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In-situ data extraction for pathway analysis in an idealized model atmosphere

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Work done as part of the profiling subthrust of Simulated Pathways Thrust of CLDERA Grand Challenge.

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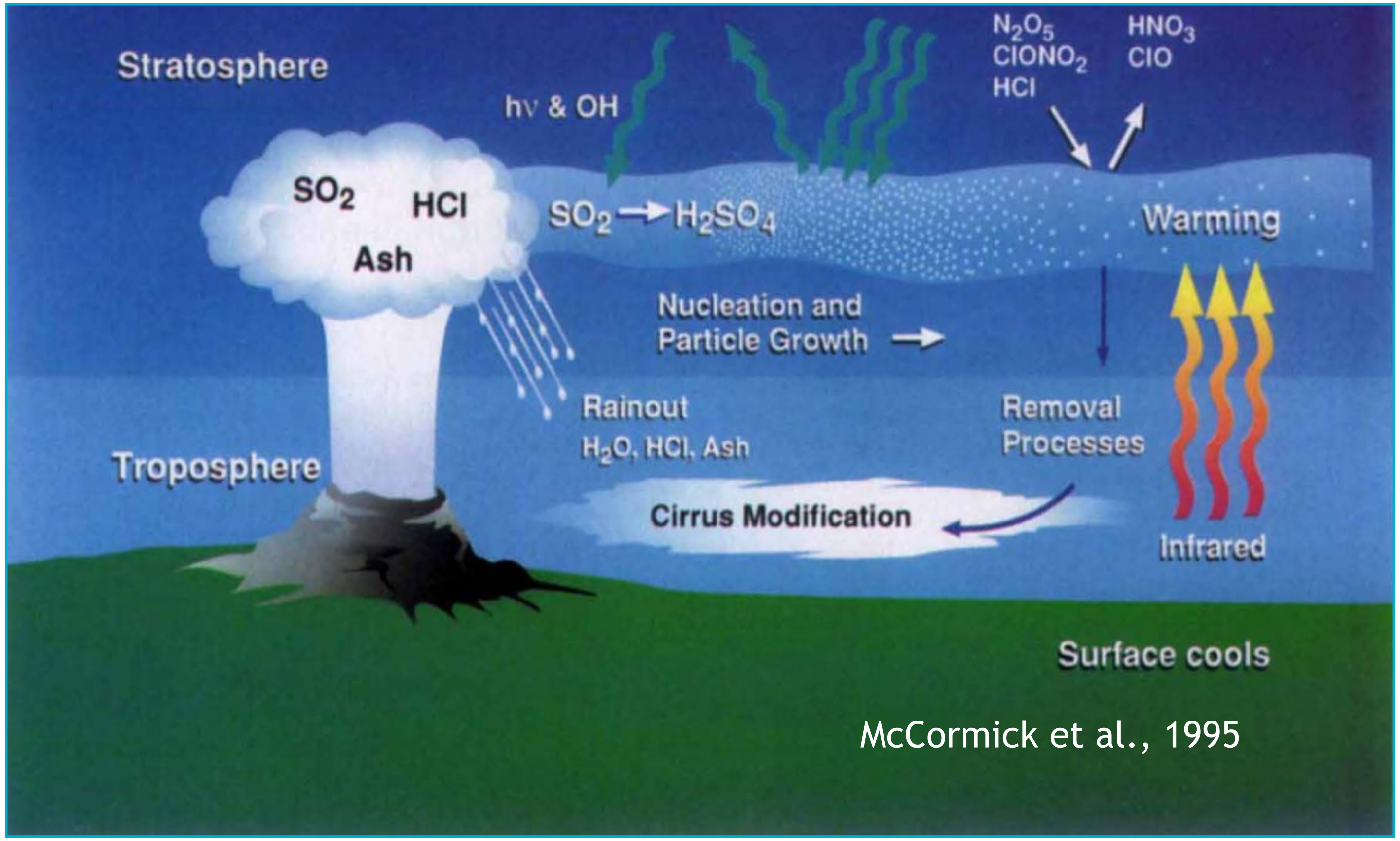
U.S. DEPARTMENT OF ENERGY

NNSA

Mount Pinatubo Eruption



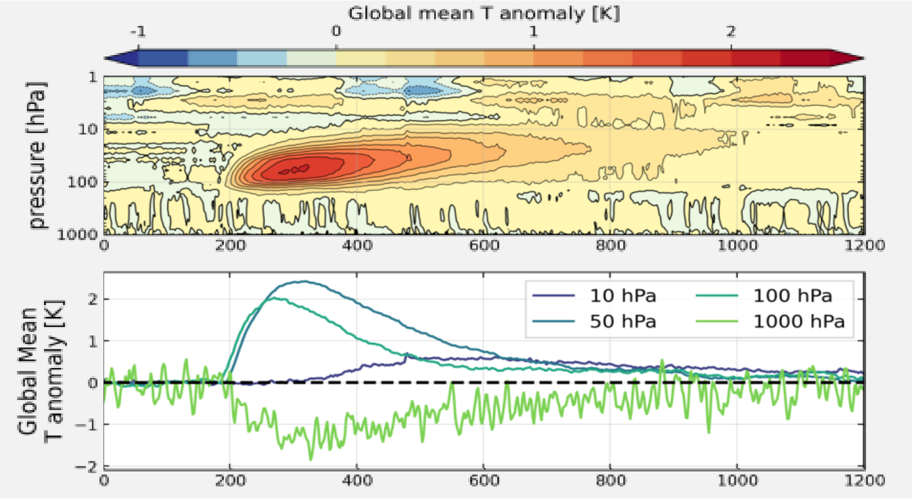
Mount Pinatubo is an active volcano in the Philippines, 54 miles northwest of Manila that erupted in June 1991. See (Ramachandran et al. 2000), (Stenchikov et al. 1998), (McCormick et al., 1995) for references on Pinatubo effects.

