In-situ analysis of Physical Pathways Activated by Aerosol Injection in E3SM

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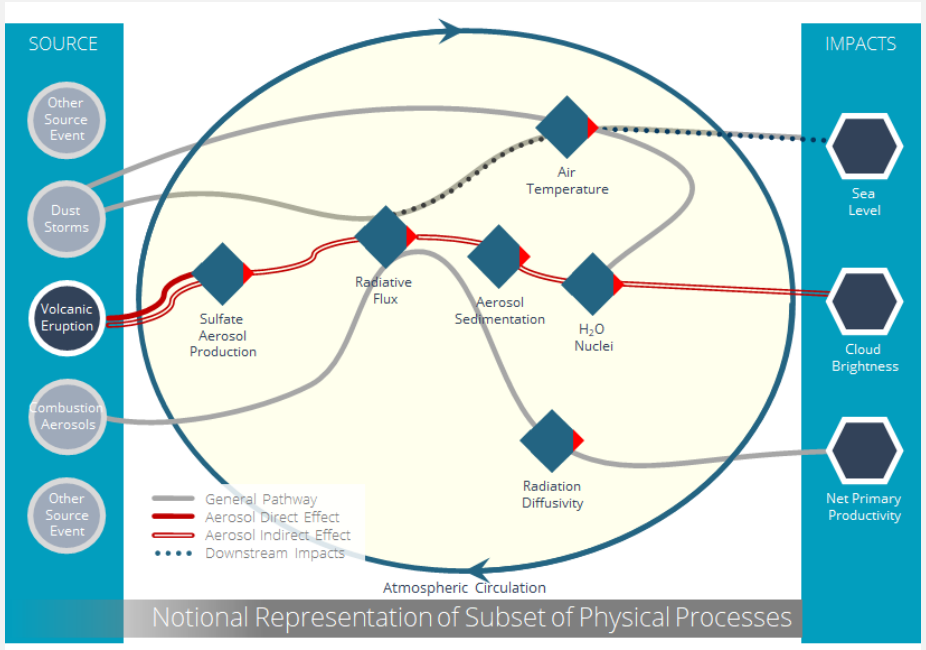
E3SM model and CLDERA

E3SM (https://e3sm.org/about/) is a fully coupled (atmosphere, ocean, land, ice, …) Earth system model developed and funded by the US Department of Energy (DOE) with focus on water cycle, biogeochemistry and energy, and the cryosphere.

Open source!: https://github.com/E3SM-Project/E3SM
Currently on v2 (released September 2021)



Notional Representation of Subset of Physical Processes

https://education.nationalgeographic.org/resource/calderas:
"A caldera is a large depression formed when a volcano erupts and collapses"

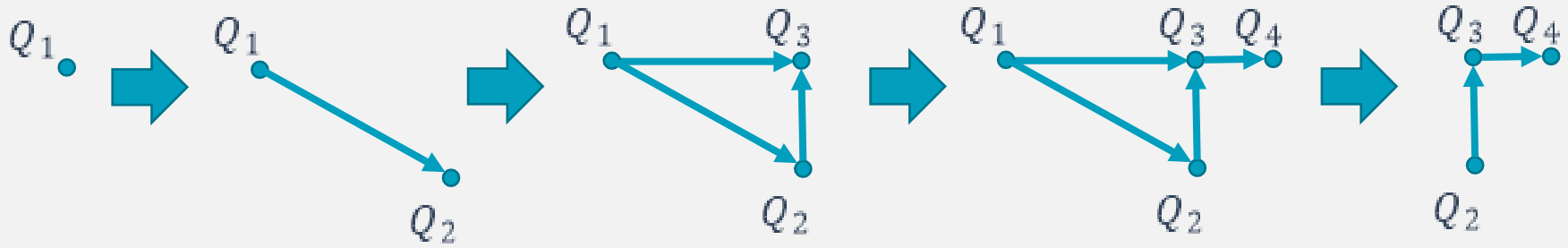
CLDERA -- CLimate impact: Determining Etiology thRough pAthways

Compute physical pathways due to sources (focus on exemplar Pinatubo eruption (see (Stenchikov et al. 1998), (Ramachandran et al. 2000)) and attribute climate impacts caused by this source.

