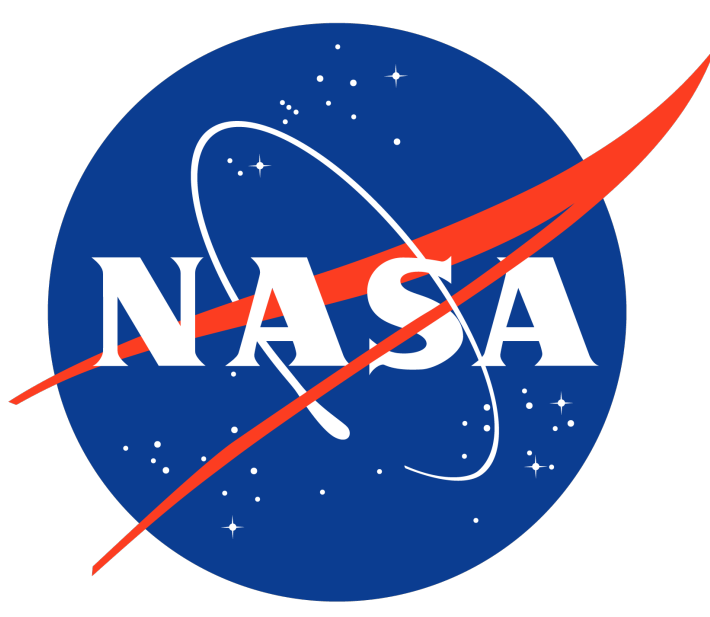




Developing methods for efficient transport and chemistry calculations in GEOS-CF

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Summary

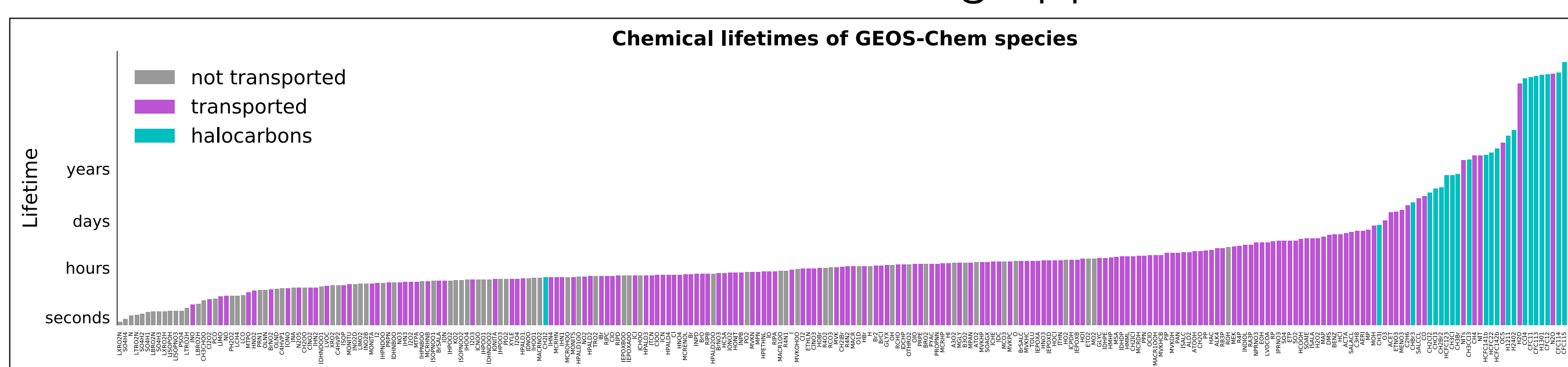
- We have identified ways to selectively reduce complexity in GEOS-CF to improve computational performance
- We explore:
 - reducing chemical complexity in transport
 - reducing spatial resolution under certain conditions
 - in replay simulations, skipping predictor chemistry
- The main slowdown originates from numerical stiffness of the chemical system under twilight conditions

Context/Significance

- A current limitation of many Earth system models (ESMs) is omission of detailed chemical mechanisms due to computational cost
- The GEOS-CF¹ system produces global predictions of atmospheric composition using the GEOS-Chem module at 0.25° resolution²
- Due to its chemical detail and high spatial resolution, GEOS-CF is computationally demanding

