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MPTRAC

Atmospheric Transport Modeling and GPU-Accelerated Simulations at Scale

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ZIH colloquium, TU Dresden, 3 November 2026

01

MPTRAC: Model Overview

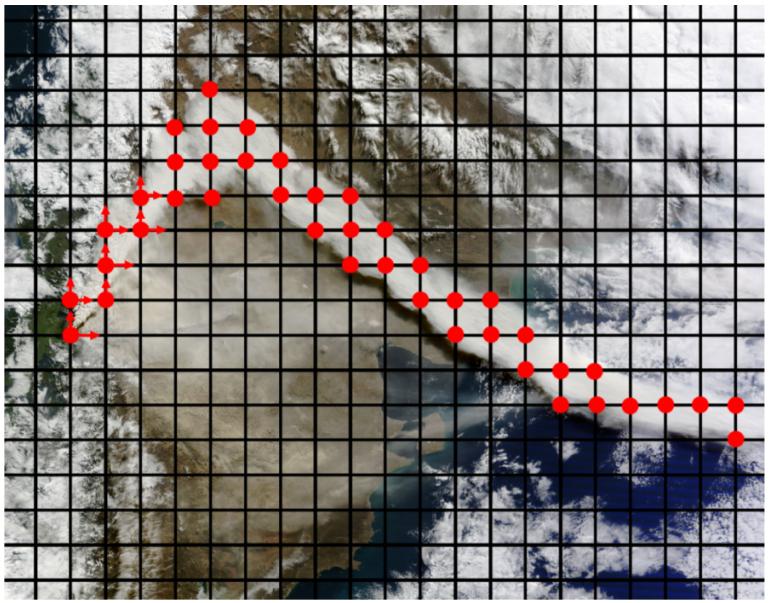
Lagrangian transport modeling

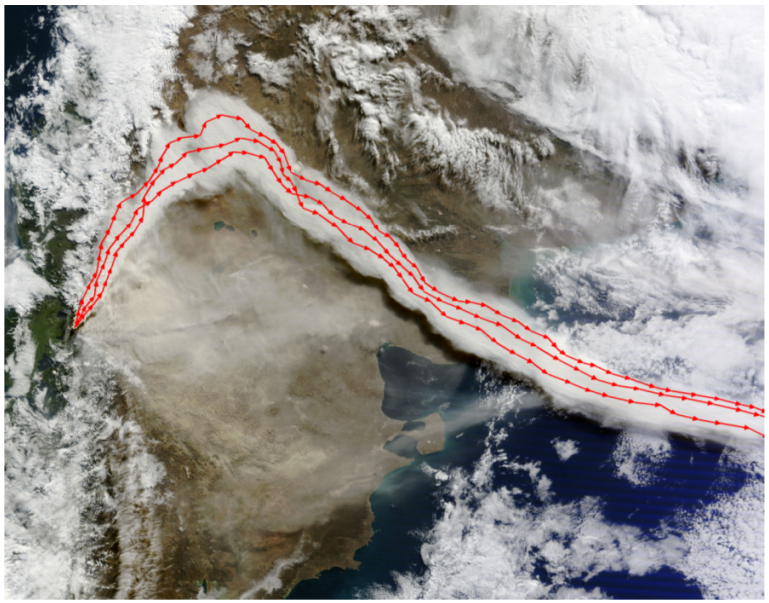
Applications of Lagrangian Transport Models



Scientific studies and operational applications involving the **transport and dispersion of atmospheric constituents**.

Eulerian and Lagrangian transport





- **Advantages:** Resolves fine-scale transport structures while minimizing numerical diffusion.
- **Challenges:** High computational cost and data demands from large meteorological datasets and particle ensembles.

MPTRAC at a glance

- **Massive-Parallel Trajectory Calculations (MPTRAC)**
- Lagrangian transport model for the **free troposphere and stratosphere**.
- Simulates **advection, diffusion, convection, sedimentation, deposition, and chemistry**.
- Processes meteorological data and derives **PBL, tropopause, CAPE, PV**, and other diagnostics.
- Provides flexible **output and visualization** (Python, ParaView, Gnuplot).
- Runs efficiently on **CPUs and GPUs**, from laptops to supercomputers.



`github.com/slcs-jsc/mptrac` `mptrac.jsc.fz-juelich.de`

Trajectory advection

- Air parcel trajectories follow the **kinematic equation of motion**:

$$\frac{d\vec{x}}{dt} = \vec{v}(\vec{x}, t)$$

- Parcel position $\vec{x} = (\lambda, \phi, p)$; wind velocity $\vec{v} = (u, v, \omega)$ from **meteorological reanalyses or forecasts**.
- **Implementation challenges:**
  - Numerical integration schemes and time steps.
  - Different vertical coordinates (p, η, ζ, ...).
  - Spherical geometry and coordinate transformations.

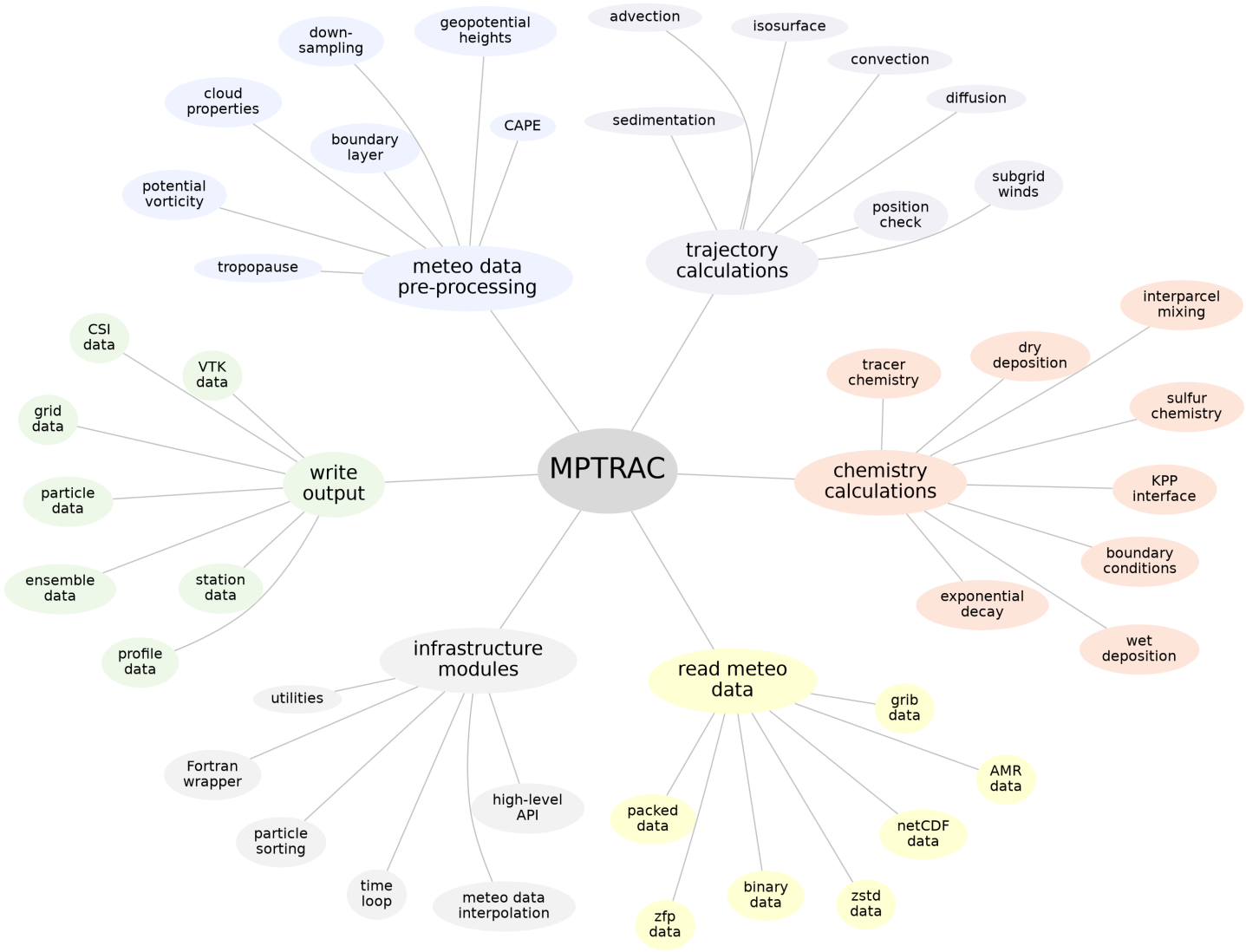
Atmospheric diffusion

- Lagrangian transport minimizes **numerical diffusion**, but **unresolved atmospheric mixing** must be parameterized.
- Turbulent wind fluctuations are modeled using a **Langevin equation**:

$$v'(t+\Delta t) = \underbrace{r\, v'(t)}_{\text{correlated part}} + \underbrace{\sqrt{(1-r^2)\sigma_v^2}\,\xi}_{\text{random component}} + \ldots$$

- Stochastic wind perturbations produce **random-walk trajectories**.
- Correlation r and fluctuation amplitude σ_v depend on the turbulence parameterization.

Physical modules and software architecture



Modular framework for physical and chemical processes, with flexible meteorological input and simulation output.

02

Scientific Applications

From observations to atmospheric processes

Superpressure balloon observations

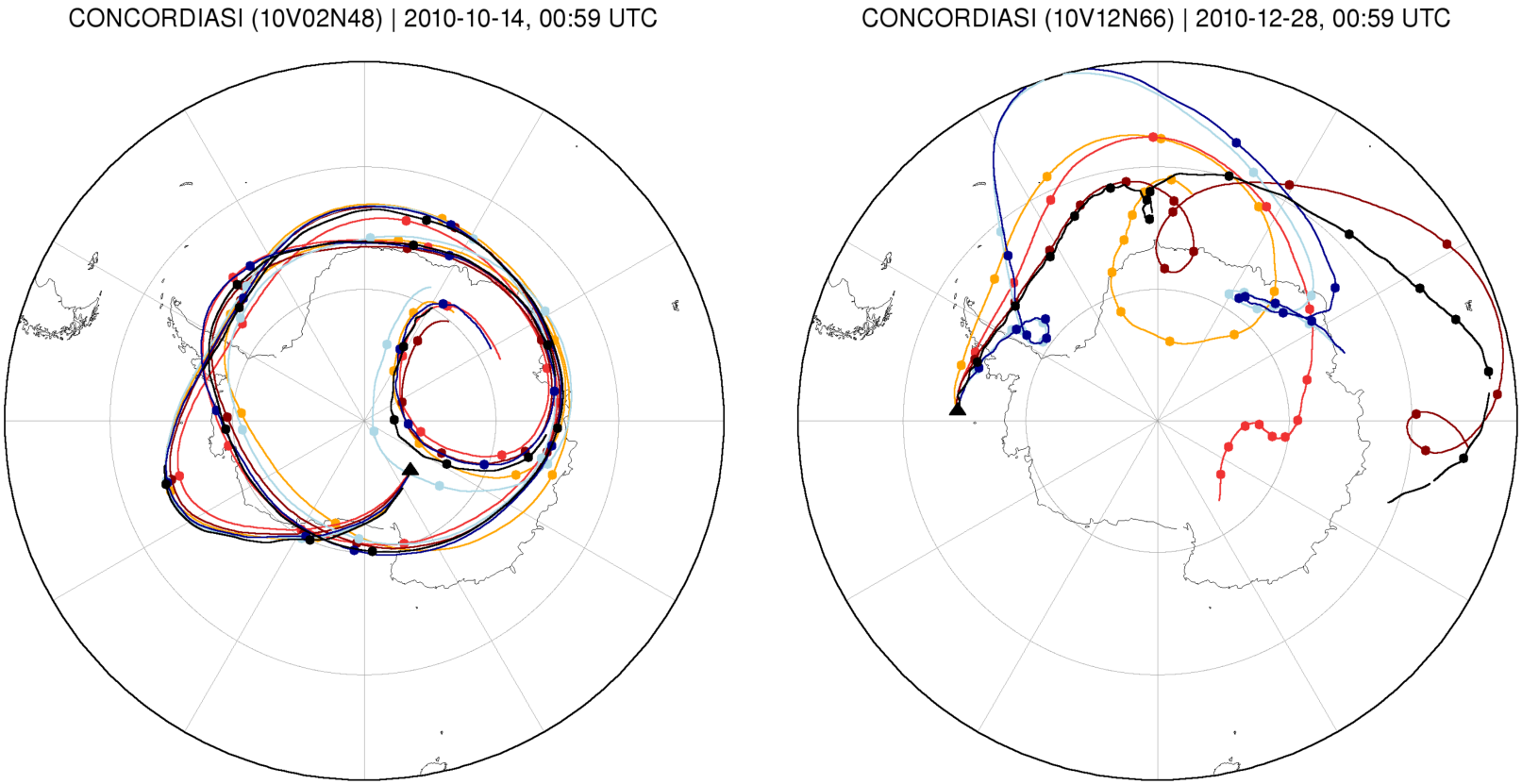
- Concordiasi campaign in Antarctica in 2010/2011:



- GPS-tracked superpressure balloons provide **valuable reference data** for trajectory evaluation.

