



Simulation of Atmospheric Particle Movement

A Framework for Modeling Air Parcel Dynamics

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Project Overview & Motivation

The Problem

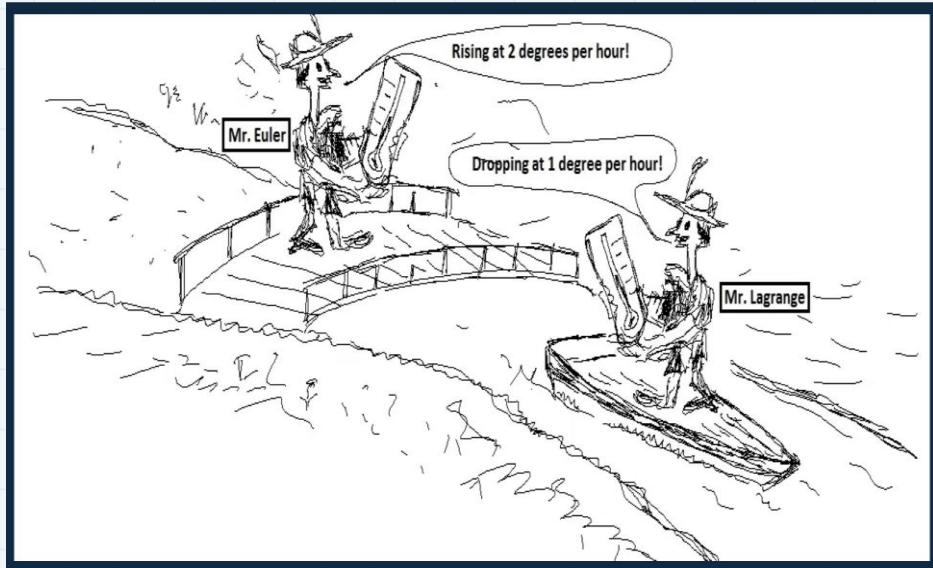
Atmospheric dynamics are complex and non-linear, making parcel tracking difficult in traditional fixed-grid systems.

The Need

Research tools that allow for controlled, parcel-scale investigation of convection and transport.

Our Solution

A Molecular Dynamics-inspired framework that tracks individual air parcels as discrete objects.



Physical Background & Global Circulation

Large-scale atmospheric flow is shaped by uneven solar heating and Earth's rotation, creating organized circulation patterns.

Hadley Cells

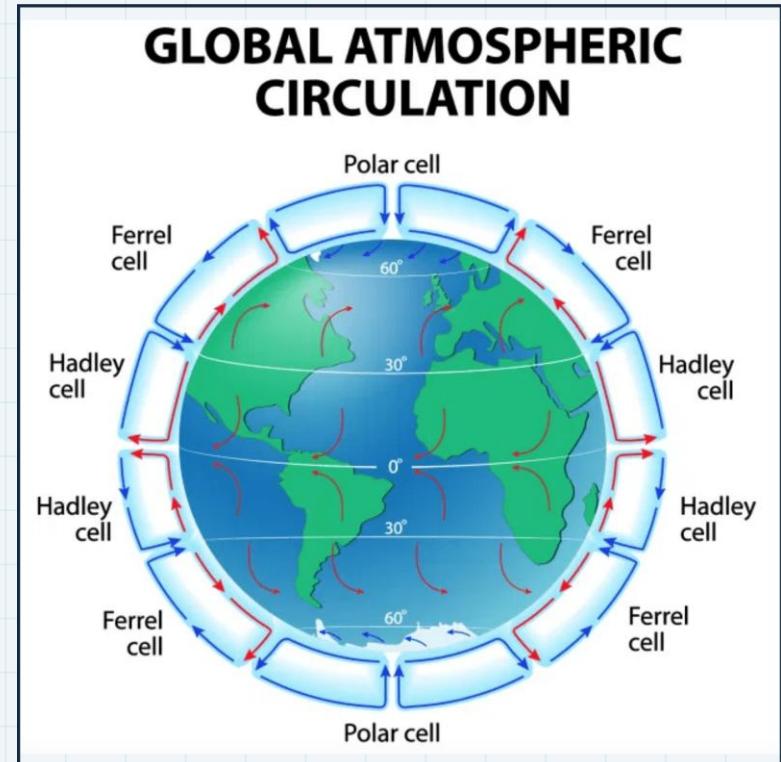
Warm air rises at the equator, moves poleward aloft, and sinks at 30° latitude.

