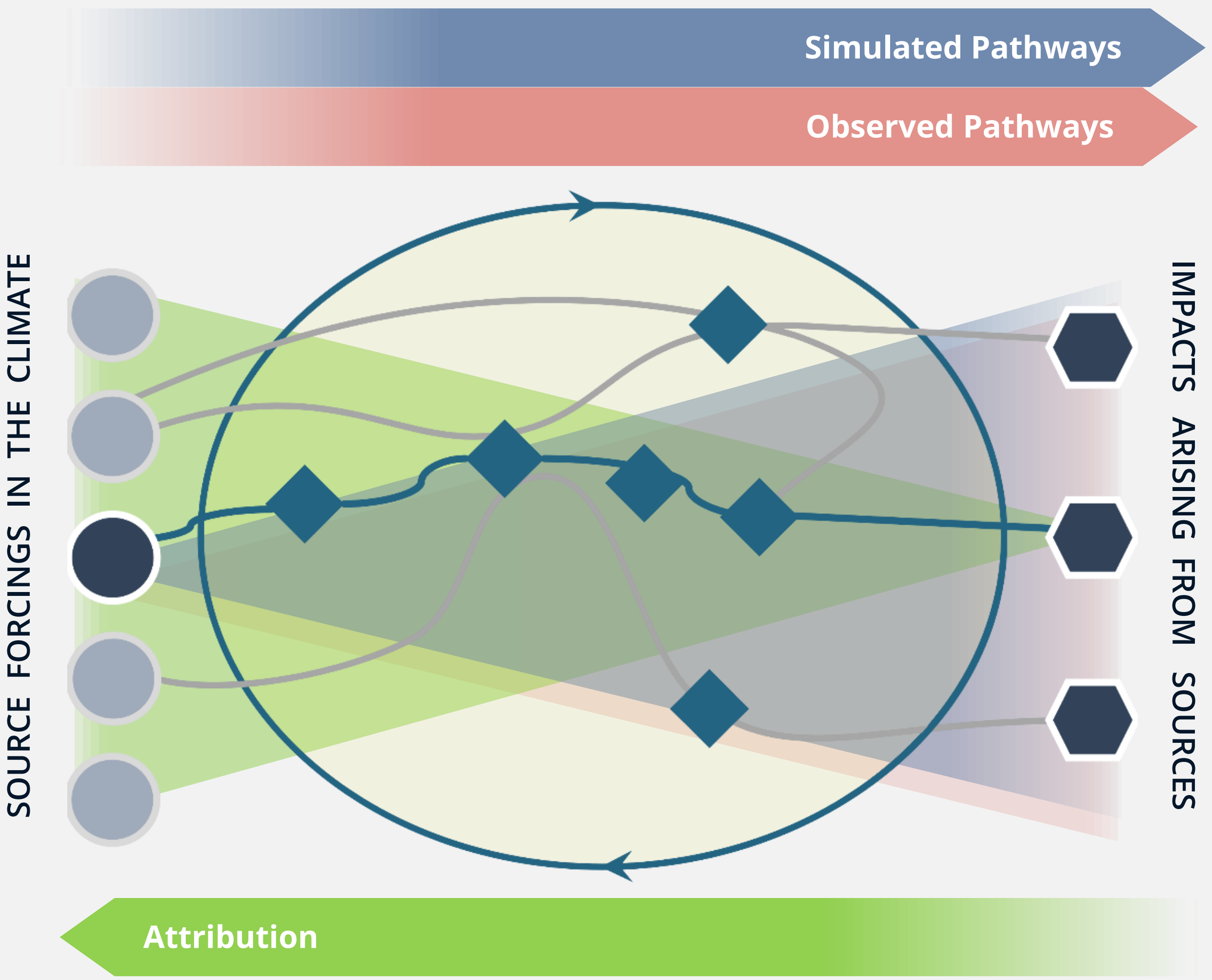


Summary of CLDERA



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.

CLDERA Team

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Observed Pathways Lead: L. Shand (5573)
Attribution Lead: L. Swiler (1400)

Thank you for your attention!





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Start of Backup Slides

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.

