Stretched Grids for Simulations of Atmospheric Chemistry with GEOS-Chem High Performance

Liam Bindle

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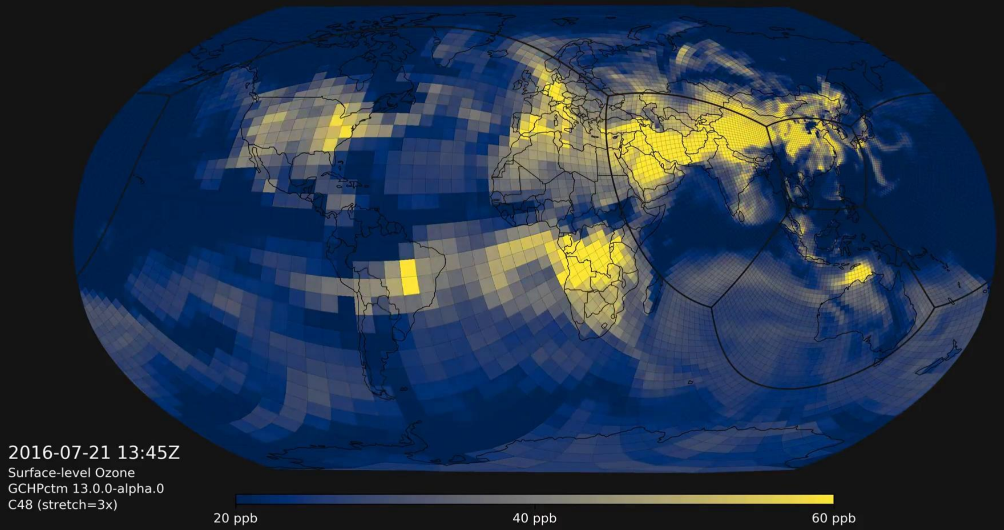


Washington University in St. Louis

Atmospheric Composition Analysis Group

Some background on GEOS-Chem

- First described in Bey et al., 2001
- Community model
  - New release every 3 months
  - 35 members on the Steering Committee
- 5 full-time support staff (Harvard + WashU)
- Multiple interfaces
  - GC-Classic
  - GEOS-Chem High Performance (GCHP)
  - GEOS-Chem in GEOS-5
  - CESM-GC
  - WRF-GC

9th International GEOS-Chem Meeting (IGC9) – Harvard University, 2019
Credit: https://geos-chem.seas.harvard.edu/geos-meetings-2019-igc9

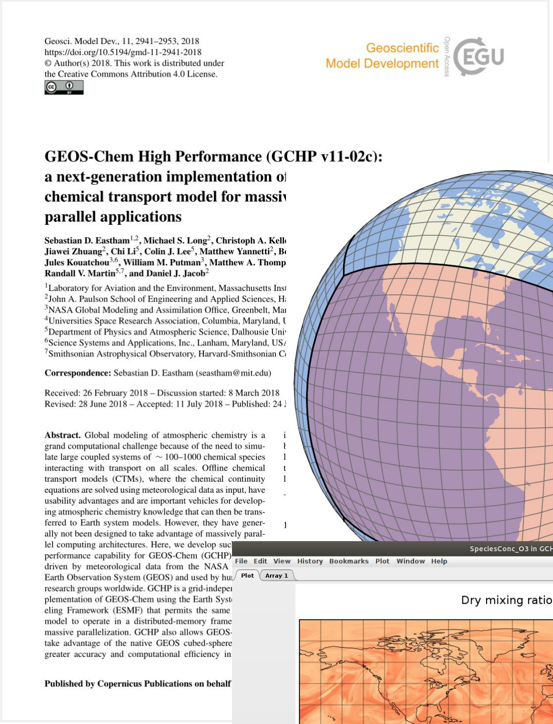
GEOS-Chem users around the world
Credit: https://geoschem.github.io/geos-chem-people-projects-map/

GEOS-Chem High Performance (GCHP)

- Offline CTM (Eastham et al., 2018, GMD)
- Capable of multi-node simulation
- Uses FV3 (similar to UFS)

- Horizontal: cubed-sphere grid
- Vertical: surface to 1 Pa

- Capable of simulations on thousands of cores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Geoscientific Model Development
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GEOS-Chem High Performance (GCHP v11-02c): a next-generation implementation o chemical transport model for massiv parallel applications

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Abstract. Global modeling of atmospheric chemistry is a grand computational challenge because of the need to simulate large coupled systems of ∼ 100–1000 chemical species interacting with transport on all scales. Offline chemical transport models (CTMs), where the chemical continuity equations are solved using meteorological data as input, have usability advantages and are important vehicles for developing atmospheric chemistry knowledge that can then be transferred to Earth system models. However, they have generally not been designed to take advantage of massively parallel computing architectures. Here, we develop suc performance capability for GEOS-Chem (GCHP) driven by meteorological data from the NASA Earth Observation System (GEOS) and used by hu research groups worldwide. GCHP is a grid-indepe plementation of GEOS-Chem using the Earth Syst eling Framework (ESMF) that permits the same model to operate in a distributed-memory frame massive parallelization. GCHP also allows GEOS take advantage of the native GEOS cubed-sphere greater accuracy and computational efficiency in

