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Numerical Issues Associated with Strongly Compensating Processes in Climate Models: an Example from ECHAM-HAM

Hui Wan[1,2], Phil Rasch[1], Kai Zhang[1,2], Jan Kazil[3,4], and Ruby Leung[1]

[1] PNNL, Richland, WA
[2] MPI-M, Hamburg, Germany
[3] CIRES, Boulder, CO
[4] NOAA ESRL, Boulder, CO

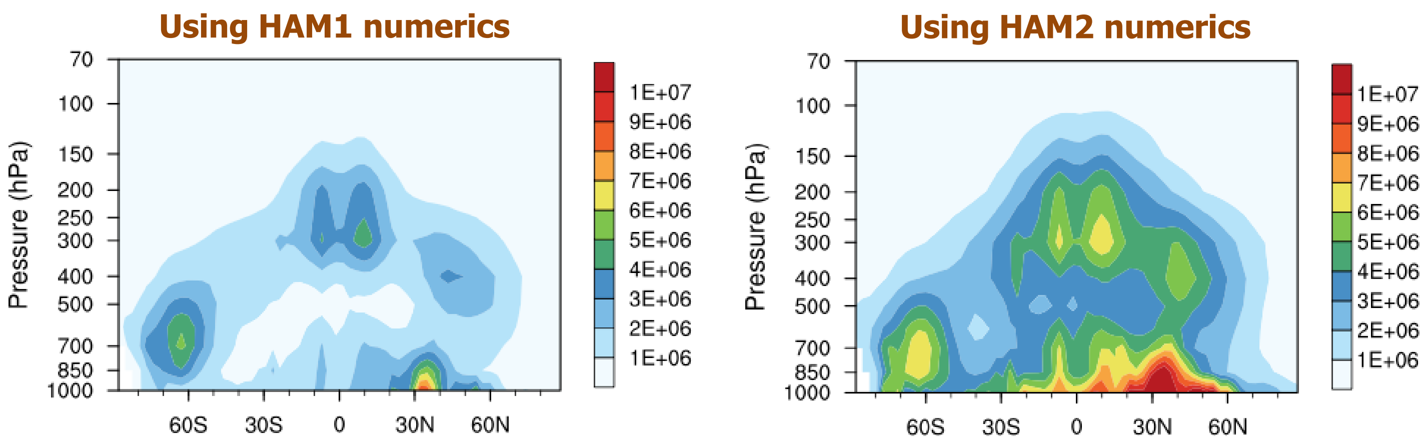
Sulfuric acid gas equation

$$\frac{dS}{dt} = \boldsymbol{P} - \boldsymbol{C} \cdot \boldsymbol{S} - \boldsymbol{N}(\boldsymbol{S})$$

- $\boldsymbol{P}$: Transport and chemical production
- $\boldsymbol{C} \cdot \boldsymbol{S}$: Condensation on pre-existing aerosol particles
- $\boldsymbol{N}(\boldsymbol{S})$: Aerosol nucleation

Motivation

H_2SO_4 gas concentration (unit: cm^{-3}), zonal and annual mean



- New scheme outperforms old scheme in box model calculations (Kokkola et al., 2009, GMD)
- There is evidence of significant positive bias in H_2SO_4 gas in HAM2 (O'Donnell, 2011, HAMMOZ Workshop)