Simulated pathways thrust: to develop a new data-science informed modeling framework to dynamically trace and rank connective relationships ("pathways") between a climate source and its impact(s) using E3SM simulations.

Challenges of pathway analysis in-situ

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



$$\dot{Q}_1 = F_1(Q_1),\ \dot{Q}_2 = F_2(Q_1, Q_2),\ \dot{Q}_3 = F_3(Q_1, Q_2, Q_3),\ \dot{Q}_4 = F_4(Q_3, Q_4)$$

In-situ pathway analysis – construct and determine properties of pathways while software executes.

- In-situ analysis lays groundwork for sensitivity/causality studies, climate intervention simulation/analysis, platform capability for diagnosing bugs or issues with modeling AMOC,ENSO, etc.

Constructing pathways in-situ is novel and challenging.

- Space-time dependence in a large and complex system – downstream effects across wide range of space and time scales.
- Need to come up with new methods, although can leverage ideas from in-situ anomaly detection (Shead et al., 2019), (Milroy et al. 2019), (Aditya et al. 2019) and software bug causes (Milroy et al., 2019).
- Everything we do needs to be computationally cheap, since running E3SM is *expensive.*
  - Avoid things like copying/reading/writing internal variables, don't add communication costs, etc.
- Software models of complex systems are themselves complex (millions of lines, thousands of variables and subroutines) so that determining indirect relationships between variables is challenging.

Pathways from stratospheric aerosol injection in E3SM

For more detailed analysis and discussion see Benjamin Wagman's talk tomorrow at 915am:
JointJ5C.4 Pre-industrial Control and Historical Simulations for CLDERA-E3SMv2: an Earth System Model with Prognostic Volcanic Aerosol

E3SM: At each model step $m = 0,1,2,\ldots$ solve for $u = u(x, t_m)$ (with initial value $u_0(x) = u(x, t_0)$):

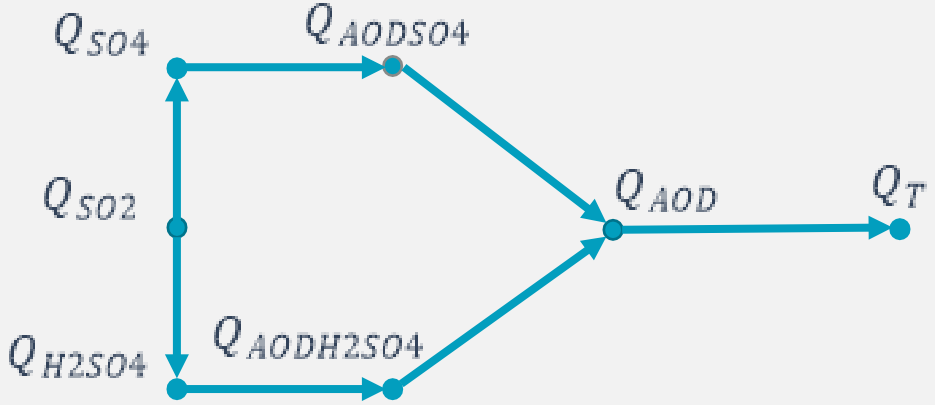
$F(u_t, u, x, t, \rho; V) = 0$, ρ - model parameters, $V = V(x, t)$ – external forcing due to SAI

The external forcing V is a source term for volcanic aerosols such as SO2 concentration Q_{SO2}:

$$\frac{\partial Q_{SO2}}{\partial t} + \vec{u} \cdot \nabla Q_{SO2} = V + S.$$

S represents the usual source/sink terms (e.g. chemistry terms).

