Verification of high-efficiency chemistry numerical solver in the global model using E3SM

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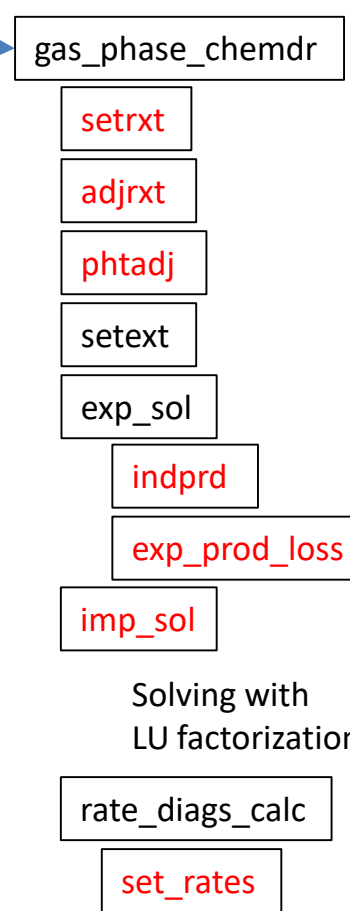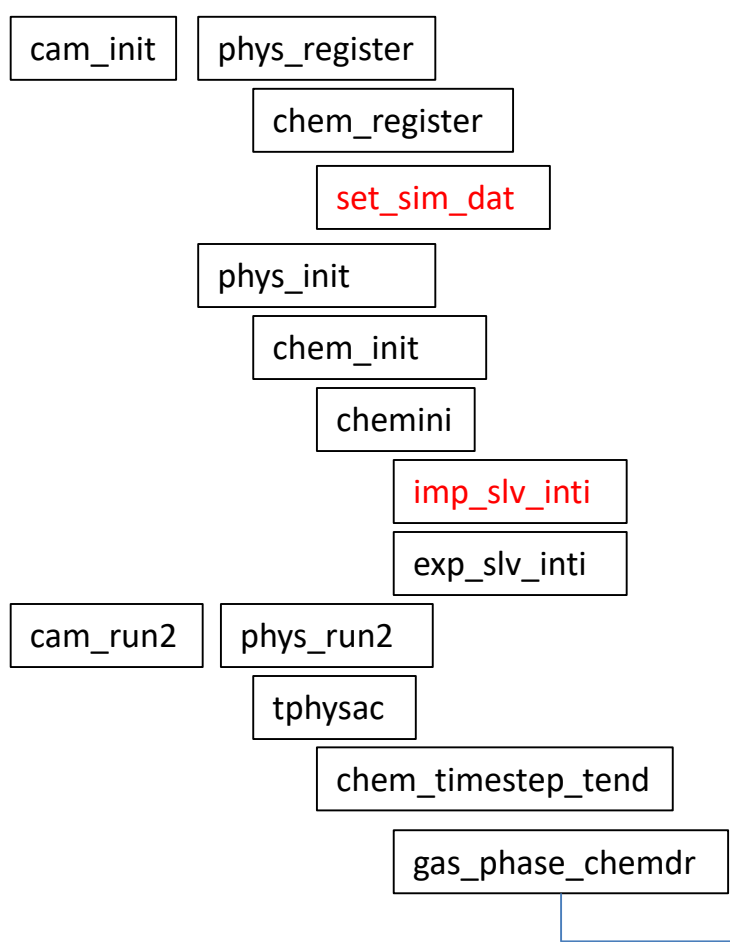TENNESSEE
KNOXVILLE

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Chemistry model in E3SM

- Chemical components are essential precursors in cloud formatting, aerosol, AOD and other processes which can affect the atmospheric radiation budget, while those chemical species are mostly pre-described in Earth system models

- Several chemistry solvers can be chosen in E3SM, while solving these chemistry reactions are time-consuming processes in solving the implicit solver

- UCI chemistry mechanism can solve most of the important species and was chose with our chemistry solver for E3SM as an example

cam_init phys_register

chem_register

set_sim_dat

phys_init

chem_init

chemini

imp_slv_inti

exp_slv_inti

cam_run2 phys_run2

tphysac

chem_timestep_tend

gas_phase_chemdr

gas_phase_chemdr

setrxt

adjrxt

phtadj

setext

exp_sol

indprd

exp_prod_loss

imp_sol

Solving with
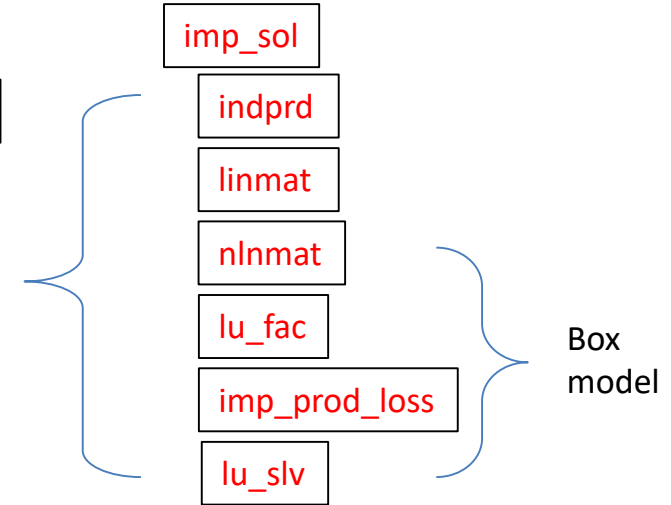LU factorization

rate_diags_calc

set_rates

$$\frac{Dy}{Dt} = F(y) = P(y) - L(y) + I(y)$$

$$(1 - h\gamma A)k_1 = F(y^n)$$

$$(1 - h\gamma A)k_2 = F(y^n + hk_1) - 2k_1$$

$$y^{n+1} = y^n + \frac{3}{2}hk_1 + \frac{1}{2}hk_2$$

imp_sol

indprd

linmat

nlnmat

lu_fac

imp_prod_loss

lu_slv

Box
model

Two stage Rosenbrock solver (ROS2)