Connection to Sandia Capabilities & Other Applications

Multi-component Sensor Systems

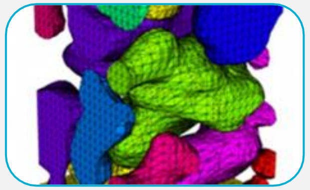
ROL
RAPID OPTIMIZATION LIBRARY

Inverse Optimization

Information Sciences

Bio-Security

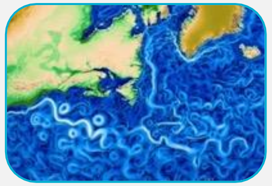
Cyber-Security



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

C L D E R A - C r i t i c a l C a p a b i l i t i e s

Bioscience

Materials Science

Engineering Science

Earth Science

Nanodevices & Microsystems

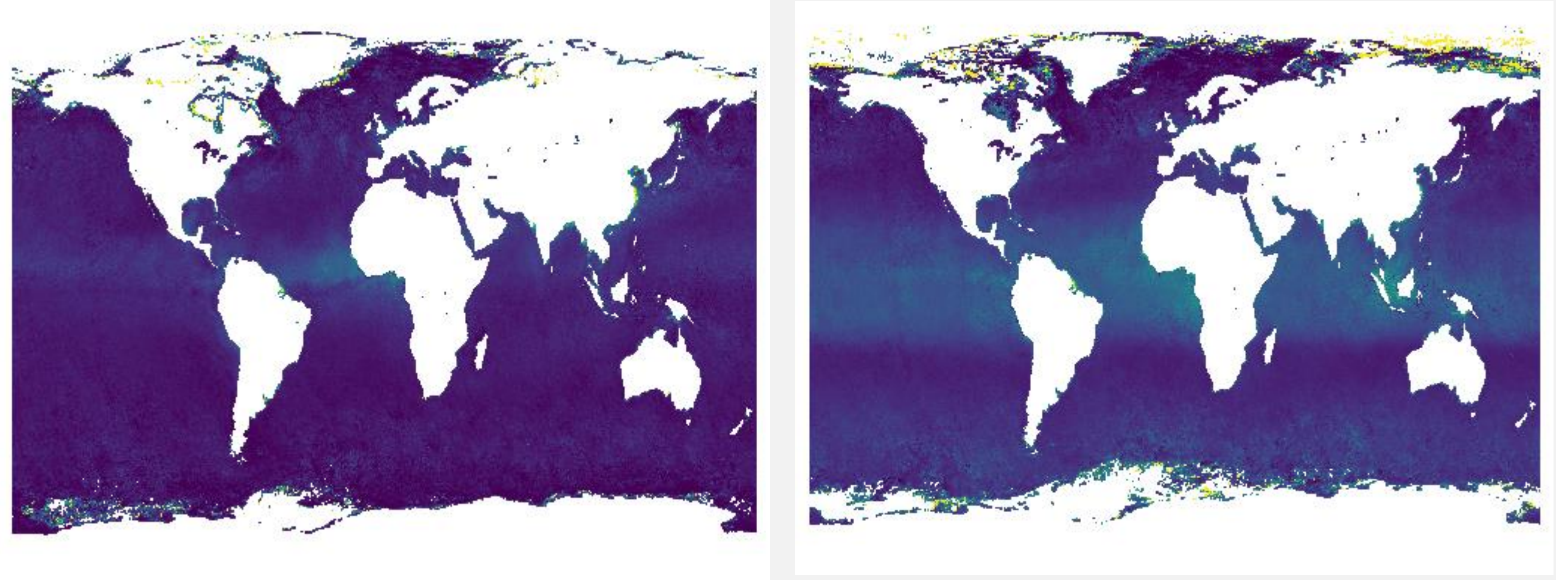
Computing & Information Science

Radiation, Electrical, & High Energy Density Science

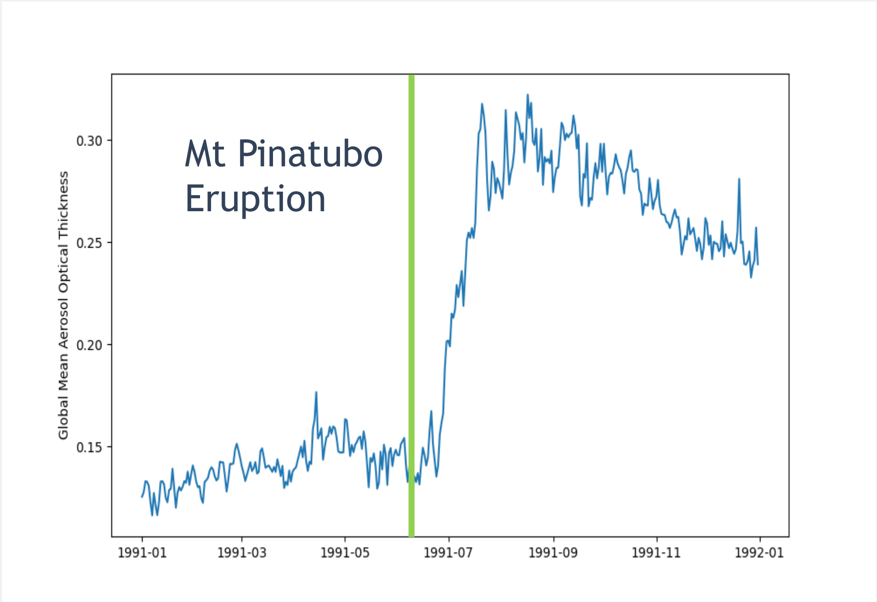
F o u n d a t i o n a l R e s e a r c h t h a t E n a b l e s C l i m a t e W o r k

Observed Pathways Thrust

Data Fusion



Aerosol optical thickness (AOT) at 0.63 micron derived from NOAA PATMOS-x AVHRR (0.1 x 0.1 degree spatial grid collected daily) before (Jan. 1- Jun. 14, 1991) and after (Jun. 15- Dec.31, 1991) eruption.



Global monthly mean AOT from January 1991 to January 1992