Ferrel Cells

Mid-latitude circulation where air flows poleward and eastward near the surface.

Polar Cells

Cold air sinks at the poles and flows equatorward at the surface.



Fundamental Force Definitions

1. Fundamental Forces

Gravity Force

Direct gravitational acceleration on each parcel mass.

Interaction Force

Parcel-to-parcel interactions – Repulsion force

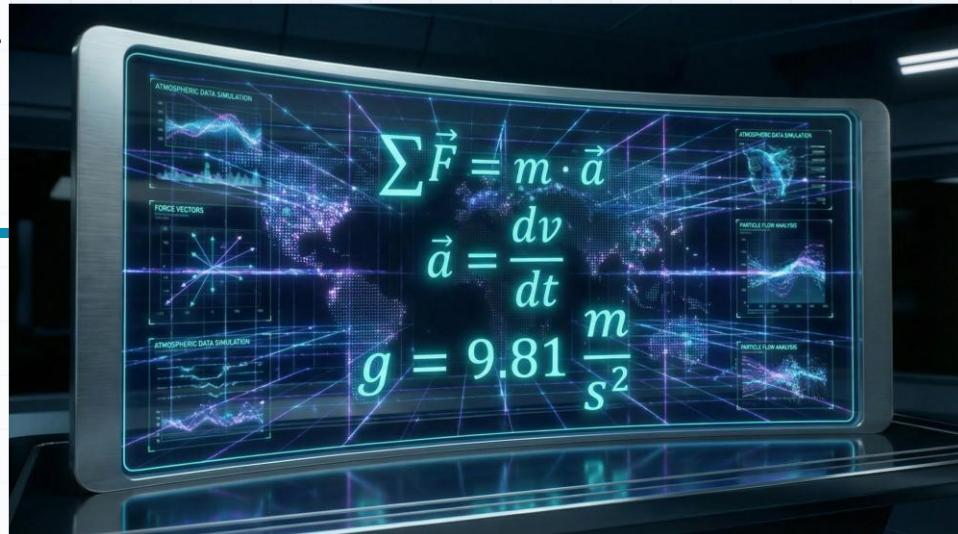
2. Emergent Forces

The following forces emerge from fundamental definitions and the rotating reference frame:

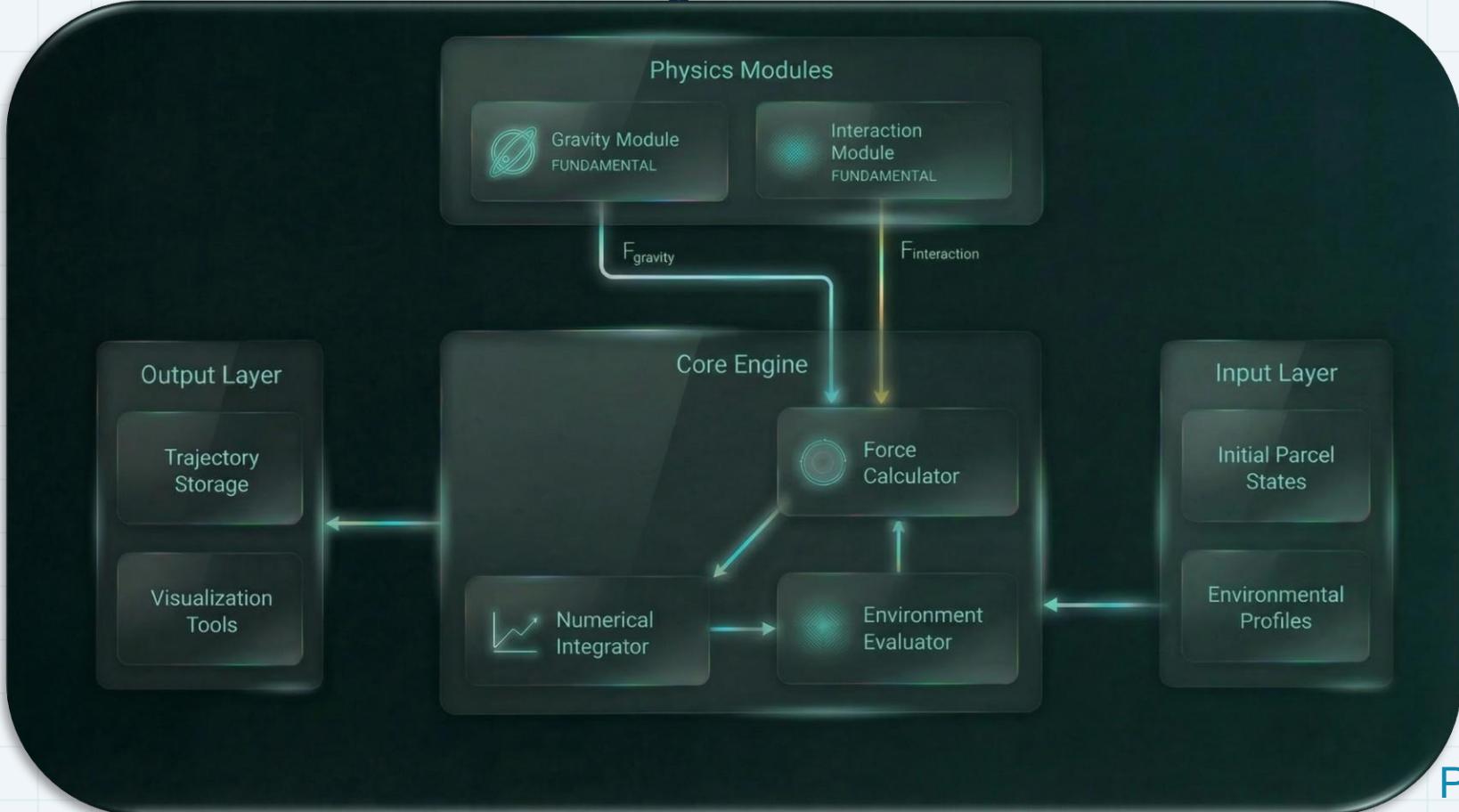
Buoyancy : Thermal density differences.

Coriolis : Earth's rotation effects.

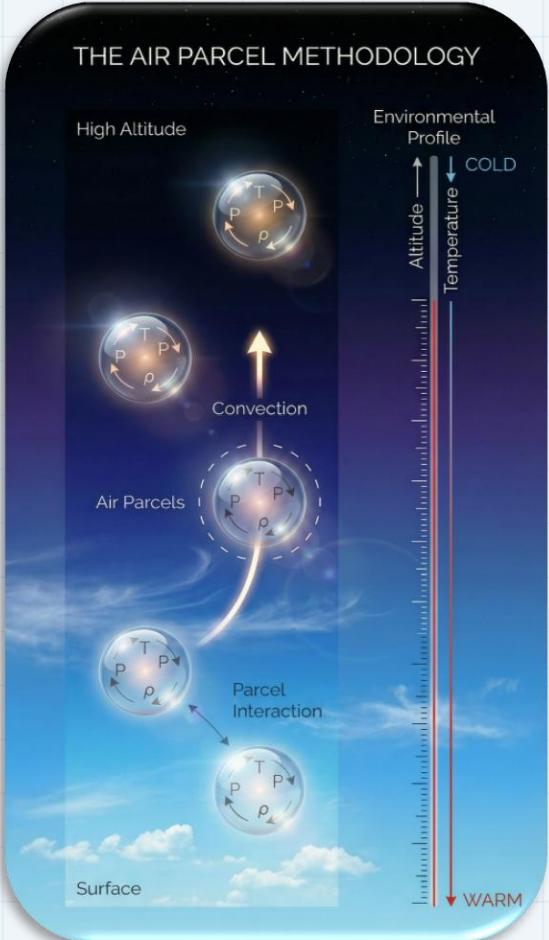
Drag: Relative motion resistance.