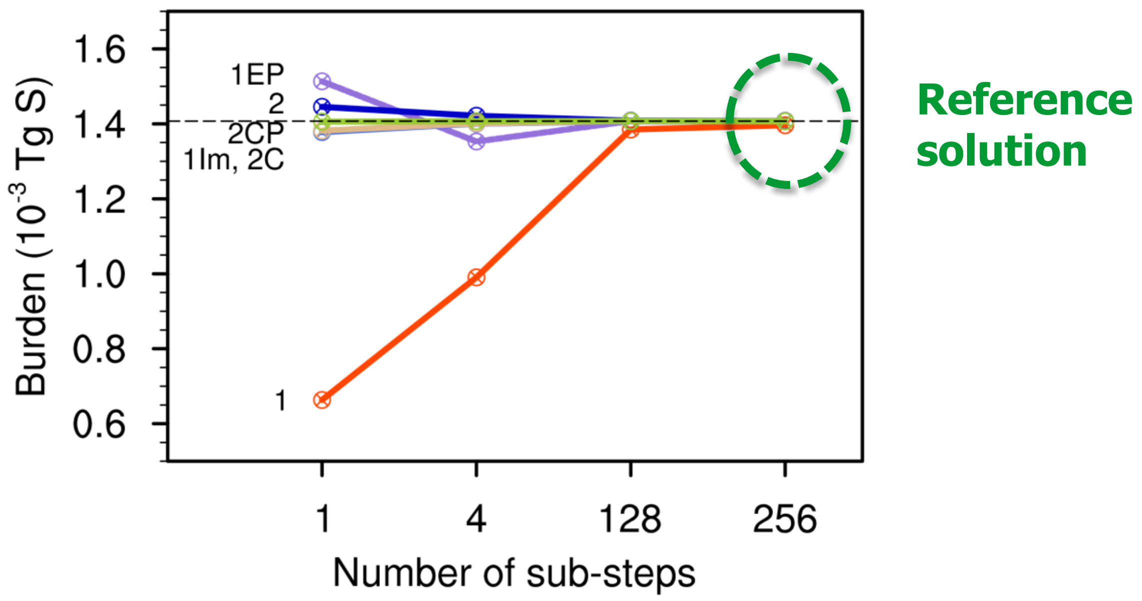
Does the new numerics really lead to model improvement?

Should we revert to the old scheme?

Numerical test

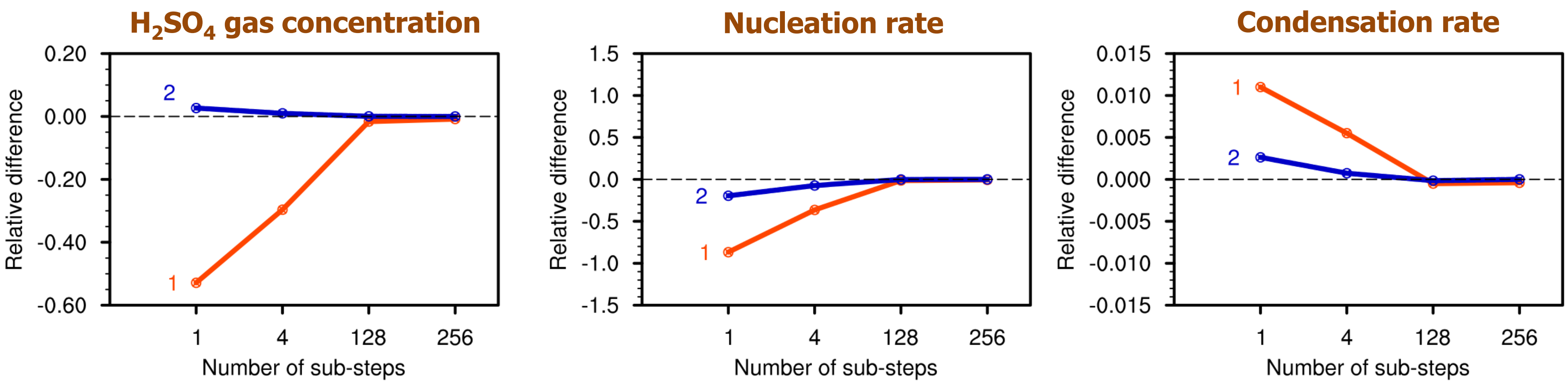
- Convergence test using sub-stepping
- Up to 256 sub-steps per each physics time step
- Using HAM1, HAM2 and a few other time stepping schemes