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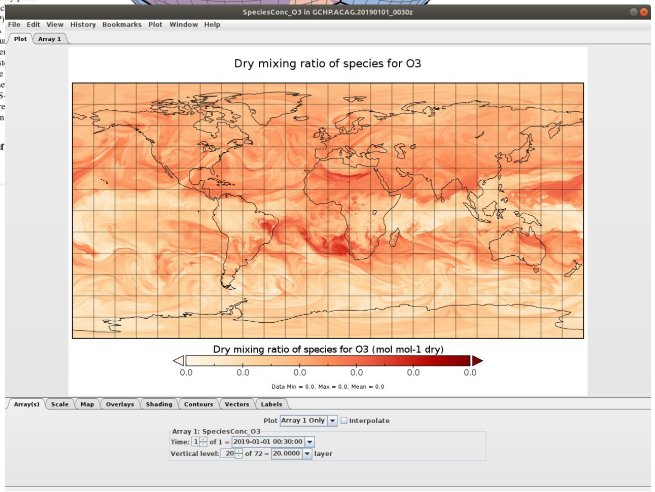
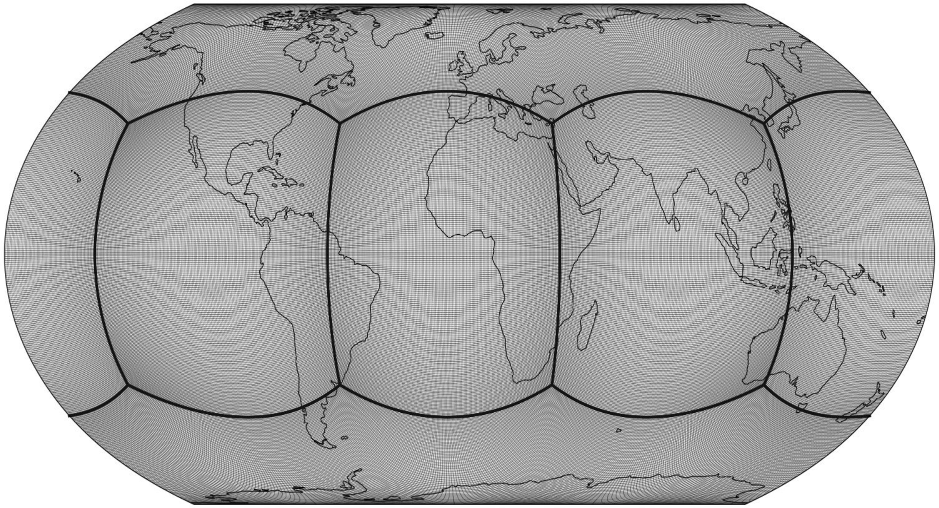
(Eastham et al., 2018,



Fine resolution output from GCHP.
Credit: https://gchp.readthedocs.io/en/latest/supplement/plotting-output.html

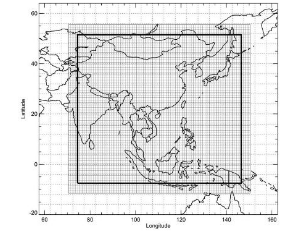
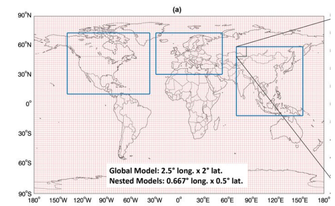
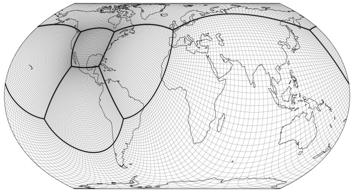
The lack of a grid refinement capability is limiting

- Global fine resolution is expensive
- C180 (~50 km)
    - 194,400 cells per level, 72 levels
    - 1-year simulation takes ~8 days with 900 cores
- 2x resolution => 4x problem size
- Studies often focus on a specific geographic region



Lots of grid cells are needed for ~50 km resolution.

There are several refinement techniques to choose from

Method	Advantages	Drawbacks	
Nested grids (1-way)	+ Simple + Multiple refined regions	– No global feedback – Needs boundary conditions	 From: Wang et al., 2004 (JGR)
Nested grids (2-way)	+ Allows for feedbacks + Multiple refined regions	– Moderate complexity (simulations are dynamically coupled)	 From: Yan et al., 2014 (ACP)
Grid stretching	+ Easy to use + No boundary conditions + Inherent 2-way coupling	– Single refinement	
Adaptive grids	+ Dynamic refinement + Most accurate (in theory)	– High complexity	< No global CTM examples >

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Why grid-stretching is well suited for GCHP

- Easy to use
  - Runtime parameters
  - No boundary conditions

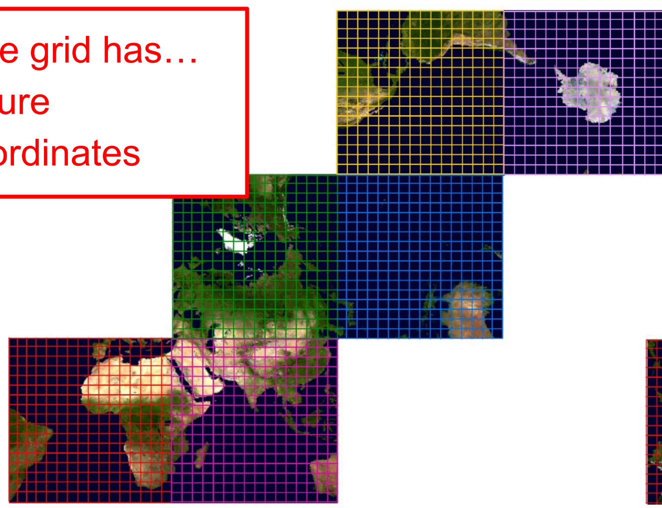
- Single refinement limitation counterbalanced by global fine res. capability

- Relatively easy to implement
  - Long et al. (2015) – Grid independent capability of GEOS-Chem
  - Harris et al. (2016) – Stretched grid capability for FV3
  - Weng et al., (2020) and GEOS-Chem 12.5.0 – Grid independent emissions

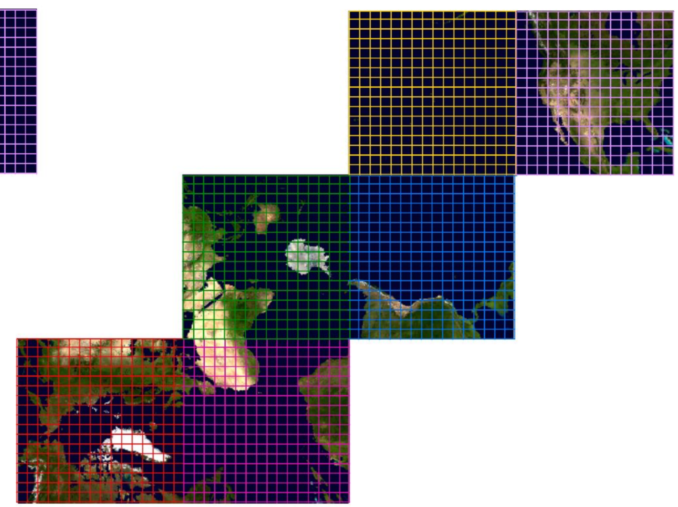
Takeaways. The grid has…
- Same structure
- Different coordinates