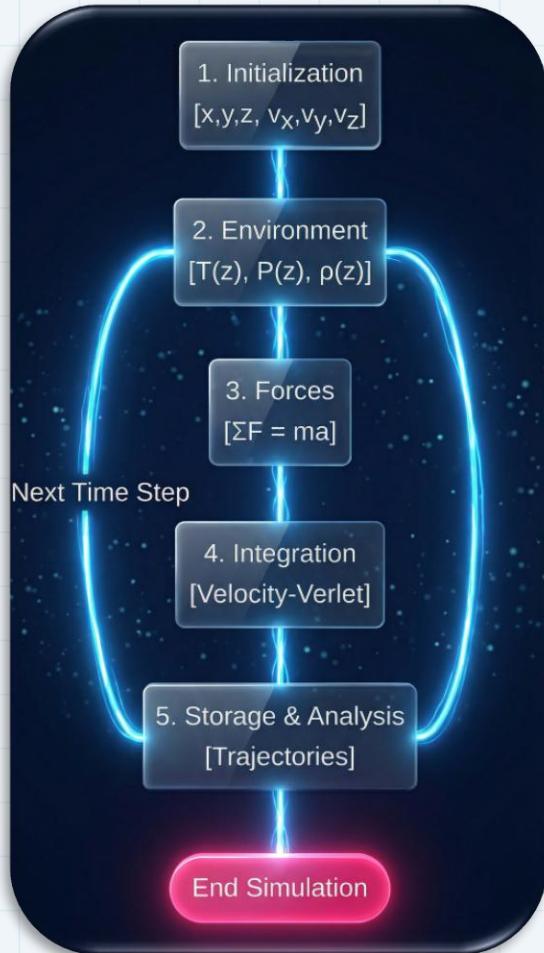
Software Architecture: Modular Design



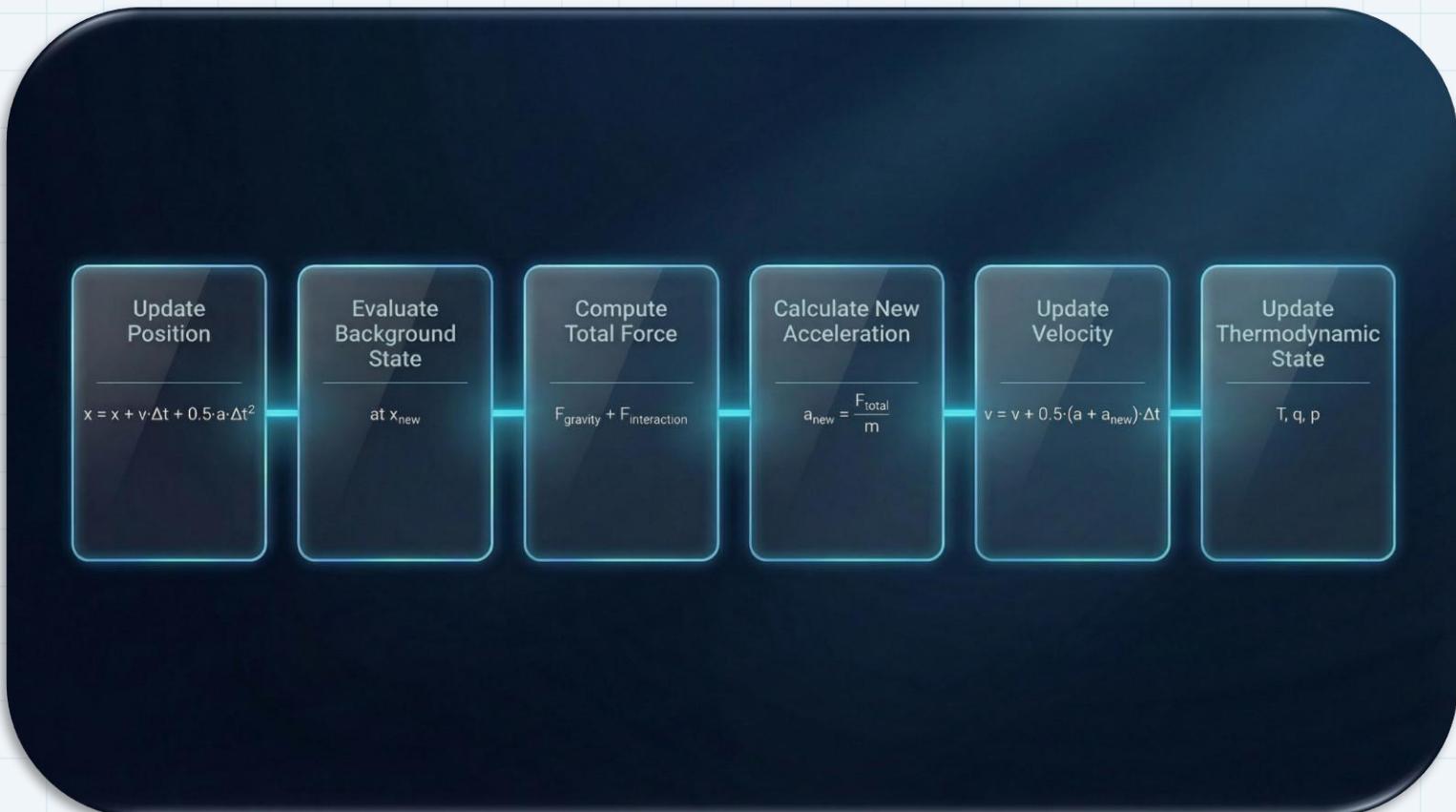
Simulation Workflow : Linear Execution



- 1. Init**
Set initial state vectors
 $[x, y, z, v_x, v_y, v_z]$
- 2. Env**
Evaluate vertical profiles
 $[T(z), P(z), \rho(z)]$
- 3. Forces**
Compute total force $\sum F = m \cdot a$
- 4. Integration**
Apply Velocity-Verlet time integration.
- 5. Storage**
Save trajectories for post-processing.



Numerical Integration: Zooming in Velocity-Verlet



Innovation & Contribution

Methodological Innovation

Applying **Molecular Dynamics integration techniques** (Velocity-Verlet) to atmospheric parcel tracking, ensuring stability.

High-Precision Trajectories

Captures detailed **thermodynamic history** of individual air masses, a feature often lost in standard grid-based meteorological models.

Research Accessibility

Provides a lightweight, **research-oriented tool** for studying idealized convection without needing dedicated computers .

Strategic Positioning

Bridges the gap between simple kinematic trajectory models and complex, resource-intensive meteorological frameworks.