Goal: develop/deploy sensor-level **data fusion techniques** to leverage high-dimensional data from at least 8 different sources.

- [Ma and Kang, 2019] proposes a **Dynamic Fused Gaussian Process (DFGP)** methodology to combine multiple datasets from different satellite instruments.
- [Nychka et al., 2015] combines **Multi-resolution Gaussian Process Model** and **Geometric Mean Fold Rise (GMRF)** approaches.

Synthetic Test Case Formulation

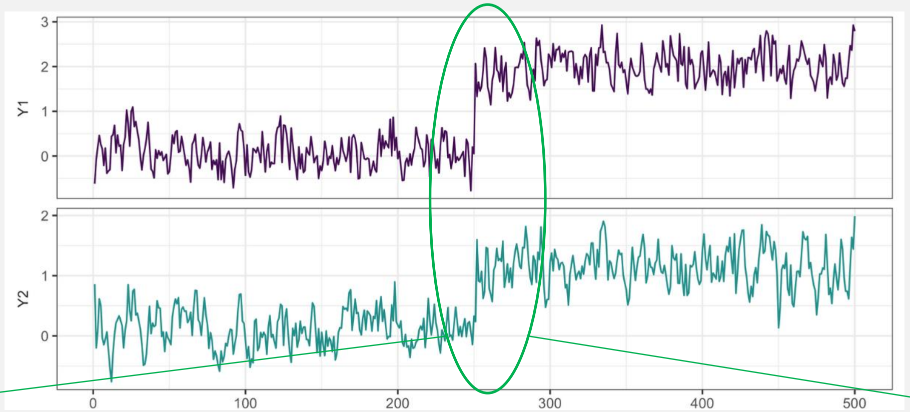
- **Tiered Datasets, four formulations across**
  - ➢ Temporal trends
  - ➢ Temporal trends on spatial grid
  - ➢ Temporal trend on linearly-trended spatial grid
- **Characteristics**
  - ➢ Distinct numbers of couplings with both linear and nonlinear relationships
  - ➢ Distinct lags
  - ➢ Quasi-periodicity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

Two Variable Changepoint Exemplar

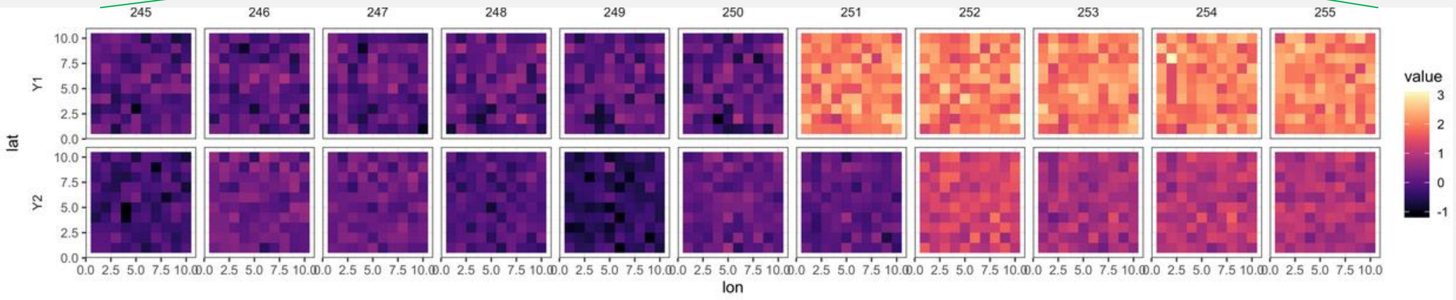
$$Y_{1,t} = 0.5Y_{1,t-1} + 2I[t > 250] + \epsilon_{Y_{1,t}}$$
$$Y_{2,t} = 0.2Y_{1,t-1} + 0.6Y_{2,t-1} + \epsilon_{Y_{2,t}}$$

