Software Engineering Department

Braude College of Engineering

Final Project—Phase A (61998)

Title: Simulation of Atmospheric Particle Movement

Subtitle: A Framework for Modeling Air Parcel Dynamics

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Link to GitHub:

https://github.com/Yasser-Saadi-7/Atmospheric-Particle-Motion-Simulation-3D-Environmental-Modeling.git

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Table of Contents

Abstract

This project develops a simulation framework to model air parcel motion in Earth's atmosphere. The main goal is to estimate atmospheric properties such as temperature, density, pressure, and moisture and to understand how changes in these properties influence atmospheric circulation. The framework uses a Lagrangian approach inspired by molecular dynamics, meaning it tracks individual air parcels as they move through the atmosphere, with each parcel carrying its own thermodynamic state. Parcel motion is driven by gravity, buoyancy, pressure-like interactions modeled through short-range parcel–parcel repulsion, and Earth's rotation, represented using a rotating reference frame. In this project, large-scale circulation is not prescribed as an external background wind field; instead, macroscopic transport patterns emerge from the collective particle dynamics under physically motivated thermal forcing and rotation and are diagnosed from particle statistics. By varying atmospheric and thermodynamic parameters, we demonstrate how dry and moist processes affect circulation strength and behavior. The simulation enables analysis of atmospheric changes and includes visualization tools to observe parcel trajectories and evaluate how transport patterns emerge under controlled forcing conditions.

Introduction

The Earth's atmosphere is a complex and continuously changing system driven by variations in temperature, pressure, density, and moisture. A fundamental aspect of atmospheric dynamics is the motion of air parcels, which are finite volumes of air with relatively uniform thermodynamic properties. This motion drives essential processes like convection and large-scale atmospheric circulation, making it critical to understand how and why they move (Seinfeld & Pandis, 2016). However, describing air parcel motion is challenging. The atmosphere is thermodynamically active and rotating, and even small changes can produce unpredictable outcomes. Parcel dynamics emerge from multiple interacting processes. Gravity and buoyancy control vertical acceleration, while large-scale circulation is not prescribed as an external wind field; instead, macroscopic transport patterns emerge from the collective particle dynamics under thermal forcing and rotation and are diagnosed from particle statistics. Local pressure-like effects are represented by parcel–parcel repulsion, friction slows motion down, and temperature variations modify density and atmospheric stability. When moisture is involved, phase changes introduce energy exchange through latent heat, further affecting parcel behavior (Pope, 2000). Numerical modeling has become essential for addressing this complexity. Numerical simulations enable the tracking of air parcels and allow systematic study of how they evolve and interact with the surroundings. Such models balance between physical accuracy and computational efficiency by using simplified but physically realistic representations of key atmospheric processes. This project adopts a molecular dynamics-based Lagrangian framework. The Lagrangian approach tracks individual air parcels as they move through the atmosphere, following their paths rather than observing fixed points in space. Each parcel represents an individual object whose motion follows Newton's laws and responds to the dominant atmospheric forces (Allen & Tildesley, 2017). While molecular dynamics methods were originally developed for molecular-scale physics, they are well-suited for simulating interacting air parcels and diagnosing emergent transport under buoyancy, gravity, drag, and rotational effects. Each parcel carries its own thermodynamic properties, including moisture content, and we account for Earth's rotation using a rotating reference frame. Lagrangian parcel-based simulations are widely used in atmospheric research because they excel at capturing detailed motion and convection processes (Crowe et al., 2011). The goal of this project is to build a simulation framework for modeling the motion and evolution of air parcels in the atmosphere. The framework enables visualization and analysis of air-parcel paths, serving as a research tool for studying buoyancy-driven convection, moisture effects, and rotation-influenced atmospheric dynamics.

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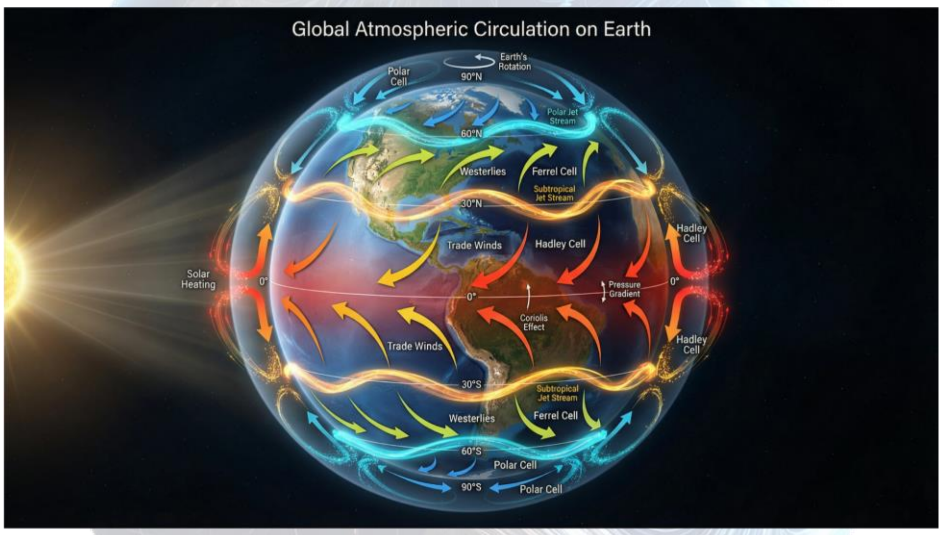
1. Literature Review

1.1 Physical Background

1.1.1 Atmospheric Flow

Atmospheric flow refers to the large-scale movement of air in the Earth's atmosphere. This movement is driven by pressure differences, uneven solar heating, and the rotation of the Earth. These processes create organized circulation patterns, including three main cells: Hadley cells near the equator, Ferrel cells in the mid-latitudes, and Polar cells near the poles. Jet streams also emerge as part of this global circulation system. These circulations determine the distribution of wind, pressure, and temperature in which air parcels move. As a result, atmospheric flow plays a major role in shaping parcel paths and atmospheric stability (Seinfeld & Pandis, 2016).