- Two stage Rosenbrock solver

- Box model performance shown that ROS2 has higher accuracy with less iterations

- Box model shown that ROS2 can save 33% computation time compare with original implicit solver

trop_morzart_mam4, Implicit solver

- Pseudo Species, 1
- Pseudo Species, 2
- Pseudo Species, 3

trop_morzart_mam4, ROS2 solver
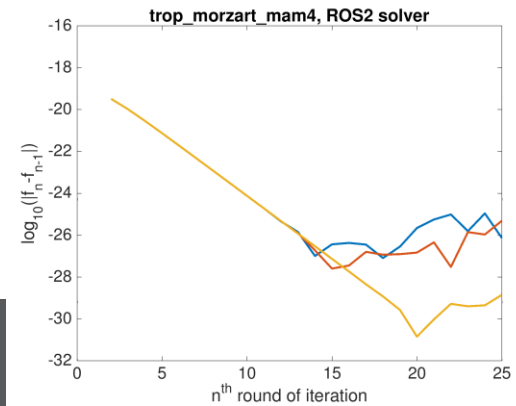
Model performance using ROS2 in E3SM_v1

- Changing different solver may converge to different solution, while the difference are still reasonable
- 20% improvement of computation time using 21 nodes with ne30 resolution in Cori
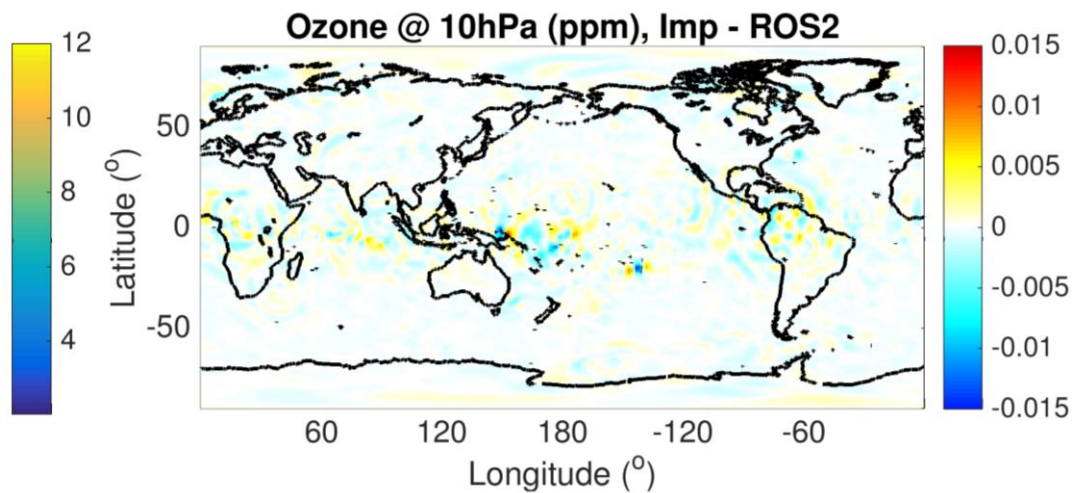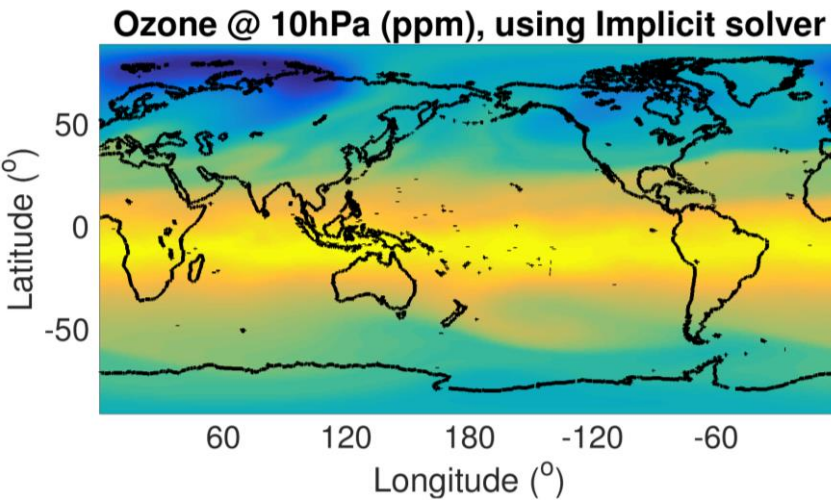
Conclusion and Future work

- E3SM_v1 using ROS2 have 20% improvement in computation time compare with implicit solver

- Currently only have 1-day results, will need to have longer experiment time

- Further test may be needed with MOZART and UCI chemistry in E3SM_v2

- Seeking the GPU for model improvement