Observed and deterministic trajectories

- 19 balloon flights lasting 8–97 days, separated into 104 trajectory samples of 15 days each.

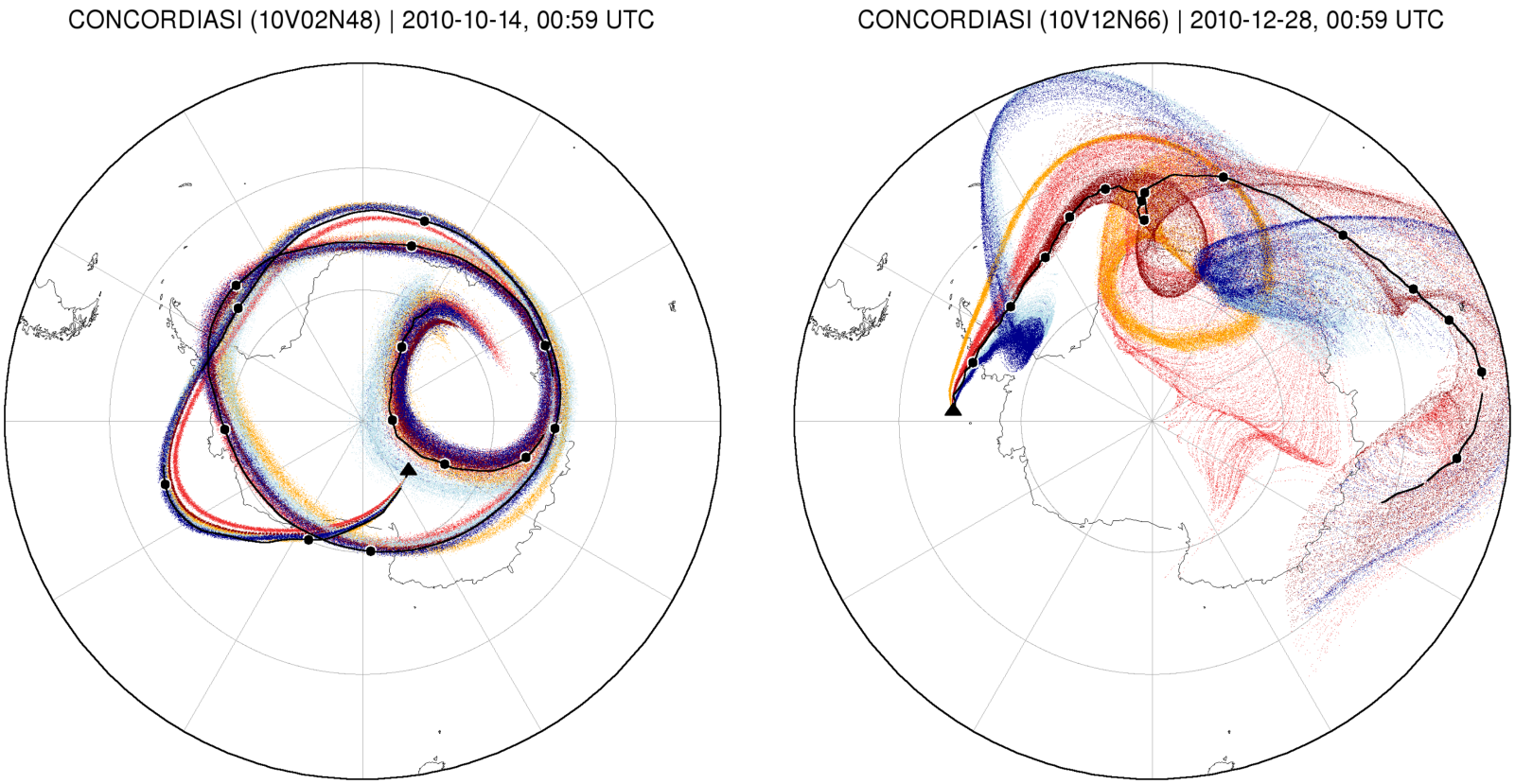


Black: balloon observations — Colored curves: different meteorological reanalyses

- **Trajectory accuracy varies substantially** between individual samples.

Trajectories including atmospheric diffusion

- The same 15-day Concordiasi samples shown as trajectory ensembles with simulated diffusion:

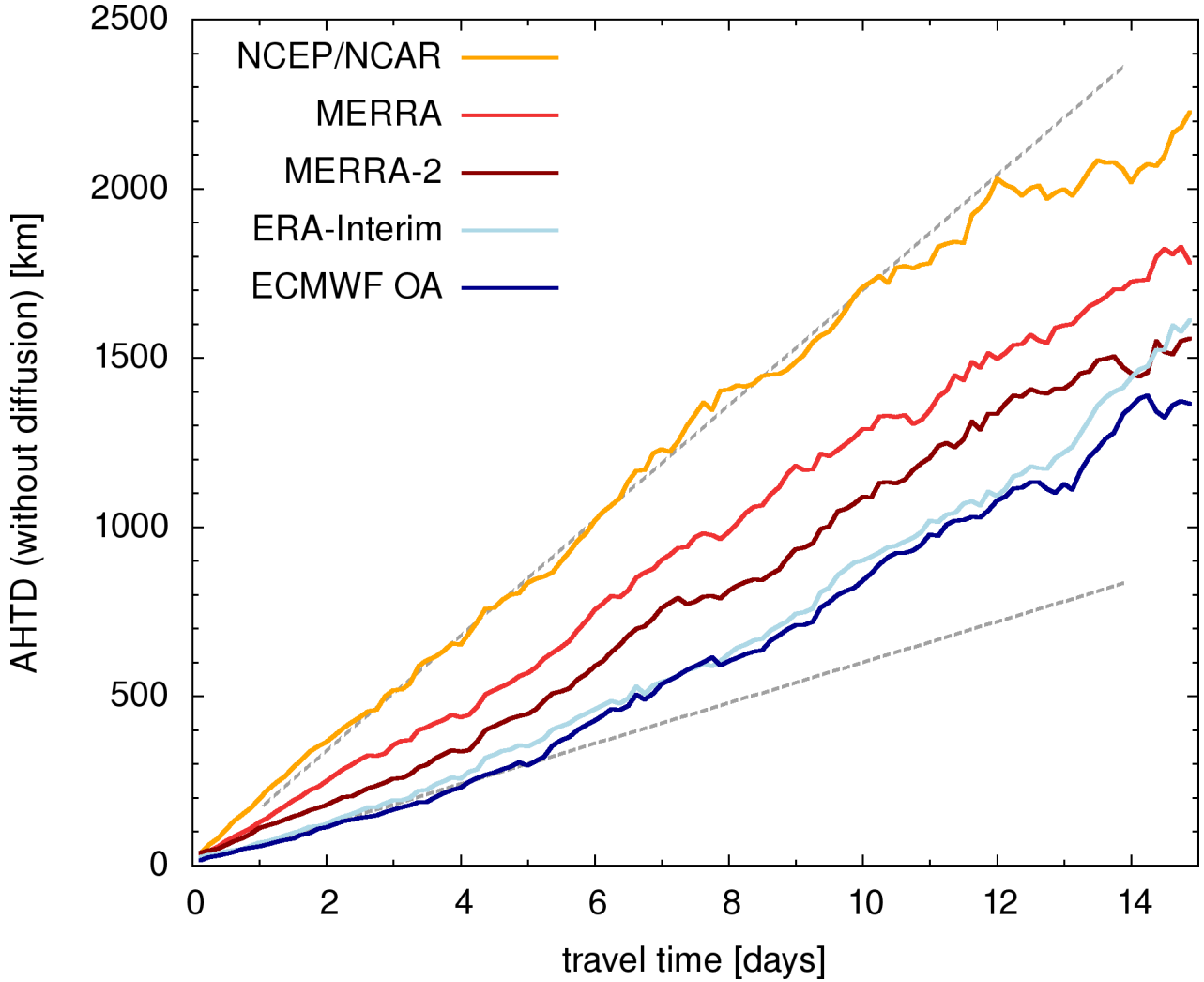


Black: balloon observations — Colored curves: different meteorological reanalyses

- Ensemble spread makes **meteorological complexity** and **transport uncertainty** visible.

Quantitative trajectory errors

- Statistical analysis of transport deviations:



- Typical error growth rates of about 60 – 170 km/day.

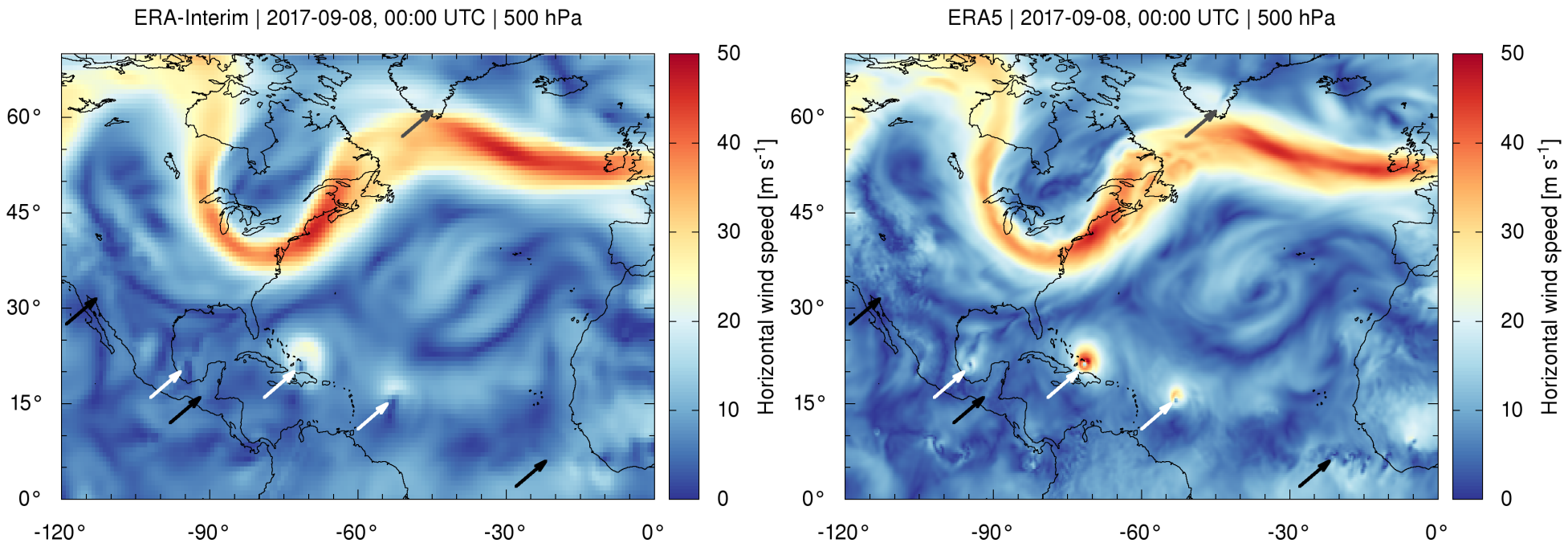
Balloon Evaluation: Key Findings

- Concordiasi balloon observations provide a **valuable reference** for evaluating atmospheric transport simulations.
- **Trajectory errors grow substantially** over time, with significant differences between meteorological reanalyses.
- Surprisingly, superpressure balloon observations were **assimilated into most of the reanalyses** investigated (except NCEP/NCAR).
- Nevertheless, differences persist, highlighting the importance of **other observations, forecast models, and data assimilation methods**.

Hoffmann et al., Atmos. Chem. Phys. 17, 8045–8061 (2017), doi:10.5194/acp-17-8045-2017.