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

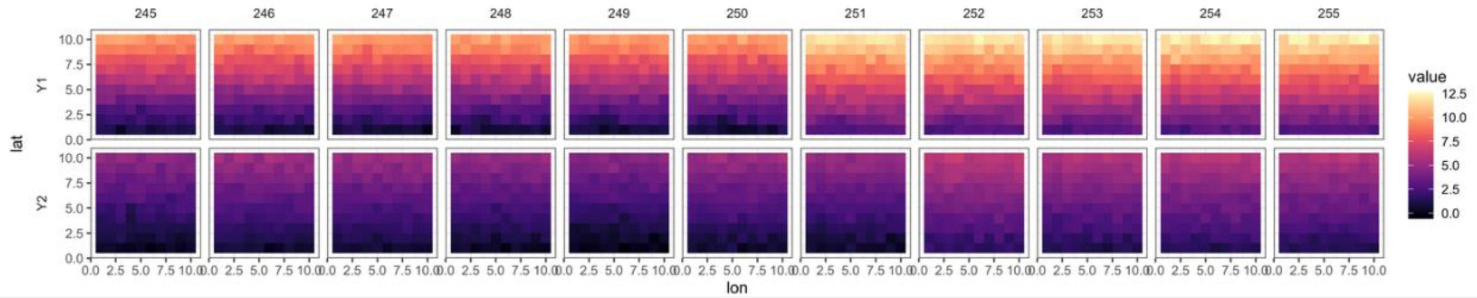
Temporal Trend



Temporal Trend in Space



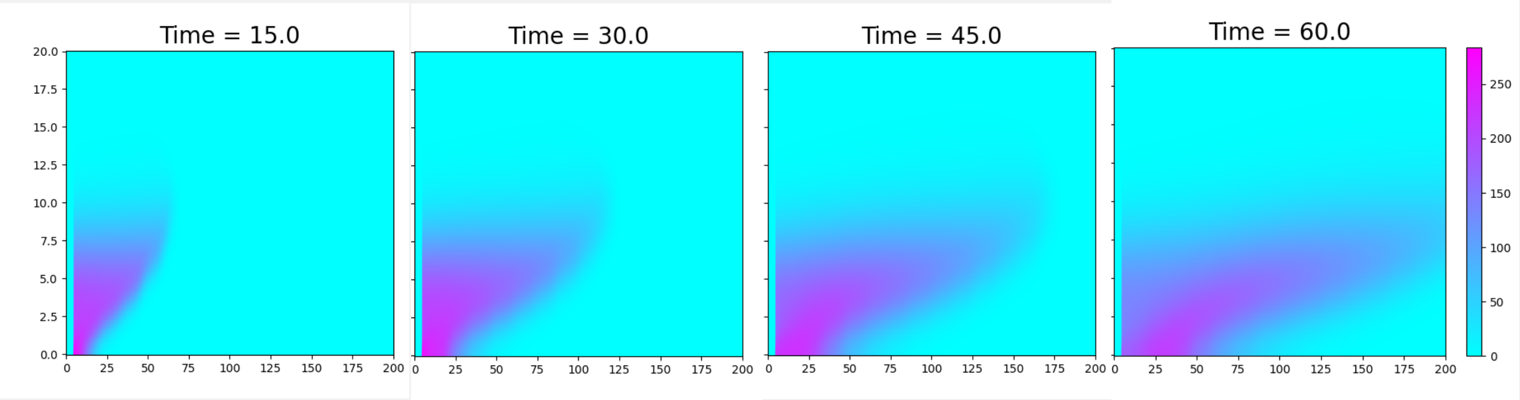
Spatio-Temporal Trend
Linearly-trended Spatial Grid



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, …