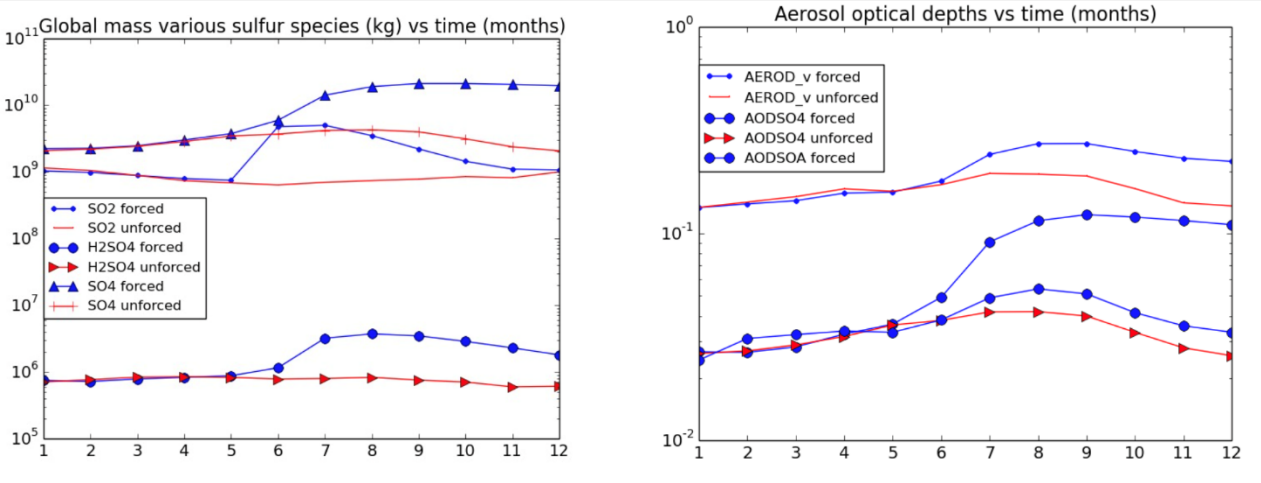
SO2 reacts into sulfate (SO4) and sulfuric acid (H2SO4), changing the aerosol optical depth (AOD) and temperature (T):

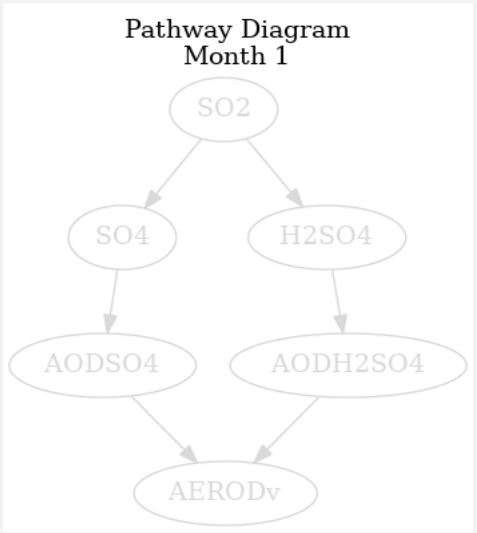


We also make use of the HSW++ configuration in E3SM: Modified idealized Held-Saurez-Williamson configuration (Held and Suarez, 1994), (Williamson et al., 1998) that includes simplified chemistry model for SO2-Sulfate-T pathway (does not include H2SO4 or other aerosols from E3SM chemistry packages).

Mathematical Paradigm for Pathways

- Heuristic: A *pathway* is the chain of physical processes from source to impacts and their evolution in space-time.
- Mathematical interpretation: A pathway is a (time-dependent) graph/network representation of dynamics.
- Potential pathways are determined by software implementation, which limits how quantities of interest (QoIs) can interact.
- Formalize pathways as time-dependent directed acyclic graphs (DAGs) living in some *base-DAG* – nodes are QOIs statistically anomalous according to some test, arrows represent direction of the impact of source.
    - The *base-DAG* represents all potential pathways supported by the software.
- Vast body of literature on relationship to dynamical systems and networks (Anderson et al., 2020), (Glass et al., 2021).