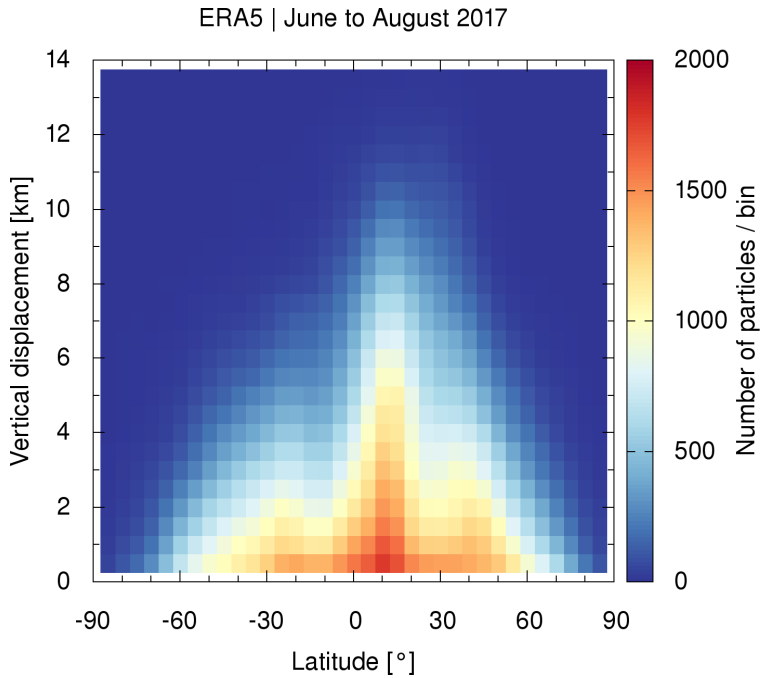
From ERA-Interim to ERA5

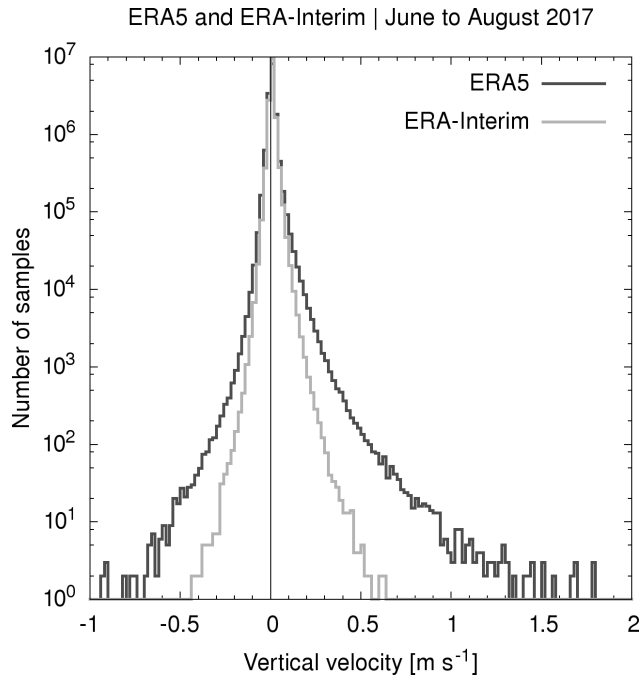
- ERA5 offers **higher resolution and physically improved meteorological modeling** compared to ERA-Interim.
- However, the increased spatial and temporal resolution leads to **85 times more data per day**, posing a major challenge for storage and I/O.



ERA5: Convective Vertical Transport

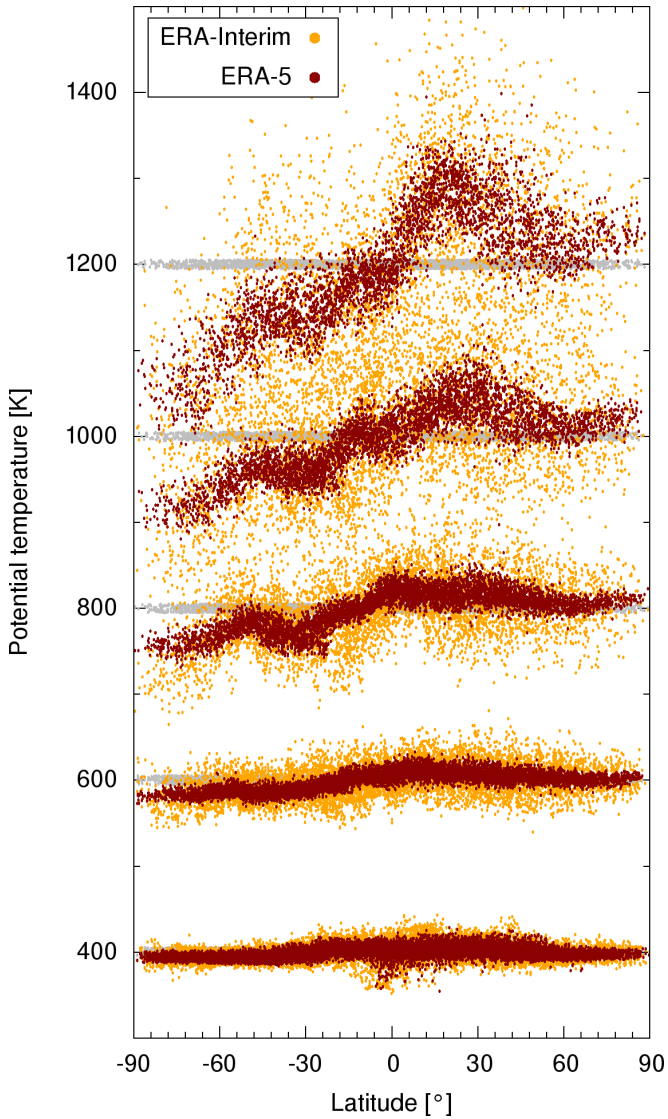
- ERA5 provides a **more realistic representation of convective vertical transport**, including stronger updrafts and finer spatial structures in the troposphere.





- However, a **convection parameterization** is still required at ∼30 km horizontal resolution.

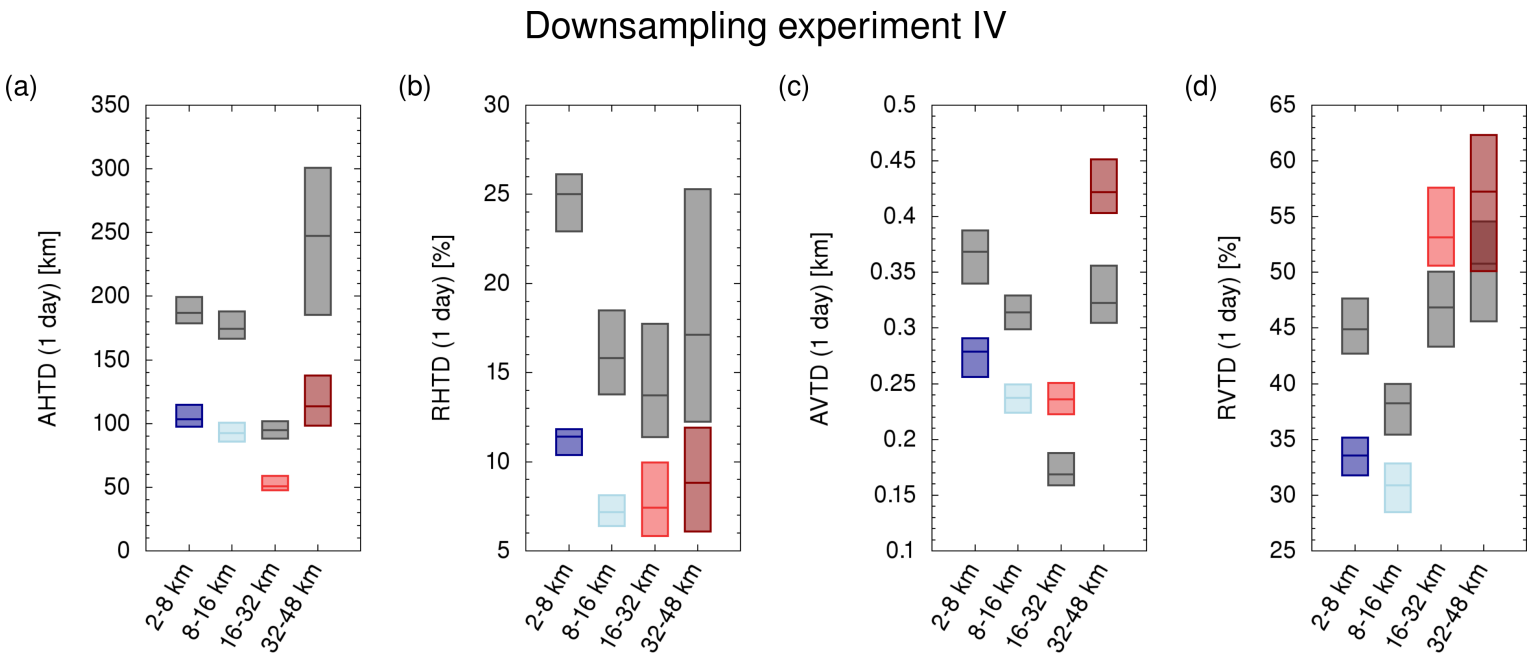
ERA5: Potential Temperature Conservation



- In the stratosphere, potential temperature θ is usually **conserved during adiabatic transport**.
- ERA5 trajectories (red) show **better conservation of** θ over 10 days compared to ERA-Interim (orange).

ERA5: Beyond Higher Resolution

- To assess the impact of resolution, we **downsampled ERA5 to the spatiotemporal resolution of ERA-Interim**.



Red/blue: ERA5 downsampling effects; gray: ERA5 vs. ERA-Interim.

- **Resolution is not the whole story:** Differences in forecast model and data assimilation scheme also affect trajectories.

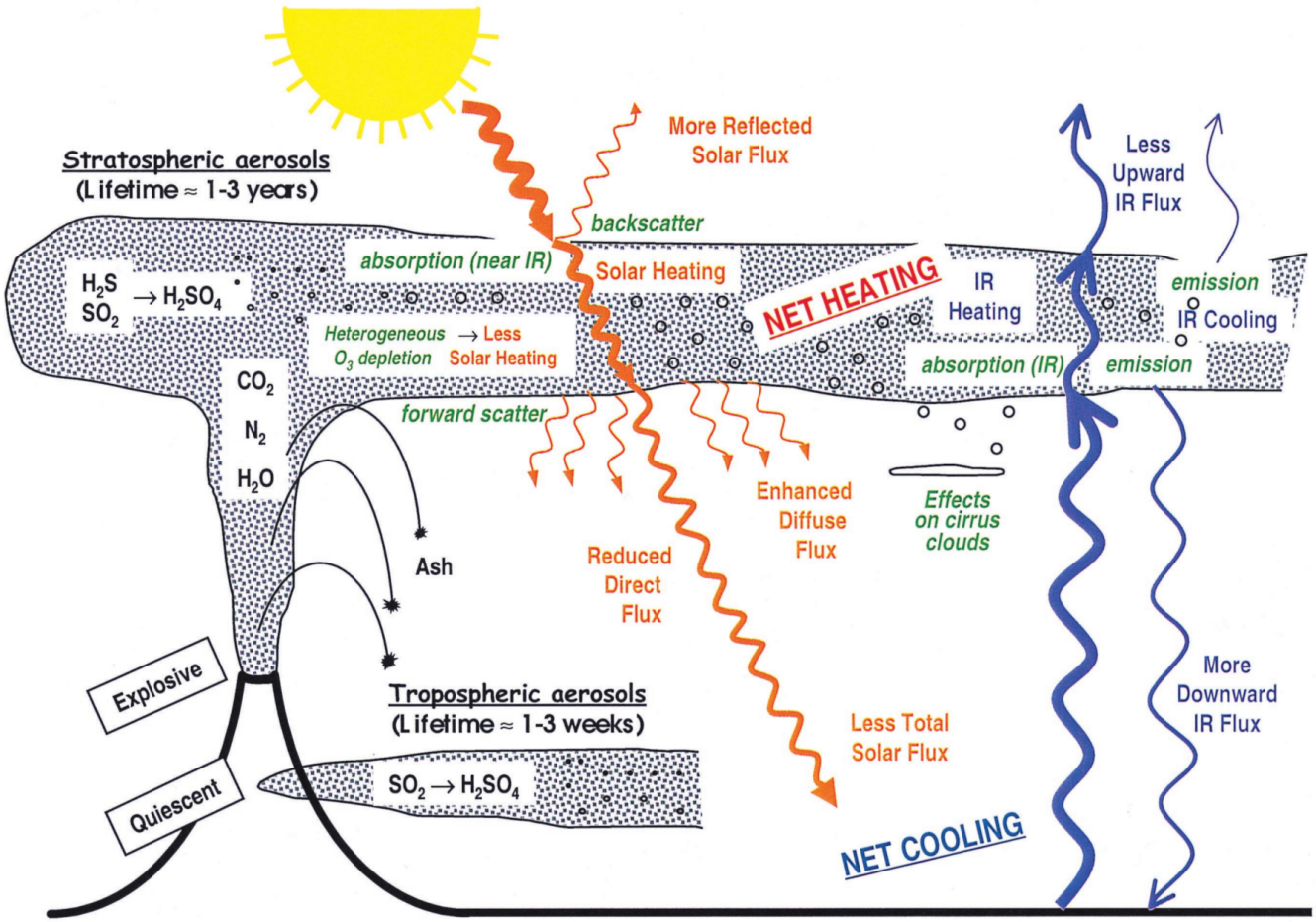
ERA5: Key Findings

- **Trajectory analyses** provide a sensitive diagnostic tool for evaluating meteorological datasets.
- ERA5 provides a **more detailed and realistic representation of atmospheric transport**, particularly convection and fine-scale structures.
- In the stratosphere, ERA5 trajectories show **better conservation of potential temperature**.
- **Higher resolution is not the only factor:** Forecast models and data assimilation also influence transport simulations.