- Second-largest eruption of the 20th century – largest perturbation to particulate content of the stratosphere.
- Volcanic plume reached over 30km high and injected 10Tg of SO2 gas into the atmosphere.
- SO2 reacts with OH to make H2SO4 (sulfuric acid) resulting in an atmospheric haze.

- Global surface temperature decreased by about 0.5 K in mid-1992, negative radiative forcing lasted into 1993.
- Stratosphere warmed by as much as 3.5 K .

Idealized E3SM configuration: HSW-v

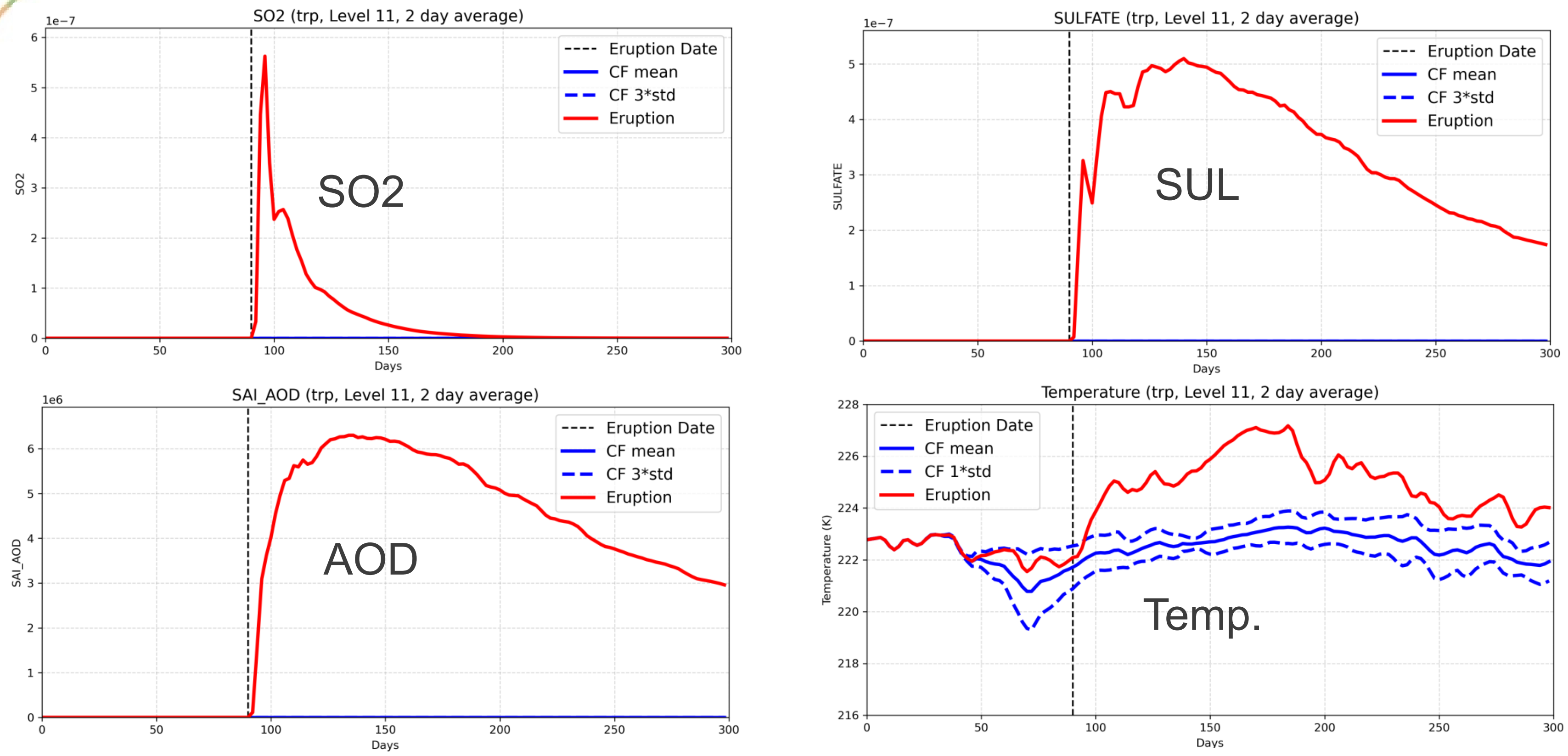
- Main code-base is fork of E3SM version 2 (Golaz et al., 2024).
  - E3SM is a fully-coupled climate model funded by the U.S. Dept. of Energy.
- We make use of an extended version (HSW-v) (Hollowed et al., 2024) of the idealized Held-Suarez-Williamson (HSW) (Held and Suarez, 1994), (Williamson et al. 1998) atmosphere configuration.
  - Dry atmosphere, aseasonal, and topography free.
  - Inject SO2 and ash tracers into the stratosphere.
  - SO2 reacts via a simple chemistry relation into sulfate (SO4).
  - Adjust radiative forcing based on total tracer content such that the stratosphere warms and the surface cools. (the atmosphere temperature is constantly nudged towards a daytime equilibrium).
  - No background concentrations of ash, SO2, SO4.