1.1.2 Parcel Transport Mechanisms

Air parcel motion is controlled by several transport mechanisms that act simultaneously. The primary processes are advection and convection. Advection describes horizontal transport associated with the emergent mean flow, while convection refers to vertical motion driven primarily by buoyancy differences caused by variations in temperature and humidity.

In addition to these processes, radiative heating and cooling modify parcel temperature and buoyancy. Phase changes of water vapor—such as condensation and evaporation—release or absorb latent heat, altering parcel density and vertical stability. Together, these mechanisms operate across a wide range of spatial and temporal scales, making air parcel transport a strongly coupled, multiscale process (Seinfeld & Pandis, 2016).

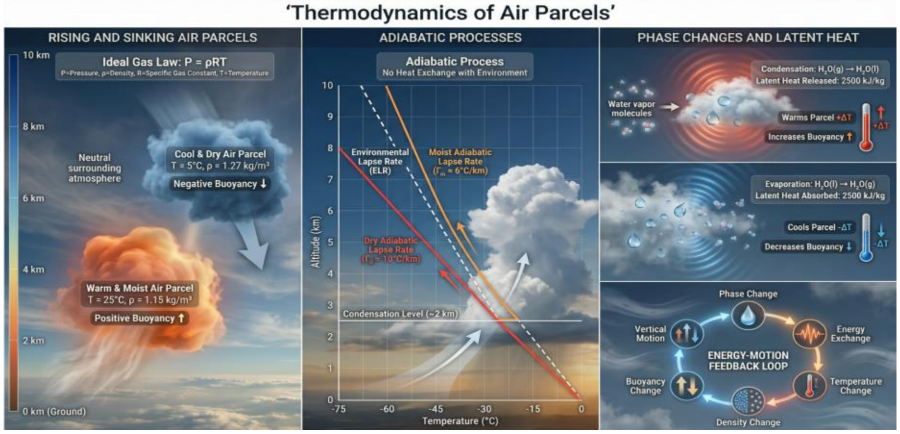
1.1.3 Forces Acting on Air Parcels

Air parcel motion is governed by forces that can be viewed as fundamental versus derived (parameterized) contributions. The fundamental forces include gravity, which pulls parcels downward toward Earth's center, and short-range repulsive interactions between parcels, which produce a pressure-like response in dense regions. The derived forces include buoyancy arising from parcel–environment density differences, drag and friction representing momentum exchange that opposes motion, and Coriolis and centrifugal effects that appear when the equations are written in Earth's rotating reference frame. In this project, pressure is not computed via an explicit grid-based pressure gradient ∇P; instead, pressure-like forcing emerges from inter-parcel repulsion, and macroscopic transport patterns arise as an emergent outcome of the particle dynamics under thermal forcing and rotation, while buoyancy and drag are implemented as explicit parameterizations based on local environmental conditions (Wallace & Hobbs, 2006; Holton & Hakim, 2013).

1.1.4 Thermodynamics of Air Parcels

The thermodynamic properties of an air parcel determine its density, stability, and whether it will rise or sink. The ideal gas law links temperature, pressure, and density, providing the basis for calculating buoyancy: a parcel that is warmer or moister than its surroundings becomes less dense and rises, while a cooler parcel becomes denser and sinks. When an air parcel moves vertically, its temperature changes adiabatically: for dry air, this follows the dry adiabatic lapse rate, while in saturated air, latent heat release during condensation slows the cooling rate, following the moist adiabatic lapse rate. Phase changes of water vapor play an important role: condensation releases latent heat (approximately 2500 kJ/kg), warming the parcel and increasing buoyancy, while evaporation absorbs heat and cools the parcel, directly linking energy exchange to vertical convection through a feedback loop (Holton & Hakim, 2013)

'Thermodynamics of Air Parcels'



1.2 Computational and Numerical Approaches

1.2.1 Eulerian and Lagrangian Air-Parcel Modeling

Atmospheric motion is commonly modeled using either Eulerian or Lagrangian frameworks. In the Eulerian approach, atmospheric variables are defined at fixed locations in space, and the governing equations are solved on a spatial grid. This method is efficient for large-scale simulations and is widely used in weather prediction and climate models but provides limited insight into the paths of individual air parcels. The Lagrangian approach, in contrast, follows individual air parcels along their paths through space and time, with each parcel carrying its own thermodynamic properties—such as temperature, humidity, and density—and interacting with the surrounding flow. This method is effective for representing convection and transport processes, though its main limitation is computational cost, which increases with the number of parcels tracked. Lagrangian frameworks offer flexibility to incorporate rotational effects from Earth's rotation through a rotating reference frame (Crowe et al., 2011).

