# Chemistry Solver in the Energy Exascale Earth System Model

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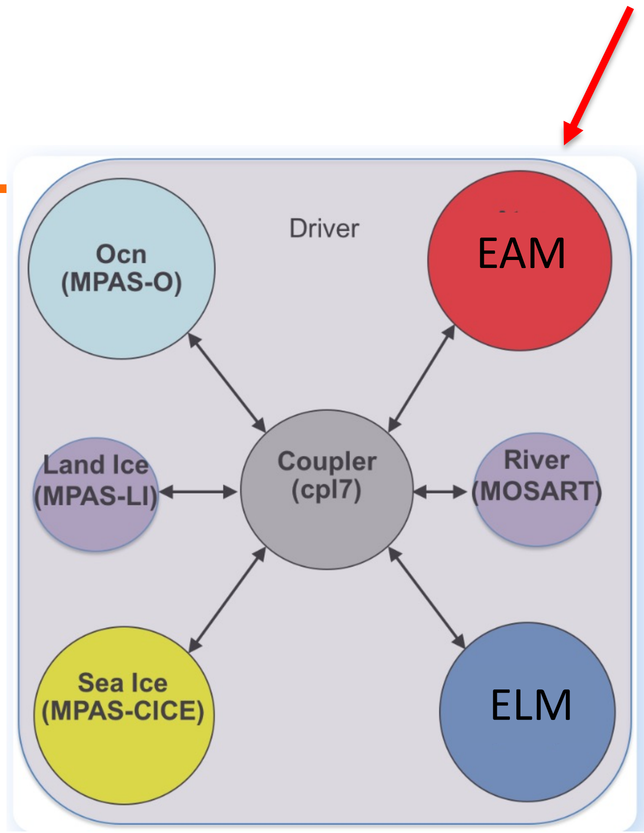
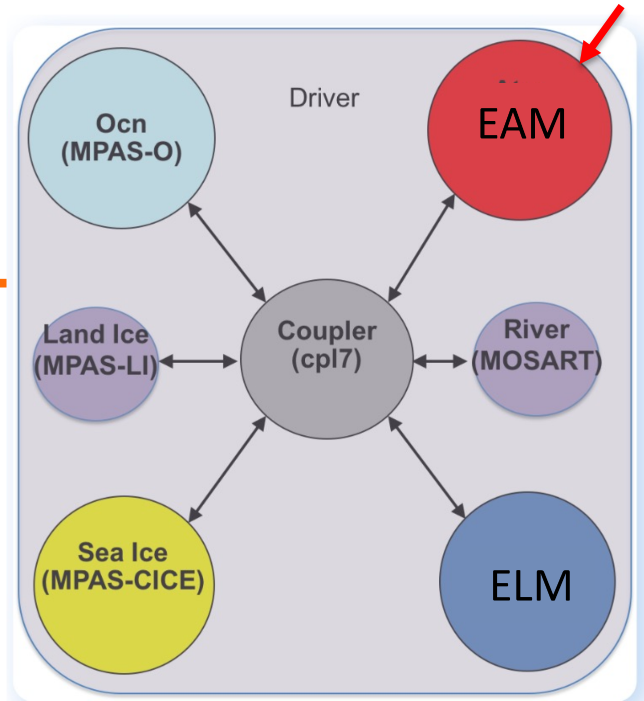
# The E3SMv1

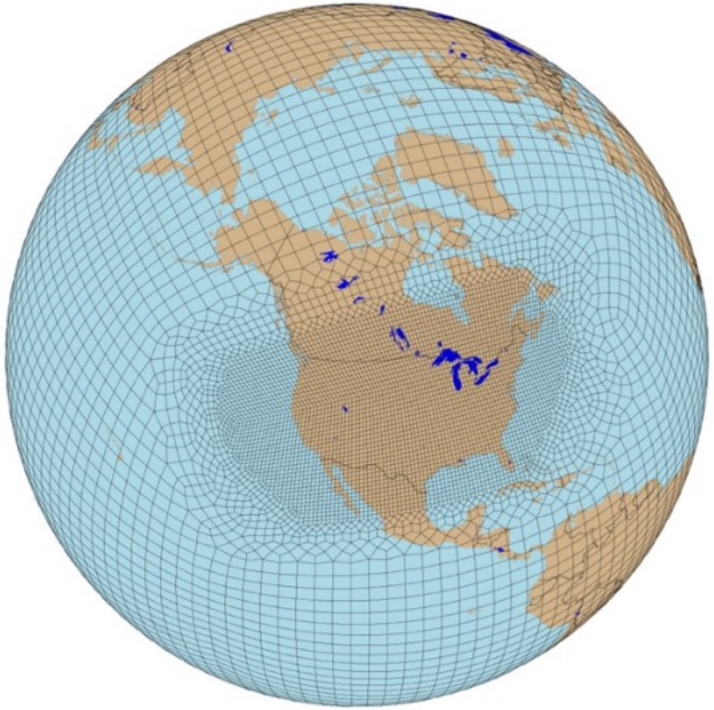
- Exascale Energy Earth System Model (E3SM) started with a version of CESM1, while notable changes occurred
  - EAM with spectral dynamic core
  - Ocean and Sea Ice based on the MPAS
  - ELM based on the CLM4.5, with more options in presenting the soil hydrology
- The E3SM present-day climate of the atmosphere showed credible compared to an ensemble of CMIP5



# The E3SMv1

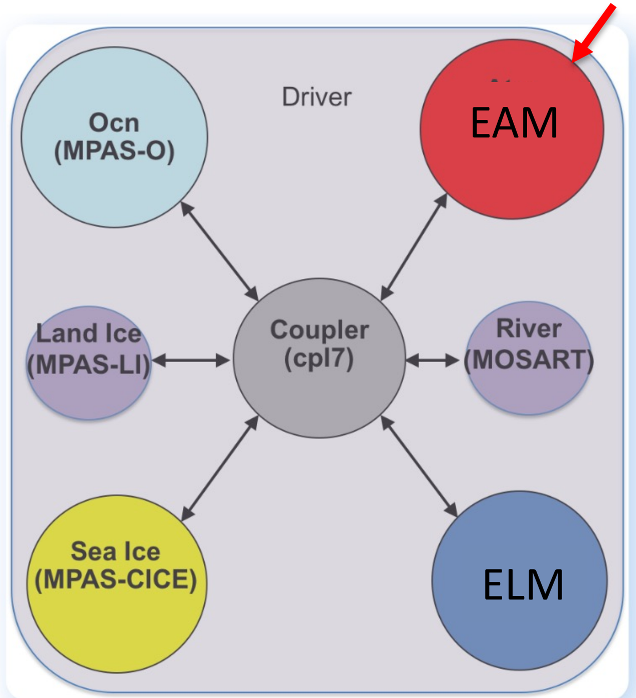
- E3SM atmosphere model (EAM) is based on the Community Atmosphere Model version 5 (CAM5): the spectral-element (SE) dynamical core was chosen as the default.
  - cloud microphysics, shallow convection, and turbulence parameterizations were replaced
  - the aerosol parameterization was enhanced substantially, and the vertical resolution was more than doubled (30 to 72 levels)
  - The physics parameterizations have been tested and well-tuned for both low- and high-resolution applications, which is important for addressing our v1 water cycle question.
- The E3SM present-day climate of the atmosphere showed credible compared to an ensemble of CMIP6