Time [days]

- Stratospheric temperature heating with peak at ~2.5 K near month 3.
- Global-mean surface temperature cooling with significant minima of ~-1.5 K near month 3.

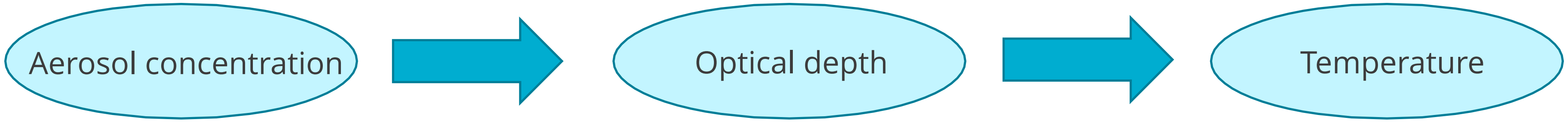
HSW-v: Downstream effects of SO_2 injection



(Left) Time-series of 2-day averages of mean values in the upper-stratosphere of the tropical region of SO_2 concentration (top left), SO_4 concentration (top right), AOD (bottom left), and temperature (bottom right).

Means values (red) are compared to baseline-statistics (blue) from an eruption-free ensemble run.

- Main contribution of our work based on this “pathway”:
  - Algorithms to formally characterize the “pathway” from source to space-time impacts in terms of time-dependent DAGs.
  - Develop in-situ methods for extracting necessary data.



Pathways and DAGs (abstract)

Consider a space-time discrete forward model:

$$u_{m+1} = F(u_m, t_m, \alpha), u_m \in \mathbb{R}^J \times \mathbb{R}^d, \alpha \in \mathbb{R}^p.$$

The variable u_m is the model state at time t_m and α are the (physical) model parameters.

Let $Q_1, \ldots, Q_r$ denote r quantities of interest (QOIs) of the model state: $Q_l: \mathbb{R}^J \to \mathbb{R}, l = 1, \ldots, r$.

The base-DAG G_B (DAG=directed acyclic graph) - nodes correspond to QOIs, edges correspond to relationship between QOIs (informed by physics/subject-matter-expertise).

A *pathway* is a sequence of DAGs $G = \{G_m\}$ where G_m is a subgraph of G_B.

- Node is "active" at time-step m if it is in the vertex set of G_m and "inactive" otherwise.

Algorithm to construct pathway from base-DAG (see Algorithm 1 in (Steyer et al., forthcoming)):

- Determine bounds-tests for each node (i.e. QOI), (bounds test = 1 if active, 0 if inactive).
- At each time-step m:
  - Set vertex set V_m as the set of all vertices in the base-DAG with a bounds-test value equal to 1.
  - Set edge set E_m to be set of all edges in base-DAG edge set whose component vertices are in V_m.
  - Set $G_m = (V_m, E_m)$.

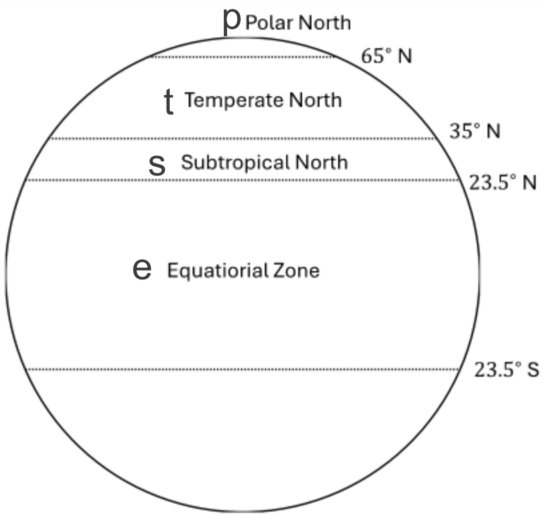
Pathways and DAGs (concrete).

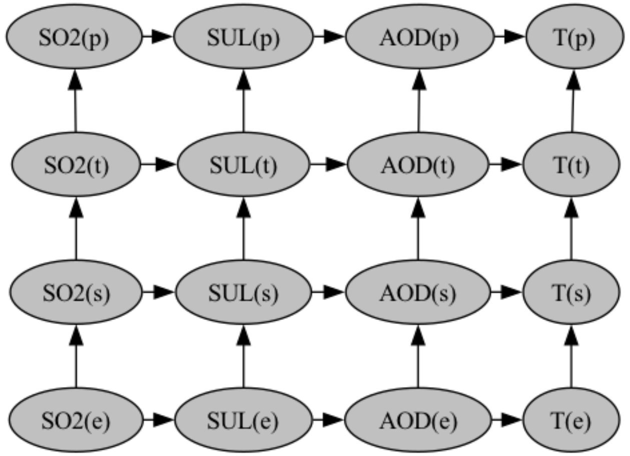
Pinatubo eruption:

- SO2 erupts into the stratosphere, erupted SO2 converts to SO4 (sulfate), SO4 increases aerosol optical depth (AOD), changes in AOD results in increase in stratospheric temperature (T).
- Effects propagate from the equatorial zone (where eruption happens) through the mid-latitudes to the poles.