(the model's pe

Standard Cubed-Sphere Layout



Stretched Cubed-Sphere Layout



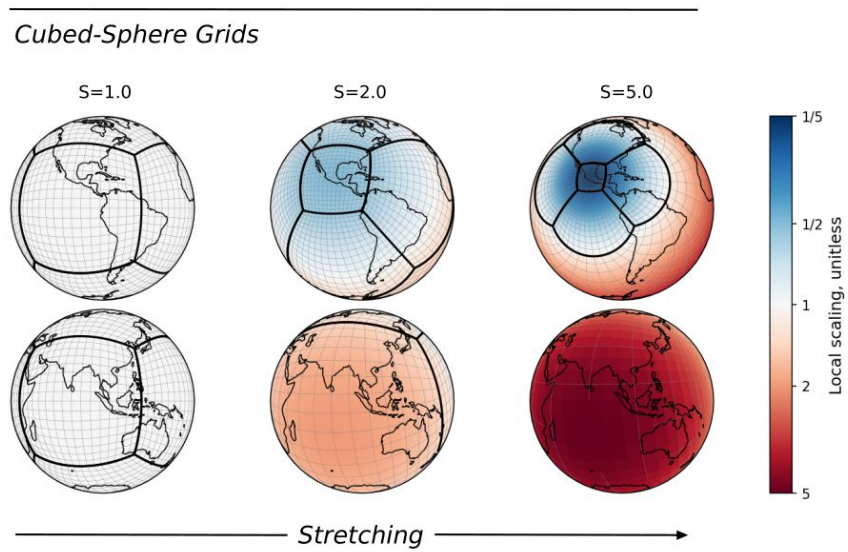
Stretched-grid parameters and notation

Runtime parameters

- S – stretch factor
- T – target point
- Cubed-sphere size (e.g., C120)

Our notation

- Standard cubed-sphere: e.g. C180-global
- Stretched cubed-sphere: C180e-US



Validating stretched-grid simulations in GCHP

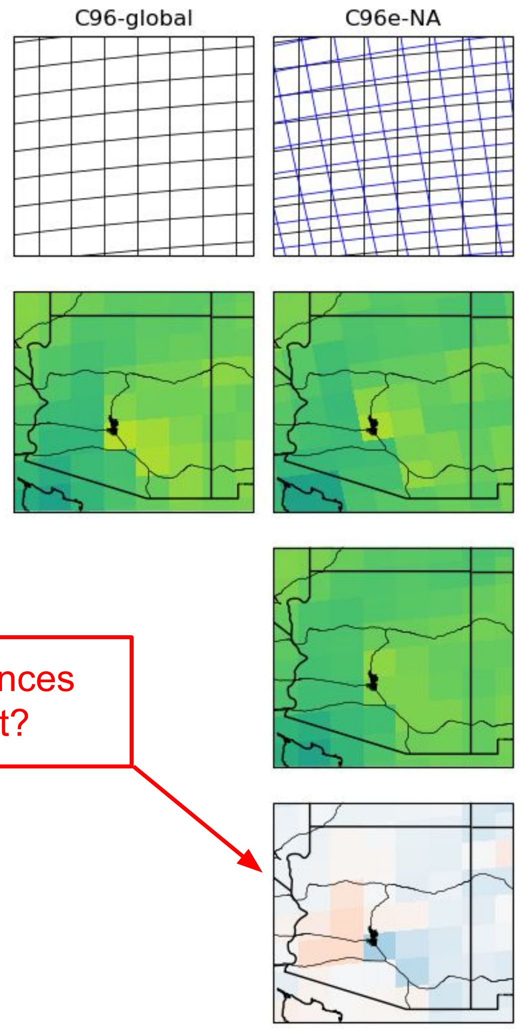
(there’s something interesting here)

How do we check if it works?

- Look through the code
- Check that the simulation runs
- **Compare output from stretched-grid and cubed-sphere simulations (via regridding)

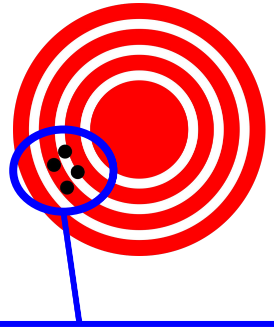
**More complicated than it seems

Aliasing effects from upscaling emissions…



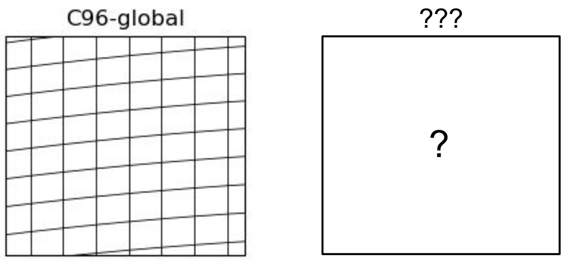
What kind of differences should we expect?

Precision (and Accuracy)



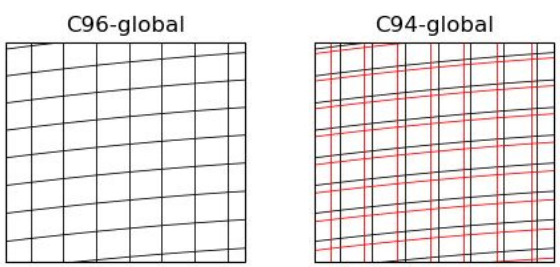
What level of precision should we expect?

We need a way to gauge expected differences



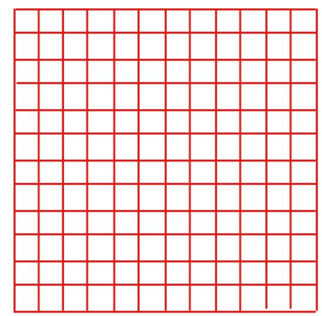
- If we were to shift the C96-global grid and rerun the simulation, what differences would we see?