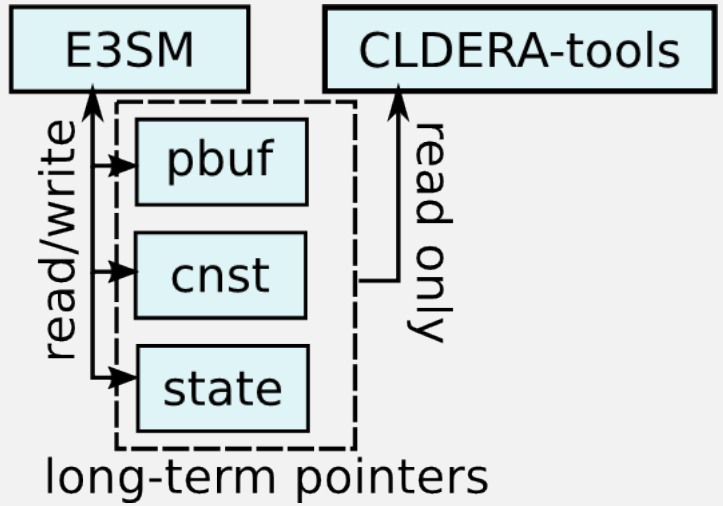


(Left) Time series of monthly means for various sulfur species and various aerosol optical depths of a 1 year low resolution E3SM simulation of a forced run with Mount Pinatubo injection 10Tg of SO2 in to the atmosphere compared to an unforced run. (Right) The time-dependent DAG representing the pathway associated to the time-series data on the left.

CLDERA-Tools: software for in-situ pathway analysis I/II

CLDERA-tools: software tool for in-situ analysis of statistics and pathways of QOIs of E3SM internal variables.

- Noninvasive– provides access to E3SM internal variables without significant code modifications.
- Cheap - Simple global stats of 20 vars in test case with ne16 atm added <1% overhead.
- Detect and track “anomalies” of internal variables and track through time and/or space.



Inputs: Fields, base-DAG, tests

- Fields: The E3SM fields to track.
- Base-DAG: DAG determining *potential* field dependencies.
- Tests: Abstract test determining anomalousness.

Output: Timestamps and values for test failures.

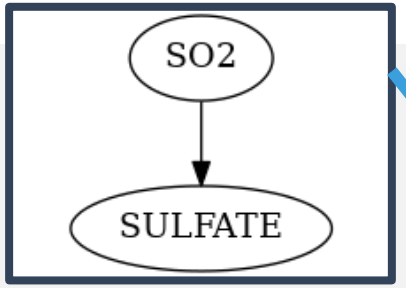
Design

1. User provides superset base DAG for physical processes; identify root QOI
2. Create tests for each QOI based on control data
   - Can use variables directly or derived quantities.
3. Forced E3SM run.
4. Track propagation in real time.

Generating tests for Step 3. can be highly non-trivial – see slide 8!

CLDERA-Tools II/II

- Configuration: HSW++ with CLDERA-tools enabled
- Input: yaml format file with simple SO2->SULFATE pathway w/ tests
  - SO2: check bounds [0, 0.0001]
  - SULFATE: check bounds [0, 0.000005]



input

```
! cldera_profiling_config.yaml
%YAML 1.0
---
Stats Output File: cldera_stats.yaml
Fields To Track: [SO2, ASH, SULFATE]

SO2:
  Compute Stats: [Min,Max]
ASH:
  Compute Stats: [Min,Max]
SULFATE:
  Compute Stats: [Min,Max]

Pathway:
  DAG:
    SO2:
      Activation Tests: ["so2bounds"]
      Affects: SULFATE
    SULFATE:
      Activation Tests: ["sulfatebounds"]
Tests:
  so2bounds:
    Field: SO2
    Type: Bounds
    Params: [0.0,0.0001]
  sulfatebounds:
    Field: SULFATE
    Type: Bounds
    Params: [0.0,0.000005]
...
```