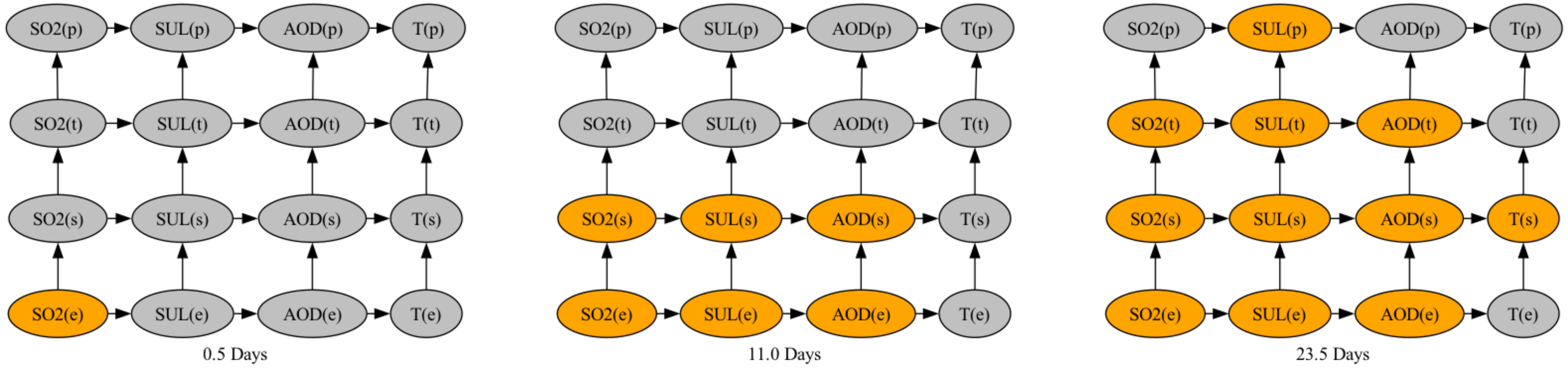
QOI	Description
SO2(x)	Integrated value of SO2 over the mid-stratosphere and zone x.
SUL(x)	Integrated value of SO4 (sulfate) over the mid-stratosphere and zone x
AOD(x)	Integrated value of AOD over zone x
T(x)	Integrated value of temperature over the mid-stratosphere and zone x

Table of QOIs. Zone x=e,s,t,p where e=equatorial zone, s=subtropical north, t=temperate north, p = polar north. Mid-stratosphere is appr. 25-75 hPa.





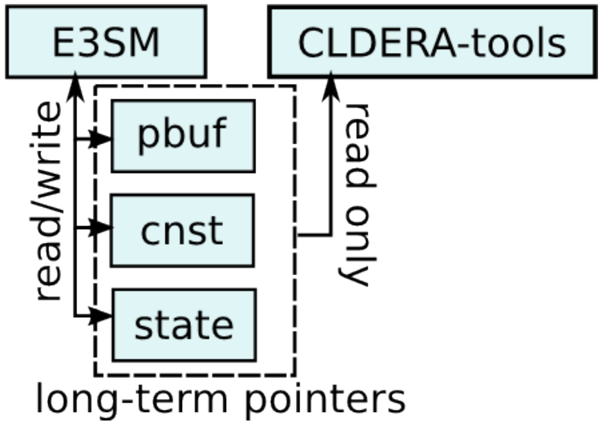
Base-DAG for Pinatubo eruption simulations.



Pathway: orange-shaded nodes are “active” and gray-shaded nodes are inactive.

In-situ coanalysis and CLDERA-Tools

- In-situ coanalysis: computing, processing, storing statistics of QOIs of internal model fields without stopping the simulation
  - In-situ methods avoid costs associated with I/O operations, movement of data in memory, or halting a simulation.
- CLDERA-Tools: software package for for in-situ coanalysis in E3SM (*or other forward model).
  - Reads in YAML file a list of all the desired QOIs to compute and analyze, along with desired configuration for I/O.
  - E3SM passes pointers to fields to CLDERA-Tools.
  - I/O is initialized and output files are readied for writing operations.
- CLDERA-Tools implementation:
  - Internal functions to compute statistics (zonal/vertical means, max. value in given region, etc.)
  - Install CLDERA-Tools separately and link in the E3SM installation process.
  - Deploy “hooks” in E3SM to gain access to internal model fields.