1.2.2 CFD-Based Atmospheric Simulations

Computational Fluid Dynamics (CFD) models solve the governing fluid dynamics equations on fixed spatial grids, providing detailed representations of atmospheric flow fields. While these models are highly effective for large-scale atmospheric simulations, their computational cost increases rapidly with higher spatial resolution, limiting their suitability for studies focused on tracking large numbers of individual air parcels in detail. In contrast, Lagrangian approaches inspired by molecular dynamics directly follow discrete air parcel paths, emphasizing parcel-scale motion, mixing, and transport rather than reconstructing the full flow field, offering greater conceptual clarity and computational flexibility for controlled studies that incorporate thermodynamic variables and rotation effects (Crowe et al., 2011).

1.2.3 Numerical Methods for Air Parcel Tracking

In Lagrangian simulations, parcel motion is computed by solving equations of motion derived from Newton's second law. These equations form a system of ordinary differential equations (ODEs), where parcel acceleration depends on the balance of forces such as buoyancy, gravity, pressure-like forcing (modeled via parcel–parcel interactions), friction, and rotation effects. Because analytical solutions are not available under realistic atmospheric conditions, numerical time-integration schemes are required. Common methods include Euler, Verlet, and velocity-Verlet algorithms. These methods are widely used in molecular dynamics because they balance accuracy, stability, and efficiency. When equations include rotation or thermodynamic terms such as latent heat release, careful time-step selection is needed to maintain numerical stability (Allen & Tildesley, 2017).

1.3 Existing Models and Research Tools

1.3.1 Research-Oriented Atmospheric Models

Several atmospheric models have been developed to simulate atmospheric flow and air mass movement on regional and global scales. The Weather Research and Forecasting (WRF) model is widely used for solving the fundamental equations governing atmospheric motion to generate high-resolution meteorological (detailed atmospheric conditions) fields. WRF is commonly applied in studies of regional weather patterns, convection, and atmospheric circulation. (Skamarock et al., 2008). For transport studies, Lagrangian modeling tools such as FLEXPART are commonly used. FLEXPART tracks the motion of air parcels using meteorological data from numerical weather prediction models or reanalysis datasets, making it widely used in studies where parcel paths and dispersion are important (Stohl et al., 2005). While these models are powerful for operational forecasting and large-scale atmospheric research, they are less suited for controlled, idealized studies focused on fundamental parcel dynamics and thermodynamic processes.

1.3.2 Existing Air-Parcel Transport Frameworks and Limitations

Research tools such as FLEXPART and similar Lagrangian dispersion models are effective for large-scale atmospheric transport studies. However, they rely on simplified force representations and pre-computed wind fields, which limits their flexibility for detailed parcel-scale studies where force interactions and thermodynamic processes are central (Stohl et al., 2005). Operational frameworks such as HYSPLIT efficiently compute paths for forecasting applications but offer limited capability for analyzing the full dynamical and thermodynamic evolution of individual air parcels. (Stein et al., 2015). More advanced atmospheric models solve the full Navier–Stokes or primitive equations and include radiative transfer and cloud dynamics. These models provide high physical realism but require high computational cost (Skamarock et al., 2008). While powerful for operational forecasting and climate research, these models are not well-suited for controlled, idealized studies focused on fundamental parcel dynamics and thermodynamic processes. These limitations motivate the development of simulation frameworks that emphasize physically based parcel dynamics within a flexible, controlled modeling environment (Holton & Hakim, 2013).

1.4 Key Atmospheric Processes and Modeling Assumptions for Realistic Air-Parcel Simulation

Realistic simulation of Lagrangian air parcel motion requires representing the main atmospheric mechanisms that govern transport and thermodynamic evolution. A full global atmospheric model that solves the complete Navier–Stokes or primitive equations with radiative transfer and cloud processes is beyond the scope of a research-oriented parcel simulator. Therefore, this project adopts a controlled modeling strategy that separates the system into (i) a thermodynamic reference state and forcing (e.g., target temperature profiles and reference stratification) without prescribing a background wind field and (ii) simplified process models that represent essential dynamics without high computational cost (Pope, 2000; Vallis, 2006).

1.4.1 Global Atmospheric Circulation as a Background Flow Field

Global atmospheric circulation provides the main transport pathway for mass, heat, and moisture, shaping how air parcels move over long distances. Large-scale features such as the Hadley, Ferrel, and Polar cells, along with jet streams, strongly influence parcel motion (Holton & Hakim, 2013; Vallis, 2006). Rather than prescribing an analytic background wind field, this project follows a molecular-dynamics-inspired Lagrangian framework in which large-scale circulation is an **emergent** outcome of the simulated particle dynamics. In this approach, the model does not impose $u(\phi, z)$ as an external input; instead, macroscopic flow structures arise from the combined effects of: (i) particle–particle interactions that produce pressure-like responses in dense regions, (ii) differential thermal forcing represented by Newtonian relaxation toward a target temperature profile $T_{eq}(\phi, z)$, (iii) gravity and drag and (iv) planetary rotation through a rotating reference frame (Pope, 2000; Vallis, 2006). To quantify circulation, the simulator diagnoses mean flow fields from particle velocities by binning parcels in latitude–altitude space and computing $v(\phi, z)$, enabling direct assessment of whether Hadley/Ferrel/Polar-like cells and jet-like structures form as statistically stable patterns. Accordingly, the project adopts a fully particle-driven formulation: global transport is not prescribed but measured as a macroscopic consequence of the underlying MD-like dynamics under controlled forcing and rotation conditions.