Hoffmann et al., Atmos. Chem. Phys. 19, 3097–3124 (2019), doi:10.5194/acp-19-3097-2019.

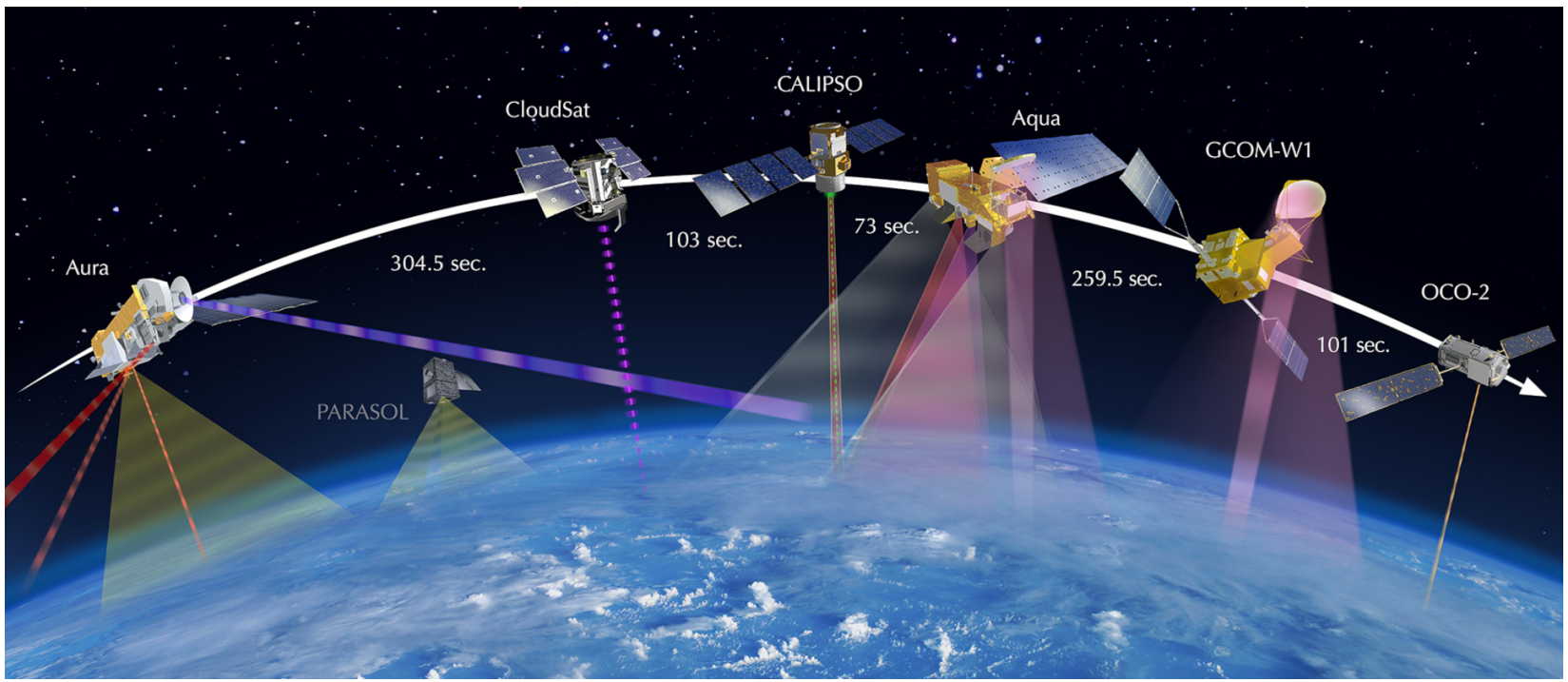
Why Volcanic SO_2 Matters

- Volcanic SO_2 can form **sulfate aerosol layers**, affecting atmospheric composition and climate.



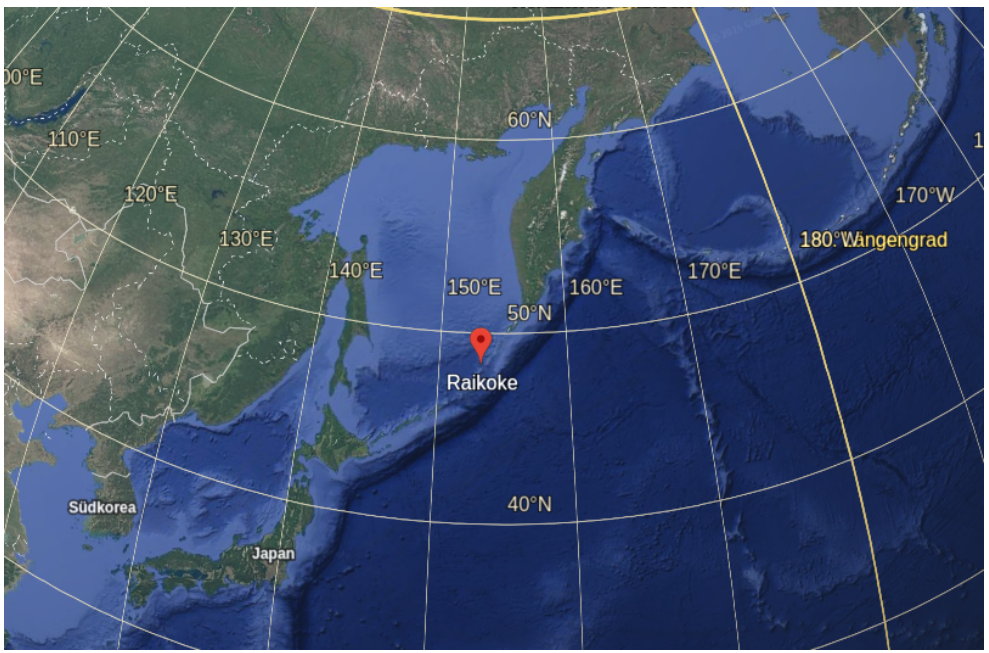
Satellite Observations of Volcanic SO_2

- **AIRS and TROPOMI** provide more than 20 years of satellite observations of volcanic SO_2.
- Satellites measure **SO_2 columns**, but not vertical profiles — the **injection altitude remains uncertain**.
- **MPTRAC backward trajectories** help reconstruct the time and altitude of volcanic SO_2 emissions.



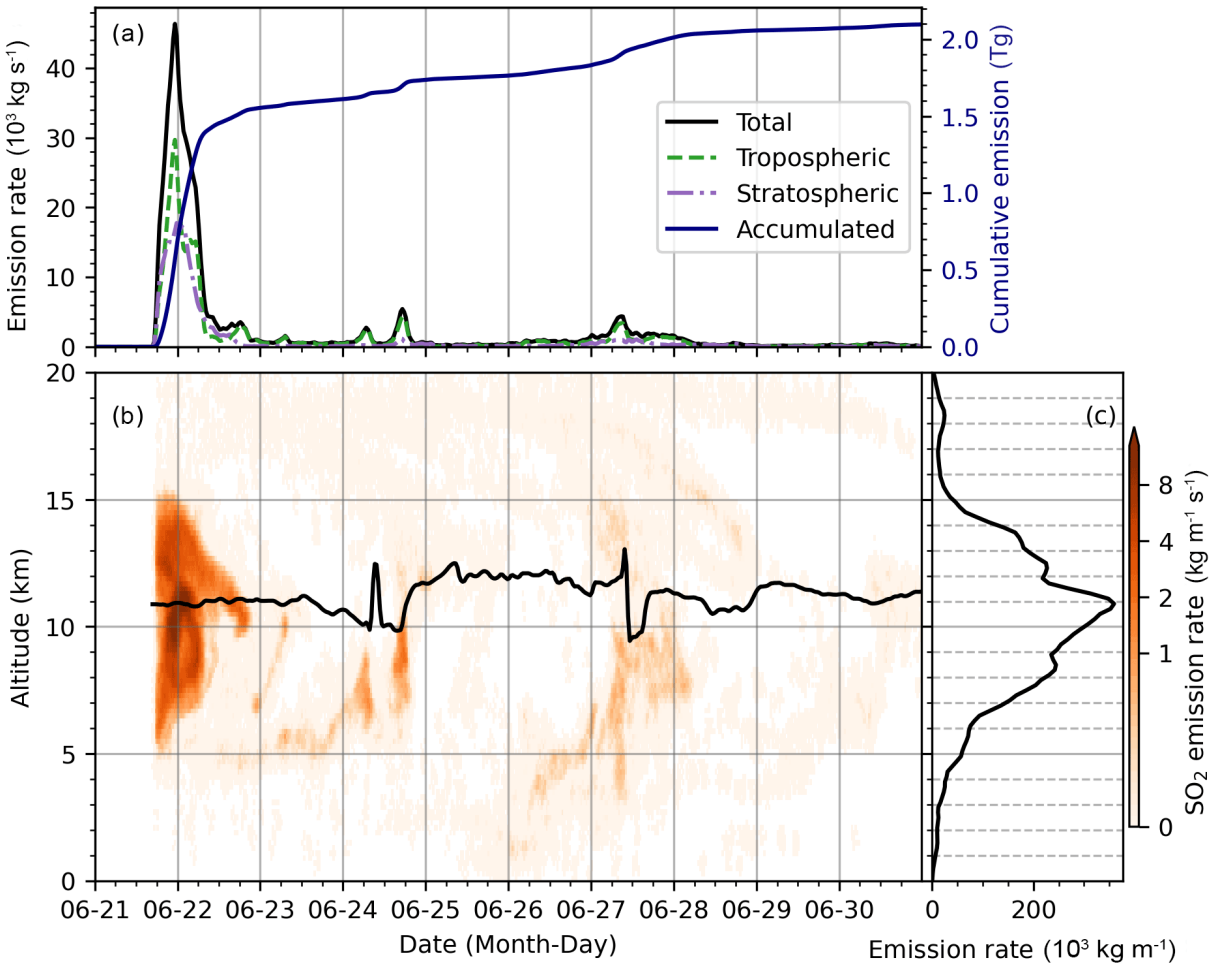
Case study: Raikoke 2019 eruption

- Remote volcanic island in the **Kuril Islands**, NW Pacific.
- Explosive eruption (VEI 4) on 21 June 2019.
- **Large SO_2 injection into the UT/LS region**.