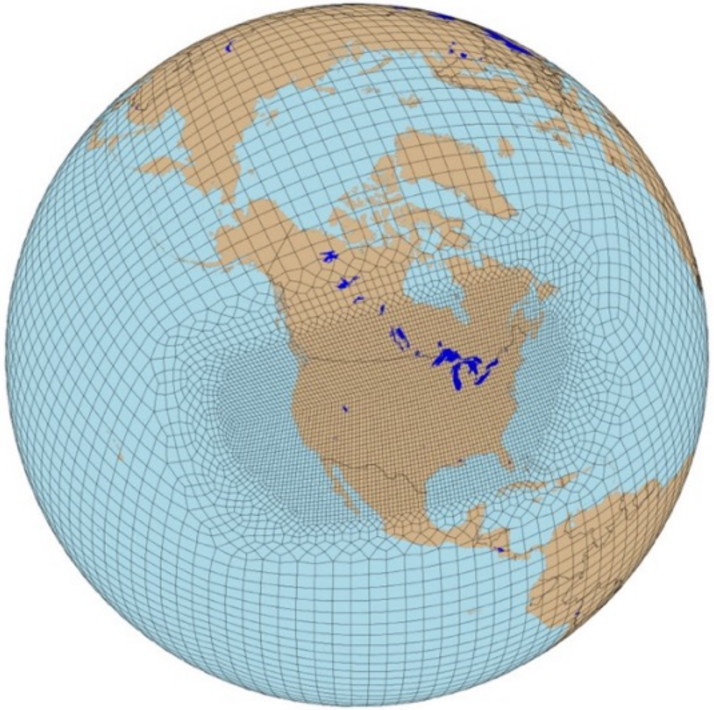


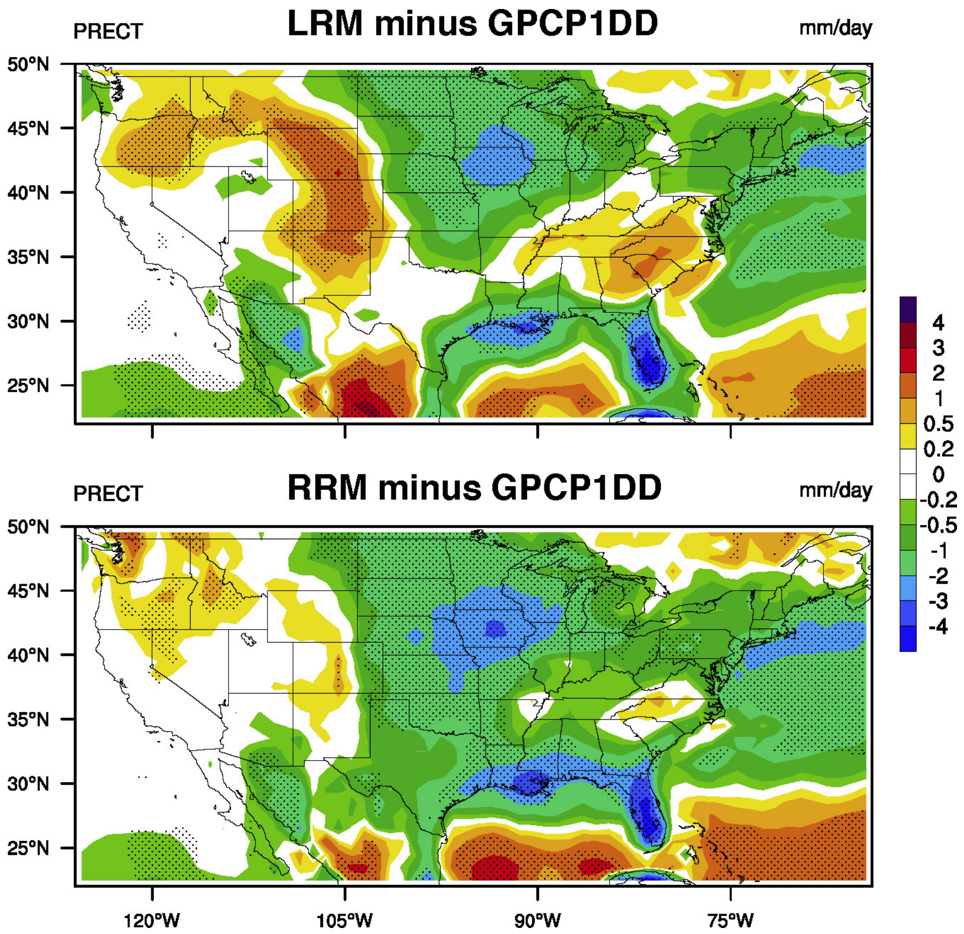
# The E3SMv1

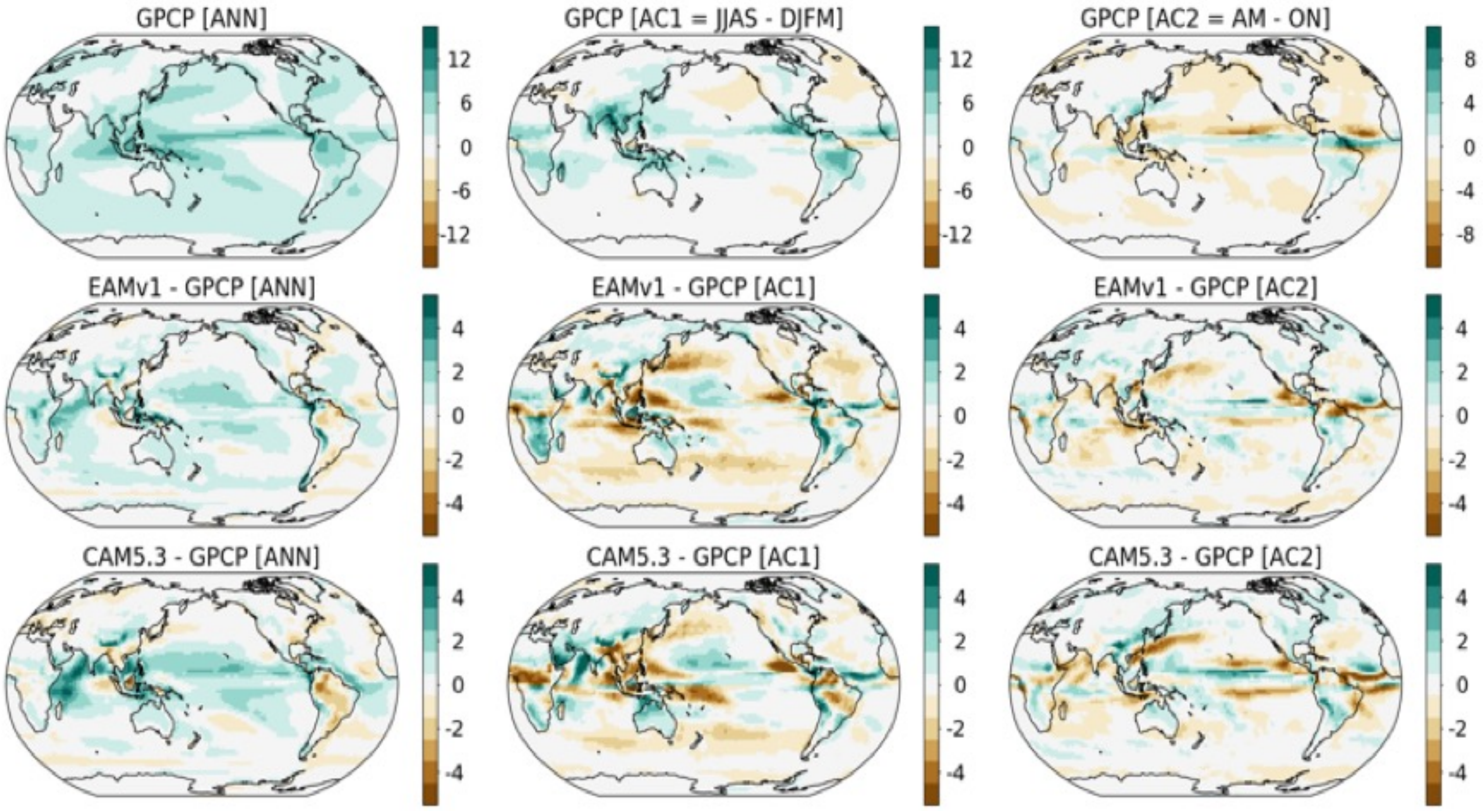
- The E3SM Atmosphere Model (EAM) is a descendant of the DOE/NSF supported Community Atmosphere Model version 5.3 (CAM5.3). EAM uses a Spectral Element Dynamical Core at low- (100km, LR) and high- (**25 km**, HR) resolution
- A variable resolution horizontal grid (termed a regionally refined model, or RRM), is sometimes used to reduce the computational cost of high resolution simulations at a region scale.