1.4.2 Thermal Forcing via Simplified Radiative Effects

Differential heating is the primary energy source driving atmospheric circulation and stability. It creates temperature differences across latitude and altitude that alter air density and buoyancy, influencing both vertical motion and horizontal flow patterns (Holton & Hakim, 2013; Vallis, 2006). These temperature gradients maintain large-scale circulation cells and establish thermal structures that control whether parcels rise, sink, or move horizontally. In this project, radiative heating and cooling are represented using a Newtonian relaxation scheme toward a prescribed target temperature profile $T_{eq}(\phi, z)$: $\frac{dT}{dt} = - \frac{T - T_{eq}}{\tau}$

where T is the parcel temperature, T_{eq} is the target temperature at latitude ϕ and altitude z, and τ is the relaxation timescale.

This provides a computationally efficient way to impose thermal forcing without solving radiative transfer equations. This approach provides a computationally efficient way to include thermal forcing without solving complex radiative transfer equations and is widely used in idealized atmospheric models (Vallis, 2006; Holton & Hakim, 2013).

1.4.3 Rotating Reference Frame Formulation

Planetary rotation shapes atmospheric dynamics, creating zonal jets, vortices, and large-scale wave patterns that cannot be captured in non-rotating models. To represent these effects, the simulation is formulated in a reference frame that rotates with the planet rather than in a fixed (inertial) frame. When Newton's laws are expressed in a rotating coordinate system, rotation-induced effects emerge naturally from the frame transformation. These include the Coriolis acceleration: $F_{coriolis} = -2m(\Omega \times v)$ and the centrifugal acceleration: $-m(\Omega \times (\Omega \times r))$
Where m is parcel mass, Ω is the planetary rotation vector, **v** is parcel velocity, and **r** is position. The centrifugal term can be absorbed into an effective gravitational potential, so rotational effects are represented consistently without adding extra force terms. The rotating frame formulation is implemented by specifying the planetary rotation vector Ω and expressing parcel positions and velocities relative to the rotating frame. Initial conditions are transformed accordingly, and the approach is validated by recovering the non-rotating solution when Ω→0. This framework enables realistic emergence of rotation-driven structures such as zonal jets and vortices within a computationally efficient model (Vallis, 2006; Holton & Hakim, 2013).

1.4.4 Spherical Geometry and Metric-Aware Transport

Earth's spherical shape influences air parcel motion by affecting distances, area calculations, and the latitude dependence of forces like the Coriolis effect, which in turn affects global paths and transport patterns (Vallis, 2006). The simulator accounts for this spherical geometry by performing calculations in Cartesian coordinates (a standard x, y, z coordinate system) while consistently mapping to spherical coordinates (latitude, longitude, altitude) for physical forcing terms, or by using regional flat-Earth (f-plane) approximations where appropriate. Diagnostic measures such as great-circle distances are used to ensure correct interpretation of parcel paths and prevent geometric distortions. Path visualization and averaging use geometry-consistent methods. Simple Cartesian averaging of parcel positions can produce physically unrealistic results on a spherical planet. To avoid these artifacts, trajectory statistics are computed using spherical coordinate representations and proper geometric averaging techniques that account for Earth's curvature.

1.4.5 Moisture and Moist Convection

Moist processes modify atmospheric dynamics through the release of latent heat during condensation, providing an additional energy source absent in dry models. Water vapor enhances buoyancy and vertical motion, making it essential for representing the intensification of convection associated with clouds and large-scale circulation features. In this project, moisture is carried by each parcel as specific humidity q, with initial values prescribed from idealized profiles. Saturation is diagnosed using a Clausius–Clapeyron/Tetens-type approximation for saturation vapor pressure $e_{sat}(T) = e_0 exp(\frac{L_v}{R_v}(\frac{1}{T_0} - \frac{1}{T}))$, from which the saturation mixing ratio is computed as $q_{sat}(T,P) = \varepsilon\, e_{sat}(T)/(P - e_{sat}(T))$. Condensation occurs when $q > q_{sat}$; the excess vapor is converted to condensate q_c using a relaxation formulation $dq_c/dt = (q - q_{sat})/\tau_{relax}$ (and $dq/dt = -dq_c/dt$), where τ_{relax} is a prescribed timescale. Latent heating is then applied as $dT/dt += (L_v/c_p) dq_c/dt$, which warms the parcel, reduces its density, and increases buoyancy. Condensed water may be tracked as a passive tracer or removed to represent precipitation, enabling controlled comparisons between dry and moist simulations and their impact on convective intensity.

2. Project Description and Research Methodology

2.1 Project Goals and Objectives

This project develops a research-oriented simulation framework for studying how air parcels move and evolve in Earth's atmosphere. We aim to model and analyze parcel paths under physically realistic atmospheric conditions, with emphasis on understanding buoyancy-driven motion and convection rather than producing an operational forecasting system. The specific objectives of the project are to:

1. Formulate a physically consistent model for air parcel motion based on Newtonian mechanics.
2. Simulate parcel paths using a Lagrangian approach inspired by molecular dynamics methods.
3. Incorporate dominant atmospheric forces: pressure gradients, buoyancy, gravity, Coriolis acceleration, and friction.
4. Examine how environmental processes such as temperature structure and radiative effects influence parcel motion and stability.
5. Study the influence of moisture and latent heat release on buoyancy-driven parcel motion under rotating atmospheric conditions.
6. Provide visualization and analysis capabilities for studying air parcel dynamics.

The project serves as a flexible research tool for exploring how air parcels behave under controlled atmospheric conditions.