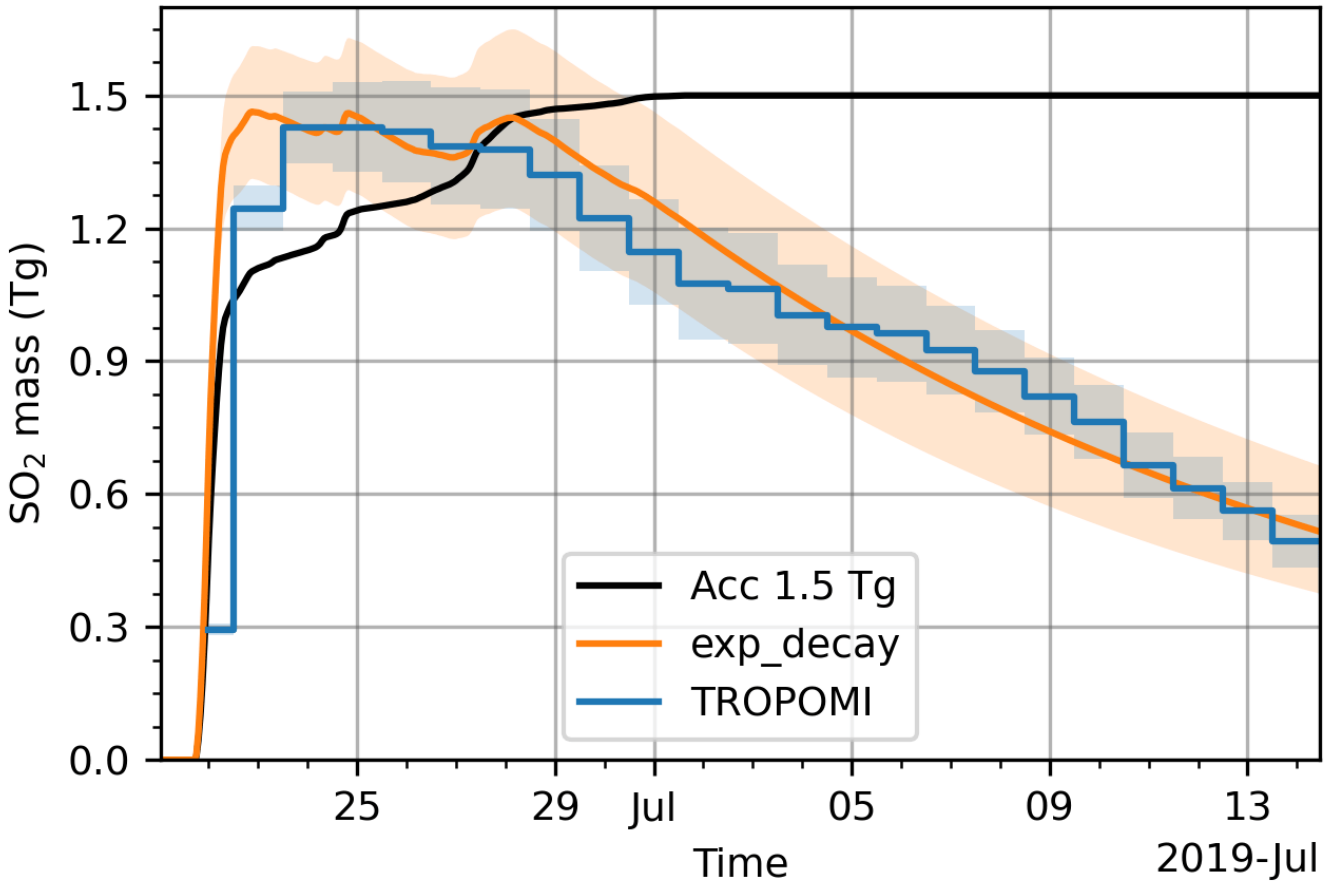
Reconstructing Raikoke SO_2 Emissions



- **Observations:** TROPOMI detects the SO_2 plume.
- **Backward trajectories:** MPTRAC traces transport from satellite locations at different altitudes.
- **Emissions:** Reconstruct injection time, altitude, and SO_2 emission rates.

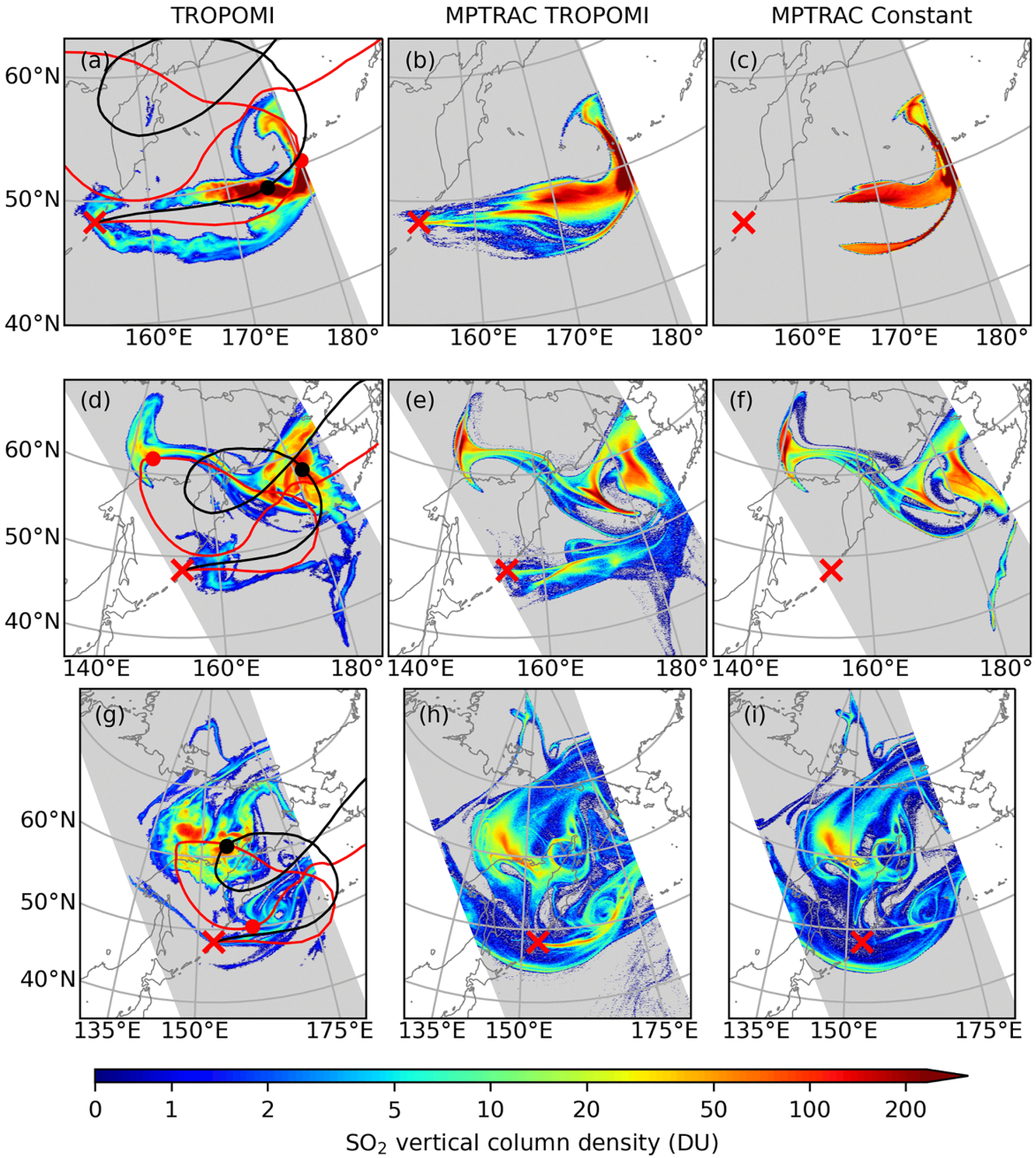
SO_2 Mass Evolution

- MPTRAC simulations reproduce the **SO_2 mass evolution** observed by TROPOMI.



- Earlier SO_2 mass estimates adjusted from **1.5 to 2.1 Tg**.
- Assumed SO_2 e-folding lifetime of **15 days**.

Raikoke: Simulated SO_2 Transport



- **Excellent agreement** with TROPOMI after 1–6 days.
- **Good skill scores** (POD, FAR) up to ~10 days.

Raikoke Study: Key Findings

- **Satellite observations and backward trajectories** enable reconstruction of volcanic SO_2 emissions in time and altitude.
- The Raikoke eruption injected about **2.1 Tg of SO_2**, with a substantial fraction reaching the stratosphere.
- **Forward MPTRAC simulations** successfully reproduce the observed SO_2 plume evolution over several days.
- **Remaining limitations:** Excessive dispersion of compact SO_2 clouds occurs at longer transport times.

Cai et al., Atmos. Chem. Phys. 22, 6787–6809 (2022), doi:10.5194/acp-22-6787-2022.

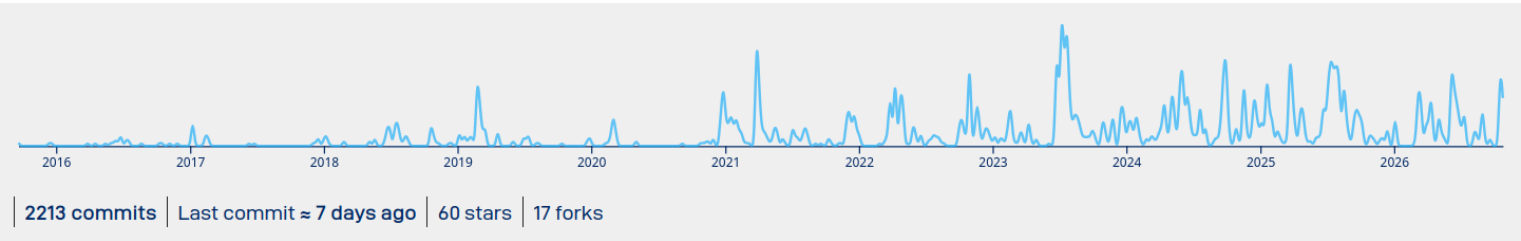
03

High-Performance Computing

GPU acceleration and efficient data handling

MPTRAC: Scalable Research Software

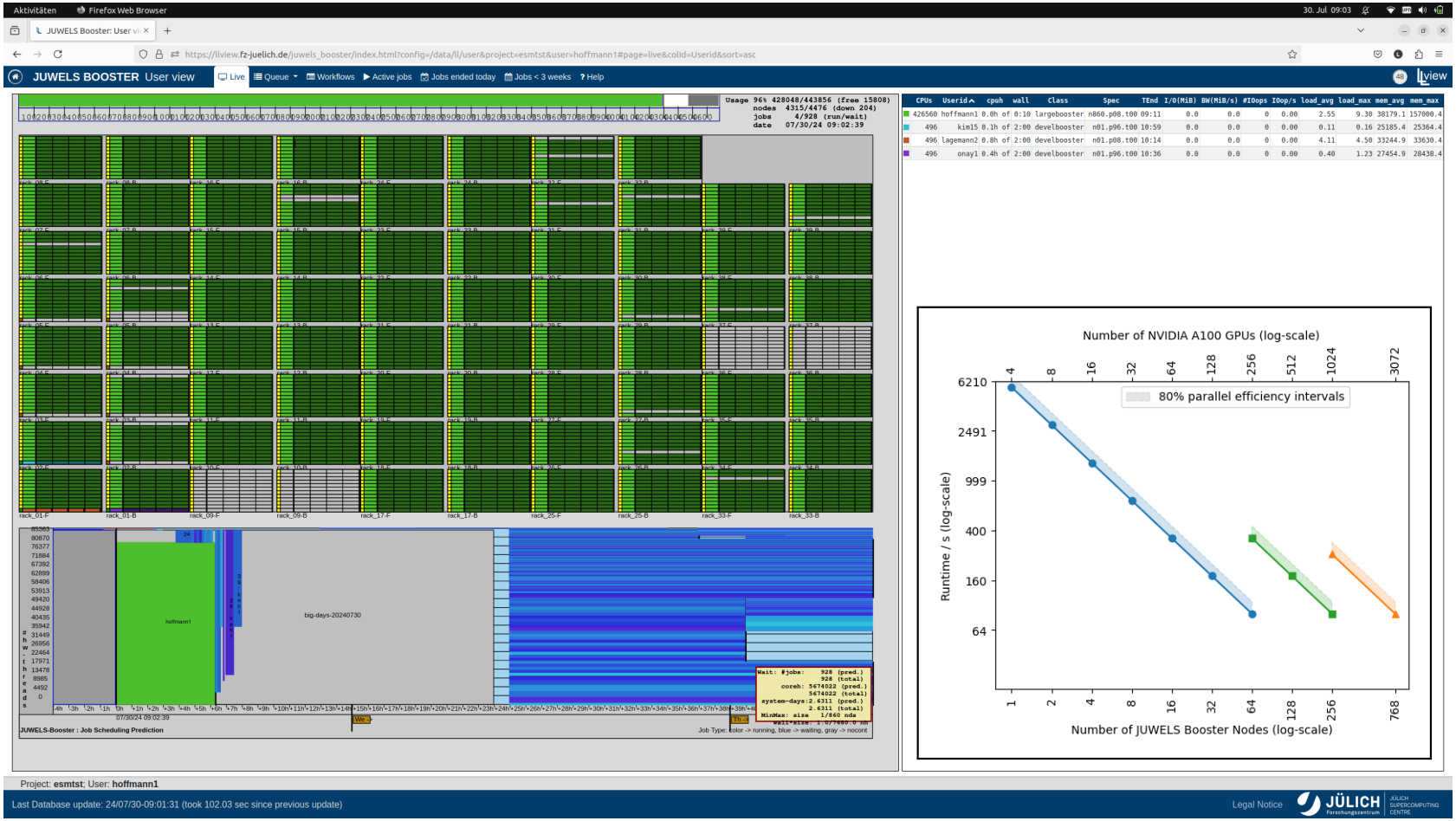
- **Scalable and portable:** From laptops to GPU-accelerated supercomputers, with containerized deployment options.
- **Hybrid parallelization:** MPI, OpenMP, and OpenACC.
- **Active development:** Maintained since 2015, with about 30,000 lines of C code.



- **RSE best practices:** Version control, testing, CI/CD, code review, documentation, and AI-assisted development.
- **Scientific impact:** About 30 peer-reviewed publications.