- Improved or new satellite and ground-based cloud and aerosol simulators were developed to better evaluate clouds, aerosols, and aerosol-cloud interactions.



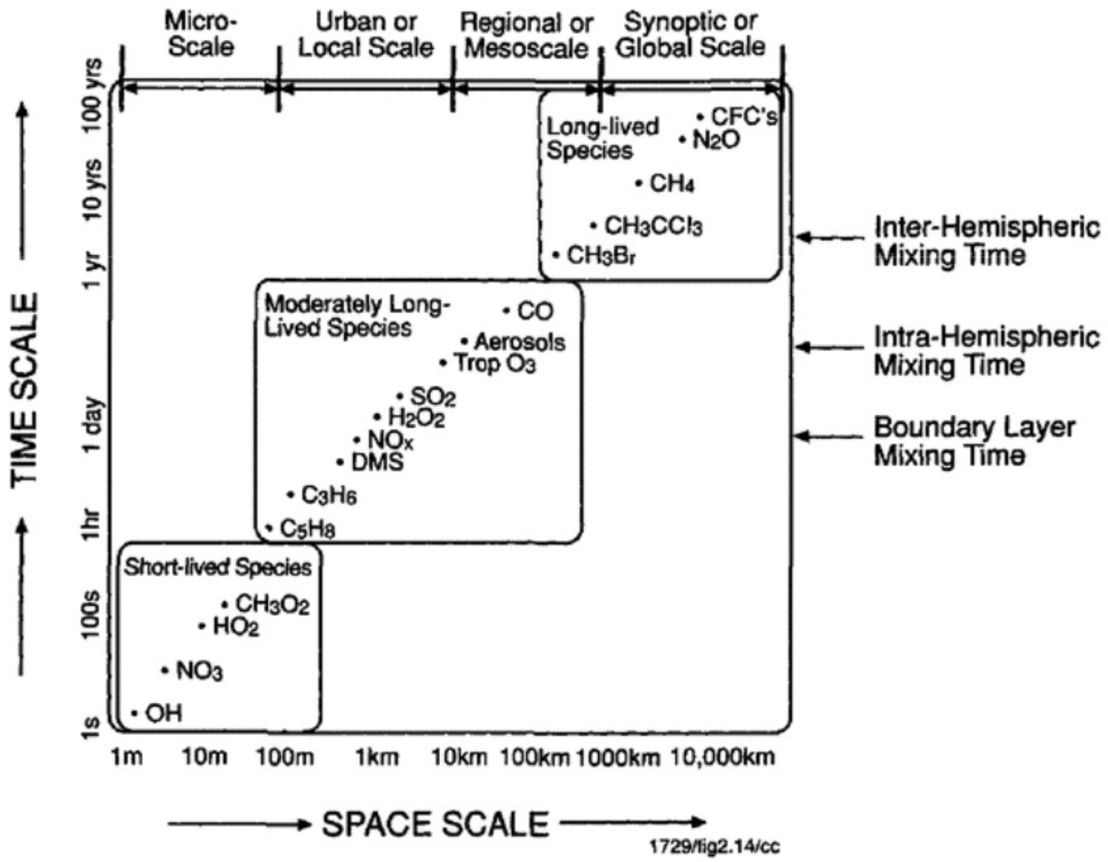
# The E3SMv1 Improvement



# Chemistry species in the global climate

- Atmospheric chemistry is important, yet for most non-fully coupled global model, the chemistry interaction within the model is not included
- Only 8 of 23 CMIP3 model contain black carbon, while less than half included the future tropospheric ozone
- Due to the wild range of chemical reaction rate and species lifetime, thus the chemical reaction system would be stiff and hence limited the choice of integral method