2.2 Project Requirements

2.2.1 Functional Requirements

The proposed system is required to:

- Simulate the motion of individual air parcels within a defined spatial domain.
- Compute time-dependent parcel paths by numerically integrating the equations of motion.
- Represent key atmospheric forces acting on parcels: gravity, buoyancy, pressure-like forcing via short-range parcel–parcel repulsion, and friction.
- Support configurable environmental conditions, including temperature profiles, atmospheric stability, rotation effects, and parcel properties.
- Enable visualization of parcel paths and vertical convection to support qualitative and quantitative analysis.
- Track moisture content as a dynamic property of each parcel.
- Account for latent heat effects on parcel temperature and buoyancy during phase changes.
- Simulate parcel motion within a rotating reference frame to capture Earth's rotation effects.

2.2.2 Non-Functional Requirements

The system must also satisfy the following non-functional requirements:

- **Numerical stability:** Maintain stable integration under realistic time-step sizes and force magnitudes.
- **Physical consistency:** Preserve fundamental physical principles, including force balance and expected atmospheric behavior.
- **Computational efficiency:** Support simulation of large numbers of parcels with reasonable computational cost.
- **Modularity and extensibility:** Allow future extension to additional forces, moisture processes, or radiative effects.
- **Robustness:** Remain numerically stable when including rotation effects and moisture-related thermodynamic processes.

2.3 Research Methodology

The project follows a computational research methodology grounded in physical modeling and numerical simulation. The research process begins by defining a simplified but physically meaningful representation of air parcel motion. Instead of solving the complete set of atmospheric flow equations, the large-scale flow is represented conceptually while the emphasis is placed on individual parcel dynamics governed by force models. The methodology consists of four main stages. The first stage involves identifying the dominant physical mechanisms governing air parcel motion, including buoyancy, gravity, pressure-like forcing via inter-parcel interactions, and rotation effects. The second stage focuses on the mathematical formulation of the equations of motion for individual parcels based on Newtonian mechanics. The third stage involves selecting appropriate numerical methods for time integration, using molecular dynamics approaches such as the Verlet and velocity-Verlet algorithms. The fourth stage is the design of a simulation workflow that enables controlled experimentation and analysis of parcel behavior under different atmospheric conditions. This methodology allows isolation of parcel-scale dynamics while maintaining physical relevance.

2.4 Proposed Simulation Model

2.4.1 Physical Model Formulation

Air parcel motion is modeled using Newton's second law in a rotating reference frame, where each parcel is treated as a Lagrangian particle that carries its own kinematic and thermodynamic state. The primary state variables are the parcel position $x(t)$ and velocity $v(t)$, and (when thermodynamics are enabled) parcel temperature $T(t)$, specific humidity $q(t)$, pressure $P(t)$, and density $\rho(t)$. In this project, large-scale circulation is not prescribed as a background wind field; instead, macroscopic transport patterns emerge from particle dynamics under physically motivated forces and are diagnosed from particle statistics. The equations of motion are written as an explicit system of ordinary differential equations (ODEs):

v = $\frac{dx}{dt}$, $F_g + F_b + F_d + F_{cor} + F_{int} = m\frac{dv}{dt}$, gravity is modeled as $F_g = -mg\hat{k}$.

Where g is gravitational acceleration and $\hat{k}$ is the upward vertical unit vector.

Buoyancy is computed from the parcel–environment density contrast:

$F_b = -V(\rho_{parcel} - \rho_{env})g\hat{k}$, where V is the parcel volume, ρ_{parcel} is the parcel density, and ρ_{env} is the environmental density evaluated at the parcel location (same latitude and altitude).

Frictional effects are represented by a linear drag (damping) model: $F_d = -C_d v$

Where C_d is a drag coefficient (units: kg/s). C_d is chosen via a damping timescale τ_d as $C_d = \frac{m}{\tau_d}$, giving $a_d = \frac{F_d}{m} = -\frac{v}{\tau_d}$.

Rotation is incorporated through the Coriolis force: $F_{cor} = -2m(\Omega \times v)$

Where Ω is the planetary rotation vector, evaluated at each time step using the current velocity.

Pressure-like effects are represented in an MD-inspired way through short-range repulsive parcel–parcel interactions: $F_{int,i} = \sum_{j\neq i} -\Delta_{x_i} V(r_{ij}), r_{ij} = \|x_i - x_j\|$, using a purely repulsive potential $V(r)$ with a cutoff radius r_c to keep interactions local. Thermodynamic variables are carried with each parcel to support buoyancy and moist processes; density is computed using the ideal gas law $\rho_{parcel} = \frac{P_{parcel}}{R_d T}$, while temperature and humidity are updated using the simplified radiative and moist parameterizations described in Sections 1.4.2 and 1.4.5 .These ODEs are integrated in time using a Velocity-Verlet scheme with an initial time step $dt = 0.1s$ (scaled), as described in Section 2.4.3. (Allen & Tildesley, 2017).