Approach 1: Advecting a reduced set of species

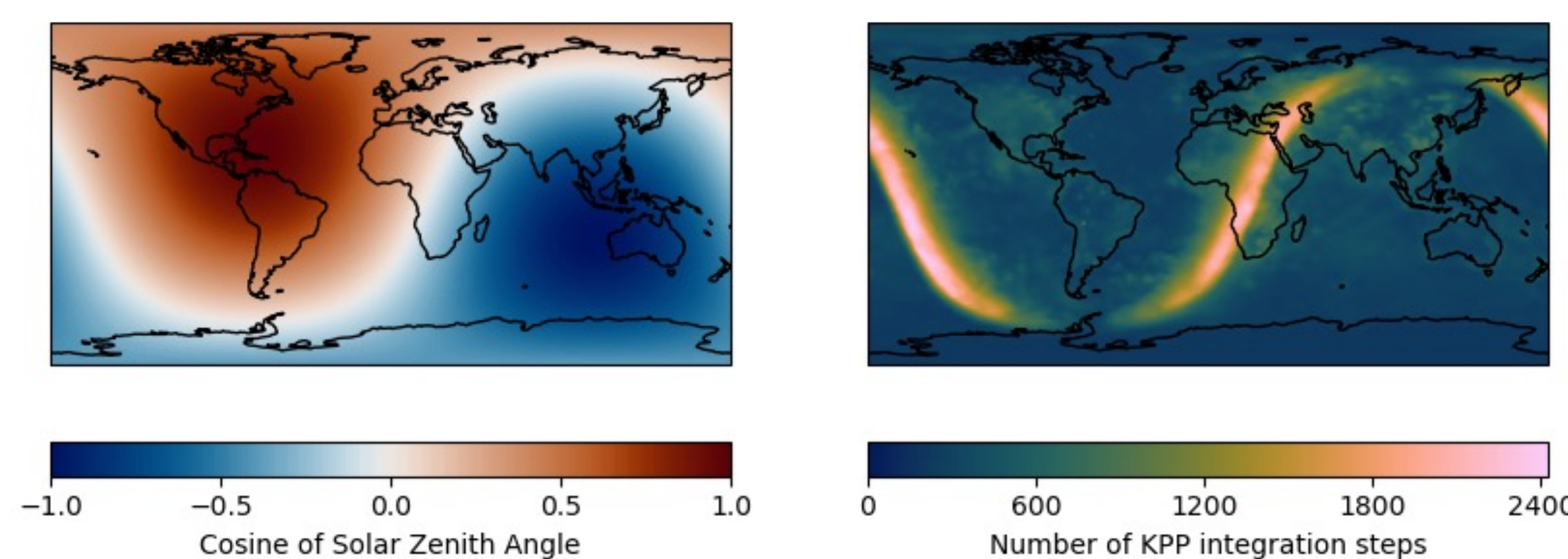
- Prior work has explored reducing the dimensionality of transported particle species³⁻⁶, motivated for a latent chemical space including gas phase species⁷
- We omit species with chemical lifetimes longer than the 5-day time horizon of interest in forecasting applications.



- Aside from species with specific emissions sources (e.g. CO), longer lifetimes can be used as a proxy for small concentration gradients, affected minimally by transport
- We find **reduced advection has a limited effect on speedup**

