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MPTRAC: A high-performance Lagrangian transport model for atmospheric air parcel dispersion

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Summary

The Massive-Parallel Trajectory Calculations (MPTRAC) Lagrangian transport model (Hoffmann et al., 2016, 2022) simulates the movement, dispersion, and chemical transformation of aerosols and trace gases in the atmosphere. Unlike grid-based models, MPTRAC tracks individual air parcels, providing high-resolution insights into transport, mixing, chemistry, and deposition. Trajectory calculations are driven by meteorological fields from data assimilation systems and forecast models. MPTRAC has been applied in various contexts, especially for tracking volcanic plumes in the troposphere and stratosphere. Optimized for high-performance computing (HPC) and graphics processing units (GPU), MPTRAC efficiently supports large-scale, high-resolution simulations, making it a powerful tool for atmospheric research.

Statement of need

Accurate atmospheric transport modeling is essential for applications such as air quality assessments, climate studies, and public health protection. Traditional Eulerian models often struggle with fine-scale resolution, limiting their ability to capture complex transport and mixing processes. Lagrangian models, such as MPTRAC and others (Jones et al., 2007; Lin et al., 2003; McKenna et al., 2002; Pisso et al., 2019; Stein et al., 2015; Stohl et al., 2005), address this limitation by tracking individual air parcels, offering fine-grained representations of atmospheric processes.

MPTRAC supports both research and operational applications requiring precise transport simulations. It models long-range transport and chemical transformations, enabling pollution studies, emission tracking, and environmental impact forecasting. MPTRAC runs efficiently on HPC and GPU systems, supporting fast, large-scale simulations that facilitate real-time decision-making and scientific analysis.

Features

MPTRAC computes air parcel trajectories using wind and vertical velocity fields from global reanalysis or forecast data (Gelaro et al., 2017; Hersbach et al., 2020). In addition to standard pressure-level input, it supports advection on forecast model levels, improving near-surface accuracy. MPTRAC accounts for eddy diffusion and subgrid-scale winds via the Langevin equation. An inter-parcel exchange module represents air mixing. MPTRAC also simulates convection, sedimentation, radioactive decay, gas and aqueous phase chemistry, and wet and dry deposition. Meteorological pre-processing routines compute boundary layer heights, CAPE, geopotential heights, and tropopause data. Figure 1 shows MPTRAC's geophysical and chemical modules and core software components.

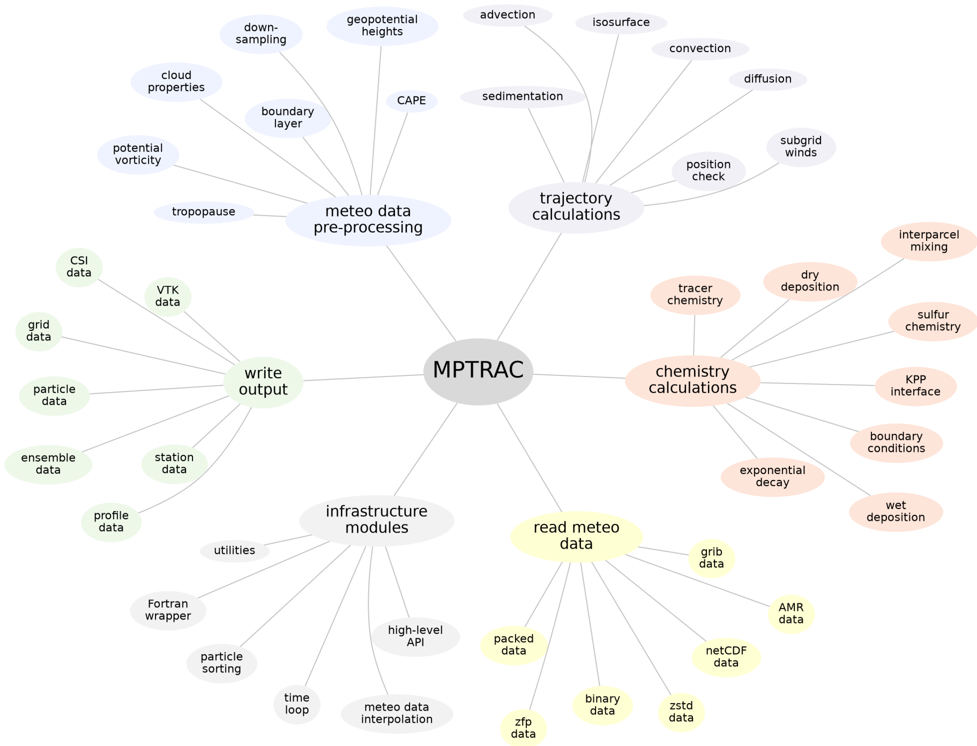

Figure 1: Geophysical and chemical modules and main software components of the MPTRAC Lagrangian transport model. Image adapted from Hoffmann et al. (2024).