Scaling on JUWELS Booster

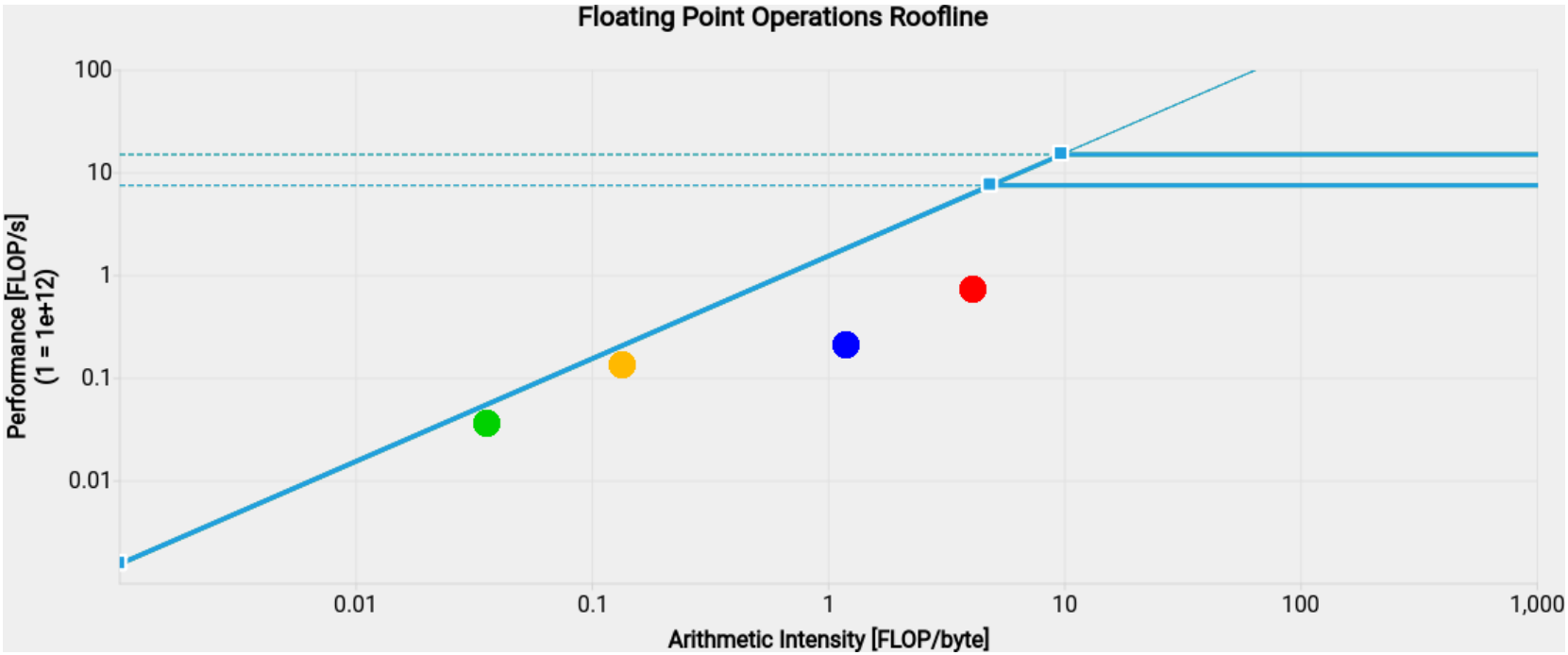
- MPTRAC scales to **3,440 NVIDIA A100 GPUs** on JUWELS Booster.



- Largely independent particle calculations enable **efficient weak and strong scaling**.

MPTRAC: GPU Performance Bottlenecks

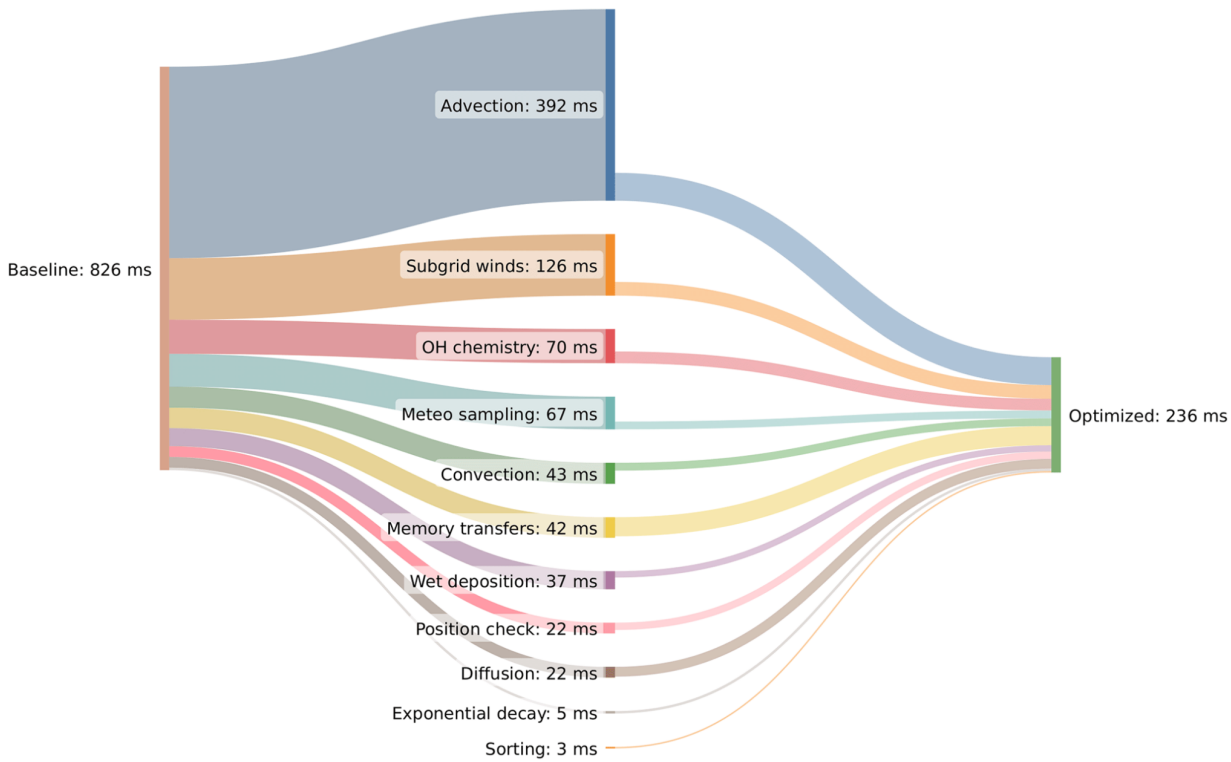
- **Advection dominates GPU runtime**, accounting for 55 % of a time step in the profiled configuration.
- **Roofline analysis reveals a memory-bound kernel**, limited by near-random access to meteorological fields.



Baseline: FP32 green, FP64 orange; optimized: FP32 blue, FP64 red.

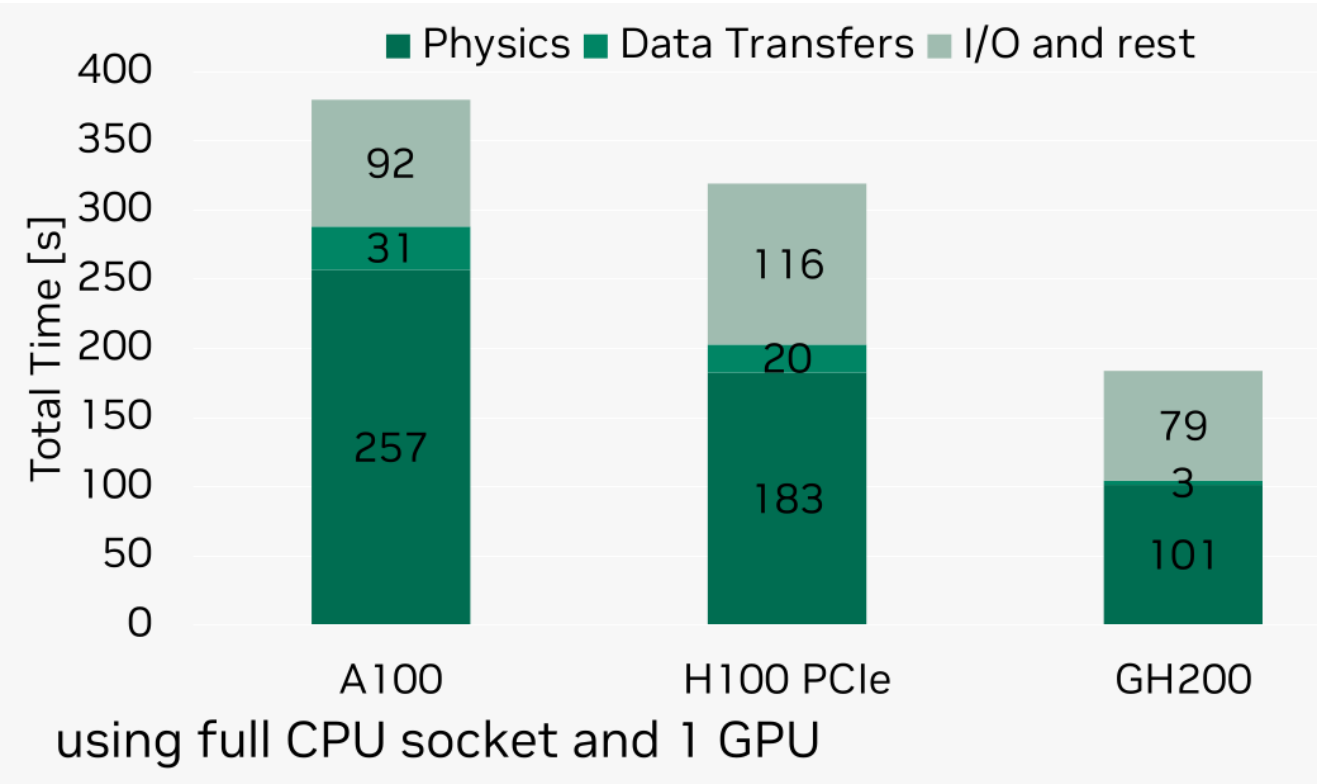
Optimizing GPU Memory Access

- **Interleaved wind fields:** Improved memory access (SoA $\rightarrow$ AoS) accelerates the advection kernel by 1.8$\times$ and total physics by 1.4$\times$.
- **Particle sorting:** Grouping particles by meteorological grid location improves data locality, accelerating advection by 5$\times$ and total physics by 3.5$\times$.



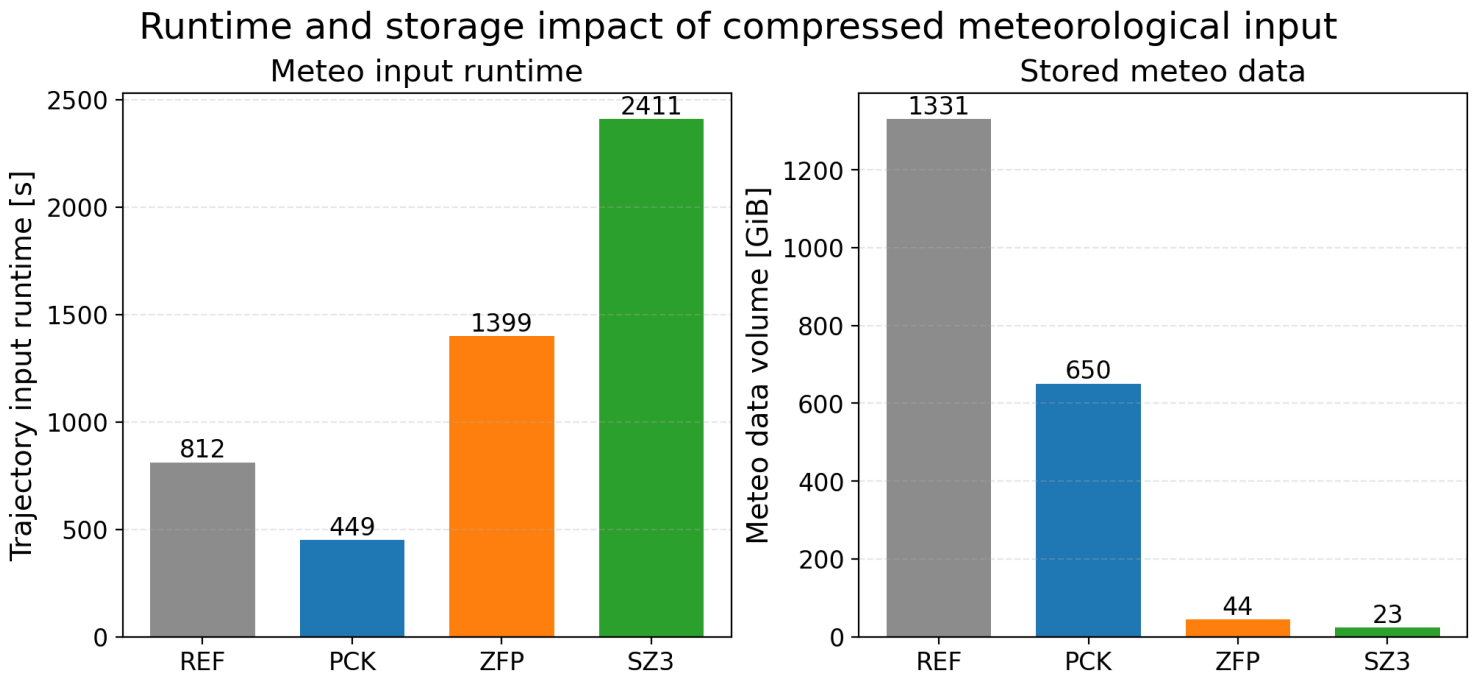
Towards Exascale: A100 to GH200

- **Preparing MPTRAC for JUPITER:** Evaluating NVIDIA GH200 (Grace CPU + Hopper GPU) for exascale computing.
- **Performance gains:** About 2× faster GPU computations, with substantially faster host-device data transfers enabled by NVLink-C2C.