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2.4.2 Scaled Virtual Environment and Geometric Assumptions

To ensure computational efficiency while preserving essential atmospheric dynamics, the simulation is designed around a scalable virtual environment with two operating modes: a small prototype configuration for debugging and stability testing and a target configuration intended to resolve large-scale circulation patterns. The model selects a planetary radius R and atmospheric depth H that keep the atmosphere relatively thin $(R/H \gg 1)$ while remaining computationally feasible. The target configuration uses a planetary radius on the order of $R = 1000\ km$ and an atmospheric depth $H = 10 - 20\ km$, which better supports the emergence and diagnosis of global-scale circulation structures compared to overly compact domains. Planetary rotation is prescribed through a rotation period P, giving $\Omega = \frac{2\pi}{P}$and being chosen to maintain dynamically relevant Rossby-scale behavior in the scaled system. The baseline particle resolution is increased to $N = 20{,}000 - 50{,}000$ parcels (or higher when feasible) to provide sufficient statistical sampling for diagnosing mean flow fields and cell-like circulation patterns. Each parcel represents a coarse-grained air volume V with mass $m = \rho_0 V$, using a reference density ρ_0 (e.g., $\rho_0 = 1.2\ kg/m^3$), and these parameters are selected to balance numerical stability, runtime, and memory constraints, with final values refined during implementation using sensitivity tests, profiling, and convergence checks to confirm that macroscopic circulation diagnostics are robust to resolution changes.

2.4.3 Numerical Integration Strategy

The equations of motion form a system of ordinary differential equations (ODEs) in time. Because analytical solutions are not available for realistic atmospheric conditions, numerical time integration is required. In this project, the simulation uses an explicit Velocity-Verlet scheme due to its stability and common use in molecular dynamics. The system advances using a fixed time step $dt = 0.1s$ (scaled) and is a prototype/debug setting and is re-tuned for the target large-scale configuration using stability and sensitivity tests, updating parcel positions and velocities from the total acceleration, including drag and rotation terms. Rotation is handled by evaluating the Coriolis acceleration $a_{cor} = -2\Omega \times v$ at each step and adding it to the total acceleration. Although no Eulerian grid is used, an analogous stability constraint is enforced by requiring that per-step displacements remain small relative to key length scales (e.g., $|\Delta x| \ll r_c$ and $|\Delta z| \ll H$). Stability is verified by repeating runs with $\frac{dt}{2}$ and requiring trajectory differences below 5% over the same simulated time, while thermodynamic tendencies are applied after each dynamics update using a forward-Euler operator-splitting step. This value is an initial choice and will be adjusted during implementation based on stability and sensitivity tests (Allen & Tildesley, 2017).

2.4.4 Simulation Workflow

The simulation workflow consists of the following stages:

1. Initialization of Parcel State

At initialization ($t = 0$), the model defines a baseline ensemble of $N = 20000 - 50000$ air parcels within the scaled spherical domain ($R = 1000\ km$, $H = 10 - 20\ km$) . Each parcel is assigned a three-dimensional position (x, y, z), velocity (v_x, v_y, v_z), and thermodynamic properties (T, P, ρ, q). Parcel positions are sampled using a reproducible random seed, with parcels distributed approximately uniformly in horizontal area and stratified in height (denser sampling near the lower atmosphere) to represent a realistic concentration of mass near the surface. Initial velocities are set to zero-mean small perturbations (e.g., $|v_0| \leq 0.1\ m/s$) to break symmetry while avoiding artificial large-scale momentum. Temperature is initialized from a prescribed stable background profile (e.g.,$T(z) = T_0 - \Gamma z$ with $T_0 = 300\ K$, $\Gamma = 6.5\ K/km$). Pressure is initialized using a hydrostatic approximation, and density is computed from the ideal gas law $\rho = P/(R_d T)$. Moisture is initialized as either a dry baseline ($q = 0$) or an idealized humidity profile (e.g., near-surface $q = q_0$ that decays with height) depending on the experiment, enabling controlled dry-versus-moist comparisons.

2. Evaluation of Environmental Conditions

In this stage, the environmental state surrounding each parcel is evaluated. The environment is represented as an idealized thermodynamic reference rather than a fully resolved Eulerian flow field and includes background temperature profiles, vertical stability structure, and reference thermodynamic conditions required for buoyancy calculations. Radiative heating and cooling are applied through simplified parameterizations, such as Newtonian relaxation toward a prescribed target temperature profile $T_{eq}(\phi, z)$. This separation between parcel properties and environmental reference conditions allows clear computation of temperature and density contrasts, which form the basis for buoyancy-driven motion and convective development. In this project, large-scale circulation is not imposed as a background wind field; instead, macroscopic transport patterns emerge from the collective particle dynamics under thermal forcing and rotation and are diagnosed from particle statistics.

3. Computation of Forces Acting on Each Parcel

Once the environmental conditions are determined, the forces and accelerations acting on each parcel are computed. These include gravitational acceleration, buoyancy derived from parcel density differences between the parcel and its environment, and friction representing interaction with the surrounding air. When the simulation is formulated in a rotating reference frame, rotation-related inertial effects such as Coriolis and centrifugal accelerations are included. In moist simulations, additional thermodynamic effects such as latent heat release during condensation contribute to parcel buoyancy. All forces are computed for each parcel at every time step, enabling a fully Lagrangian and modular representation of atmospheric dynamics. Pressure-like effects are represented through short-range parcel–parcel interactions, where repulsive (and optionally attractive) forces act only between neighbors within a cutoff radius r_c, allowing macroscopic circulation to emerge from the collective particle dynamics rather than being prescribed externally.

