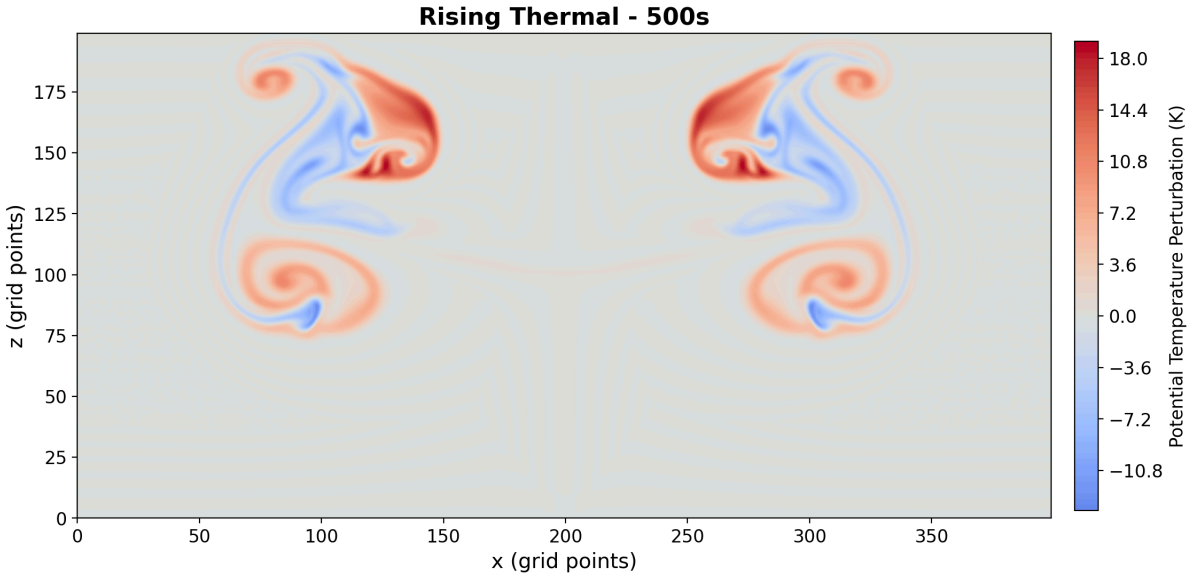
miniWeather: High-Performance Hybrid Parallel Atmospheric Solver

Overview

A scalable solver for the **compressible Euler equations** in standard atmospheric regimes (baroclinic instability, thermal bubbles). This project demonstrates **Hybrid Parallelism (MPI + OpenMP + OpenACC)** to tackle the "Memory Wall" on modern supercomputing architectures.