Adapted from Brasseur et al. (1999) Fig. 3.15

# Basic chemistry mechanism

- Take ozone formation as example

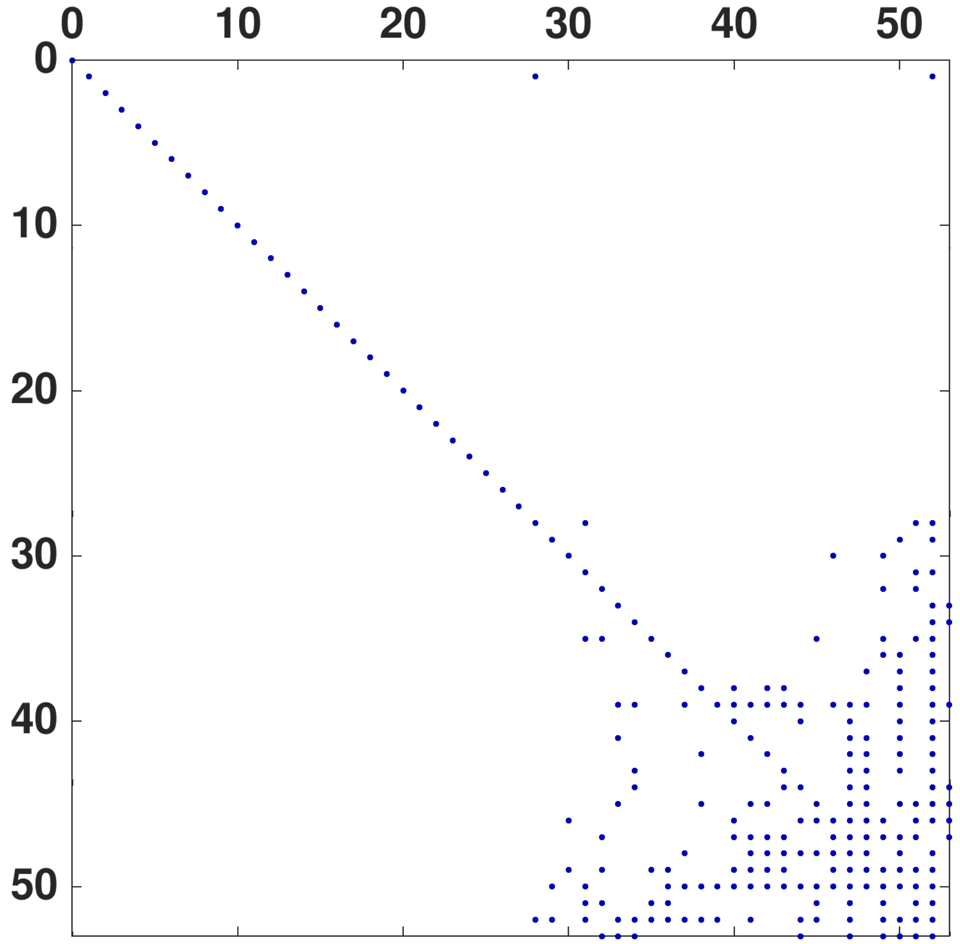
- $$\begin{cases} O_2 + hv \rightarrow O + O \\ O + O_2 \rightarrow O_3 \\ O_3 + hv \rightarrow O_2 + O \\ O + O_3 \rightarrow O_2 + O_2 \end{cases} \Rightarrow \begin{matrix} R_1 = J_1[O_2] \\ R_2 = k_2[O][O_2] \\ R_3 = J_3[O_3] \\ R_4 = k_4[O][O_3] \end{matrix}$$

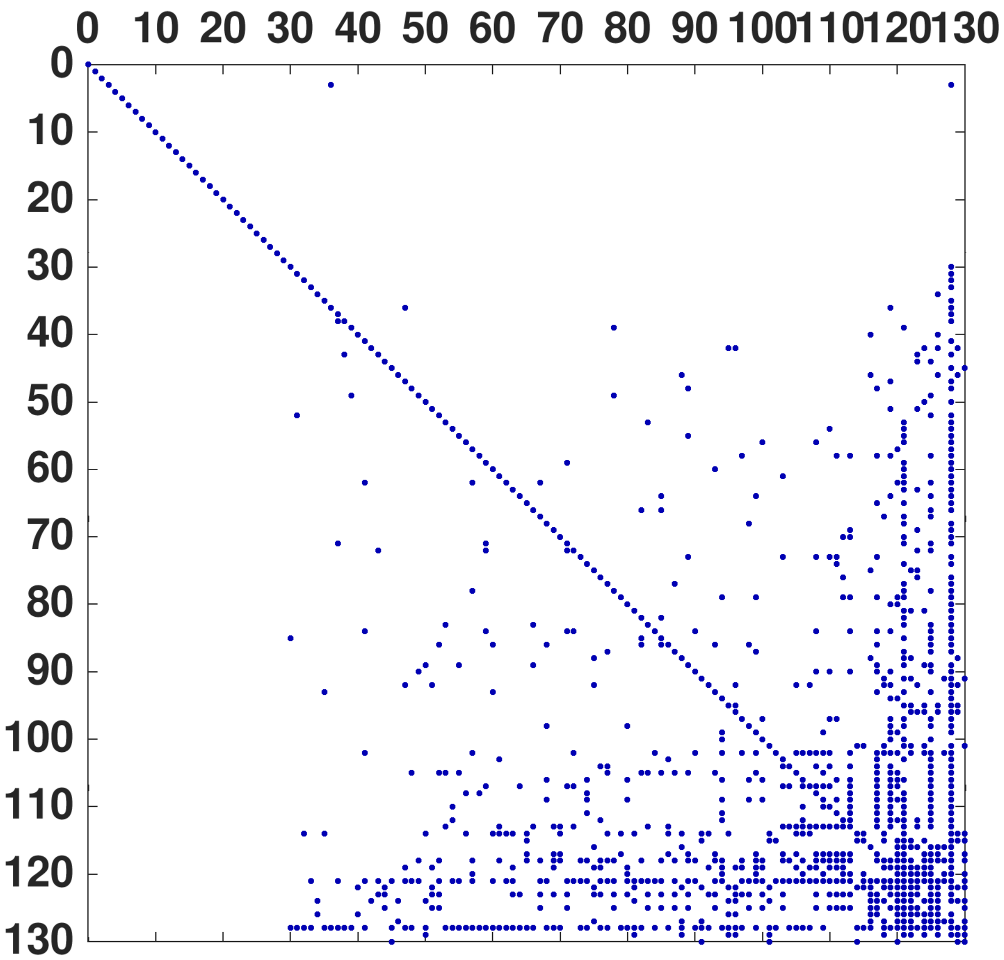
- $$\frac{d}{dt}\begin{bmatrix}[O_3] \\ [O] \\ [O_2]\end{bmatrix} = \begin{bmatrix} -J_3 - k_4[O] & k_2[O_2] - k_4[O_3] & k_2[O] \\ J_3 - k_4[O] & -k_2[O_2] - k_4[O_3] & 2J_1 - k_2[O] \\ J_3 + 2k_4[O] & -k_2[O_2] + 2k_4[O_3] & -J_1 - k_2[O] \end{bmatrix}\begin{bmatrix}[O_3] \\ [O] \\ [O_2]\end{bmatrix}$$