4. Numerical Time Integration

The temporal evolution of the system is advanced by numerically integrating the equations of motion using a time-stepping scheme. In this project, the dynamics are advanced with a Velocity-Verlet integrator due to its stability and common use in molecular dynamics simulations. At each time step, the total acceleration (including gravity, buoyancy, drag, rotation, and inter-parcel interaction terms) is used to update velocities and then positions; large-scale transport is not applied through an imposed background wind field, but emerges from the collective particle dynamics under thermal forcing and rotation. Thermodynamic variables are updated after the dynamics step using an operator-splitting approach, where radiative and moist tendency terms are applied with a forward-Euler update. The time step dt is chosen to balance numerical accuracy, stability, and computational efficiency and is refined during implementation based on stability and sensitivity tests, especially when rotation and moisture-related processes are included. Boundary conditions are enforced after each time step to keep parcels inside the domain $0 \leq z \leq H$. At the ground $(z = 0)$, parcels are prevented from penetrating the surface using an inelastic reflection: if $z < 0$, set $z = 0$ and update $v_z \leftarrow \alpha v_z (0 < \alpha < 1)$, with optional damping of horizontal velocity to represent surface friction. Near the top boundary $(z = H)$, a simple sponge layer applies additional damping to vertical motion to reduce artificial reflections; parcels that cross $z > H$ are removed (or clamped) depending on the experiment. Horizontal transport is treated as periodic in longitude (wrap-around), while positions and updates are performed in Cartesian coordinates to avoid polar singularities.

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5. Data Storage, Visualization, and Analysis

During and after the simulation, parcel path data and thermodynamic variables are stored for post-processing and analysis. This includes three-dimensional parcel paths, time series of temperature, altitude, and humidity, and derived statistical measures of motion and mixing. Visualization tools are used to identify physically meaningful patterns such as buoyant ascent, convective overturning, and rotation-induced path curvature. This stage supports both qualitative validation of physical behavior and quantitative comparison between different simulation scenarios, such as dry and moist or rotating and non-rotating configurations.

This workflow enables systematic experimentation under controlled and repeatable conditions.

2.5 Tools and Technologies

The project uses scientific computing tools suitable for large-scale particle-based numerical simulation, diagnostics, and visualization. The entire framework is implemented in C++ to ensure high performance and scalability for MD-style force evaluation with tens of thousands of parcels. Parallel execution is supported using OpenMP for efficient multi-core computation during neighbor-based force calculations and time integration (Velocity-Verlet). The implementation uses standard C++ data structures and optimized routines for vector operations and neighbor-search acceleration (e.g., cell lists). Tool selection prioritizes numerical stability, computational efficiency, reproducibility, and suitability for research-oriented simulation tasks.

2.6 Software Architecture and Implementation Structure

The implementation is divided into three independent but interconnected components: a simulation program, a data analysis program, and a visualization program. Each component handles a distinct stage of the workflow and communicates with the others through data files. This modular architecture follows best practices in computational physics, allowing independent development, testing, and modification of each component.

2.6.1 Simulation Program (Numerical Simulation Engine)

The simulation program forms the computational core of the project and is responsible for the numerical implementation of the physical air parcel model. Its primary role is to solve the equations governing air parcel motion under prescribed atmospheric conditions using a Lagrangian, molecular dynamics-based framework. At the beginning of a simulation run, the program initializes the state of each air parcel, including its position, velocity, and thermodynamic properties such as temperature, pressure, density, and specific humidity. Environmental reference conditions, such as background temperature structure and stability, are evaluated based on the parcel location. During the simulation, the program computes the physical and thermodynamic forces acting on each parcel: gravity, buoyancy, short-range parcel-parcel repulsive interactions (pressure-like coupling), friction, rotation-related inertial effects, and simplified moist-process contributions when enabled.

Parcel states are then advanced in time using numerical integration schemes. The simulation program operates independently of visualization and post-processing tasks. Its sole output consists of structured data files containing time-resolved parcel paths and thermodynamic evolution. This strict separation ensures numerical stability, reproducibility, and transparency of the physical model implementation.

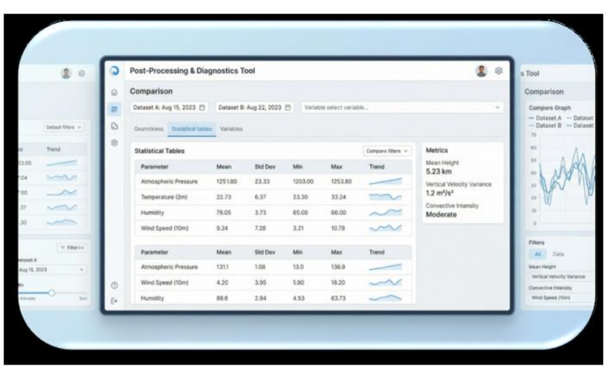
2.6.2 Analysis Program (Post-Processing and Diagnostics Tool)

The analysis program is designed to perform a quantitative evaluation of the simulation outputs generated by the numerical engine. Rather than participating in the time integration of parcel motion, this component operates entirely in a post-processing mode, reading simulation data from stored output files. Its purpose is to extract physically meaningful metrics and diagnostic quantities that characterize the simulated atmospheric behavior. Using the raw path and thermodynamic data, the analysis program computes statistical measures such as mean parcel height, vertical velocity distributions, temperature and humidity evolution, and indicators of convective intensity. It also enables systematic comparison between different simulation conditions, such as dry and moist cases or rotating and non-rotating scenarios. By isolating quantitative analysis from the simulation runtime, this program allows repeated evaluation of the same dataset under different diagnostic perspectives, supporting validation, sensitivity analysis, and objective assessment of model performance.