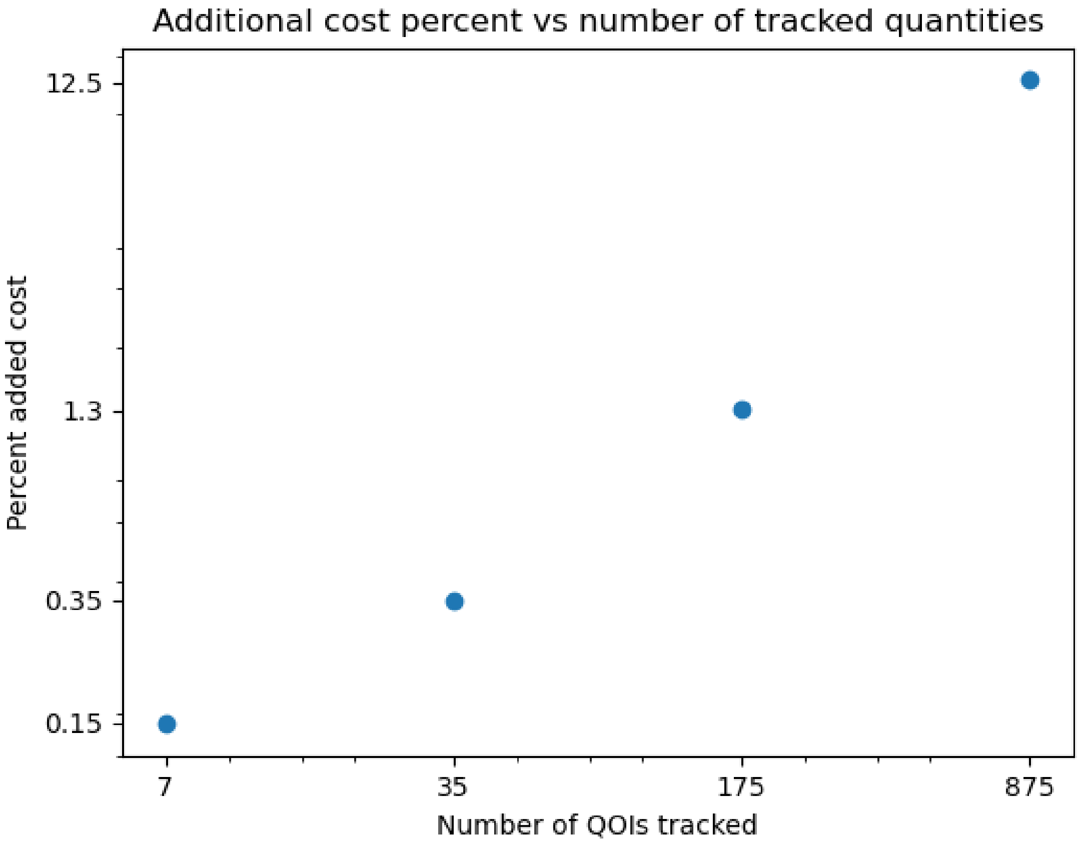

```
                  !  Output fluxes at 200 mb
                  call vertinterp(ncol, pcols, pverp, state%pint, 20000._r8, fnl, fln200)
                  call vertinterp(ncol, pcols, pverp, state%pint, 20000._r8, fcnl, fln200c)
                  ! Dump longwave radiation information to history tape buffer (diagnostics)
                  call outfld('QRL'//diag(icall),qrl (:ncol,:)/cpair,ncol,lchnk)
                  call outfld('QRLC'//diag(icall),qrlc(:ncol,:)/cpair,ncol,lchnk)
                  call outfld('FLNT'//diag(icall),flnt  ,pcols,lchnk)
                  call outfld('FLUT'//diag(icall),flut  ,pcols,lchnk)
                  call outfld('FLUTC'//diag(icall),flutc ,pcols,lchnk)
                  call outfld('FLNTC'//diag(icall),flntc ,pcols,lchnk)
                  call outfld('FLNS'//diag(icall),flns  ,pcols,lchnk)

                  call outfld('FLDSC'//diag(icall),fldsc ,pcols,lchnk)
                  call outfld('FLNSC'//diag(icall),flnsc ,pcols,lchnk)
                  call outfld('LWCF'//diag(icall),lwcf  ,pcols,lchnk)
                  call outfld('FLN200'//diag(icall),fln200,pcols,lchnk)
                  call outfld('FLN200C'//diag(icall),fln200c,pcols,lchnk)
                  call outfld('FLDS'//diag(icall),cam_out%flwds ,pcols,lchnk)

#if defined(CLDERA_PROFILING)
                  if (icall == 0) then ! profile climate calculation
                     call cldera_set_field_part_data('FLNT',lchnk-begchunk+1,flnt)
                     call cldera_set_field_part_data('FLUT',lchnk-begchunk+1,flut)
                     call cldera_set_field_part_data('FLUTC',lchnk-begchunk+1,flutc)
                     call cldera_set_field_part_data('FLNS',lchnk-begchunk+1,flns)
                  endif
#endif
```

Hooks are ”minimally invasive”, involving a short call to the appropriate CLDERA-Tools subroutine.

CLDERA-Tools Cost Study



- Form baseline of 10 1-day simulations without using CLDERA-Tools in-situ analysis.
- Run 10 1-day simulations with CLDERA-Tools to compute the integral of 1,5,25,125 fields in 7-zonal regions over the mid-stratosphere (resulting in 7,35,175,875 QOIs).
- Compare the additional time in the CPL_ATM_RUN timer of each set of 10 CLDERA-Tools simulation with the baseline.

Experiments run on single node of a local cluster, featuring a dual-socket Intel Xeon Gold processor with 18 cores per socket, 2 hardware threads per core, and 96GB of RAM per socket.

Details of pathway experiments

We use four eruption mass sizes (0, 5, 10, 20 Tg) and a 10-element ensemble for each mass.

- Ensemble members differ by a small perturbation of the initial condition 90-days pre-eruption (eruption is on simulation day 90).

The 0 Tg "eruption" is the used to define baseline statistics for temperature.