- Alternatively, we could compare C96-global to a C94-global simulation

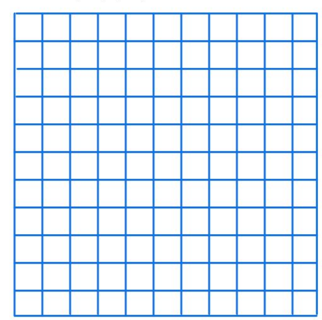


Similar regular grids overlap poorly

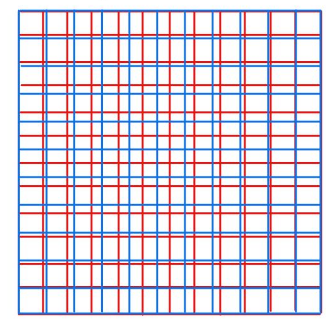
Grid #1: NxN



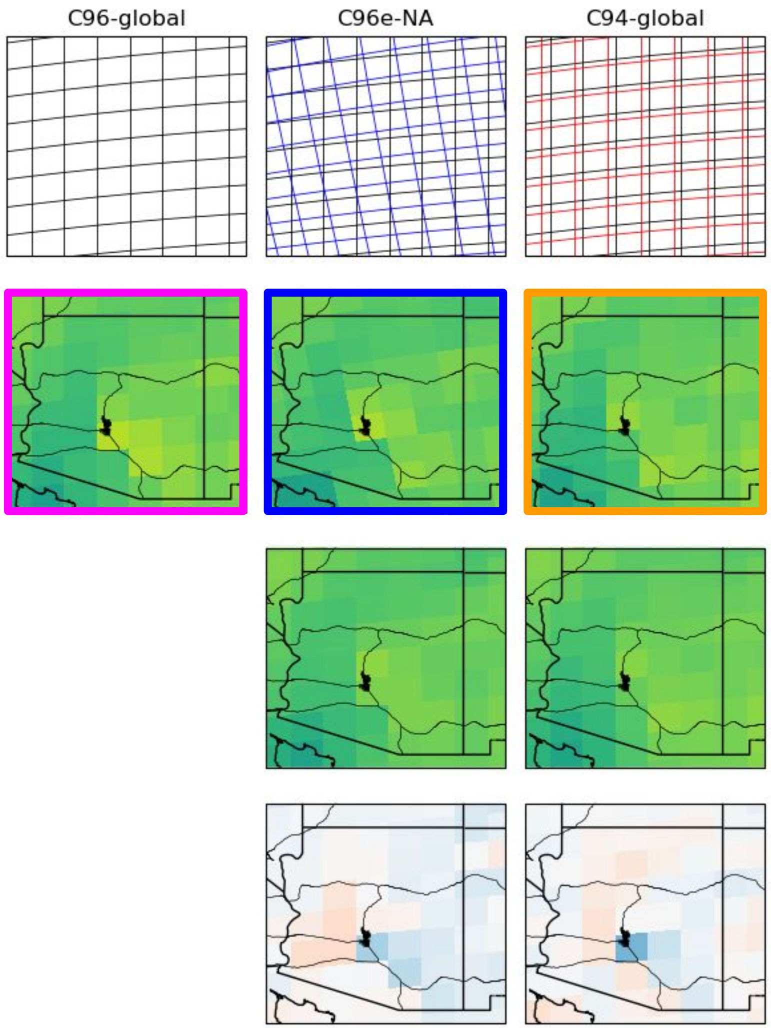
Grid #2: (N-1)x(N-1)



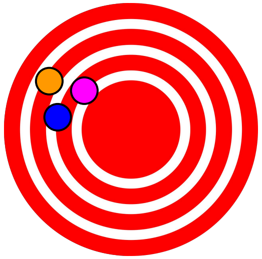
Grid-box **overlap is minimal**, but grid **resolution is similar**



Recap of the method



<u>Precision (and Accuracy)</u>



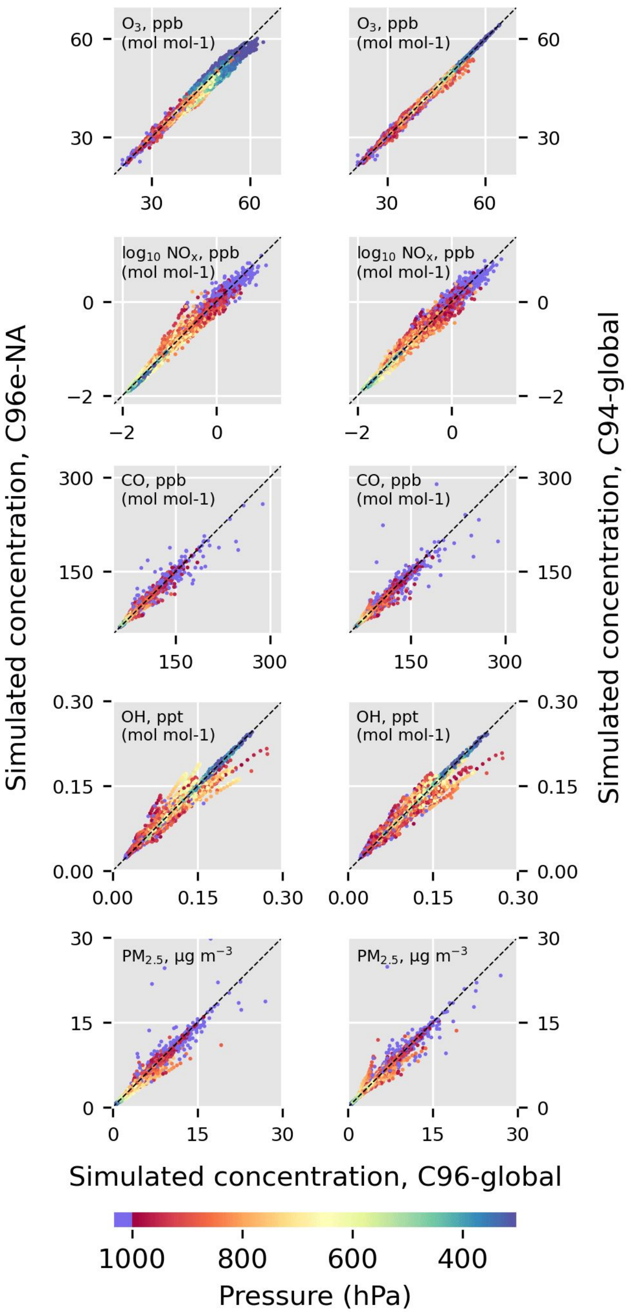
Validation experiment

3 simulation comparison

- C96-global
- C96e-NA
- C94-global

LHS: C96e-NA vs. C96-global

RHS: C94-global vs. C96-global



Conclusion

The differences in the stretched-grid simulation are consistent with what we should expect.

Stretched-Grid Simulation Demos

Two avenues to explore: efficiency and resolution

1. For efficiency (two simulations, same resolution)
2. For resolution (two simulations, same grid size)

For both, we will consider **regional comparisons** of simulated **tropospheric NO2 columns** with observations from TROPOMI.