# Target function

- Different chemistry mechanism will focus on different species, which forms an ODE system
- Solving the ODE
  - $\frac{d}{dt}y = Ay = F(y) = P(y) - L(y) + I(y)$
  - $P(y)$ is the production term, $L(y)$ is the losing term, $I(y)$ is the independent forcing term
- Current model used Newton-Raphson iteration scheme with 1800s as time step to integrate

# Two mechanisms to be tested

- 


- 

# Two stage Rosenbrock (ROS2) scheme

- For dealing with a finer time resolution, a scheme which can deal with shorter time step is needed

$$\frac{d}{dt}y = F(y) = P(y) - L(y) + I(y)$$

$$(1 - \Delta t \cdot \gamma A)k_1 = F(y^n)$$

$$(1 - \Delta t \cdot \gamma A)k_2 = F(y^n + \Delta t \cdot k_1) - 2k_1$$

$$y^{n+1} = y^n + \frac{3}{2}\Delta t \cdot k_1 + \frac{1}{2}\Delta t \cdot k_2$$

$$\gamma = 1 + 1/\sqrt{2}$$

- After solving $k_1$ and $k_2$, we can form $y^{n+1}$ for the next time step

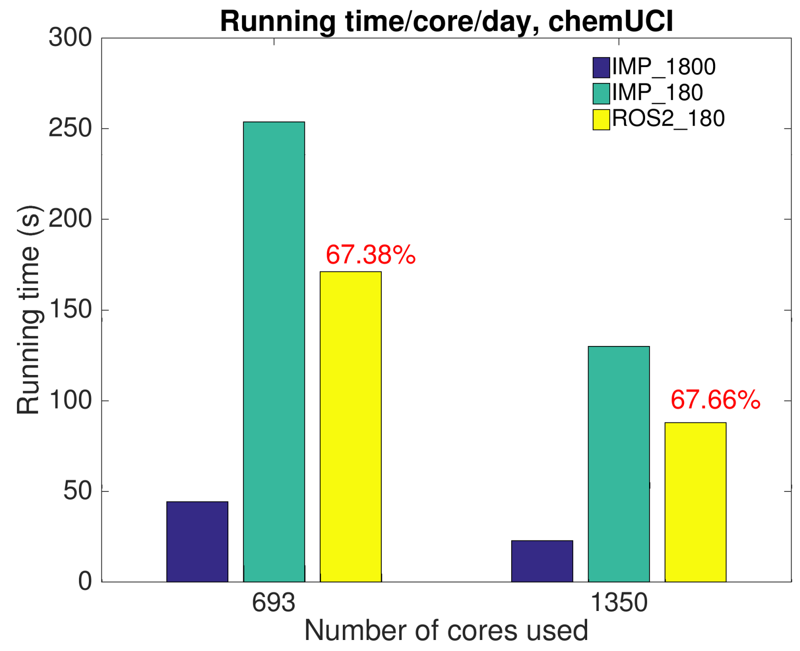
# Experiment settings and different scenarios

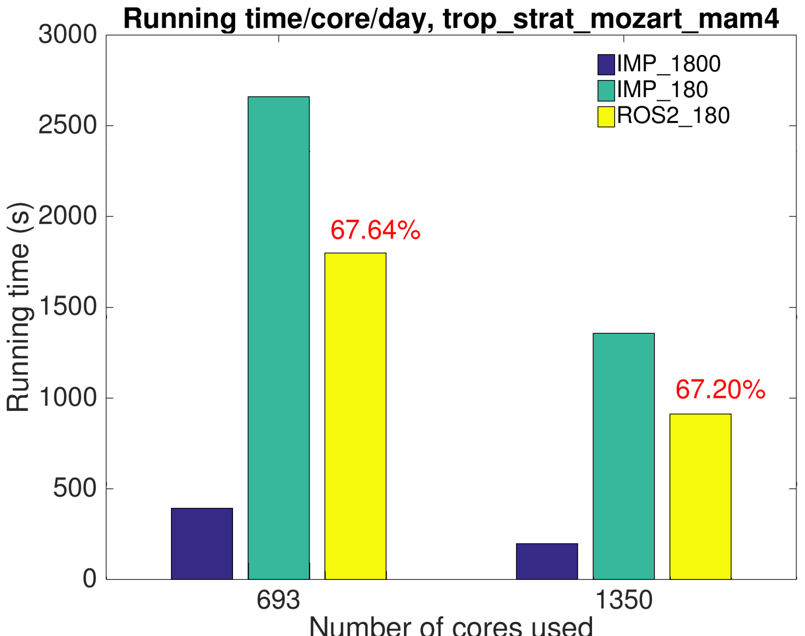
- NERSC-Cori
  - Cray XC40 with Haswell settings
  - 21 nodes with total 693 cores is used for all tests
  - 41 nodes with total 1350 cores is used for an additional efficiency test
- Model settings
  - E3SMv1, with ne30_oECv3 resolution
  - F test (only dynamic atmosphere)
- One day for an efficiency test
- One year for a diurnal cycle test
- Ten years run for a long-term test

- IMP_1800s
  - Original implicit solver with 1800s as the time step
- IMP_180s
  - Original implicit solver with 180s as the time step
- ROS2_180s
  - Two-stage Rosenbrock solver with 180s as the time step