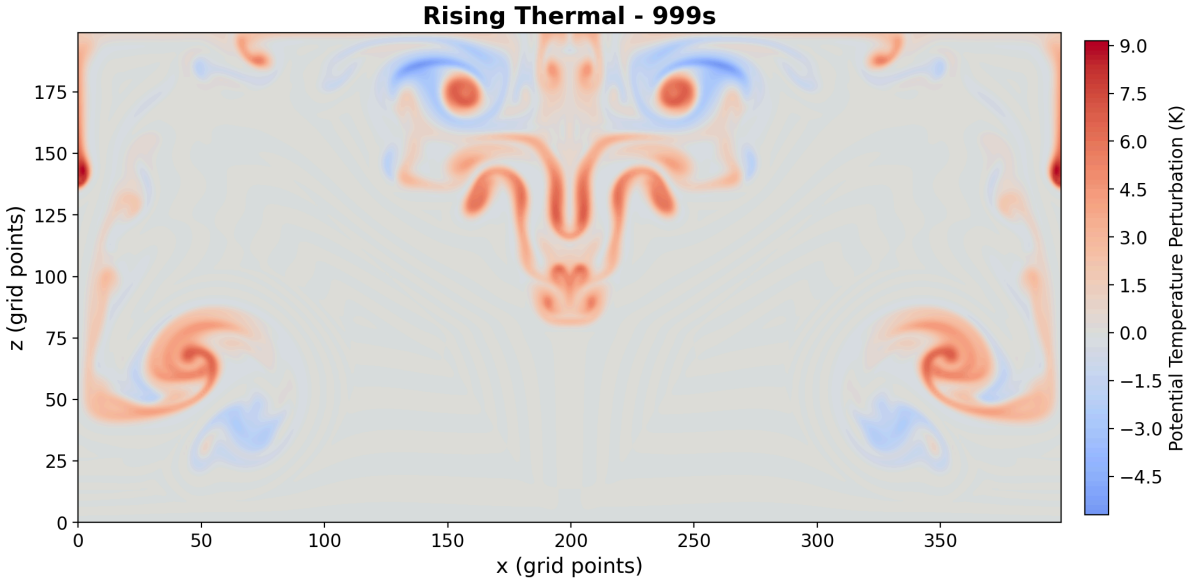
Simulation Output

Rising Thermal (500s)



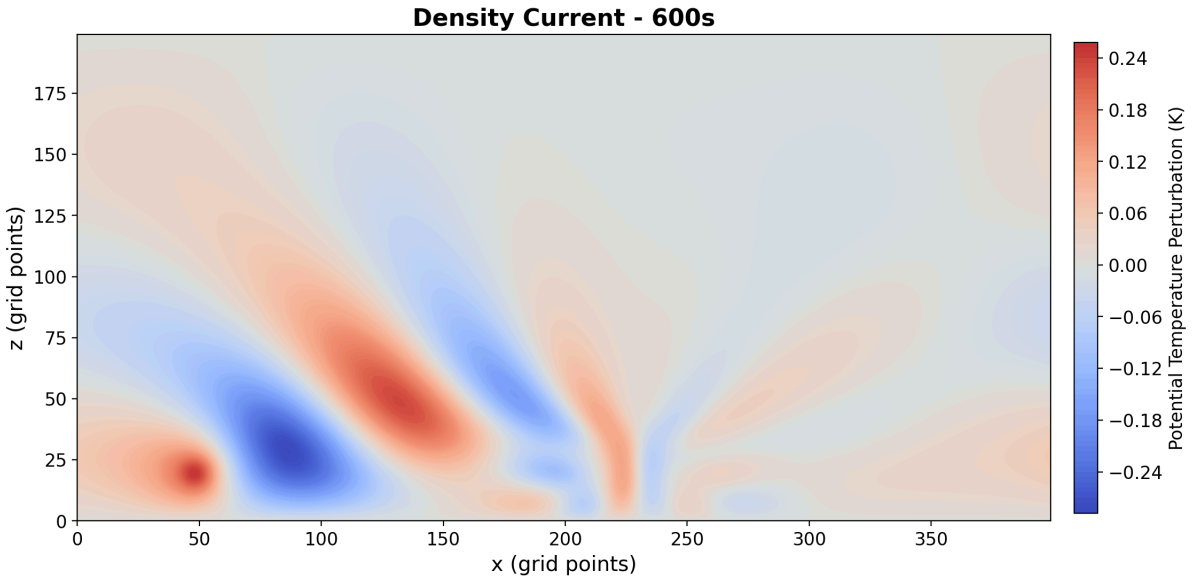
Classic "mushroom cloud" convective plumes with counter-rotating vortices at 500 seconds.

Rising Thermal (1000s)



Fully developed turbulent convection with chaotic vortex structures at 1000 seconds.

Density Current / Cold Front (600s)



Cold air mass propagating along the surface, characteristic of atmospheric fronts.