Comparing sim. and obs. NO_2 columns in CONUS (Set Up)

Two simulation comparison

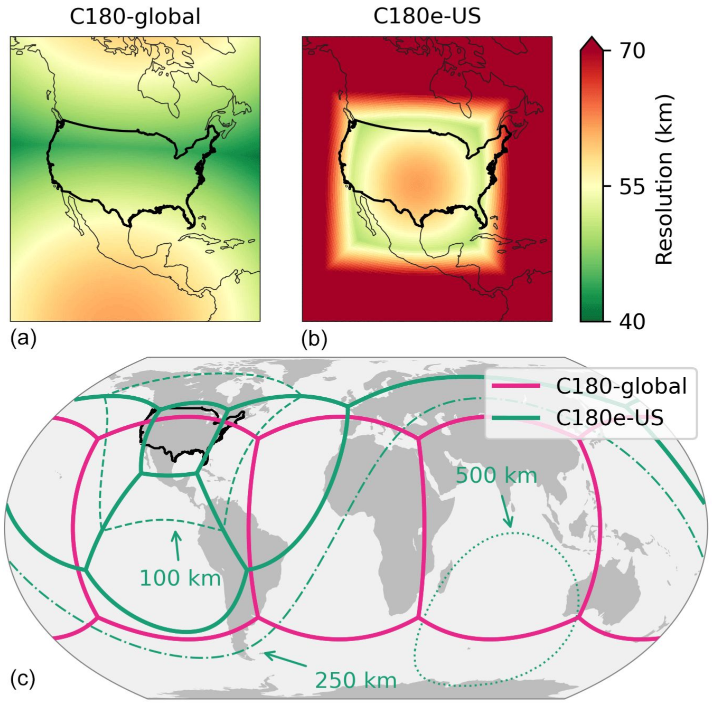
1. C180-global (48 km in US)
2. C180e-US (57 km in US; C60, S=3.0)

Similar resolutions in US,
but stretched-grid simulation has
9x fewer grid-boxes.

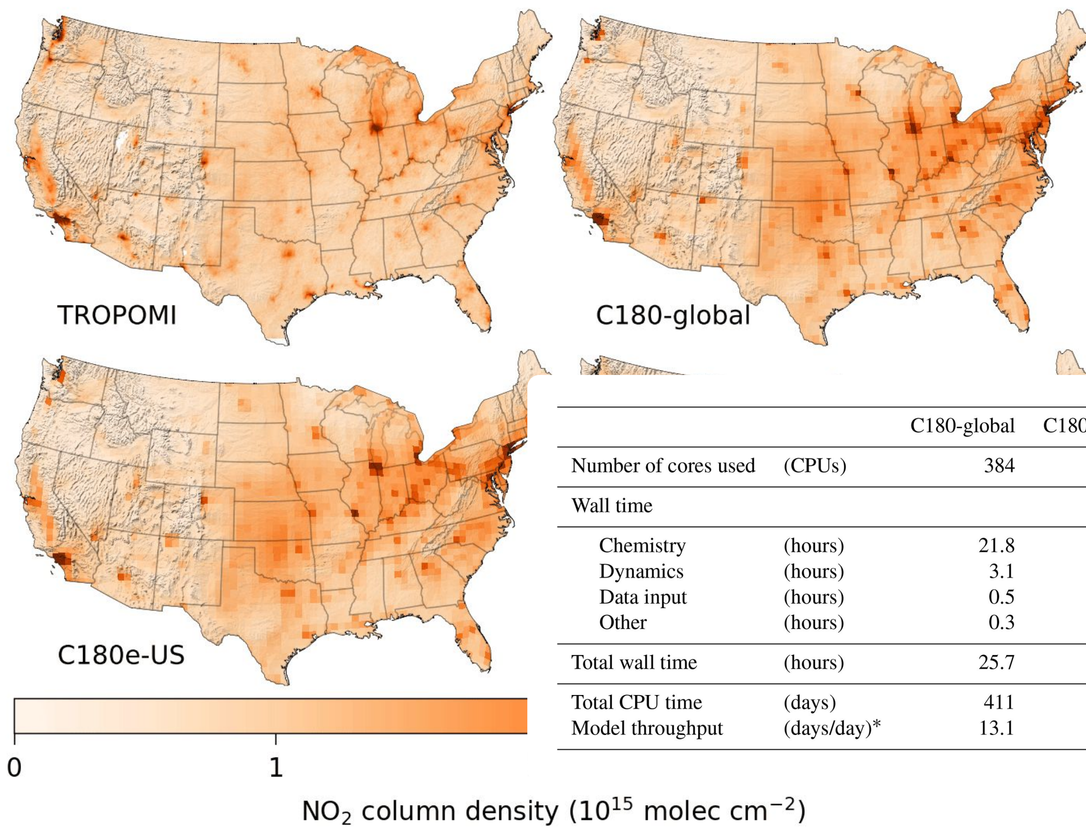
Questions

Does C180e-US produce similar results?

How does their computational compare?



Comparing sim. and obs. NO_2 columns in CONUS



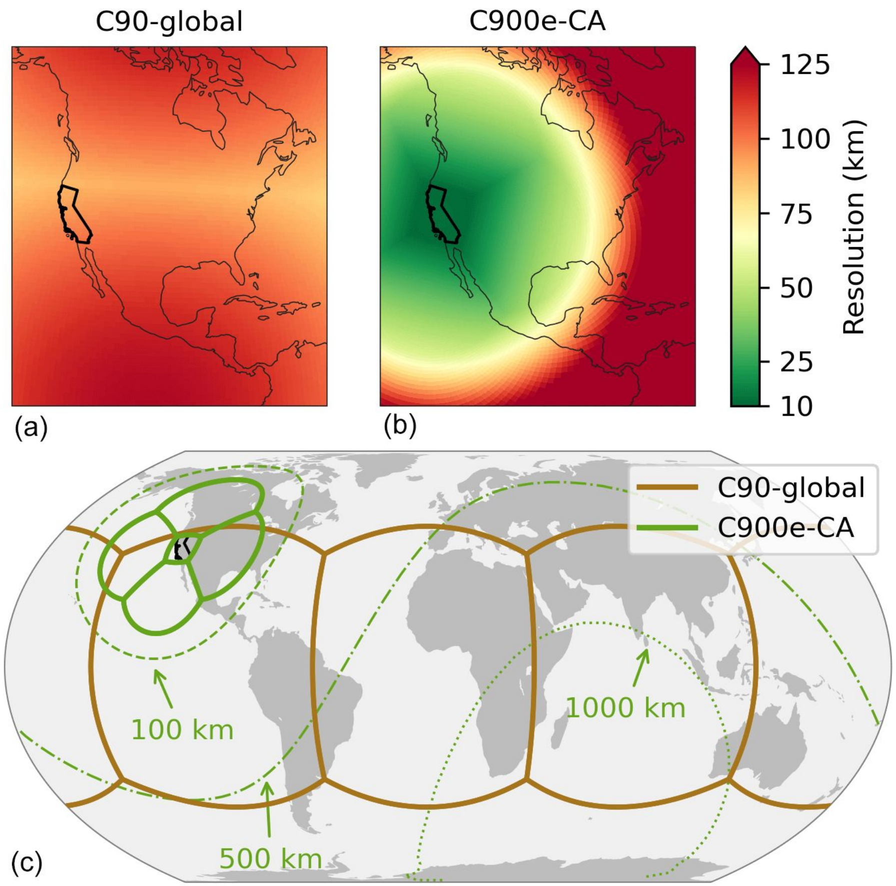
		C180-global	C180e-US	C60-global
Number of cores used	(CPUs)	384	48	48
Wall time				
Chemistry	(hours)	21.8	7.0	7.2
Dynamics	(hours)	3.1	1.7	1.7
Data input	(hours)	0.5	1.8	0.3
Other	(hours)	0.3	0.2	0.2
Total wall time	(hours)	25.7	10.7	9.4
Total CPU time	(days)	411	21.3	18.7
Model throughput	(days/day)*	13.1	31.4	35.7