Global total H_2SO_4 gas burden (unit: 10^{-3} Tg S), annual mean



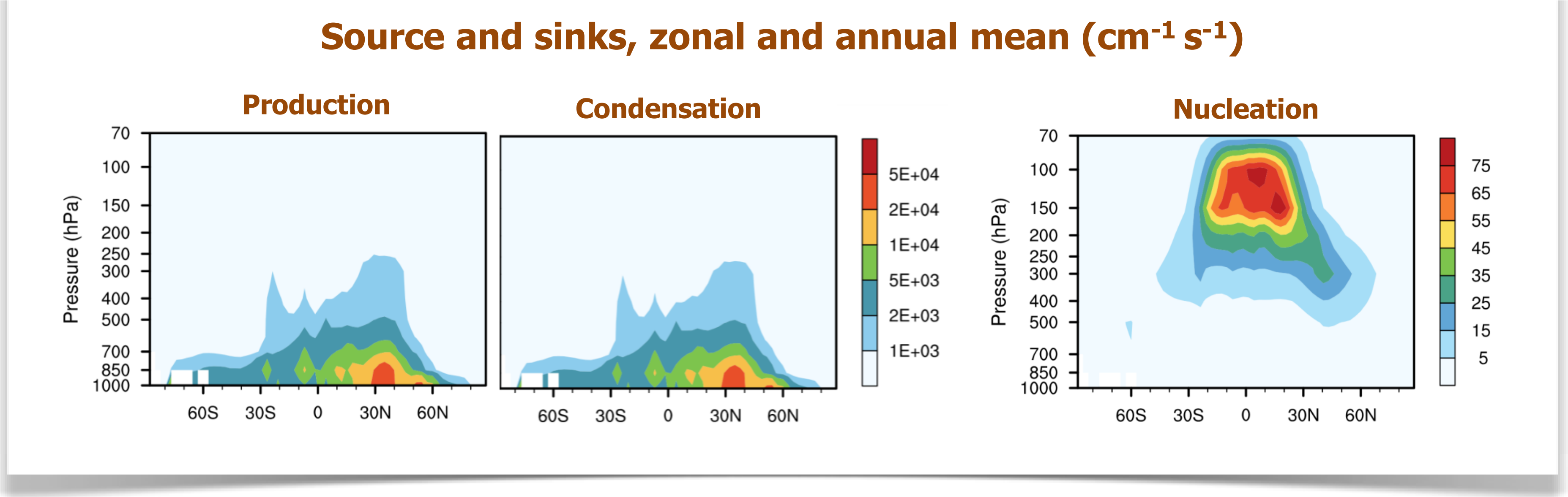
Old vs. new scheme in HAM

Relative differences of global and annual mean (w.r.t. reference solution)



- From a numerical point of view, the numerical scheme in HAM2 is much more accurate than the old one!

What was wrong with the old scheme?



Production and condensation

- are much stronger than nucleation
- nearly compensate each other

What was wrong with the old scheme?

- Production-condensation equation

$$\frac{dS}{dt} = \boldsymbol{P} - \boldsymbol{C} \cdot \boldsymbol{S}$$

- Analytical solution

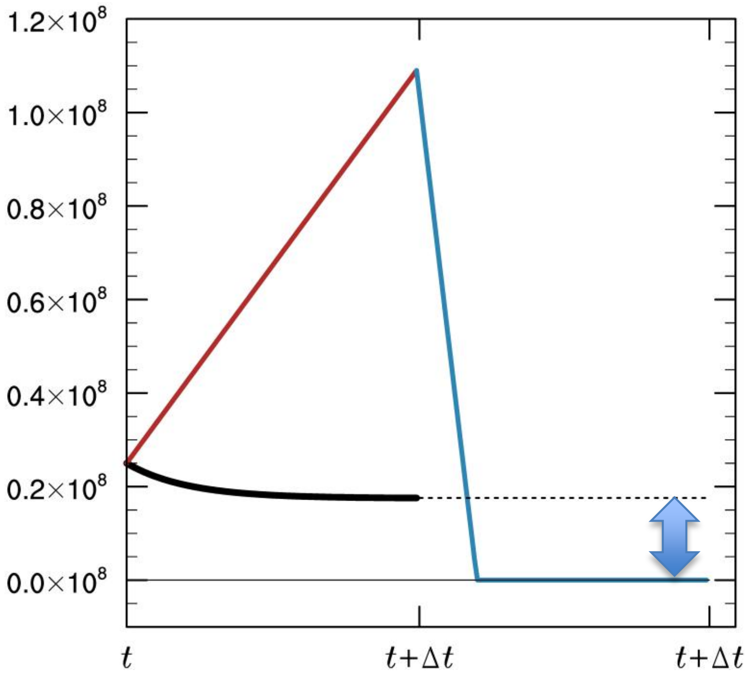
$$S_* = \left(S_t - \frac{\boldsymbol{P}}{\boldsymbol{C}}\right) e^{-\boldsymbol{C}\Delta t} + \frac{\boldsymbol{P}}{\boldsymbol{C}}$$

- Old scheme

(Sequential split, explicit method)

$$S_* = S_t + \boldsymbol{P}\Delta t$$
$$S_{**} = S_* - \boldsymbol{C} \cdot \boldsymbol{S}_* \Delta t$$

East Asia near-surface level
$P = 3.5 \times 10^5$ cm^{-1} s^{-1}
$C = 2 \times 10^{-2}$ s^{-1}
$S_t = 2.5 \times 10^{-7}$ cm^{-3}, $\Delta t = 6$ min



What was wrong with the old scheme?