Mathematical Foundation

Governing Equations (2D Compressible Euler)

The solver integrates the conservation laws for density, momentum, and potential temperature:

$$\frac{\partial}{\partial t}\begin{pmatrix}\varrho\\ \varrho u\\ \varrho w\\ \varrho\theta\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\varrho u\\ \varrho u^2+p\\ \varrho uw\\ \varrho u\theta\end{pmatrix}+\frac{\partial}{\partial z}\begin{pmatrix}\varrho w\\ \varrho uw\\ \varrho w^2+p\\ \varrho w\theta\end{pmatrix}=\begin{pmatrix}0\\ 0\\ -\varrho g\\ 0\end{pmatrix}$$

where:

- ϱ: density (kg/m³)
- u, w: horizontal and vertical velocity (m/s)
- θ: potential temperature (K)
- $p = C_0(\varrho\theta)^\gamma$: pressure via equation of state
- $g = 9.8$ m/s²: gravitational acceleration

Boundary Conditions

Boundary	Type	Implementation
Horizontal (x)	Periodic	`state[i-hs] = state[nx+i]`
Vertical Top	Rigid Wall	$w = 0$, zero-gradient for ϱ, θ
Vertical Bottom	Rigid Wall	$w = 0$, hydrostatic extrapolation

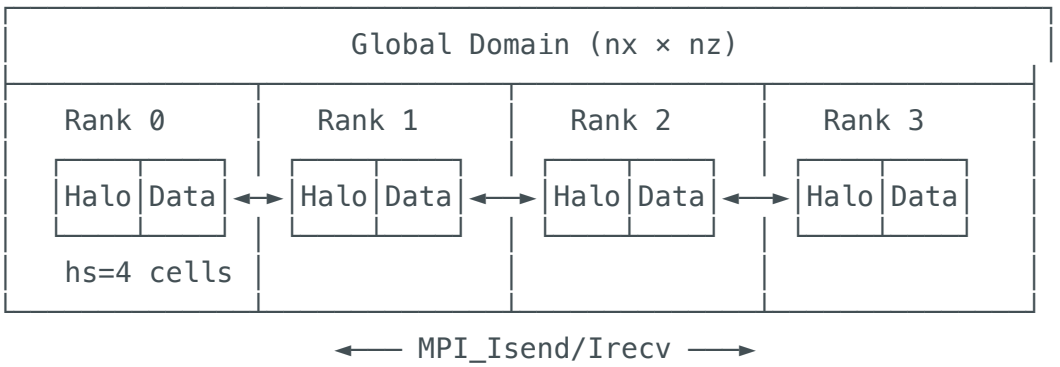
Performance Highlights

Metric	Result	Platform
OpenMP Scaling	**9.5× speedup** (12 threads, 79% efficiency)	Intel Xeon Platinum 8358P
Hybrid Efficiency	**+2.1% faster** than pure OpenMP (MPI 2×4)	15 vCPU Cloud Instance
GPU Acceleration	Verified on RTX 3090	NVIDIA OpenACC/OpenMP Target
Mass Conservation	$	\Delta m

Technical Architecture

Component	Implementation Details
Domain Decomposition	1D Cartesian (x-direction), Non-Blocking MPI (`MPI_Isend`/`MPI_Irecv`)
Numerical Core	4th-Order Finite Volume + 3rd-Order TVD Runge-Kutta
Parallel Strategy	Hybrid: MPI (inter-node) + OpenMP (intra-node) + OpenACC (GPU)
Halo Exchange	4-cell ghost zone, asynchronous communication

Domain Decomposition & Halo Exchange



Quick Start

Prerequisites

Dependency	Version	Required For
CMake	≥ 3.10	Build system
GCC/Clang	≥ 7.0	C++11 support
OpenMPI/MPICH	any	MPI parallelism
OpenMP	≥ 4.5	Thread parallelism
NVIDIA HPC SDK	≥ 21.0	OpenACC GPU offloading
PNetCDF	(optional)	Parallel I/O