Comparing sim. and obs. NO_2 columns in California (Set Up)

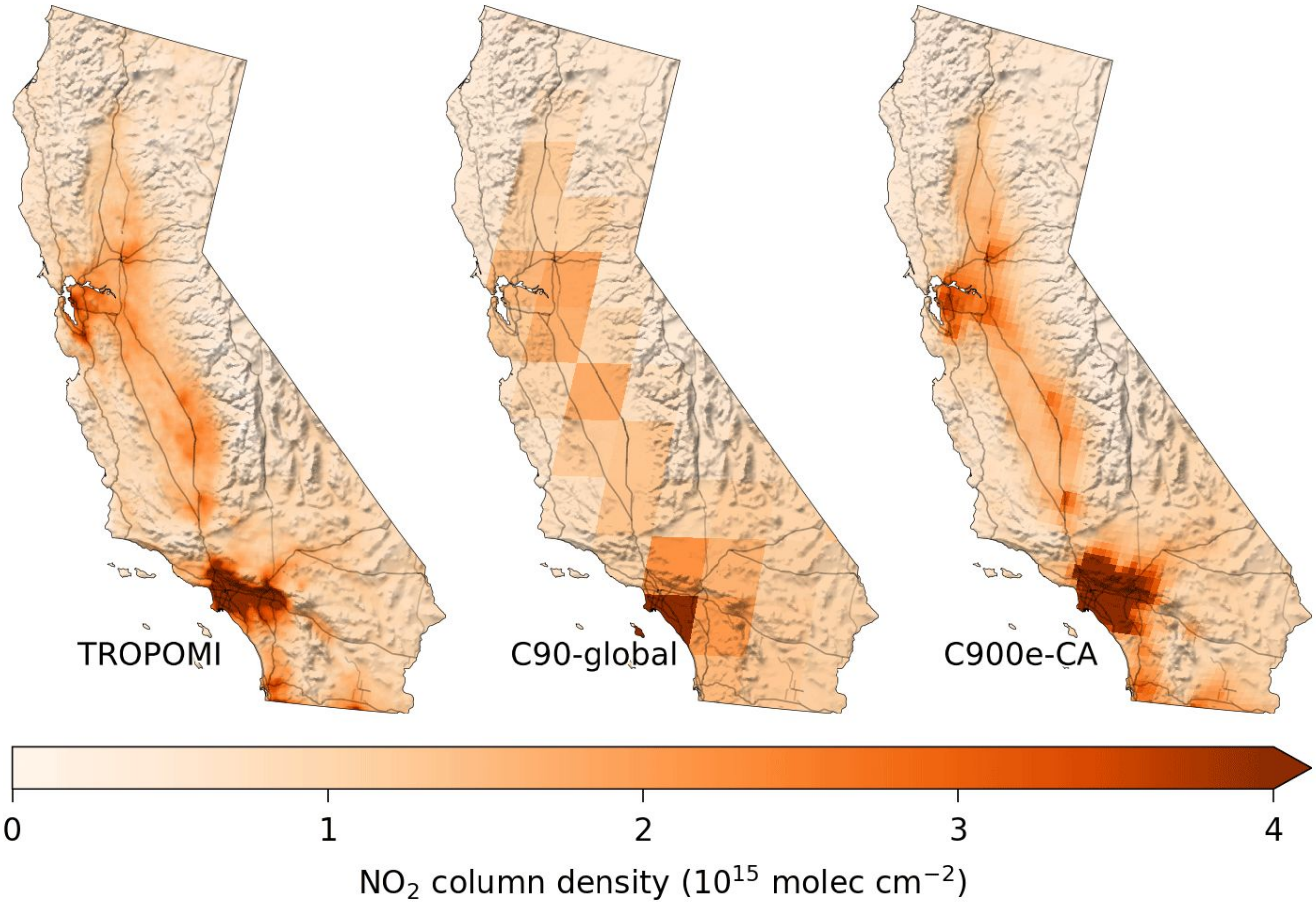
Two simulation comparison

1. C90-global
2. C900e-CA (11 km in CA; C90, S=10.0)

Same grid size (C90) but stretched-grid simulation uses S=10.