# Efficiency testing (one day)

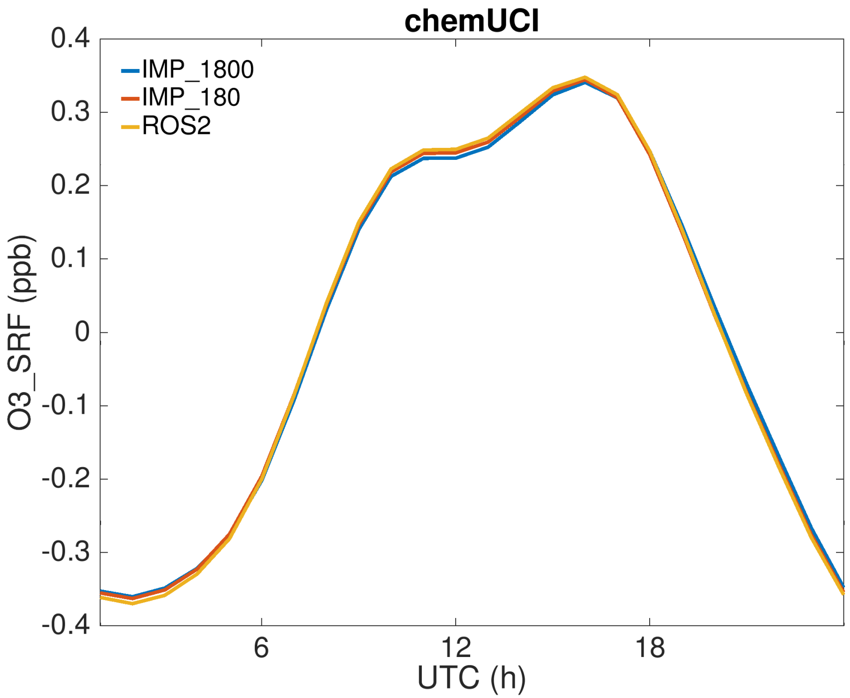
- Running time only for implicit solver
- IMP_1800 has the shortest running time
- Since IMP_180 do not need to iterate that many times, the running time for IMP_180 is not 10 times than IMP_1800
- Compared to IMP_180, the running time for ROS2_180 is 68% shorter, which means 32% more efficiency for all settings

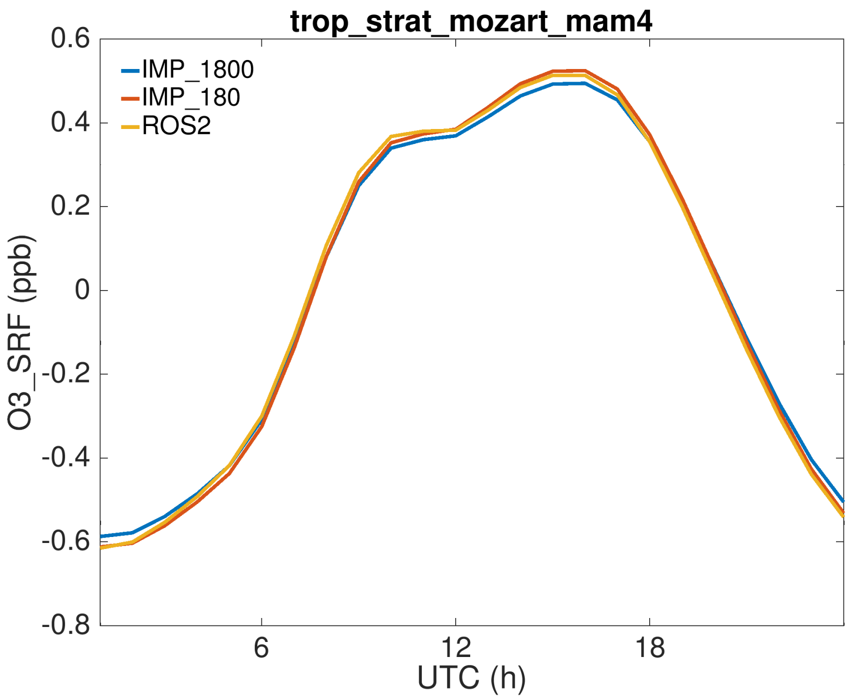


# Diurnal cycle for surface ozone (one year)

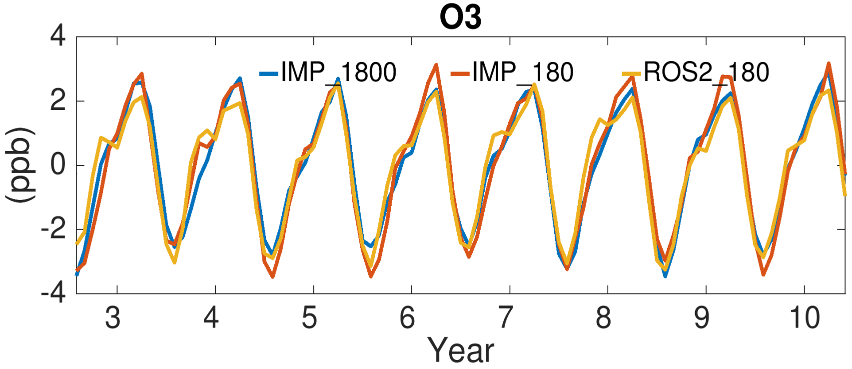
- Global mean diurnal cycle
- Not intend to compare different models results, but only compare different numerical solvers
- The IMP_1800 seems to be a little bit flatter
- Diurnal cycle shows a similar amplitude among all numerical solvers