Moisture & Latent Heat Effects

Thermodynamic Coupling

Moisture is treated as a **prognostic variable** carried by each air parcel. This coupling allows the simulation to account for humidity-driven density changes and phase transitions.

Latent Heat Release

When a parcel cools below its saturation point, condensation occurs, releasing **latent heat**. This energy source warms the parcel, significantly boosting its buoyancy compared to dry air.

Planned Testing & Validation Strategy

Numerical Stability

Planned convergence tests will confirm that air-parcel trajectories remain bounded. The target positional-norm difference between simulations with varying time steps is **below 5%**.

Sensitivity Analysis

The model will be tested for smooth and continuous parcel response to variations in initial temperature, humidity, and drag coefficients to ensure no excessive sensitivity to small perturbations.

Physical Consistency

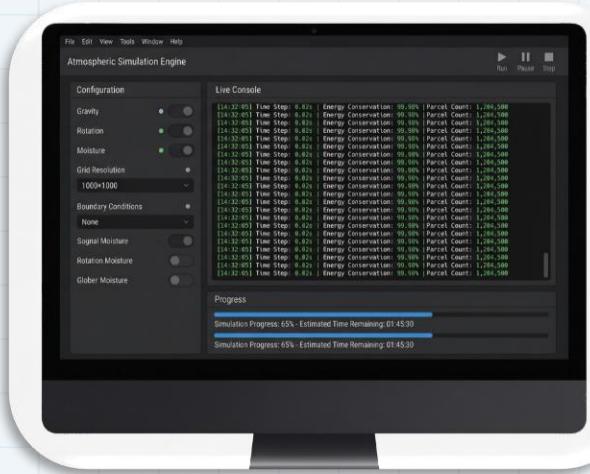
Planned comparison with analytical solutions for buoyant rise and Coriolis deflection aims for a relative error **below 10%** in idealized atmospheric test cases.