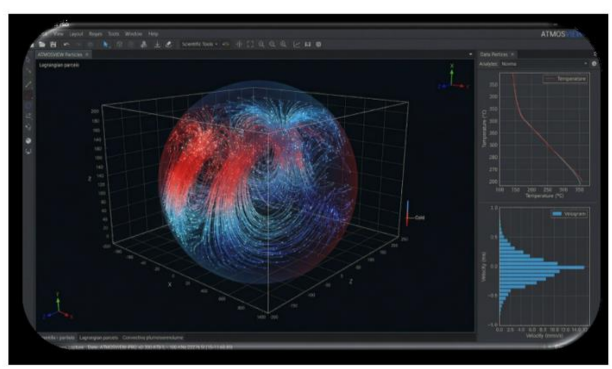
2.6.3 Visualization Program (Scientific Visualization Tool)

The visualization program provides graphical representation of air parcel dynamics and thermodynamic evolution, supporting qualitative interpretation and scientific communication of simulation results. This component operates independently of both the numerical simulation and the quantitative analysis, focusing exclusively on transforming simulation data into clear and understandable visual outputs. The visualization tool reads either raw simulation outputs or processed analysis data and generates figures such as three-dimensional parcel paths, height-time plots, and color-coded representations of temperature or humidity. These visualizations enable intuitive assessment of physical behaviors, including buoyancy-driven ascent, atmospheric layering, and rotation-induced trajectory deflection. By separating visualization from computation and analysis, the project ensures that graphical presentation does not influence numerical results and that figures can be refined or regenerated without rerunning the simulation.

Post-Processing & Diagnostics



3D Visualization



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2.7 Expected Challenges

Several challenges are anticipated during the development and analysis. Numerical stability is a key concern, as maintaining stable time integration when forces vary requires careful attention to minimize error accumulation, while parameter selection presents another challenge in identifying realistic values for parcel properties and environmental conditions. Computational efficiency must also be considered, as managing cost and memory usage when simulating many parcels may require optimized algorithms, and addressing these challenges requires careful model design, systematic testing, and validation against theoretical predictions and observational data.

3. Use of AI Tools in the Project

In this project, artificial intelligence tools were used to support the academic writing process in accordance with course guidelines and academic integrity principles, serving as writing assistants to refine structure, clarity, and technical language while all core research decisions—including physical model design, methodological choices, numerical implementation, and interpretation of results—were performed independently by the students and verified with the academic supervisor to ensure accuracy and consistency with atmospheric science principles.

4. Validation Approach

The simulation is validated using numerical stability checks, physically motivated benchmark tests, and sensitivity analysis. Numerical stability is assessed by repeating the same scenario with $dt/2$ and requiring convergence, measured by a maximum trajectory difference below 5% over the same simulated time. Physical consistency is verified using deterministic test cases with known theoretical behavior: (i) free fall with gravity only, where $z(t) = z_0 - \frac{1}{2}gt^2$ and $v_z(t) = -gt$; (ii) linear-drag relaxation, where $v(t) = v_0 e^{-t/\tau_d}$ with $\tau_d = m/C_d$; (iii) Coriolis-only inertial motion, where horizontal speed remains constant and motion exhibits inertial rotation; and (iv) moist saturation adjustment, where condensation is triggered when $q > q_{sat}(T, P)$ and latent heating follows $\Delta T = (L_v/c_p)/\Delta q_c$. Each case is evaluated with quantitative tolerances (typically 1–5% relative error) against its analytic or identity-based reference, in addition to visual inspection for non-physical drift. Sensitivity analysis then varies key parameters (e.g.,C_d, Ω, thermal relaxation timescale, and τ_{relax}) to confirm smooth, interpretable model response without excessive instability. Computational efficiency is monitored by increasing the number of parcels and verifying near-linear runtime growth in the particle-driven configuration when neighbor interactions are limited to a cutoff radius $r_c$and accelerated using neighbor-search methods, while documenting the cost of interaction evaluation when enabled.

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Conclusion

This Phase A book defined the motivation and full design of a molecular-dynamics-inspired Lagrangian framework for simulating atmospheric air-parcel motion. Unlike trajectory tracking in a prescribed wind field, the proposed model is fully particle-driven: large-scale transport patterns are not imposed as an external background flow but are expected to emerge from collective parcel dynamics under thermal forcing and planetary rotation and are diagnosed from particle statistics. The physical formulation is based on Newton's second law in a rotating reference frame and includes gravity, buoyancy, drag, Coriolis effects, and short-range inter-parcel interactions that provide pressure-like coupling. Thermodynamic evolution is supported through simplified parameterizations, including Newtonian relaxation toward a target temperature profile and optional moisture processes with condensation and latent heating. The project also defined a scalable virtual environment with a target configuration that increases particle count and maintains a thin-atmosphere regime to enable meaningful circulation diagnostics. Numerically, the simulator advances the system using an explicit Velocity-Verlet scheme with stability and convergence checks. The implementation plan commits to a high-performance C++ solution with OpenMP parallelization to support efficient neighbor-limited interaction evaluation. A modular architecture separates simulation, analysis, and visualization components, enabling reproducible experiments and clear diagnostics. The validation approach combines analytic benchmark tests, sensitivity analysis, and emergent circulation measures derived from binned velocity statistics. Phase B will focus on implementing the engine, tuning parameters via stability/convergence tests, and producing quantitative evidence that macroscopic circulation structures can arise as a statistically stable emergent outcome of the model.

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