output

```
! cldera_pathway_history.yaml
%YAML 1.1
---
SO2:
  Timestamps: [10101.10800, 10101.12600, 10101.14400, 10101.16200, 10101.18000, 10101.19800, 10101.21600, 10101.23400,
  10101.25200, 10101.27000, 10101.28800, 10101.30600, 10101.32400, 10101.34200, 10101.36000, 10101.37800, 10101.39600,
  10101.41400, 10101.43200, 10101.45000, 10101.46800, 10101.48600, 10101.50400, 10101.52200, 10101.54000, 10101.55800,
  10101.57600, 10101.59400, 10101.61200, 10101.63000, 10101.64800, 10101.66600, 10101.68400, 10101.70200, 10101.72000,
  10101.79200, 10101.81000, 10101.82800, 10101.84600, 10102.0, 10102.1800]
  Values: [0.00010329699284272, 0.00011176368785696, 0.00011975218965903, 0.0001273112128658, 0.00013448061930178, 0.
  00014130105016061, 0.00014780304098874, 0.00015401584735621, 0.00015996155127454, 0.0001656572945609, 0.
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  00028601482130648989, 0.00029137222079619816, 0.00029670924925631073, 0.00030197467863524, 0.0003072445338943, 0.0003100223717694 3,
  0.00031099073334981, 0.00031414606190033, 0.00031715030302244 4, 0.00032012319463076 1, 0.00032306302247873 7]
SULFATE:
  Timestamps: [10102.10800, 10102.12600, 10102.14400, 10102.16200, 10102.18000, 10102.19800, 10102.23400, 10102.25200,
  10102.27000, 10102.28800, 10102.30600, 10102.32400, 10102.34200, 10102.36000, 10102.37800, 10102.39600, 10102.41400,
  10102.43200, 10102.45000, 10102.46800, 10102.48600, 10102.50400, 10102.52200, 10102.54000, 10102.55800, 10102.57600,
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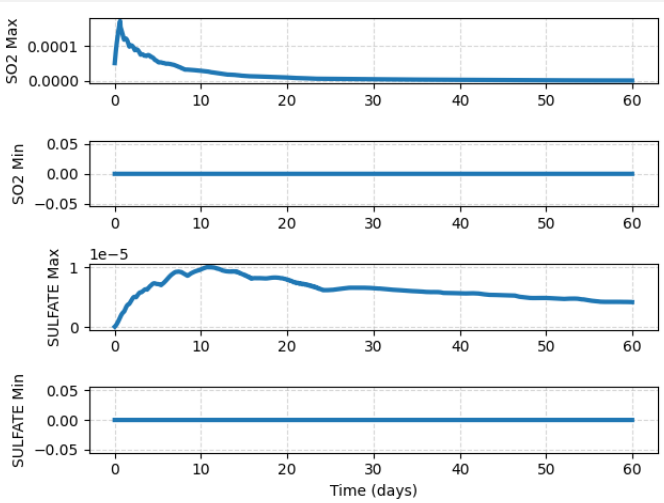
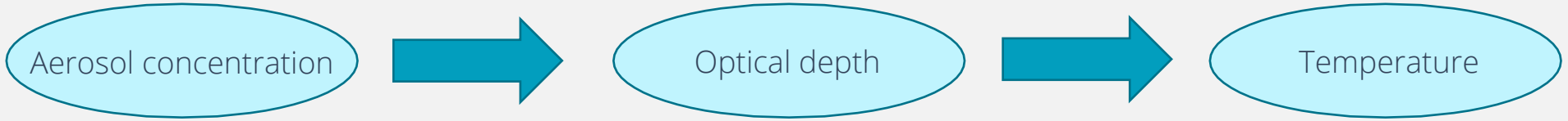
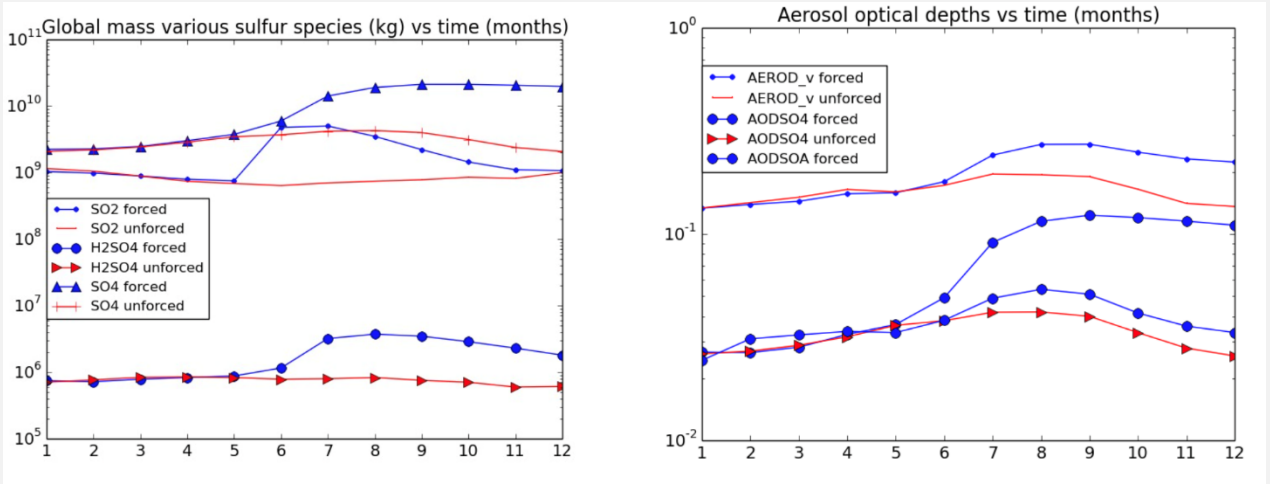


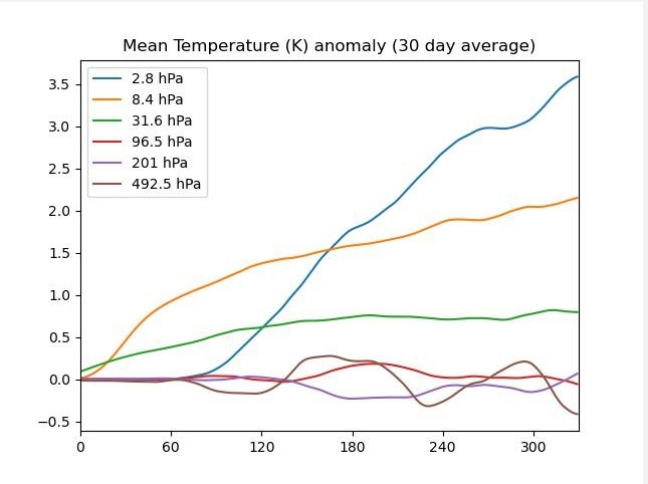
CLDERA-Tools Test Design

Each QOI requires its own CLDERA-Tools test.