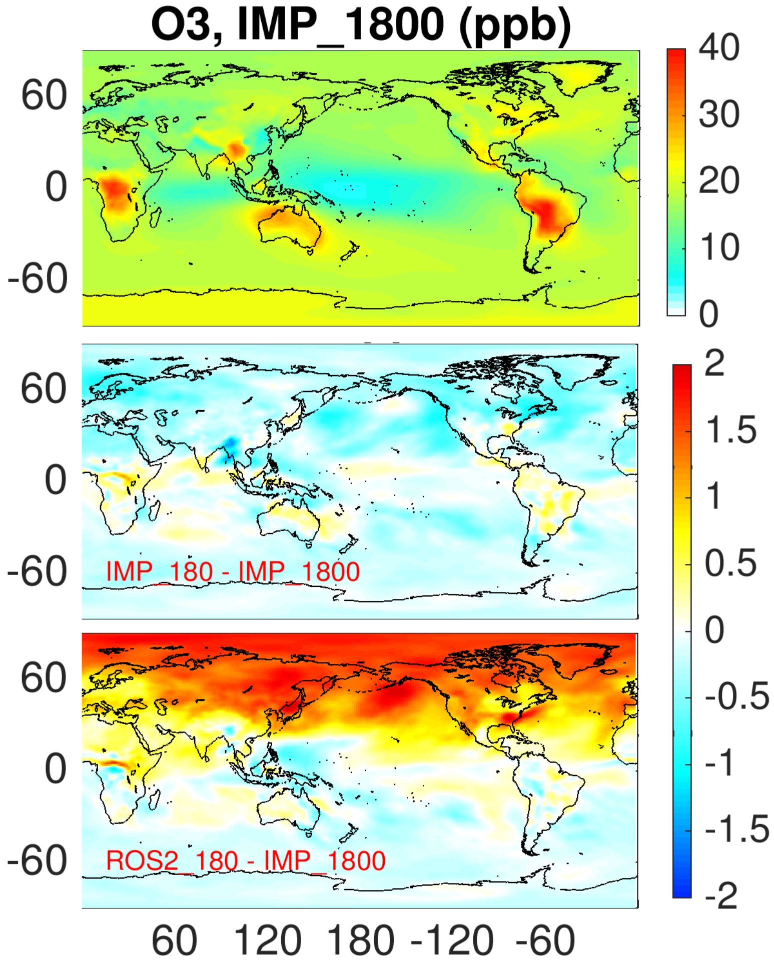



# Results for ten years

- First two years was discarded due to the spin-up
- IMP_180 has weaker surface ozone, compare to ROS2_180



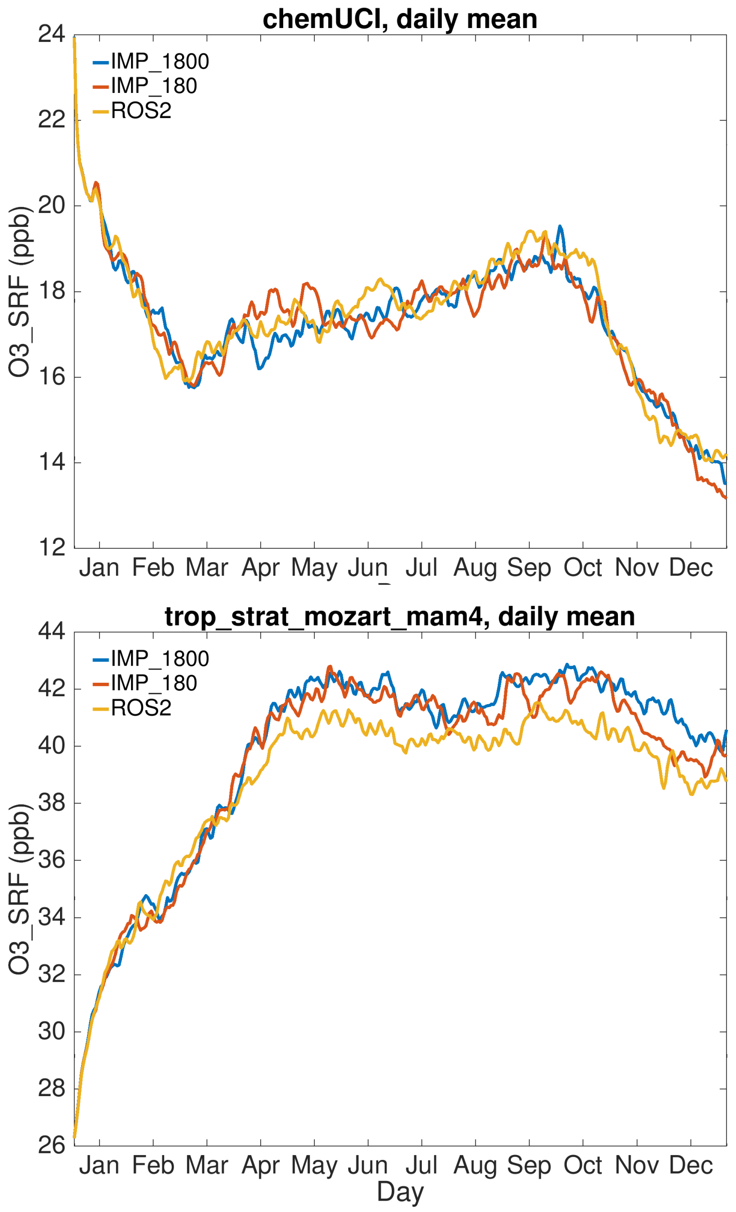

| (ppb) | IMP_1800 | IMP_180 | ROS2_180 |
|---|---|---|---|
| MEAN | 17.1008 | 16.9235 | 17.4449 |
| STD | 1.7989 | 1.9507 | 1.7046 |