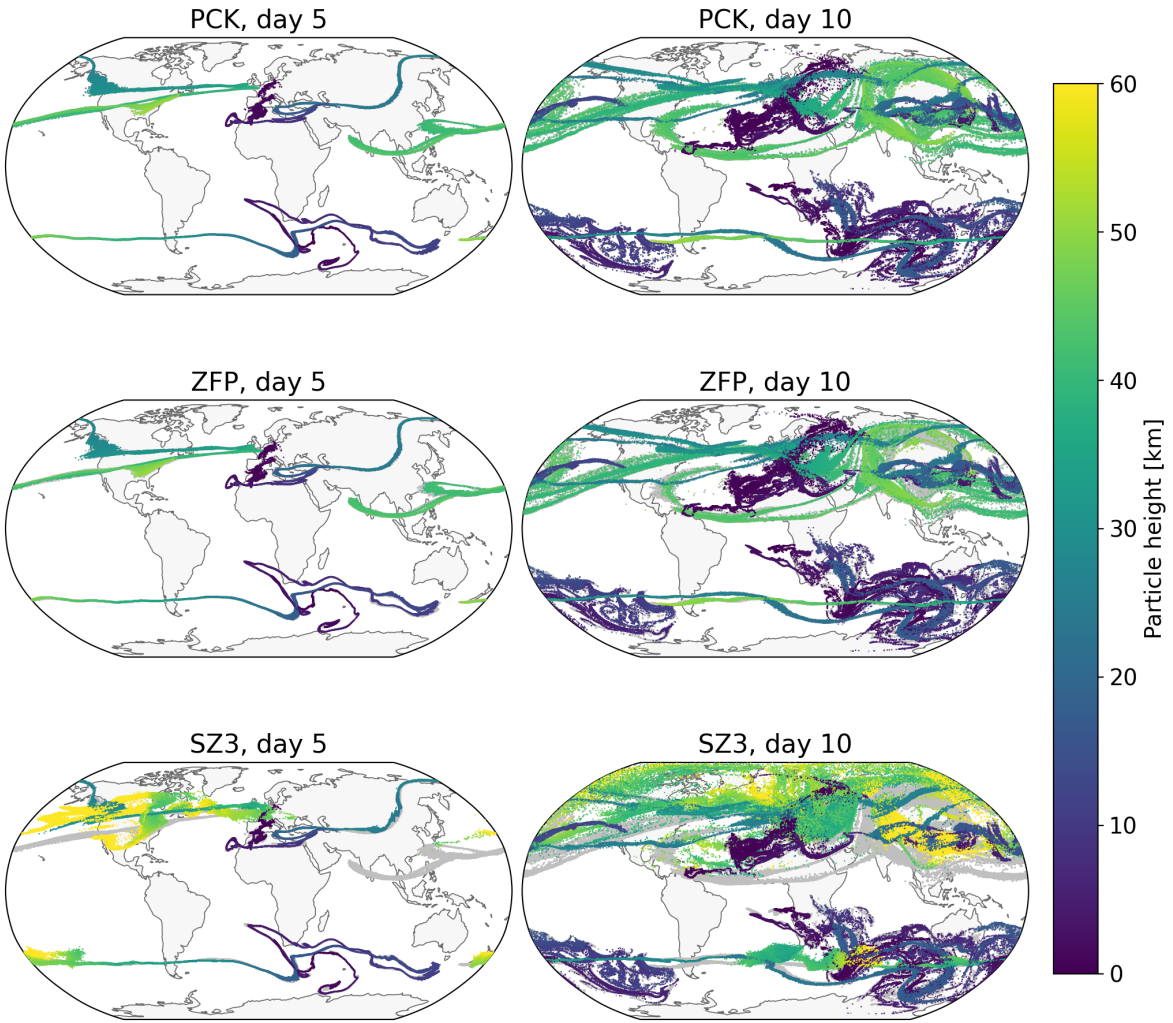


Reducing the ERA5 Data Footprint

- **Challenge:** Large meteorological datasets increase storage, data transfer, and I/O costs.
- **Approach:** Evaluate lossless and lossy compression of ERA5 in terms of data reduction, I/O performance, and trajectory accuracy.



How Does Lossy Compression Affect Trajectories?



Colored: compressed ERA5; Gray: uncompressed reference.

10-day MPTRAC experiment

- 100,000 particles, evaluated after 5 and 10 days.

Findings:

- PCK: small deviations.
- ZFP: promising compromise.
- SZ3: requires further tuning.

High-Performance Computing: Key Findings

- **Massive parallelism:** MPTRAC scales efficiently to thousands of GPUs, enabling large particle simulations.
- **Memory access matters:** Optimized data layouts and particle sorting substantially improve GPU performance.
- **Towards exascale:** New GPU architectures offer further gains, particularly in host-device data transfers.
- **Data efficiency:** Meteorological data compression offers substantial storage savings, but requires careful evaluation of performance and accuracy.

Hoffmann et al., Geosci. Model Dev. 17, 4077–4094 (2024), doi:10.5194/gmd-17-4077-2024.

04

Current Developments and Outlook

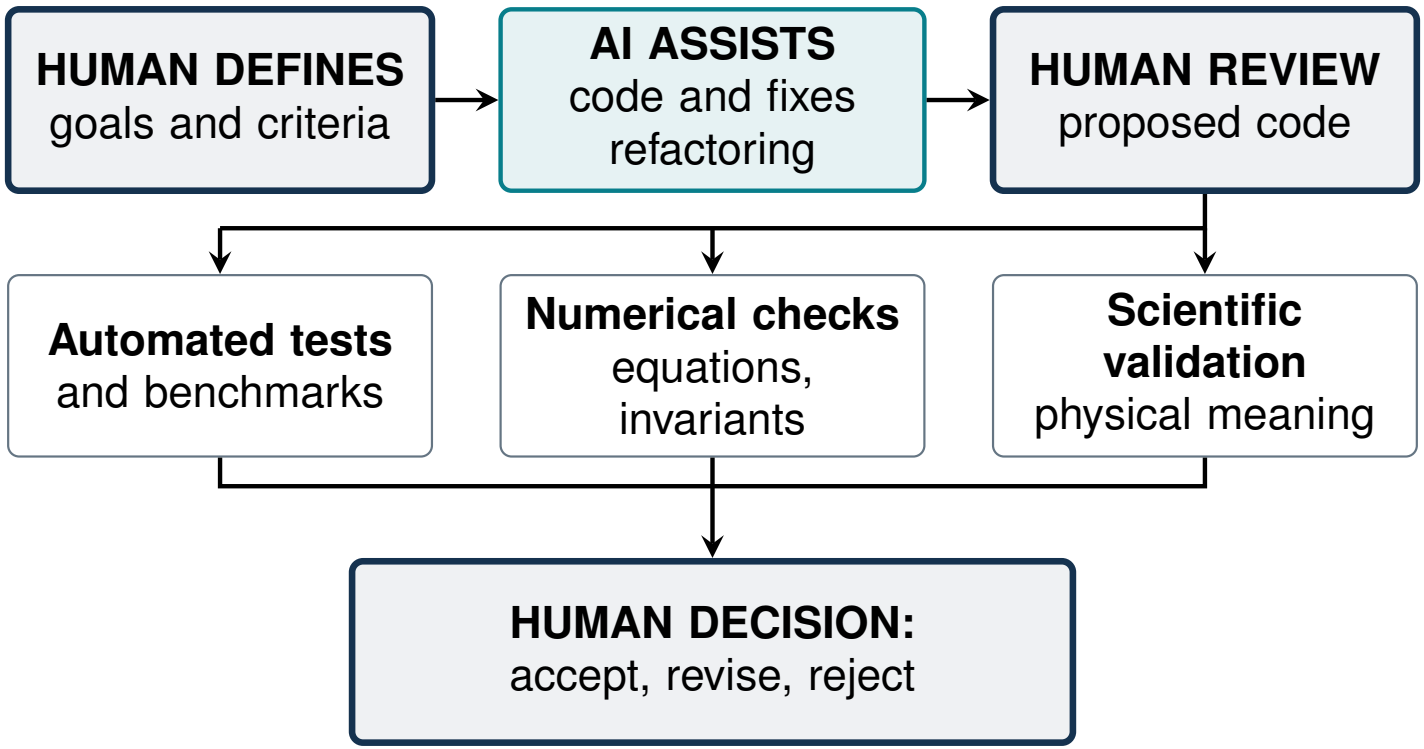
AI-assisted research software engineering

A New Approach to Research Software Engineering



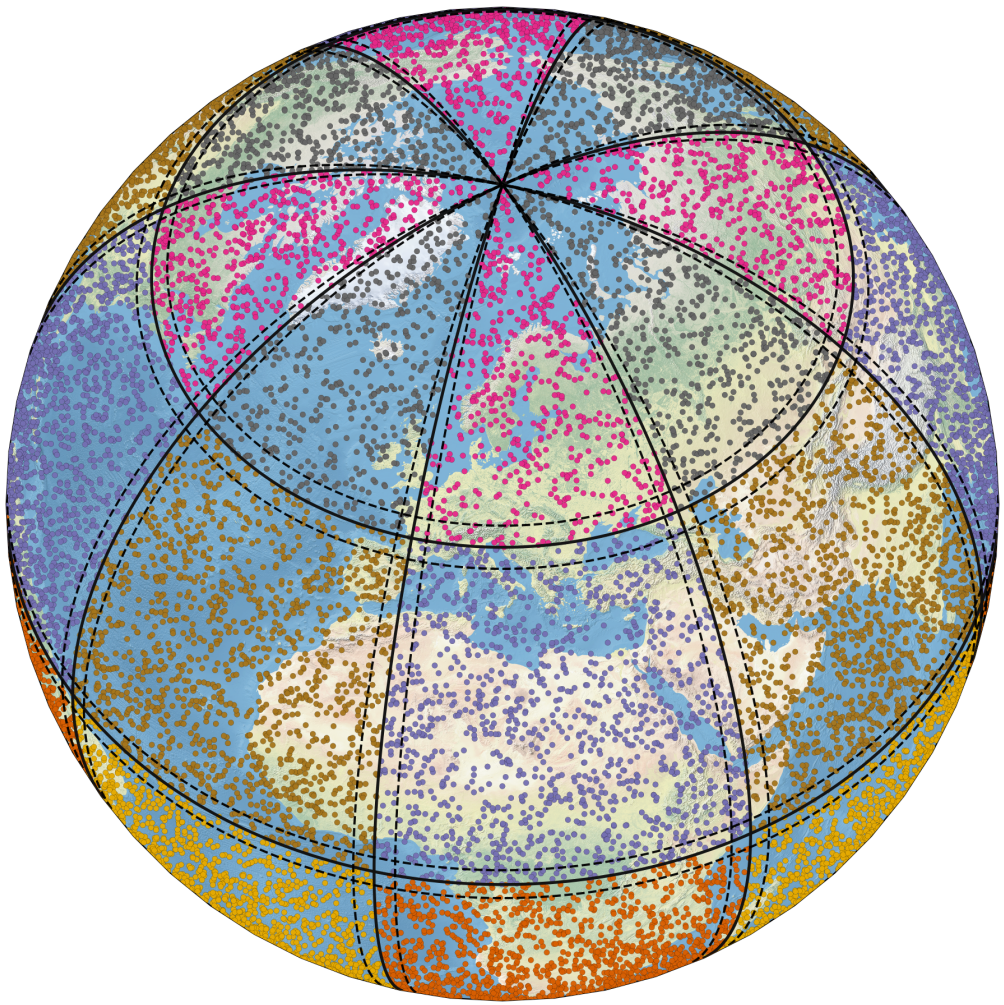
What used to be science fiction now feels surprisingly familiar.

AI-Assisted Research Software Engineering



AI accelerates development;
humans remain responsible for scientific results.