Comparing sim. and obs. NO_2 columns in California



Considerations for Stretched-Grid Simulations

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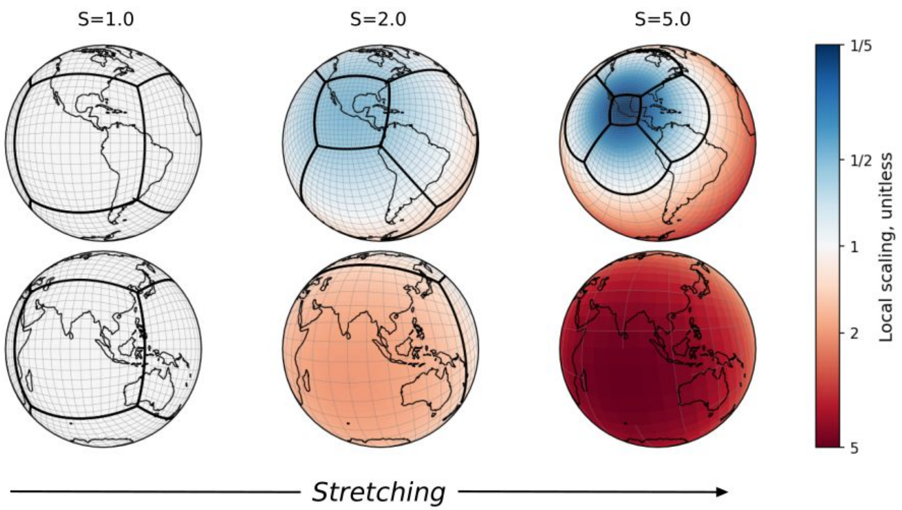
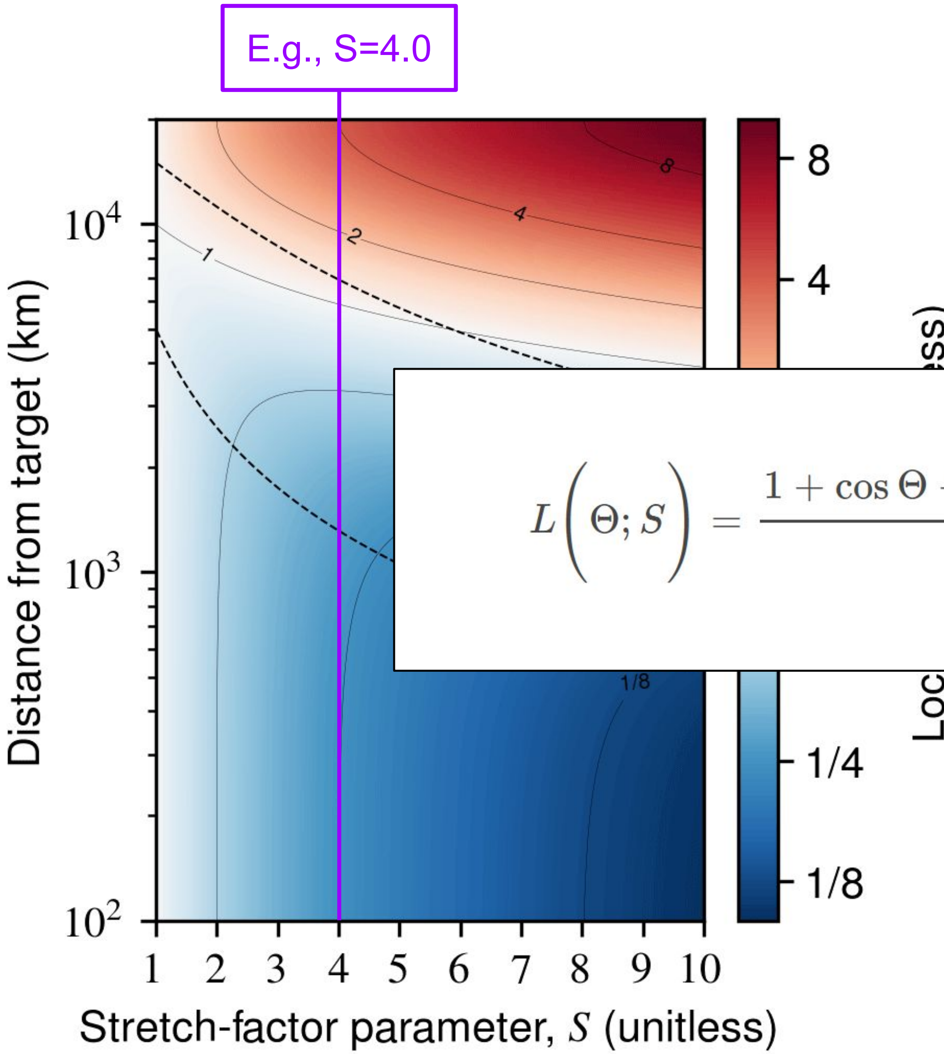
How can one choose appropriate stretching parameters?

- As stretch factor increases
  a. refined domain gets smaller
  b. grid-boxes opposite target face expand
- Implications are application specific – how can one determine an appropriate stretch factor?



Understanding how stretching changes with distance



$$L\left(\Theta; S\right) = \frac{1 + \cos\Theta + S^2\left(1 - \cos\Theta\right)}{2S}$$

Napkin calculation for choosing an appropriate stretch-factor

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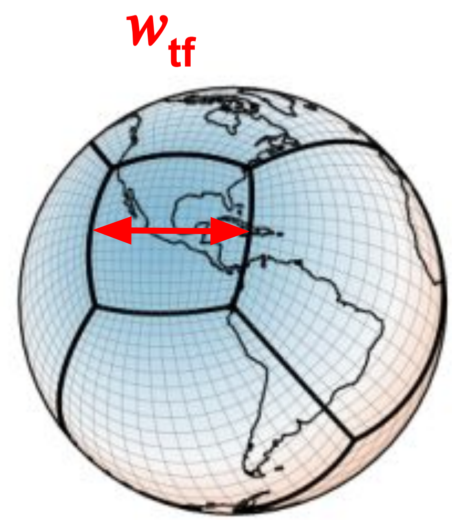
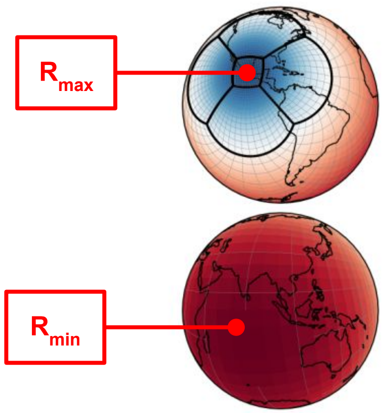
Constraint #1: Pick a width for the target face.

$$S \leq 0.414 \ \cot(w_{\mathrm{tf}}/4\ r_{\mathrm{E}})$$



Constraint #2: Pick a max & min resolution.

$$S \leq \sqrt{R_{\max}/R_{\min}}$$



Example

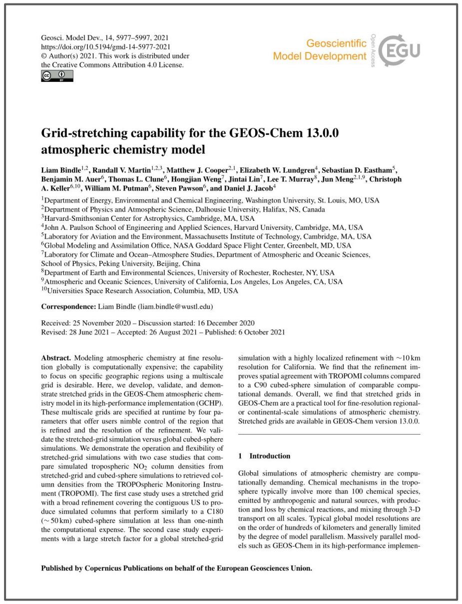
1. CONUS is ~4200 km across. w_{tf}= 4200 km
=> S ≤ 2.5
2. R_{min}=C360e (~25 km), R_{max}=C48e (~200km)
=> S ≤ 2.7