Rediagnosing slowdown: Chemistry in the twilight zone

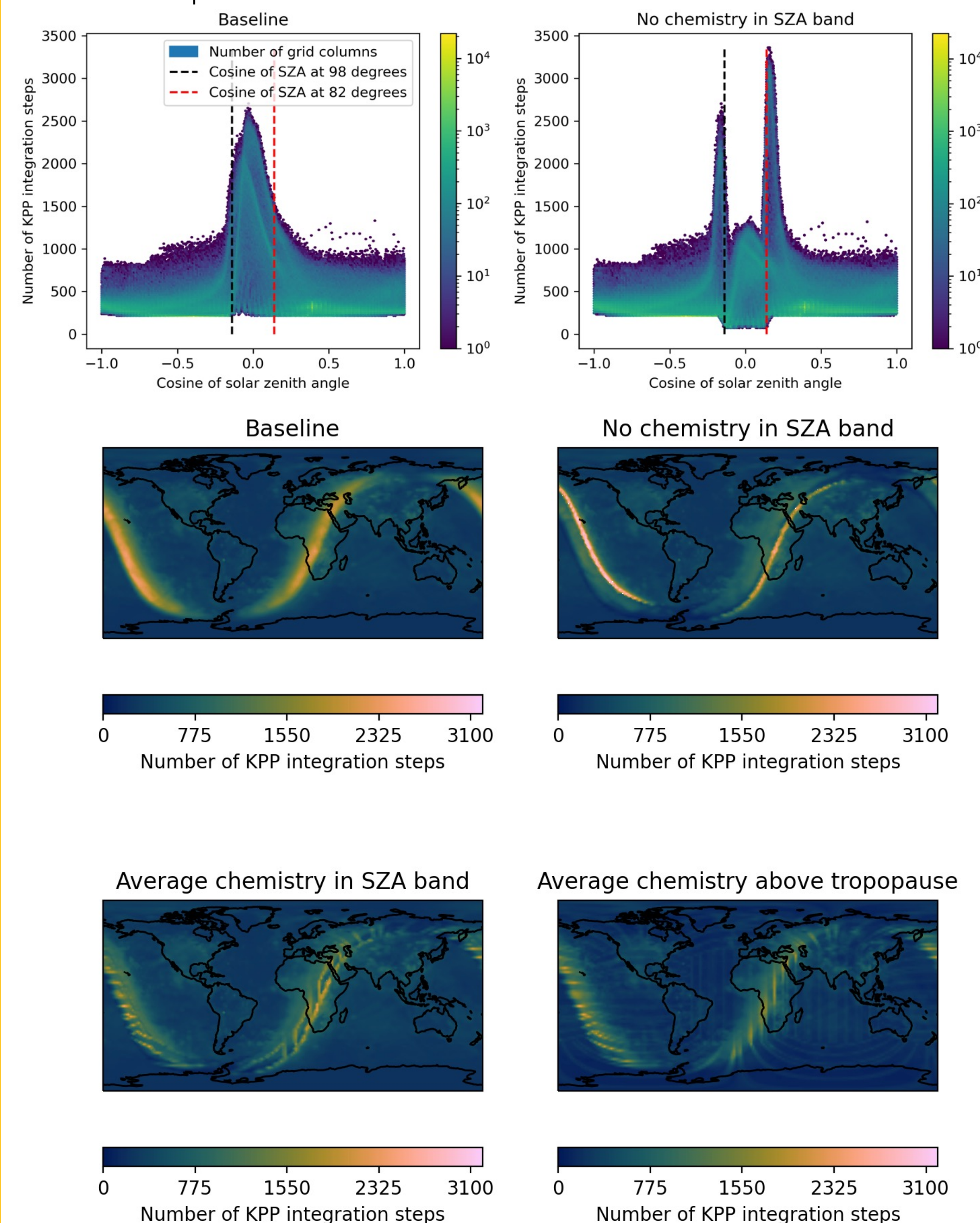
- Slowdown arises from a **load imbalance caused by twilight chemistry**, previously attributed to advection due to a parallel computing barrier
- All computing nodes must wait for nodes with a larger fraction of grid cells near the day/night terminator
- 13% of grid cells take up over 30% of the integration steps**



Approach 2: Chemistry at coarser spatial resolution

We try several approaches to even the load balance:

- 1) skipping twilight stratospheric chemistry terminator,
- 2) computing **stratospheric chemistry on a coarser grid** near the terminator, by averaging values of grid cells
- 3) computing chemistry on a coarser grid in the entire stratosphere



Approach 3: No chemistry in replay predictor step

- With a focus on chemistry as the source of slowdown, we identify a redundancy in the operator sequence during replay simulations⁸
- We **skip** the call to **chemistry during the predictor step** with a negligible effect on composition
- Over a 5-day simulation window 99% percent of ozone concentrations remained within 0.14 ppb with a maximum error of 4 ppb in the stratosphere