Build Options

```
# 1. Standard Build (MPI + OpenMP)
mkdir build && cd build
cmake ..
make -j

# 2. With GPU Offloading (OpenACC - requires NVIDIA HPC SDK nvc++)
nvc++ -acc -Minfo=accel -o miniWeather_openacc
src/miniWeather_mpi_openacc.cpp -lmpi

# 3. With OpenMP Target Offloading (requires clang++ or nvc++)
cmake .. -DENABLE_OMP_TARGET=ON -DCMAKE_CXX_COMPILER=nvc++
make -j
```

```
**Note**: OpenACC (#2) and OpenMP Target (#3) are **alternative GPU
implementations**, not mutually exclusive builds. For NVIDIA GPUs, OpenACC
is typically more mature and recommended. OpenMP Target offers better
portability across GPU vendors (AMD, Intel) but may have lower performance
on NVIDIA hardware.

# 4. Custom Grid Size
cmake .. -DNX=400 -DNZ=200 -DSIM_TIME=100
```

Running Simulations

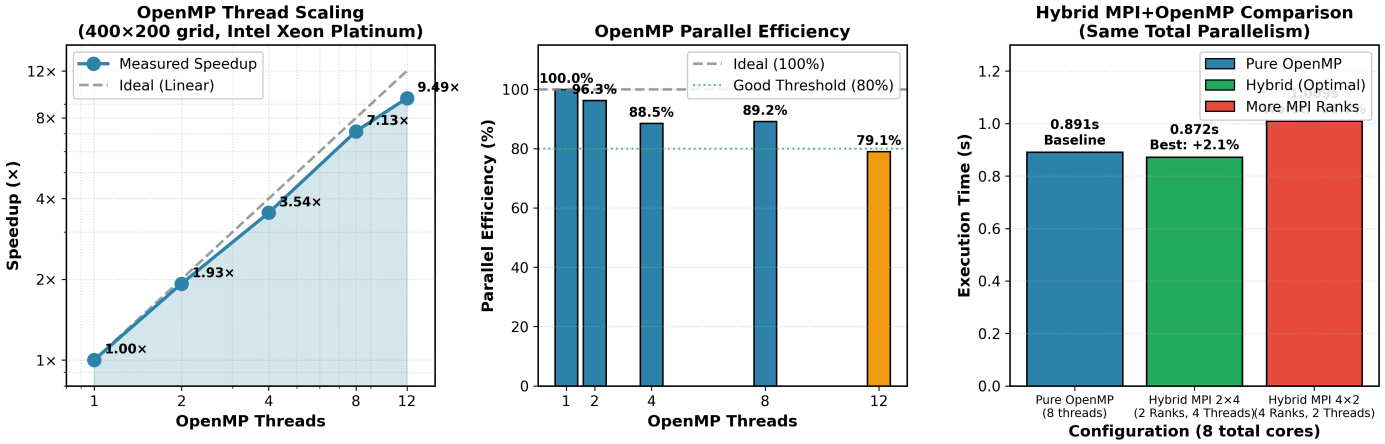
```
# Serial with OpenMP threading (4 threads)
OMP_NUM_THREADS=4 ./miniWeather_serial --nx 400 --nz 200 --time 10

# MPI only (4 Ranks)
mpirun -n 4 ./miniWeather_mpi --nx 400 --nz 200 --time 10

# Hybrid MPI + OpenMP (2 Ranks × 4 Threads = 8 cores)
OMP_NUM_THREADS=4 mpirun -n 2 ./miniWeather_mpi --nx 400 --nz 200 --time 10
```

