

TOWARDS ENABLING DIGITAL TWINS CAPABILITIES FOR A CLOUD CHAMBER

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ABSTRACT

Particle-resolved direct numerical simulations (PR-DNS), which resolve not only the smallest turbulent eddies but also track the development and motion of individual particles, are arguably an essential tool for exploring aerosol-cloud-turbulence interactions at the fundamental level. For instance, PR-DNS may complement experimental facilities designed to study key physical processes in a controlled environment and therefore serve as digital twins for such cloud chambers. In this poster we present our ongoing work aimed at enabling the use of a PR-DNS model for this purpose. We consider two approaches: traditional HPC techniques and emerging machine learning methods. Future research directions are outlined as well.

Keywords: modeling and simulation, PETSc, MPI, CUDA, neural operator learning

CLOUD CHAMBER

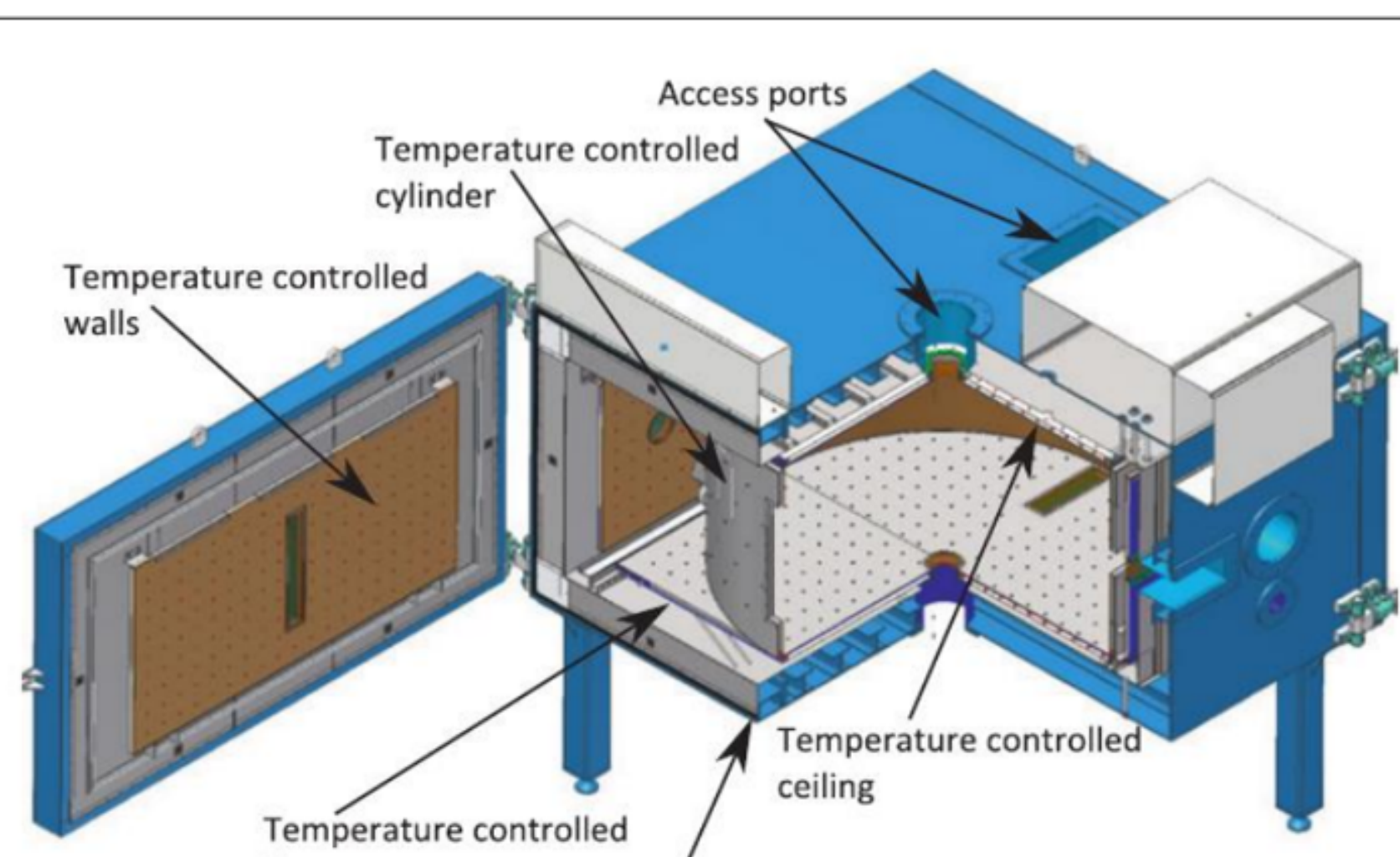


Fig. 1. A cutaway schematic of the cloud chamber with one door open and the cylindrical thermal panel in place.