- $T_\mu(x)$ and $T_\sigma(x)$ are the ensemble mean and standard deviation of $T(x)$ in the 0 Tg eruption, x=e,s,t,p.
- $T_Z(x) = (T(x) - T_\mu(x))/T_\sigma(x)$ where $T(x)$ corresponds to 5,10, or 20 Tg eruption QOI.

Bounds-tests for QOIs $0 < T_l < T_u$:

$$\tau_{T(x),m} = \begin{cases} 0 & T_Z(x)_m \leq T_l \\ 1 & T_Z(x)_m \geq T_u \\ \tau_{T(x),m-1} & T_z(x)_m \in (T_l, T_u) \end{cases}$$

$$\tau_{AOD(x),m} = \begin{cases} 0 & AOD(x)_m \leq 0.0075 \\ 1 & AOD(x)_m \geq 0.015 \\ \tau_{AOD(x),m-1} & AOD(x)_m \in (0.0075, 0.015) \end{cases}$$

$$\tau_{SO2(x),m} = \begin{cases} 0 & SO2(x)_m \leq 4 \cdot 10^{-10} \\ 1 & SO2(x)_m \geq 8 \cdot 10^{-10} \\ \tau_{SO2(x),m-1} & SO2(x)_m \in (4 \cdot 10^{-10}, 8 \cdot 10^{-10}) \end{cases}$$

$$\tau_{SUL(x),m} = \begin{cases} 0 & SO2(x)_m \leq 4 \cdot 10^{-10} \\ 1 & SO2(x)_m \geq 8 \cdot 10^{-10} \\ \tau_{SUL(x),m-1} & SO2(x)_m \in (4 \cdot 10^{-10}, 8 \cdot 10^{-10}) \end{cases}$$

Values $T_l < T_u$ for $T(x)$ used to study sensitivity of pathways w.r.t. the bounds-test. We use $T_l = 0.5$, $T_u = 0.75, 1.0, 1.5, 2.0$.

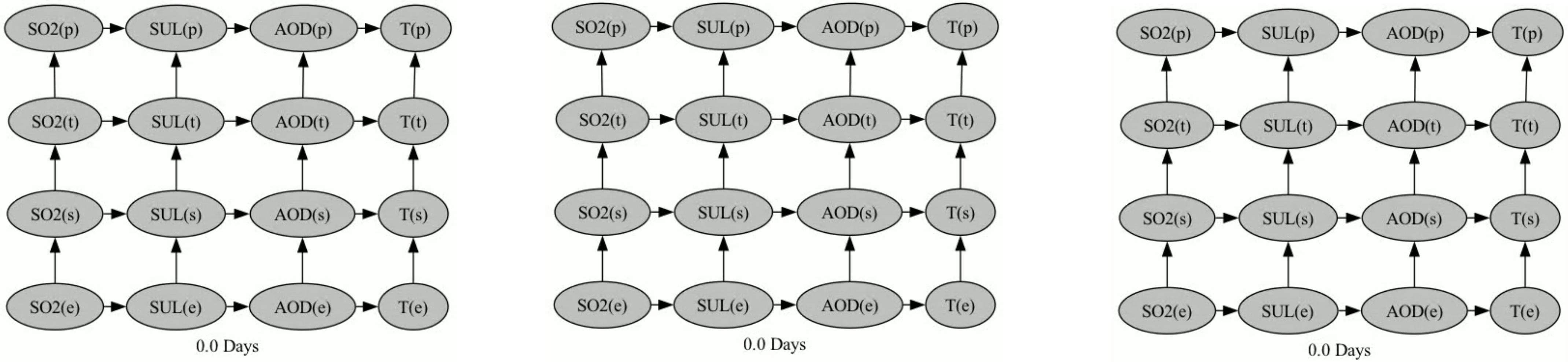
- Ex1 is $T_u = 0.75$, Ex2 is $T_u = 1.0$, Ex3 $T_u = 1.5$, Ex4 $T_u = 2.0$

Fixed bounding values for SO2, SUL, AOD are based on the size of the eruption and the expected concentration of aerosol quantities.

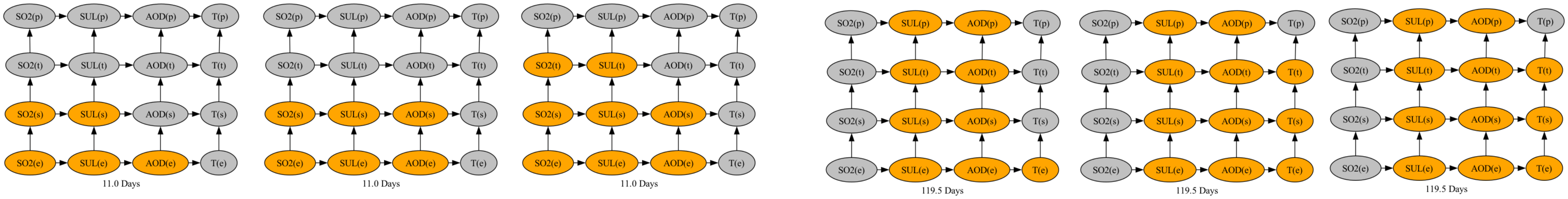
- No baseline to compare to (SO2, SUL, AOD all zero in HSW-v with mass size = 0 Tg).

Right now: DAGs are constructed as post-process using data that is extracted in-situ.