Some final thoughts

- Interactive tool for playing with stretching parameters: https://gchp.readthedocs.io/en/latest/stretched-grid.html
- Don’t disregard moderate stretch factors
- Keep the backside in mind; too coarse => STE issues (wind gradients whittled away)

Conclusions

- We added grid stretching to GCHP 13.0
- Stretched-grids are nimble and conceptually simple
- We used an estimate of expected differences from upscaled emissions to validate the capability
- We developed a simple method for estimating an appropriate upper limit for S



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Geoscientific Model Development

Grid-stretching capability for the GEOS-Chem 13.0.0 atmospheric chemistry model

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Abstract. Modeling atmospheric chemistry at fine resolution globally is computationally expensive; the capability to focus on specific geographic regions using a multiscale grid is desirable. Here, we develop, validate, and demonstrate stretched grids in the GEOS-Chem atmospheric chemistry model in its high-performance implementation (GCHP). These multiscale grids are specified at runtime by four parameters that offer users nimble control of the region that is refined and the resolution of the refinement. We validate the stretched-grid simulation versus global cubed-sphere simulations. We demonstrate the operation and flexibility of stretched-grid simulations with two case studies that compare simulated tropospheric NO_2 column densities from stretched-grid and cubed-sphere simulations to retrieved column densities from the TROPOspheric Monitoring Instrument (TROPOMI). The first case study uses a stretched grid with a broad refinement covering the contiguous US to produce simulated columns that perform similarly to a C180 (~50 km) cubed-sphere simulation at less than one-ninth the computational expense. The second case study experiments with a large stretch factor for a global stretched-grid simulation with a highly localized refinement with ~10 km resolution for California. We find that the refinement improves spatial agreement with TROPOMI columns compared to a C90 cubed-sphere simulation of comparable computational demands. Overall, we find that stretched grids in GEOS-Chem are a practical tool for fine-resolution regional- or continental-scale simulations of atmospheric chemistry. Stretched grids are available in GEOS-Chem version 13.0.0.

1 Introduction

Global simulations of atmospheric chemistry are computationally demanding. Chemical mechanisms in the troposphere typically involve more than 100 chemical species, emitted by anthropogenic and natural sources, with production and loss by chemical reactions, and mixing through 3-D transport on all scales. Typical global model resolutions are on the order of hundreds of kilometers and generally limited by the degree of model parallelism. Massively parallel models such as GEOS-Chem in its high-performance implemen-

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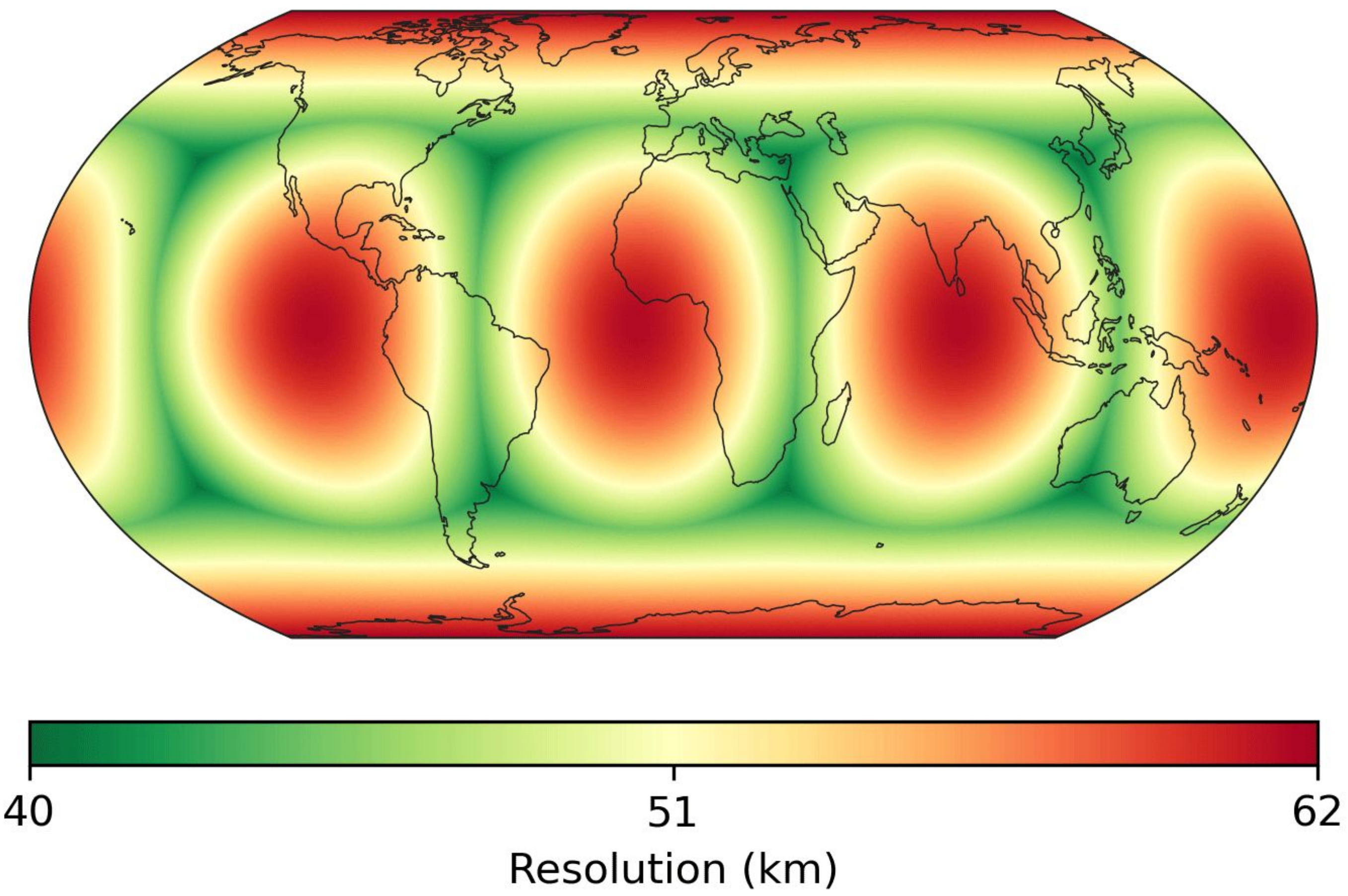
Future work that's needed

- Finer resolution meteorology and emissions data
- General purpose regridding method for C-grid vector fields

Link to our paper

Extra slides


40
51
62
Resolution (km)