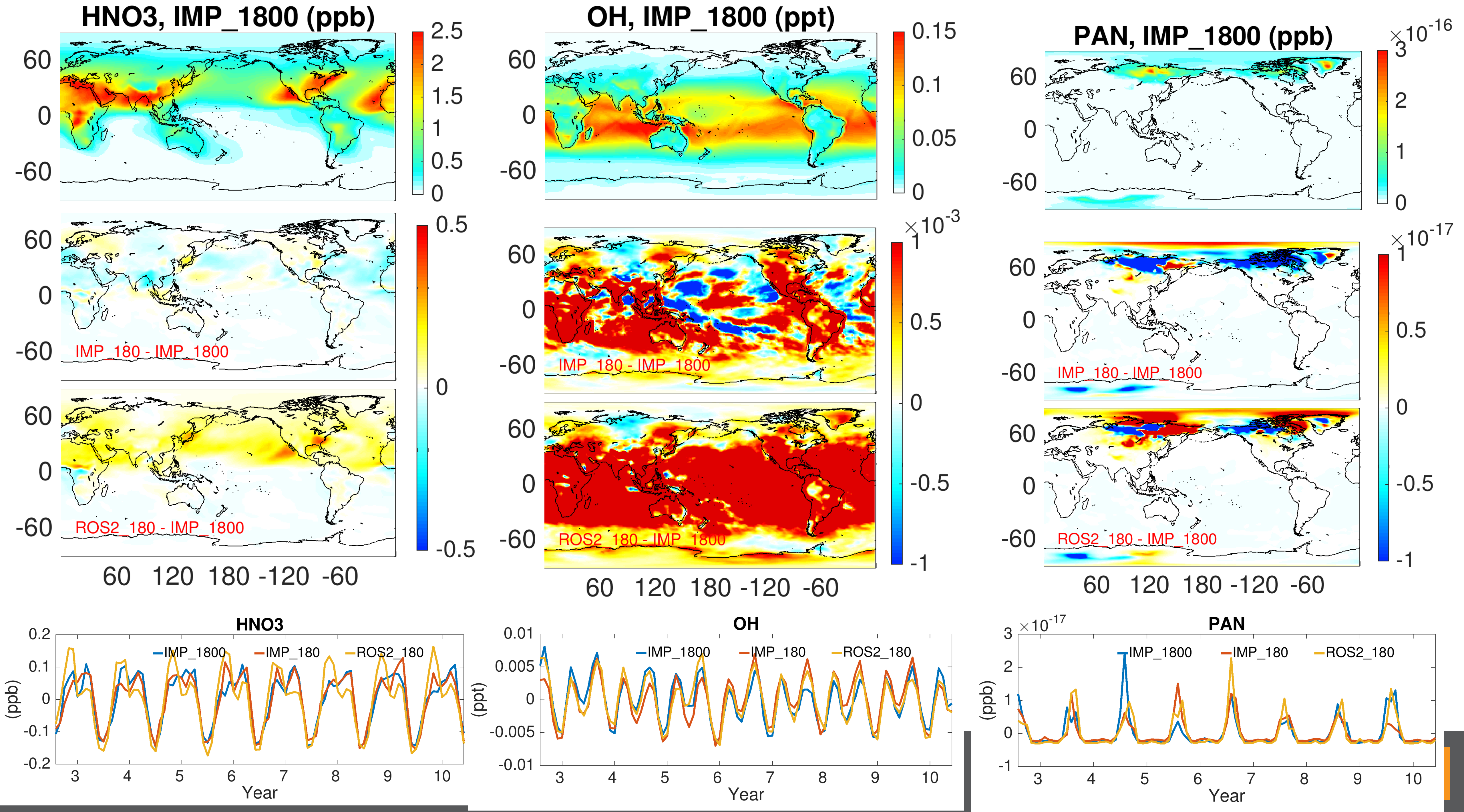


# Discussion and future work

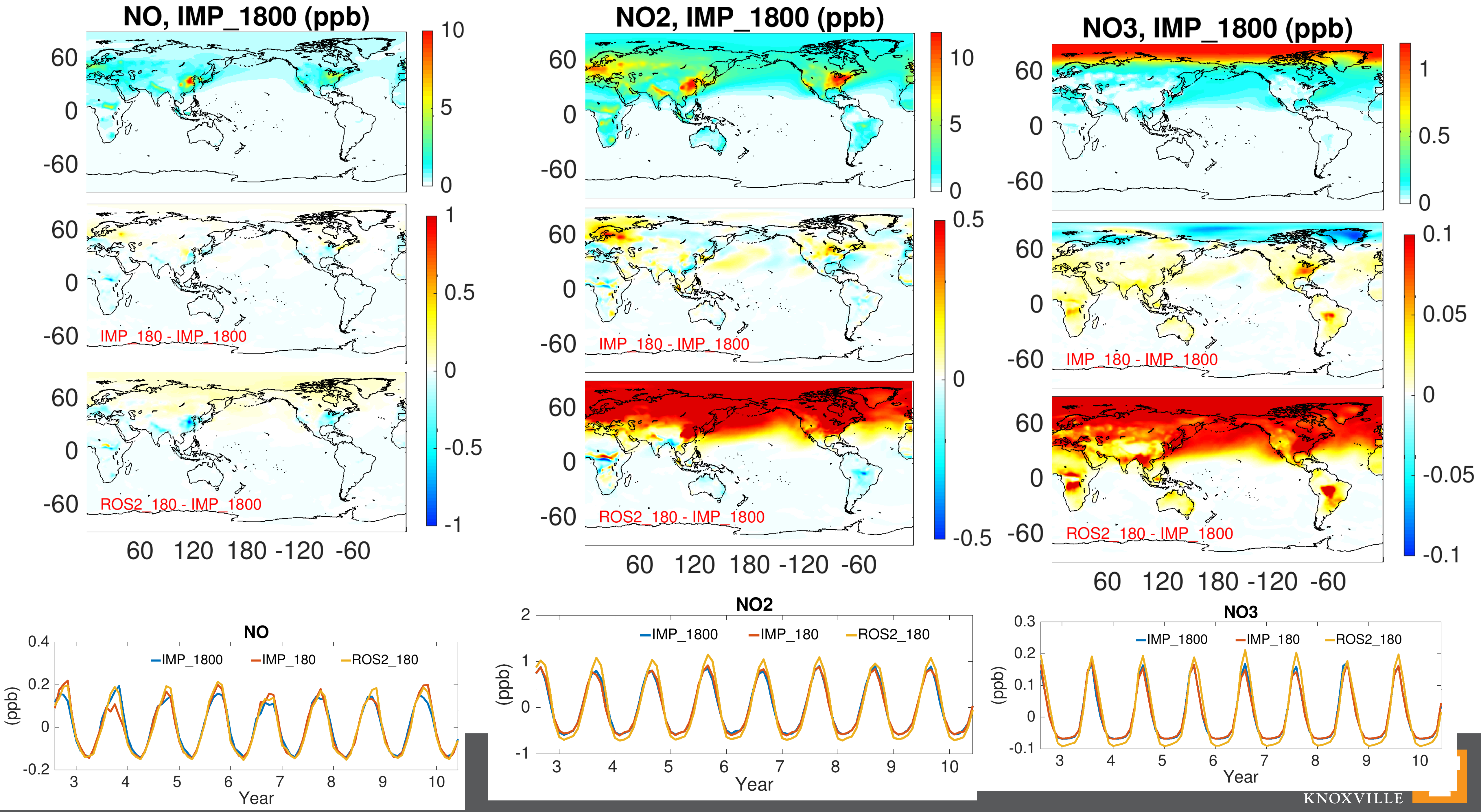
- Our numerical solvers showed that using ROS2 with 180s as the timestep, would have a higher efficiency for approximately 33%, compare to the IMP solver with 180s
- Although the solver is slower than the current IMP solver with 1800s, the benefit would come when we need a smaller timestep for those short-lived species
- From the diurnal cycle and annual cycle, the difference of the three experimental settings is probably small
- The ROS2_180 solver can be used in the future when we need a more delicate simulation and also can be used to put more short-lived species
- We are now trying the ROS3 (three stage Rosenbrock scheme) in a box model (CPU based), and GPU if possible

- Not intend to compare between different chemical mechanism





HNO3, IMP_1800 (ppb)
OH, IMP_1800 (ppt)
PAN, IMP_1800 (ppb)
IMP_180 - IMP_1800
ROS2_180 - IMP_1800
HNO3
OH
PAN
IMP_1800
IMP_180
ROS2_180
(ppb)
(ppt)
Year


NO, IMP_1800 (ppb)
NO2, IMP_1800 (ppb)
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IMP_180 - IMP_1800
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