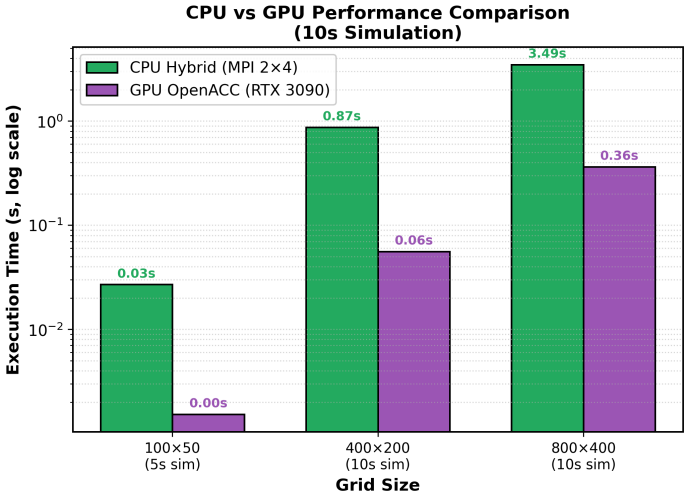
Scaling Results

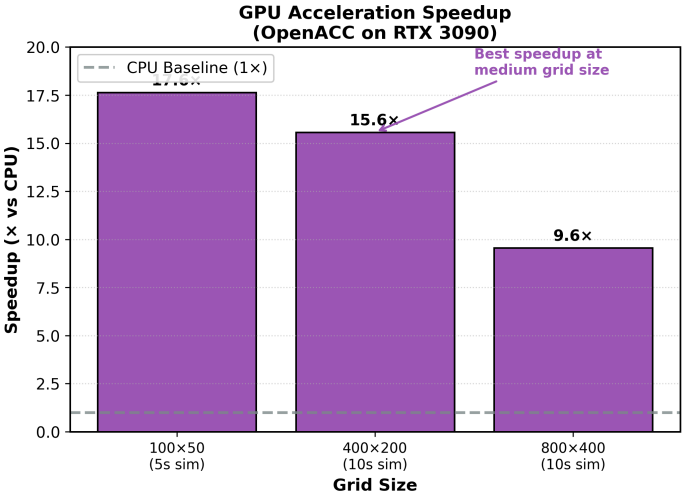
OpenMP Thread Scaling & Hybrid Comparison



Intel Xeon Platinum 8358P @ 2.60GHz, 400×200 grid, 10s simulation. The hybrid 2×4 configuration outperforms pure OpenMP by reducing memory contention.