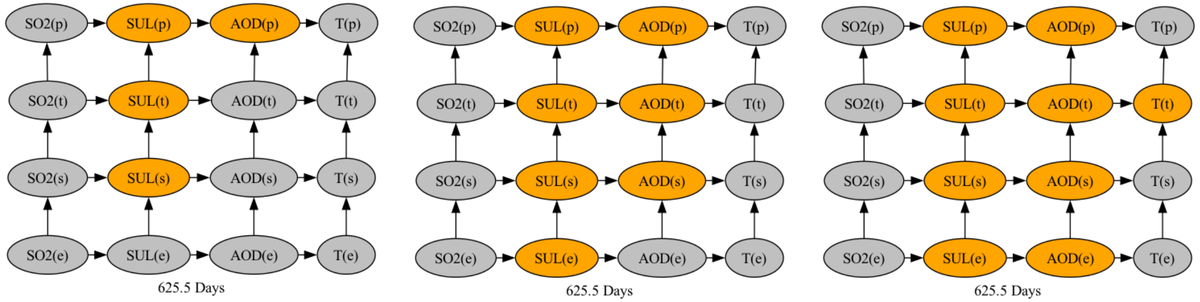
Space-time evolution of pathways.



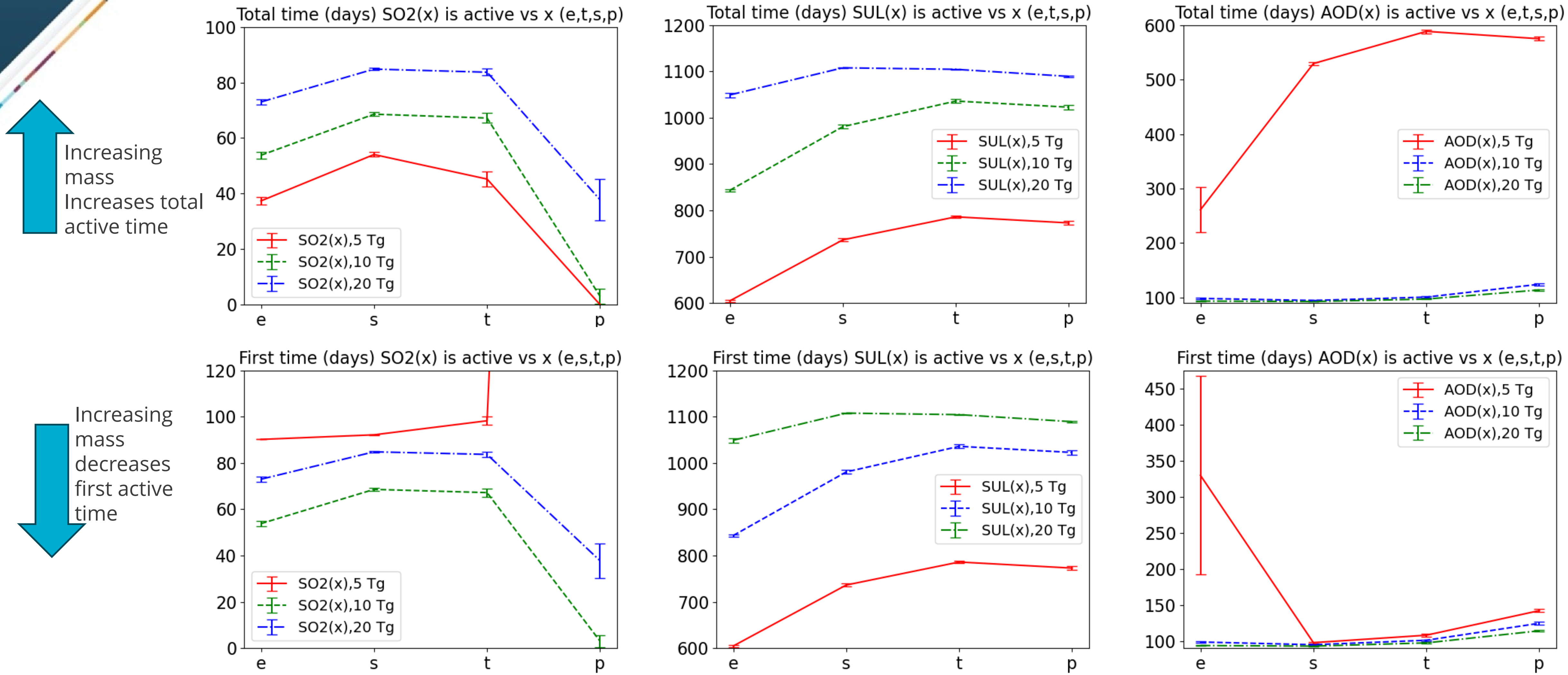
Pathways using bounding values $T_l = 0.5, T_u = 1.0$ for the 5 Tg eruption (left), 10 Tg eruption (center), and 20 Tg eruption (right). Gray-shaded nodes are inactive and orange-shaded nodes are active. "Days" label denotes days post-eruption (happens on sim. day 90).



Snapshots post eruption
days 11, 119.5, 625.5 –
5 Tg (left), 10 Tg (center),
20 Tg (right).