References

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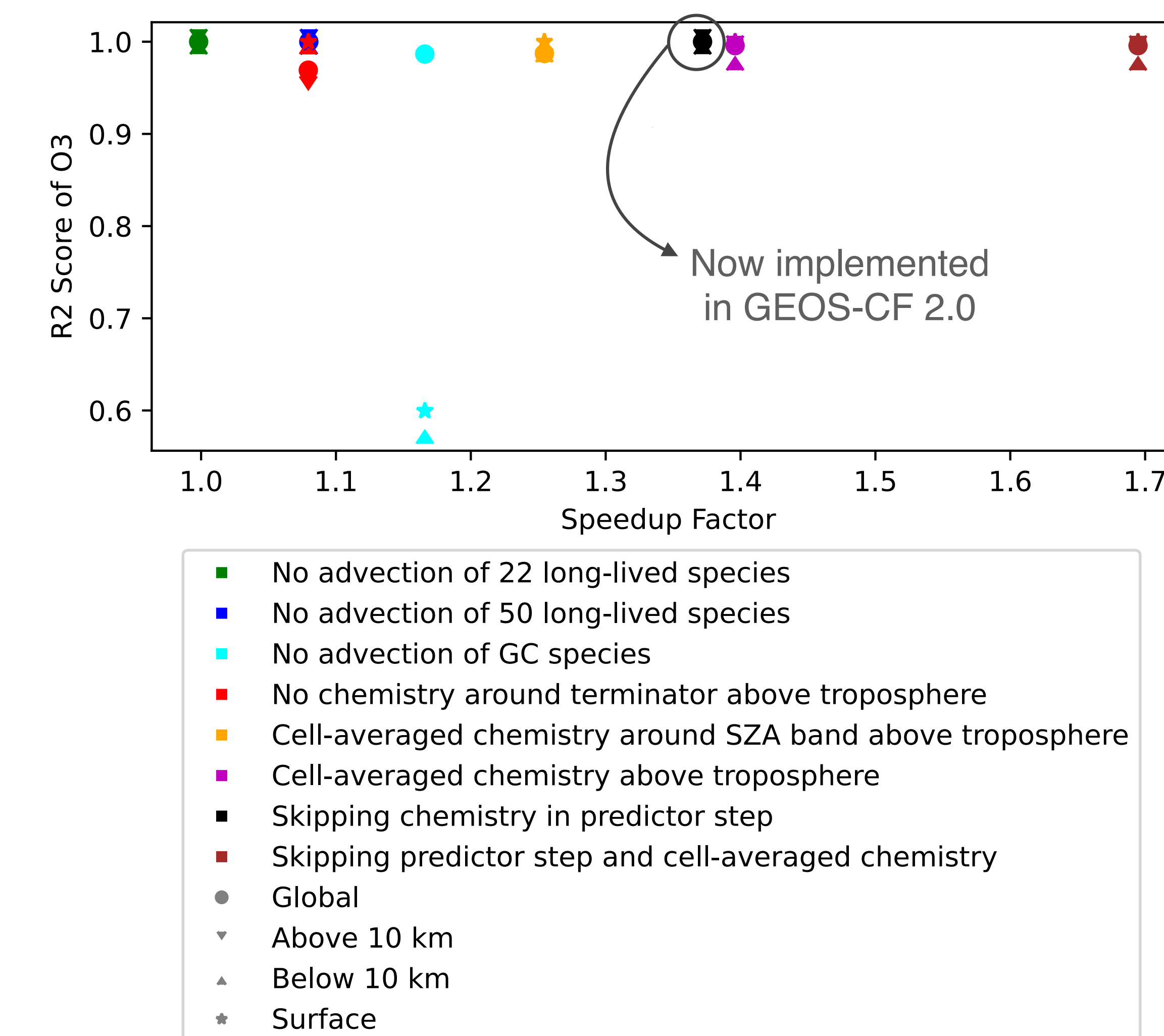
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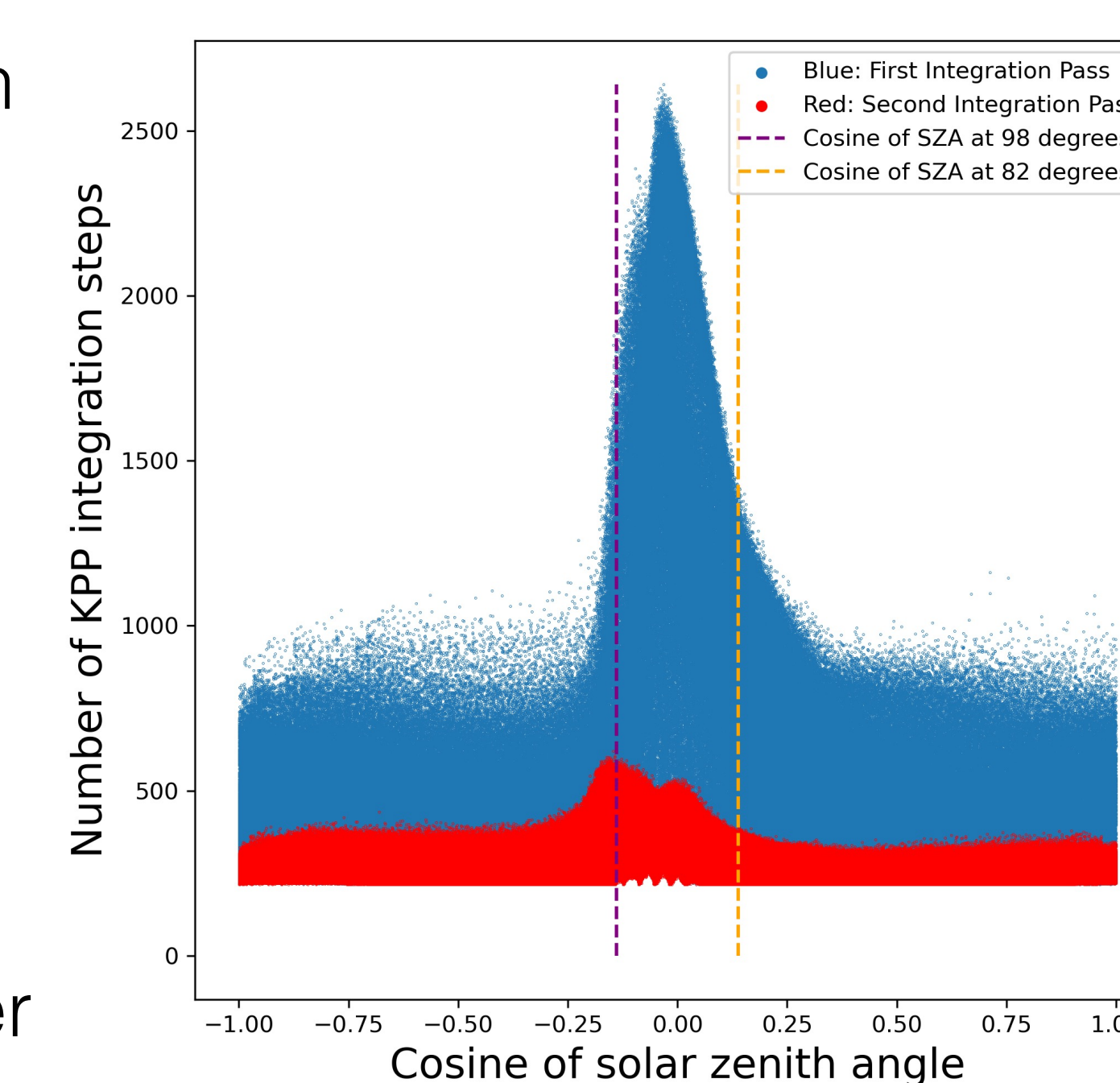
Overview: Speedup versus accuracy

- Reduced transport approaches were bounded by a speedup of 17%
- Skipping terminator chemistry delayed difficult chemistry, led to high error with only 8% speedup
- Cell-averaged stratospheric chemistry led to a speedup of 25% when applied around the terminator, and 39% when done throughout.
- Approach 3 led to a speedup of 37% with a negligible effect on ozone concentration



Next steps: Precondition the chemical state?

- Can we precondition the chemical state using machine learning⁹
- Would a “perfect guess” reduce integration counts?
- In GEOS-CF a 2nd call to the KPP integration routine converges with fewer integration counts



- We use a box model of KPP 3.0¹⁰ to explore **which species contribute to computational intensity**