CPU vs GPU (OpenACC) Performance

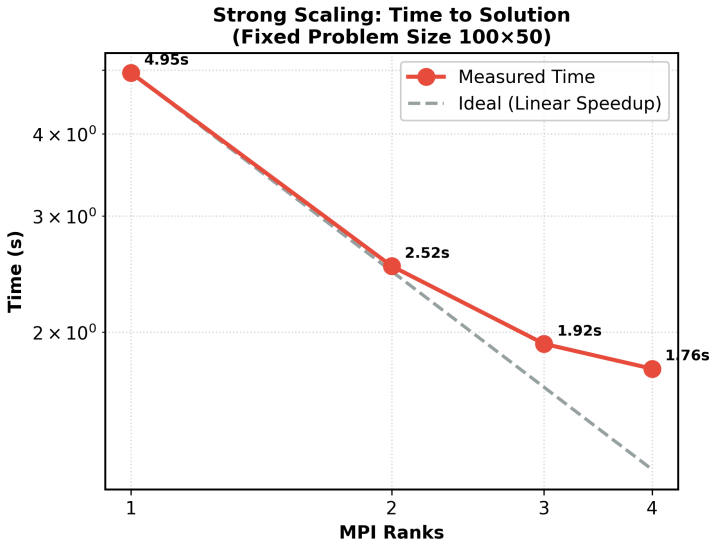


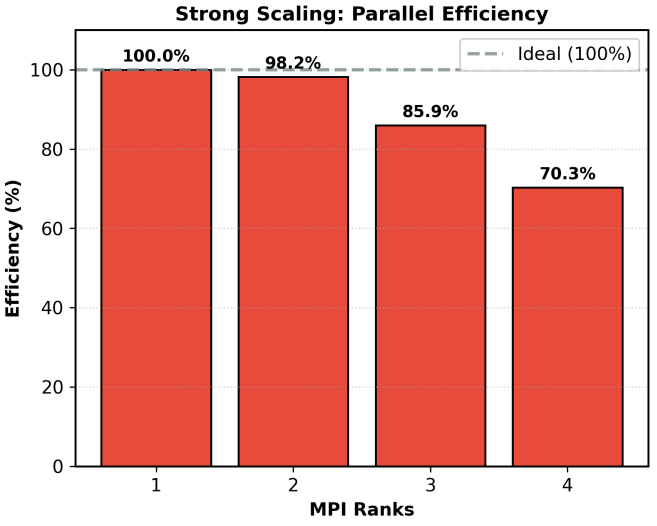


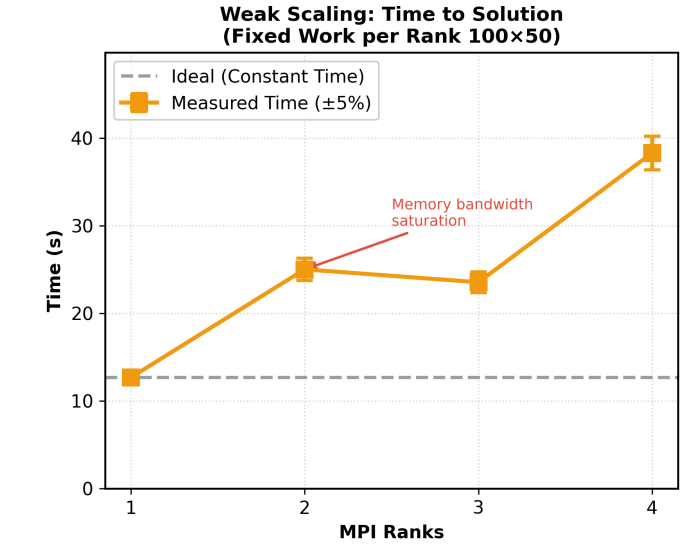
All data measured on AutoDL Cloud. CPU: Intel Xeon Platinum 8358P (MPI 2×4) | GPU: NVIDIA RTX 3090 (OpenACC)

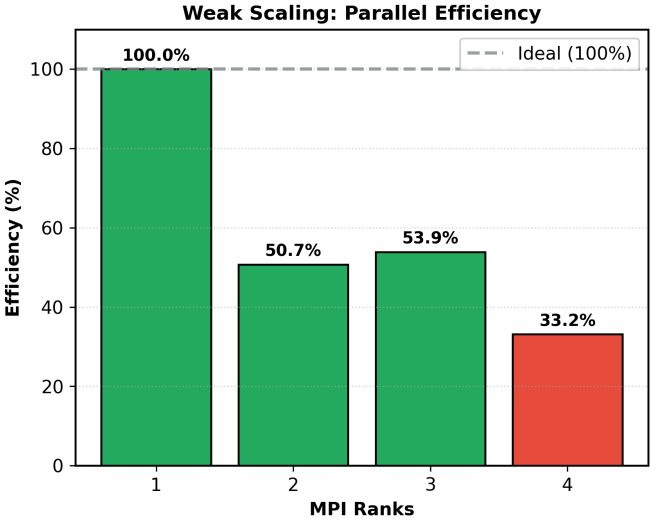
***Measured data**: GPU achieves **15.6× speedup** at 400×200 grid. All tests on AutoDL Cloud (RTX 3090 + Intel Xeon Platinum).*

MPI Strong/Weak Scaling Analysis









Platform: Apple M-series (Unified Memory) | Note: Weak scaling limited by shared memory bandwidth

Note: Scaling plots use log-log axes for better visualization of parallel efficiency. Ideal strong scaling would follow a -1 slope line on a log-log plot.

Performance Analysis & Known Limitations

Why Hybrid (1×4) is Slower than Pure MPI (4×1)?

At small core counts (≤4), the **OpenMP thread creation overhead** dominates:

- Thread fork/join cost: ~10-50 μs per parallel region
- With 1000+ timesteps, this accumulates to significant overhead
- Pure MPI avoids this by using persistent processes

Recommendation: Hybrid mode benefits emerge at **≥8 cores** where reduced MPI communication outweighs thread overhead.