- Prod.-cond. equation

$$\frac{dS}{dt} = \boldsymbol{P} - \boldsymbol{C} \cdot \boldsymbol{S}$$

- Analytical solution

$$S_* = \left(S_t - \frac{\boldsymbol{P}}{\boldsymbol{C}} \right) e^{-\boldsymbol{C}\Delta t} + \frac{\boldsymbol{P}}{\boldsymbol{C}}$$

- Sequential split, analytical solution

$$S_* = S_t + \boldsymbol{P}\Delta t$$

$$S_{**} = S_* - \boldsymbol{C} \cdot \boldsymbol{S}_* \Delta t$$

$$S_{**} = S_* e^{-\boldsymbol{C}\Delta t}$$

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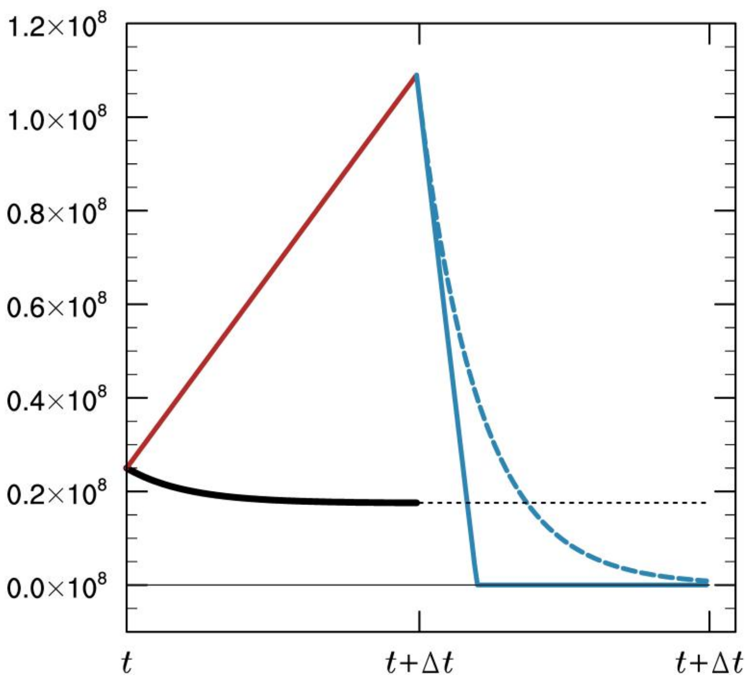

What was wrong with the old scheme?

- Prod.-cond. equation

$$\frac{dS}{dt} = \boldsymbol{P} - \boldsymbol{C} \cdot \boldsymbol{S}$$

- Analytical solution

$$S_* = \left(S_t - \frac{\boldsymbol{P}}{\boldsymbol{C}}\right) e^{-\boldsymbol{C}\Delta t} + \frac{\boldsymbol{P}}{\boldsymbol{C}}$$