Computational Efficiency

Planned benchmarks will verify **linear scalability O(N)**. The goal is to ensure that doubling the number of simulated air parcels results in a proportional increase in computation time.

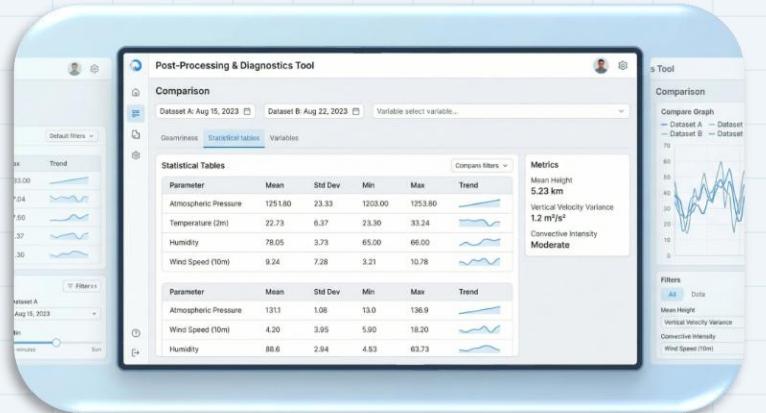
Simulation Program: Numerical Engine

- Acts as the **Computational Core** of the project.
- Numerically solves equations of motion for air parcels.
- Responsible for **Time Integration** and Force Computation.
- Operates as a batch-style program with structured data output.
- Ensures physical correctness and numerical stability.



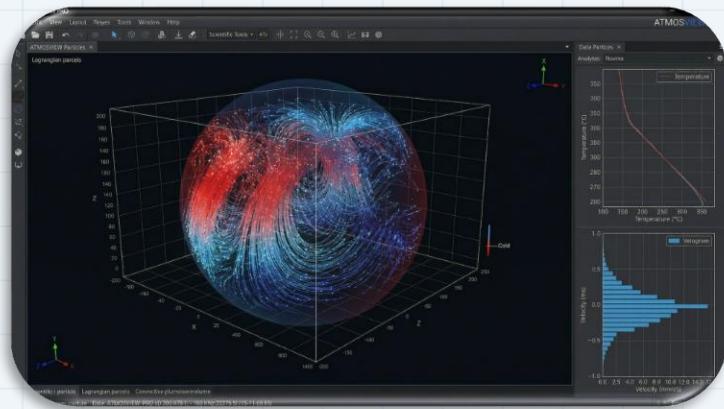
Analysis Program: Diagnostics Tool

- Performs **Quantitative Evaluation** of simulation outputs.
- Computes statistical measures and physical diagnostics.
- Transforms raw trajectory data into meaningful metrics.
- Enables **Sensitivity Analysis** and model validation.



Visualization Program: Scientific Tool

- Provides **Graphical Representation** of parcel dynamics.
- Generates 3D trajectories and thermodynamic evolution plots.
- Produces publication-quality figures and animations.
- Supports **Qualitative Validation** of physical behavior.



Anticipated Implementation Challenges

Numerical Stiffness

Rapid phase changes in moisture (latent heat release) can create stiff ODEs that challenge standard explicit integrators.

Boundary Conditions

Ensuring physical consistency at the surface and top-of-atmosphere boundaries in a scaled virtual world.

Computational Scalability

Tracking thousands of parcels with high-frequency force evaluations requires significant CPU/Memory resources.

Data Management

Storing and processing high-resolution 3D trajectory data for long-duration simulations.

Thank You

Questions & Discussion