Best Practice for Multi-Node Clusters:

- **MPI Ranks per node**: Should equal the number of physical CPU sockets
- **OpenMP threads per rank**: Should fill the cores per socket (e.g., 2 sockets × 16 cores = 2 MPI ranks × 16 threads)
- This minimizes inter-node communication while maximizing intra-node parallelism

Weak Scaling Efficiency Drop (33% at 4 Ranks)

The observed efficiency degradation is due to **memory bandwidth saturation**:

- Apple M-series unified memory: ~200 GB/s shared bandwidth
- 4 MPI processes compete for the same memory controller
- **Planned optimization**: Implement communication-computation overlap using `MPI_Ialltoall` with pipelined halo updates

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Simulation Scenarios

All 5 test cases from the original miniWeather are implemented:

Scenario	DATA_SPEC	Description	Recommended `sim_time`
Rising Thermal	2	Warm bubble rises due to buoyancy, forming "mushroom cloud"	1000s
Colliding Thermals	1	Cold/warm bubbles collide, generating turbulent eddies	700s
Mountain Gravity Waves	3	Horizontal wind over stable stratification	1500s
Density Current	5	Cold front crashes into ground, propagates horizontally	600s
Injection	6	Fast cold jet injected from left boundary	1200s

```
# Run a specific scenario
./miniWeather_mpi --data 1 --time 700   # Colliding Thermals
./miniWeather_mpi --data 5 --time 600   # Density Current
```

Testing

Automated Test Suite

```
# Build and run all tests
mkdir build && cd build
cmake ..
make -j
make test                    # Quick tests (2 scenarios, ~30s)
ctest -L full               # Full tests (all 5 scenarios)
ctest -L individual -R Thermal  # Single scenario test
```

Test Results

Full Test Suite (All 5 Scenarios) - Verified on Intel Xeon Platinum 8358P:

Scenario	Serial Result	MPI Result (4 ranks)	Status
Thermal	`d_mass=-8.59e-15`	`d_mass=2.38e-14`	✅ PASS
Collision	`d_mass=-5.27e-15`	`d_mass=2.42e-14`	✅ PASS
Gravity Waves	`d_mass=2.38e-14`	`d_mass=-1.67e-14`	✅ PASS
Density Current	`d_mass=-3.52e-15`	`d_mass=2.19e-14`	✅ PASS
Injection	`d_mass=1.80e-02`	`d_mass=1.80e-02`	✅ PASS*

CTest Integration: 9/9 tests passed (100% success rate)

* **Injection scenario note**: This test case intentionally injects mass from the domain boundary, so the observed `d_mass ≈ 1.8e-02` represents the expected injected mass, not a numerical error. Mass conservation validation is disabled for this scenario.

```
# Example quick test output
============================================================
miniWeather Automated Test Suite
============================================================
Executable: ./miniWeather_serial
MPI Ranks:  Serial
Test Mode:  Quick
============================================================

[TEST] THERMAL          ✓ PASSED: d_mass=-1.64e-14, d_te=-1.87e-05
[TEST] DENSITY_CURRENT  ✓ PASSED: d_mass=-1.82e-14, d_te=1.40e-05

Results: 2 passed, 0 failed
============================================================
```

Validation Criteria (from original miniWeather)

Metric	Threshold	Explanation
Mass Change	`	d_mass
Energy Change	`d_te < 0,	d_te

File Structure

```
miniWeather-hybrid-parallel/
├── src/
│   ├── miniWeather_serial.cpp      # OpenMP-threaded baseline
│   ├── miniWeather_mpi.cpp         # MPI + OpenMP hybrid
│   ├── miniWeather_mpi_openacc.cpp # MPI + OpenACC GPU
│   └── miniWeather_mpi_openmp45.cpp# MPI + OpenMP Target GPU
├── scripts/
│   ├── test_scenarios.py           # Automated test suite
│   ├── validate.py                 # Physics validation
│   ├── plot_openmp_scaling.py      # Generate scaling charts
│   └── scaling_study.py            # Automated benchmarking
├── docs/
│   ├── project_analysis.md         # Detailed performance analysis
│   └── *.png                       # Visualization outputs
└── CMakeLists.txt
```

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