- Parallel split, explicit method
- Implicit method

East Asia near-surface level
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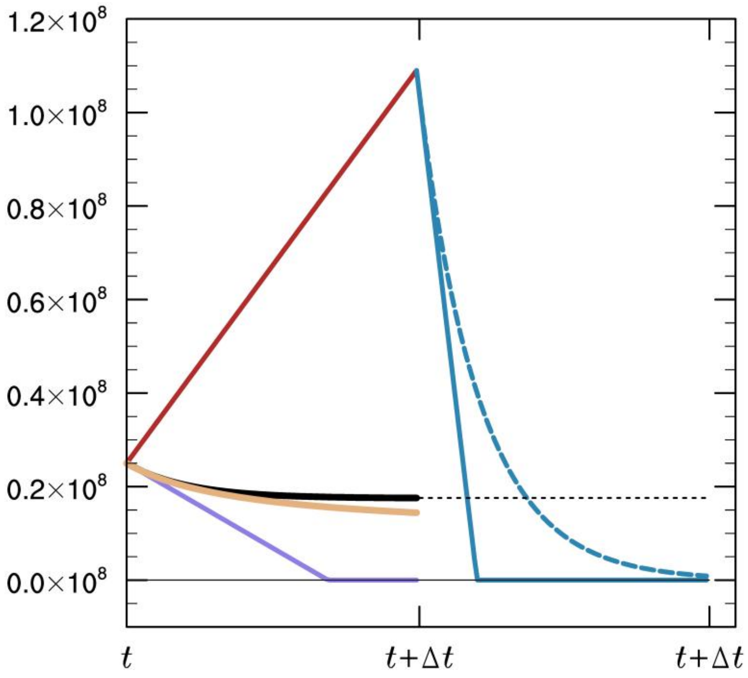


Lessons learned

- When there are strongly compensating processes, sequential split + explicit scheme+ long time step is a dangerous combination!

- Numerical instability, no crash, but large error!

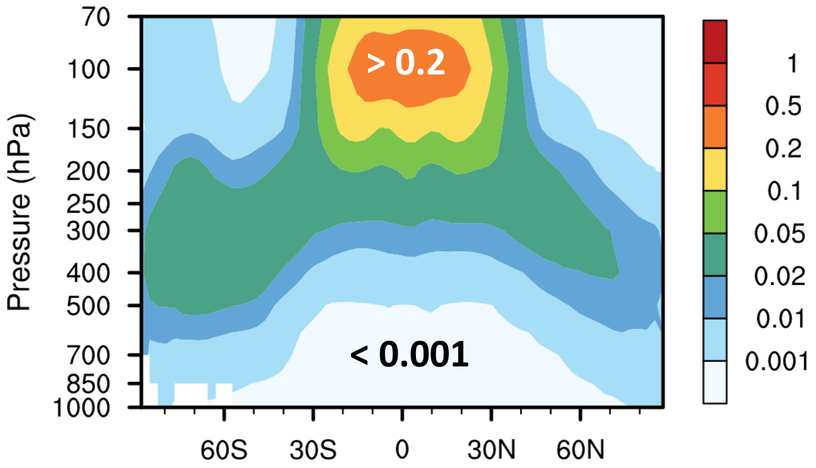
- Our recommendation
  - Analytical solution if possible
  - Implicit method if affordable
  - Process-based, sufficiently small time step

- Positive biases in H_2SO_4 gas in HAM2
  - Need further investigation
  - Should not revert to the old numerics
  - Possible biases in production and nucleation rate

Aerosol nucleation in HAM2

- Parameterization of Kazil and Lovejoy (2007)
- Sequential splitting with production and condensation
- Numerical correction (Kokkola et al., 2009)

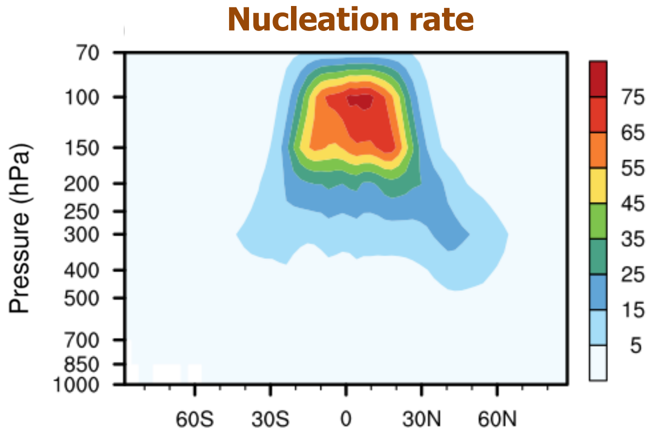
Nucleation : condensation (ratio)

