Data for Idealized Particle-Resolved Large-Eddy Simulations to Evaluate the Impact of Emissions Spatial Heterogeneity on CCN Activity

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This dataset contains all material required to produce the figures found within the manuscript submitted to Aerosol Chemistry and Physics entitled "Idealized Particle-Resolved Large-Eddy Simulations to Evaluate the Impact of Emissions Spatial Heterogeneity on CCN Activity". The archived dataset consists of:

- `data.zip`: WRF-PartMC-MOSIAC-LES simulation data in Section 3
- `scripts.zip`: Python notebooks for generating figures in Section 2 and 3, and scripts used to compile the normalized spatial heterogeneity metric as described by Mohebalhojeh et al. 2025.

Software requirements/recommendations

All figures in the paper were run with Python 3.9.23. This older version is required due to a dependency of `f2py` (used to compile Fortran code for the spatial heterogeneity metric calculation into an object which can be imported as a Python module) which has since been deprecated. Users should run the `create_env.sh` script in `scripts.zip` to create a conda environment which contains all the necessary packages.

Required packages are as follows with the version used for this manuscript:

- numpy (2.0.2)
- scipy (1.13.1)
- matplotlib (3.9.2)
- netCDF4 (1.7.2) - available at https://unidata.github.io/netcdf4-python/
- pandas (2.3.1)
- ipykernel (6.30.1)

- setuptools (59.8.0)
- gfortran (15.1.0)

Directory structure of archived simulation data for Section 3.1

Upon downloading and untarring `partmc_simulations.tar.gz`, it may be explored as follows:

- Input data files for conducting the set of three simulations:
  - `camp.spec` and relevant input files
  - `tchem.spec` and relevant input files
  - `tchem_gpu.spec` and relevant input files
- Output data in the `out/` directory consists of netCDF files per output time:
  - CAMP output: `camp_0001_*`
  - PartMC-TChem CPU output: `tchem_cb05cl_ae5_*`
  - PartMC-TChem GPU output: `tchem_gpu_cb05cl_ae5_*`
- `simulation_notebook.ipynb`: Python Jupyter notebook for producing Fig. 5 and analysis of error.

Directory structure of archived numerical experiment data for Section 3.2

Upon downloading and untarring `timings.tar.gz`, it may be explored as follows:

- `data/`: directory containing all the timing results. The descriptions of the individual directories are described in Table 1.
- `scripts/`: directory containing the following scripts:
  - `solver_plots.ipynb`: Python Jupyter notebook for producing Fig. 6, 7.
  - `rhs_plots.ipynb`: Python Jupyter notebook for producing Fig. 8.

Cluster	Experiment	Platform	Path relative to data directory
DeltaAI	RHS	NVIDIA H100 GPU	deltaAI/CB05CL_AE5_w_simpolSOA/CUDA/rhs-no_sacado
DeltaAI	Jacobian	NVIDIA H100 GPU	deltaAI/CB05CL_AE5_w_simpolSOA/CUDA/rhss-no_sacado
DeltaAI	TrBDF2	NVIDIA H100 GPU	deltaAI/CB05CL_AE5_w_simpolSOA/CUDA/trbdf-no_sacado
DeltaAI	Sundials CVODE	NVIDIA H100 GPU	deltaAI/CB05CL_AE5_w_simpolSOA/CUDA/sundials_dense-no_sacado
DeltaAI	Sundials CVODE-GMRES	NVIDIA H100 GPU	deltaAI/CB05CL_AE5_w_simpolSOA/CUDA/sundials_gmres-no_sacado
Frontier	RHS	AMD MI250X GPU	frontier/CB05CL_AE5_w_simpolSOA/HIP/rhs-no_sacado
Frontier	Jacobian	AMD MI250X GPU	frontier/CB05CL_AE5_w_simpolSOA/HIP/jac-no_sacado
Frontier	TrBDF2	AMD MI250X GPU	frontier/CB05CL_AE5_w_simpolSOA/HIP/trbdf-no_sacado
Frontier	Sundials CVODE	AMD MI250X GPU	frontier/CB05CL_AE5_w_simpolSOA/HIP/sundials_dense-no_sacado
Frontier	Sundials CVODE-GMRES	AMD MI250X GPU	frontier/CB05CL_AE5_w_simpolSOA/HIP/sundials_gmres-no_sacado
Perlmutter	RHS	AMD 7763 CPU	perlmutter/CB05CL_AE5_w_simpolSOA/HOST/rhs-no_sacado
Perlmutter	Jacobian	AMD 7763 CPU	perlmutter/CB05CL_AE5_w_simpolSOA/HOST/jac-no_sacado
Perlmutter	TrBDF2	AMD 7763 CPU	perlmutter/CB05CL_AE5_w_simpolSOA/HOST/trbdf-no_sacado
Perlmutter	Sundials CVODE	AMD 7763 CPU	perlmutter/CB05CL_AE5_w_simpolSOA/HOST/sundials_dense-no_sacado
Perlmutter	Sundials CVODE-GMRES	AMD 7763 CPU	perlmutter/CB05CL_AE5_w_simpolSOA/HOST/sundials_gmres-no_sacado

Table 1. Experiment configurations across different clusters and platforms