Optimized for computational efficiency, MPTRAC features an MPI-OpenMP-OpenACC hybrid parallelization for scalable deployment on workstations, HPC systems, and GPU platforms (Hoffmann et al., 2022, 2024; Liu et al., 2020). It supports multiple output formats for diverse data types, enabling visualization and analysis using Gnuplot, ParaView, or Python. MPTRAC is open-source, distributed under the GNU GPL v3 license. Code and documentation are available in a GitHub repository, with software releases archived on Zenodo.

Applications

MPTRAC simulates the transport and dispersion of atmospheric constituents from natural and anthropogenic sources. For volcanic eruptions, it helps estimate emissions and track the spread of volcanic ash and sulfate aerosols, which impact air traffic, climate, and ecosystems (Cai et al., 2022; Heng et al., 2016; Mishra et al., 2022; Wu et al., 2017, 2018). Similarly, MPTRAC models the dispersion of wildfire emissions, including vertical ascent and widespread transport into the upper atmosphere (Liao et al., 2024). Other studies examined the long-range transport of aerosols and trace gases in the troposphere and stratosphere (Clemens et al., 2024; Smoydzin & Hoor, 2022; Wu et al., 2023).

Figure 2 illustrates MPTRAC's use in studying convective transport of air from the planetary boundary layer (PBL) into the free troposphere (Hoffmann et al., 2023). The simulation tracks air parcels lifted by updrafts from tropical storms and mid-latitude systems, revealing how air and pollutants spread aloft, improving understanding of atmospheric circulation and pollutant distribution at regional and global scales.

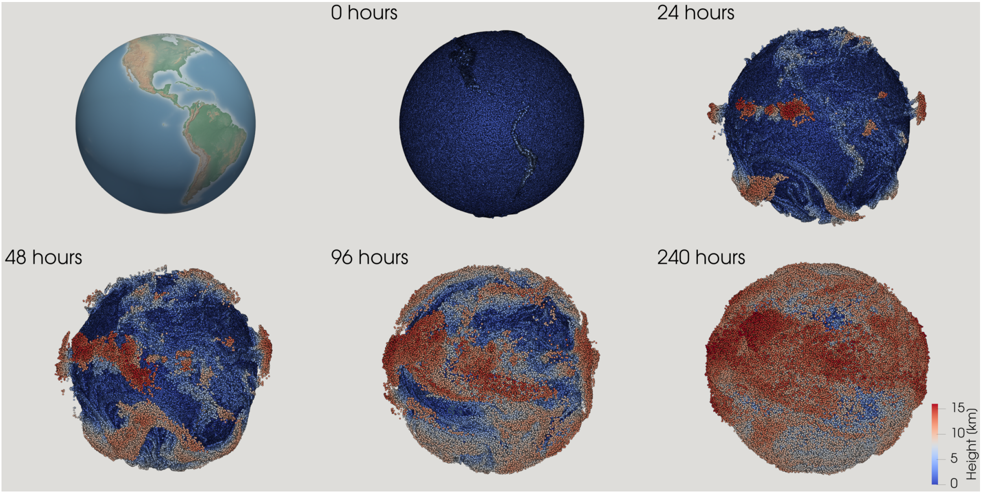

Figure 2: Lagrangian transport simulation of convective transport from the PBL into the free troposphere. One million trajectories are initialized near the surface on 1 July 2017, 00:00 UTC, and tracked over 10 days using ERA5 reanalysis data. Color coding indicates the geopotential height of the air parcels. Video available via Zenodo (Hoffmann, 2025).

MPTRAC is primarily designed for the free troposphere and stratosphere, but support for PBL processes is under active development. While not yet evaluated using controlled tracer release experiments such as ANATEX (Draxler et al., 1991) or ETEX (Van dop et al., 1998), these offer a valuable framework for future validation. Current validation focuses on real-case scenarios, including long-range transport comparisons with balloon and satellite observations.

Evolution and Future Directions

MPTRAC has evolved since 2013, designed for HPC applications. Initially using OpenMP for multi-core CPUs, it later incorporated MPI for large-scale ensemble simulations. In 2019, OpenACC offloading boosted performance by porting all geophysical modules to NVIDIA GPUs. In 2023, we explored GPU offloading using OpenMP for AMD GPUs, broadening portability. MPTRAC is now ready for simulations on the Exascale JUPITER system.

Recent technical efforts have improved documentation and usability. Written in C, MPTRAC includes a Fortran wrapper and high-level API, enabling seamless integration of Lagrangian transport simulations into other models. Continuous testing via GitHub Actions and multiple HPC systems, including the JUPITER Exascale Development Instrument (JEDI), ensures robust performance and reliability.

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