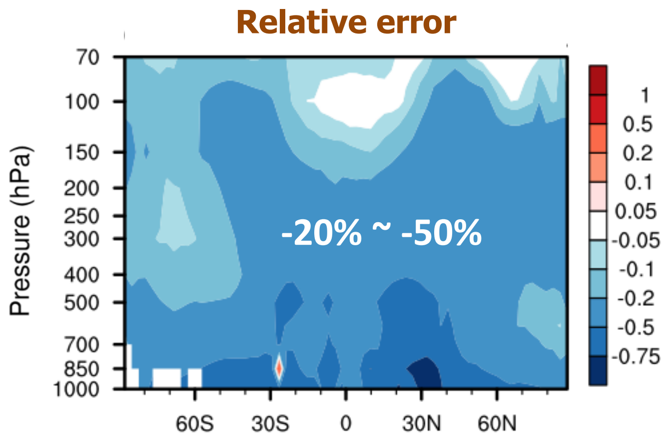


$$S_{t+\Delta t} = S_* - \frac{N(S_*)}{1 + C\Delta t}\Delta t$$

Aerosol nucleation

Using HAM2 numerics





$$S_{t+\Delta t} = S_* - \frac{\boldsymbol{N}(\boldsymbol{S}_*)}{1 + C\Delta t} \Delta t$$

Aerosol nucleation

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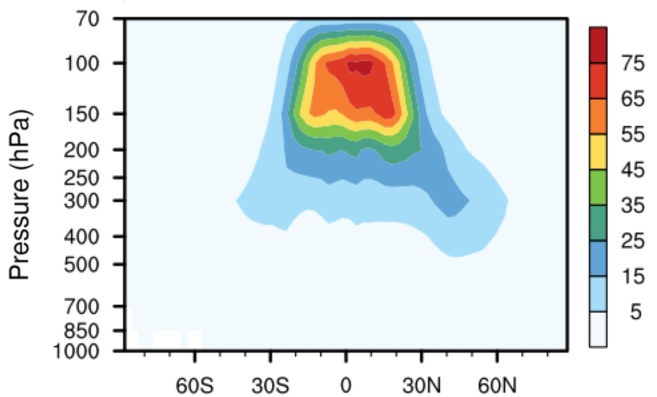
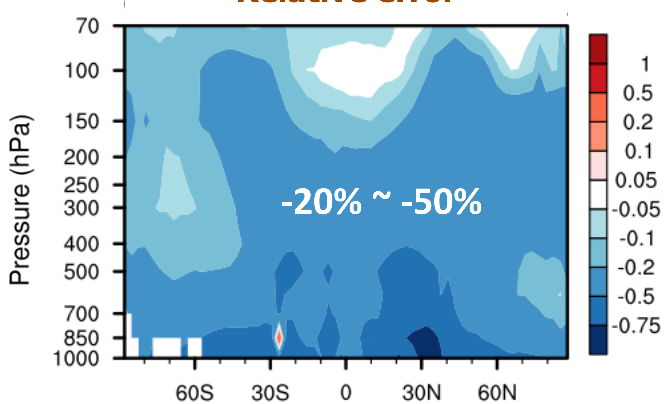
Using HAM2 numerics

Nucleation rate

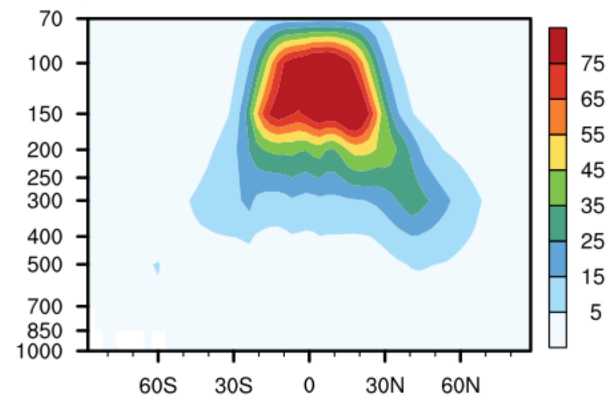


Relative error

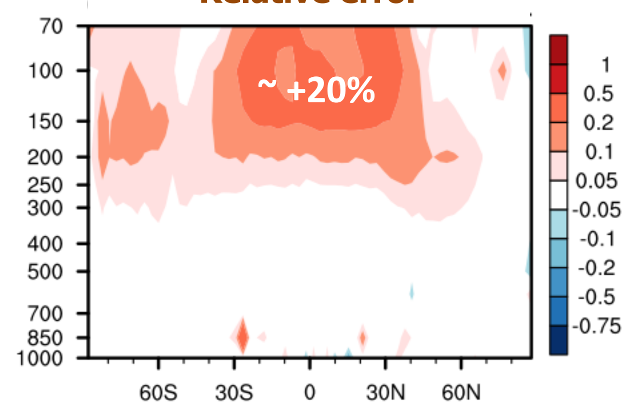


W/O artificial correction

Nucleation rate



Relative error



Can we do better?