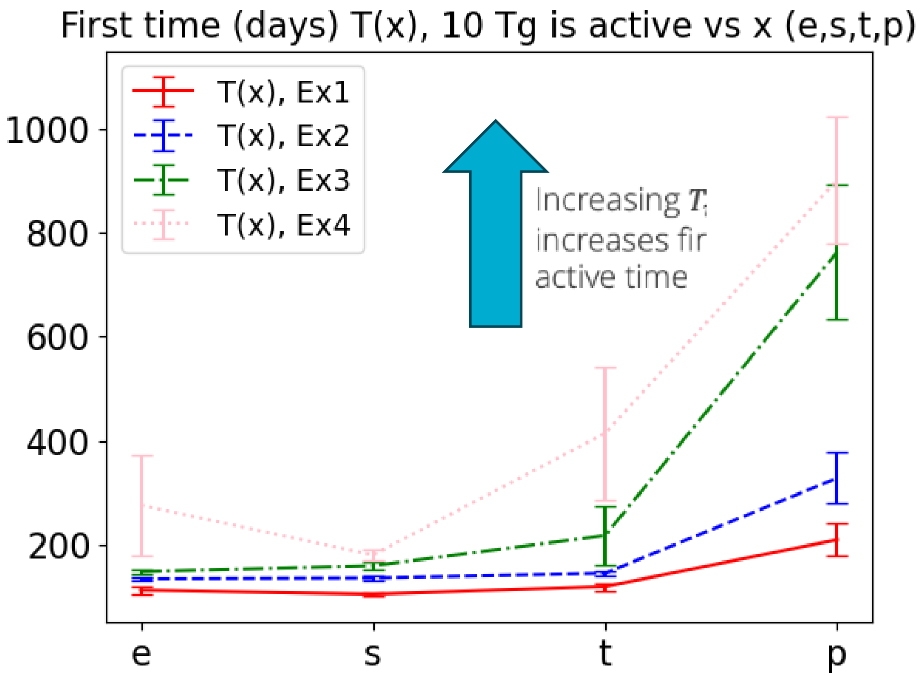


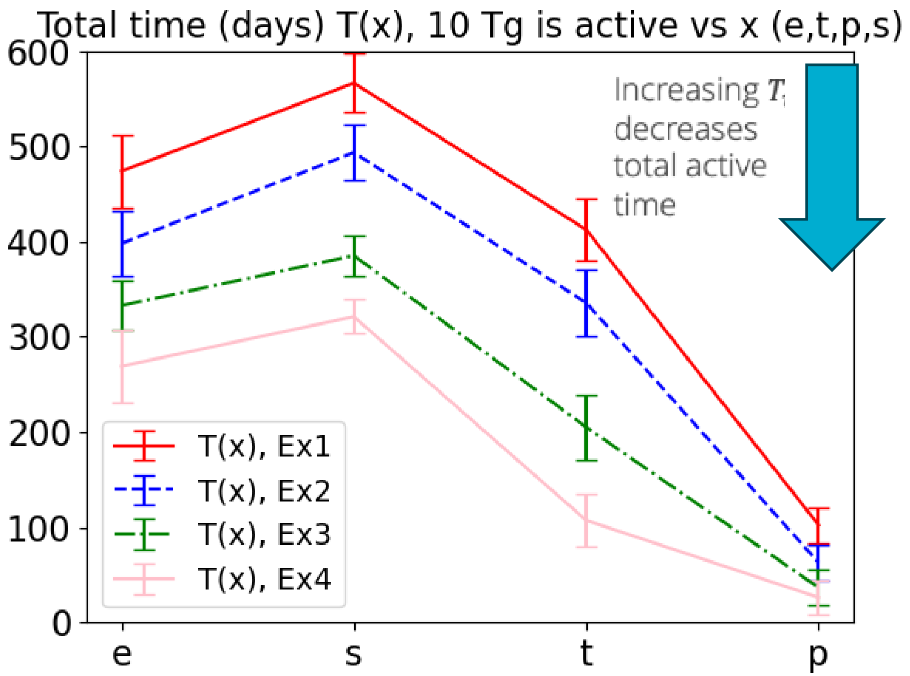
DAG statistics: SO_2, SUL, AOD



- Graphs show mean value of 10-element ensemble, error bars denote standard error.
- Effects of eruption felt sooner and longer with increasing eruption size.
- First activation time set to 1200-days if node never becomes active (First time of SO_2(p) 5 Tg is always 1200 days).

DAG statistics: T





Same story:

- Graphs show mean value of 10-element ensemble, error bars denote standard error.
- Effects of eruption felt sooner and longer with increasing eruption size.
- Decreasing the sensitivity of bounds test (i.e. increasing T_u) results in:
  - Effects felt later and with shorter duration.

- Ex1 is $T_u = 0.75$, Ex2 is $T_u = 1.0$, Ex3 $T_u = 1.5$, Ex4 $T_u = 2.0$.

$T_l = 0.5$ in all experiments

Conclusions and future work

- More complex simulations (fully-coupled E3SM) and pathways:
  - Temperature effects in non-idealized configurations with background SO2, SUL, AOD.
  - Pinatubo effects on agricultural yields, biogeochemistry (incorporating land model).
  - Changes in cirrus clouds due to aersol concentration affecting ice-nucleation processes.
- Entropy methods:
  - Hope you saw Jerry Watkins' talk "Entropy-based feature selection for capturing impacts in earth system models with extreme forcing" on June 10!
- Capability to modify pointers in CLDERA-Tools:
  - Enables implementing various control-algorithms.
  - Sensitivity, perturbation analysis; causality.

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