- Tests depend on a number of factors: QOI statistical properties, type of problem, control data, desired accuracy.
- SAI injection: effects on QOIs that are farther “downstream” (e.g. temperature) can be more difficult to characterize.

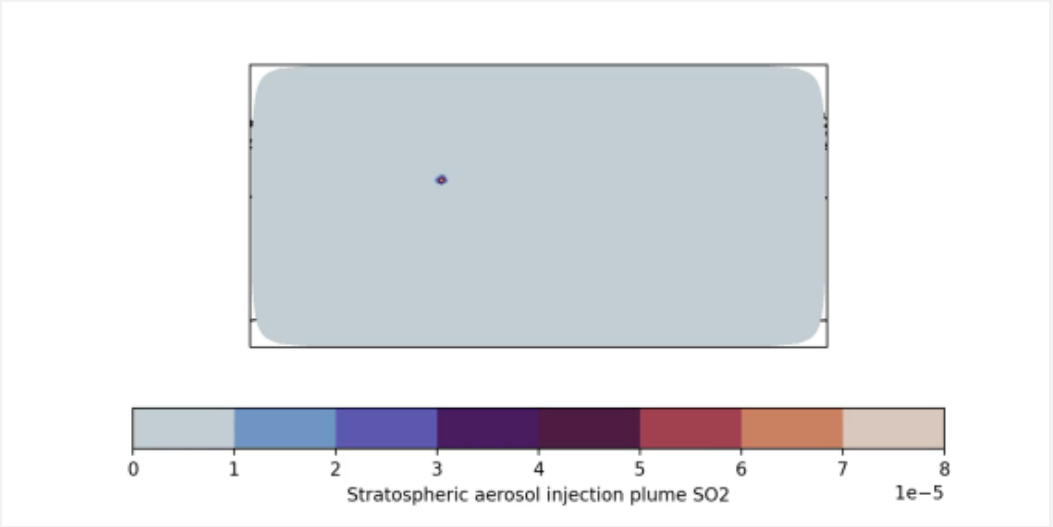


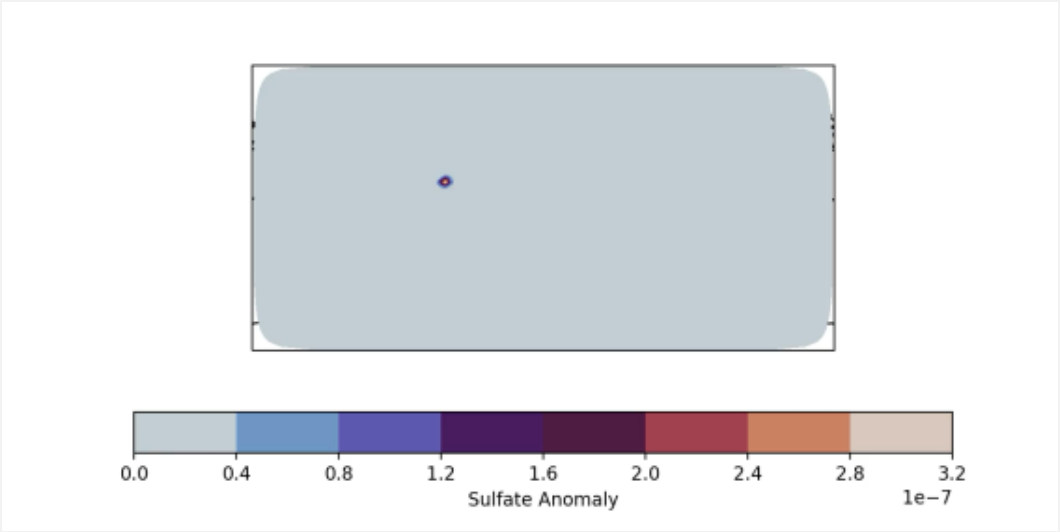




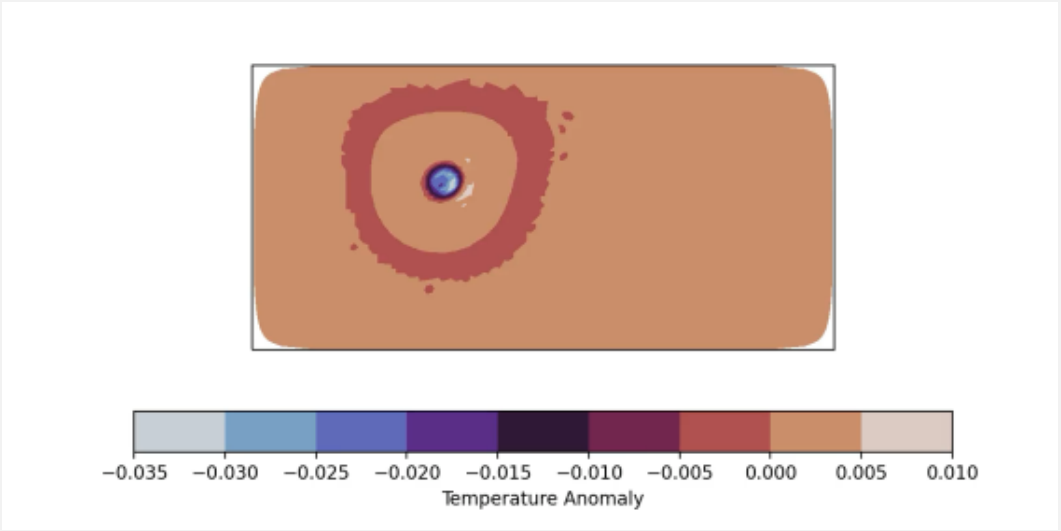
(Left) Time series of monthly means for various sulfur species and various aerosol optical depths of a 1 year low resolution E3SM simulation of a forced run with Mount Pinatubo injection 10Tg of SO2 in to the atmosphere compared to an unforced run. (Right) Time-series of 30-day time average of global mean temperature from HSW++ run.

HSW++ Results





Lat-lon plots of various QOIs for the HSW++ configuration with Pinatubo Eruptions.



Thanks!

Questions?

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