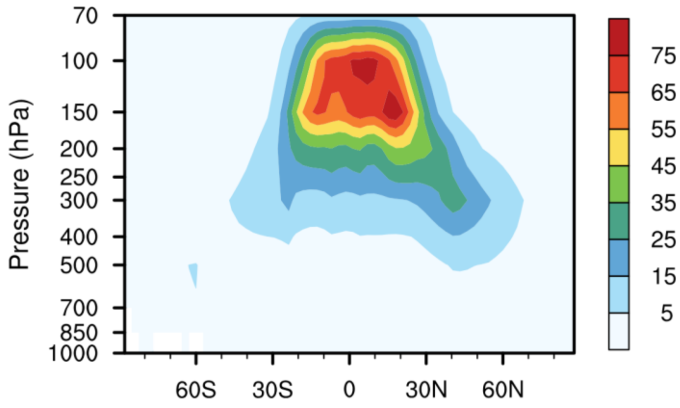
- Simple explicit scheme

$$S_* = S_t + \Delta t\,(P - C \cdot S_t)\,,$$
$$S_{t+\Delta t} = S_* - \Delta t\,N(S_*)\,.$$

- Dynamically chosen time step

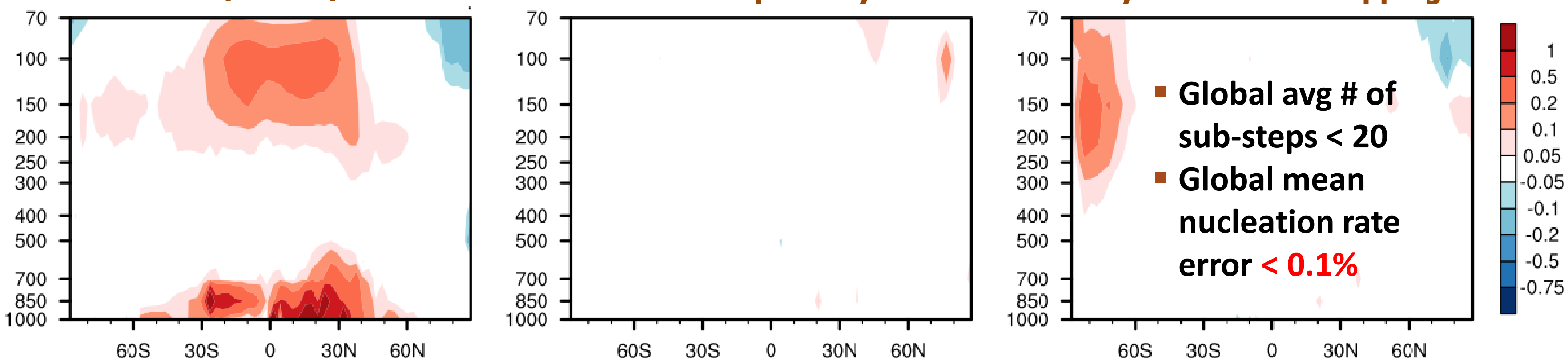
$$\Delta t < 1/C$$

Nucleation rate



Relative error w.r.t. reference solution

4 sub-steps everywhere | **128 sub-steps everywhere** | **Dynamical sub-stepping**



Conclusions

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- Microphysical processes typically have much shorter time scales than large-scale atmosphere dynamics ➔ multi-scale stiff system
- Rich experience in CTM and AQ community, but very limited attention (so far) by climate modelers

- Climate models typically use long time step and crude numerics in parameterizations ➔ numerical instability, large error
- The ubiquitous positive definite clipping can also cause problem

- Connecting parameterization schemes using a simply “USB-hub” may not work
- Caution is needed when treating compensating and competing processes

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Condensation time scale

Near-surface condensation coefficient (unit: s^{-1}), January mean