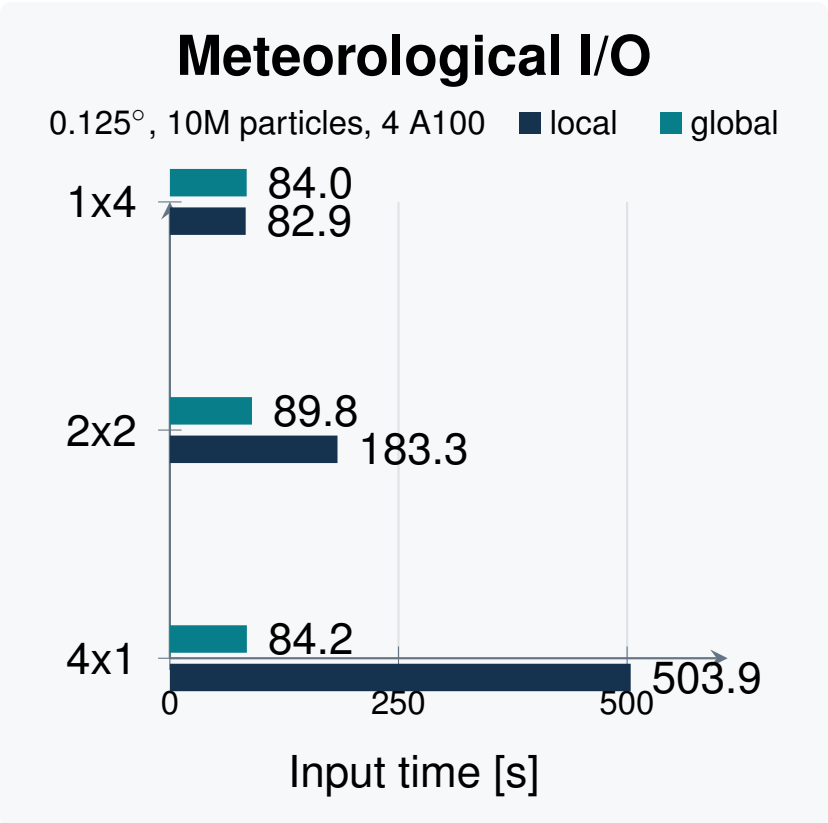
Example: Domain Decomposition for MPTRAC

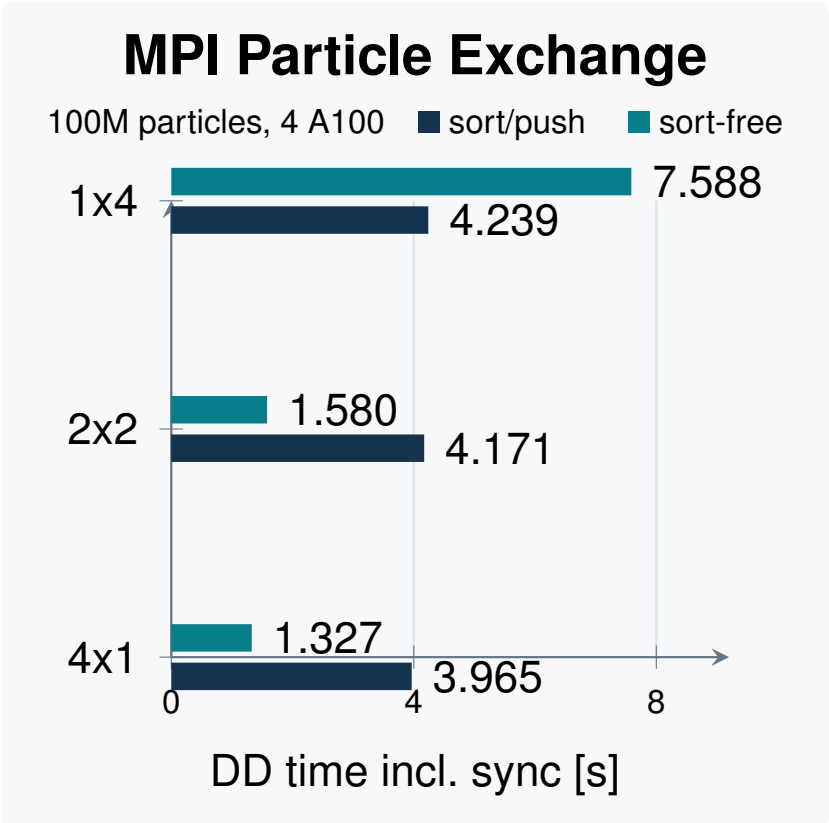


- **Motivation:** Distribute particles and meteorological fields across MPI ranks, enabling km-scale simulations (ICON, IFS).
- **Challenge:** Efficient and correct particle exchange across domain boundaries.
- **Development:** Initially developed by a researcher, later reviewed and improved with AI assistance.

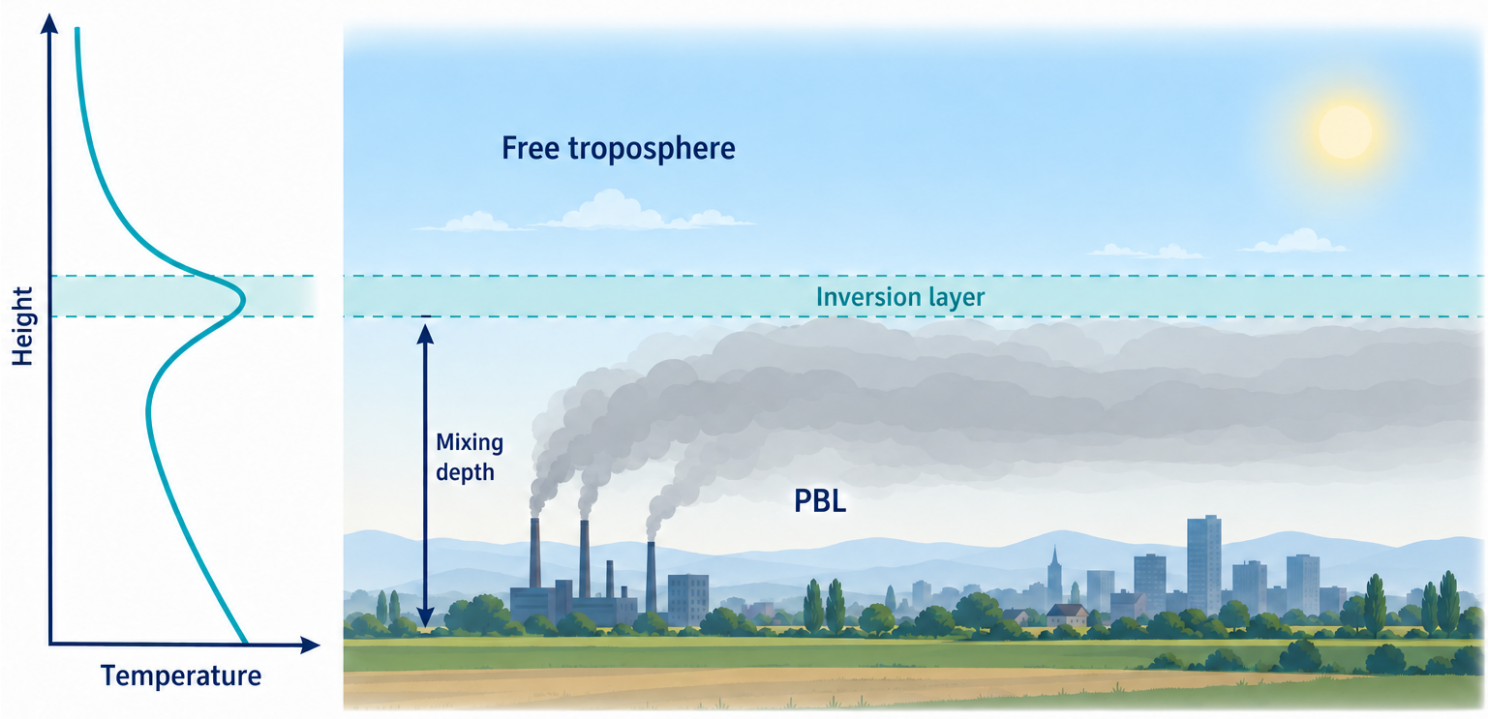
Domain Decomposition: AI-Assisted Improvements

- **Correctness:** Fixed MPI communication near the poles.
- **Performance:** Faster I/O and sort-free MPI exchange.
- **Maintainability:** Bug fixes, refactoring and documentation.





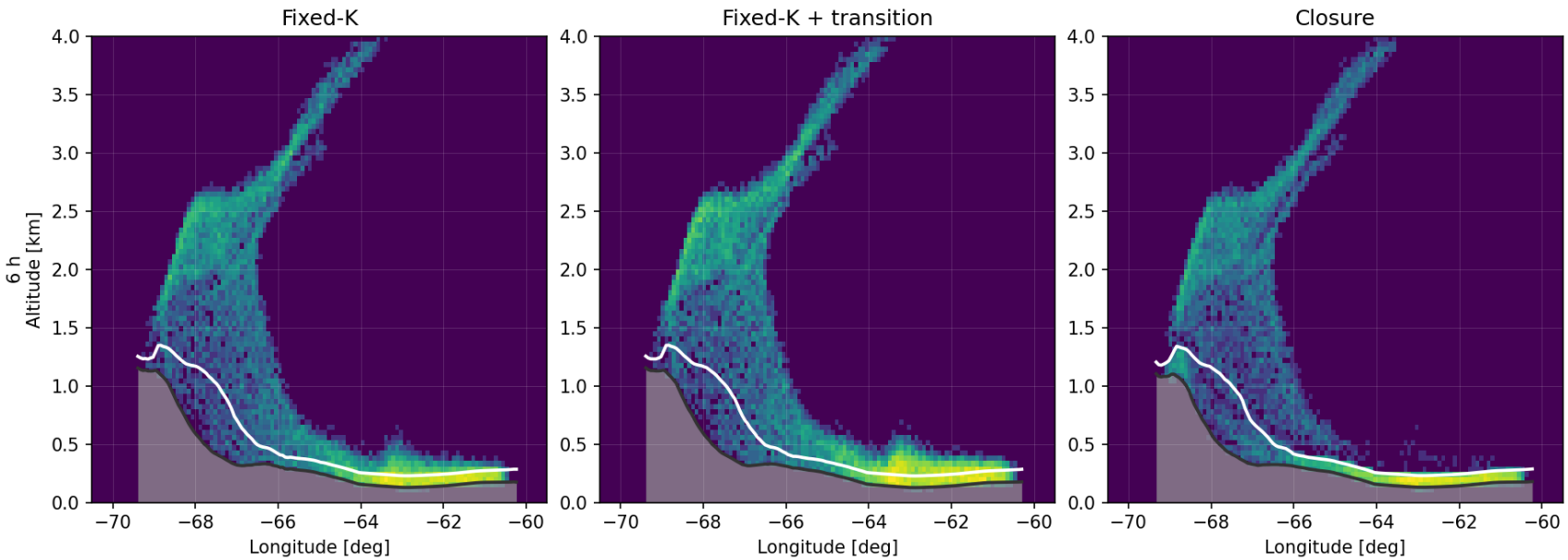
Example: Extending MPTRAC into the PBL



- **Motivation:** Many important atmospheric emission sources are located in the planetary boundary layer.
- **Challenge:** Limited PBL transport and mixing physics restricts MPTRAC applications near the surface.
- **Development:** From manually implemented basic PBL treatment to AI-assisted extensions.

Hanna PBL Closure: Stable Shallow Land

- **AI-assisted implementation:** Hanna's stability-dependent turbulence parameterization, using FLEXPART's open source implementation as a reference.



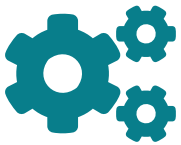
- **Comparison:** Fixed-K, modified fixed-K, and Hanna closure after 6 hours of transport.
- **Finding:** Hanna closure reduces excessive upward spreading in regions with stable boundary layer.

Lessons Learned: AI for Scientific Software



Productivity

Faster debugging, refactoring, documentation and implementation.



Complexity

Help navigating large codebases and sophisticated algorithms.



Responsibility

Human review, tests, benchmarks and scientific validation.

AI is a powerful RSE assistant,
but scientific judgment remains essential.

Summary

- **Atmospheric science:** MPTRAC enables accurate and flexible Lagrangian transport simulations, evaluated against observations.
- **High-performance computing:** GPU acceleration and scalable algorithms enable massive particle simulations with large meteorological datasets.
- **Data efficiency:** Meteorological data compression can greatly reduce storage requirements, but must be balanced against I/O performance and accuracy.
- **AI-assisted development:** AI accelerates research software engineering, while human review and scientific validation remain essential.



Thank you!

Questions?

github.com/slcs-jsc/mptrac

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