Figure 1 source: K. Chang *et al.* A Laboratory Facility to Study Gas-Aerosol-Cloud Interactions in a Turbulent Environment: The Π Chamber. *Bull. Amer. Meteor. Soc.*, 97, 2343-2358, 2016. <https://doi.org/10.1175/BAMS-D-15-00203.1>
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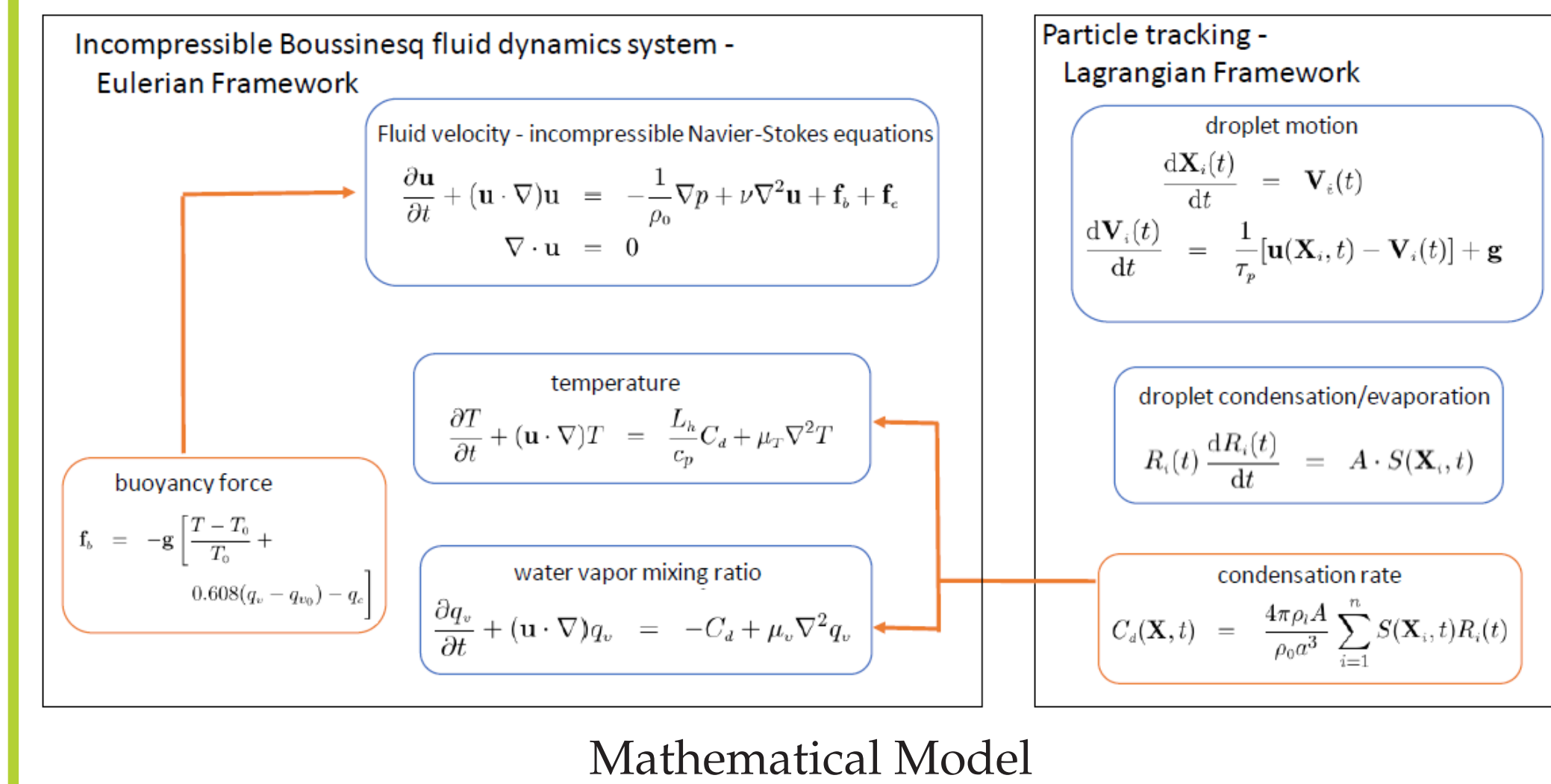
Fig. 2. Photograph of the cloud chamber with scientists for scale. Photo credit: S. Bird, Michigan Technological University.

Figure 2 source: K. Chang *et al.* A Laboratory Facility to Study Gas-Aerosol-Cloud Interactions in a Turbulent Environment: The Π Chamber. *Bull. Amer. Meteor. Soc.*, 97, 2343-2358, 2016. <https://doi.org/10.1175/BAMS-D-15-00203.1>
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Pi Chamber @ Michigan Tech

METHODOLOGY

PR-DNS: Particle-Resolved Direct Numerical Simulation



Investigating Traditional HPC Aspects

- Krylov subspace methods from PETSc employed for required linear systems solves for discretized fluid mechanics equations
- Profile PETSc operations within PR-DNS code with different preconditioners
- CPU & GPU scaling analysis carried out to assess parallel performance for various components of PR-DNS model

Exploring Potential Benefits of Machine Learning Techniques

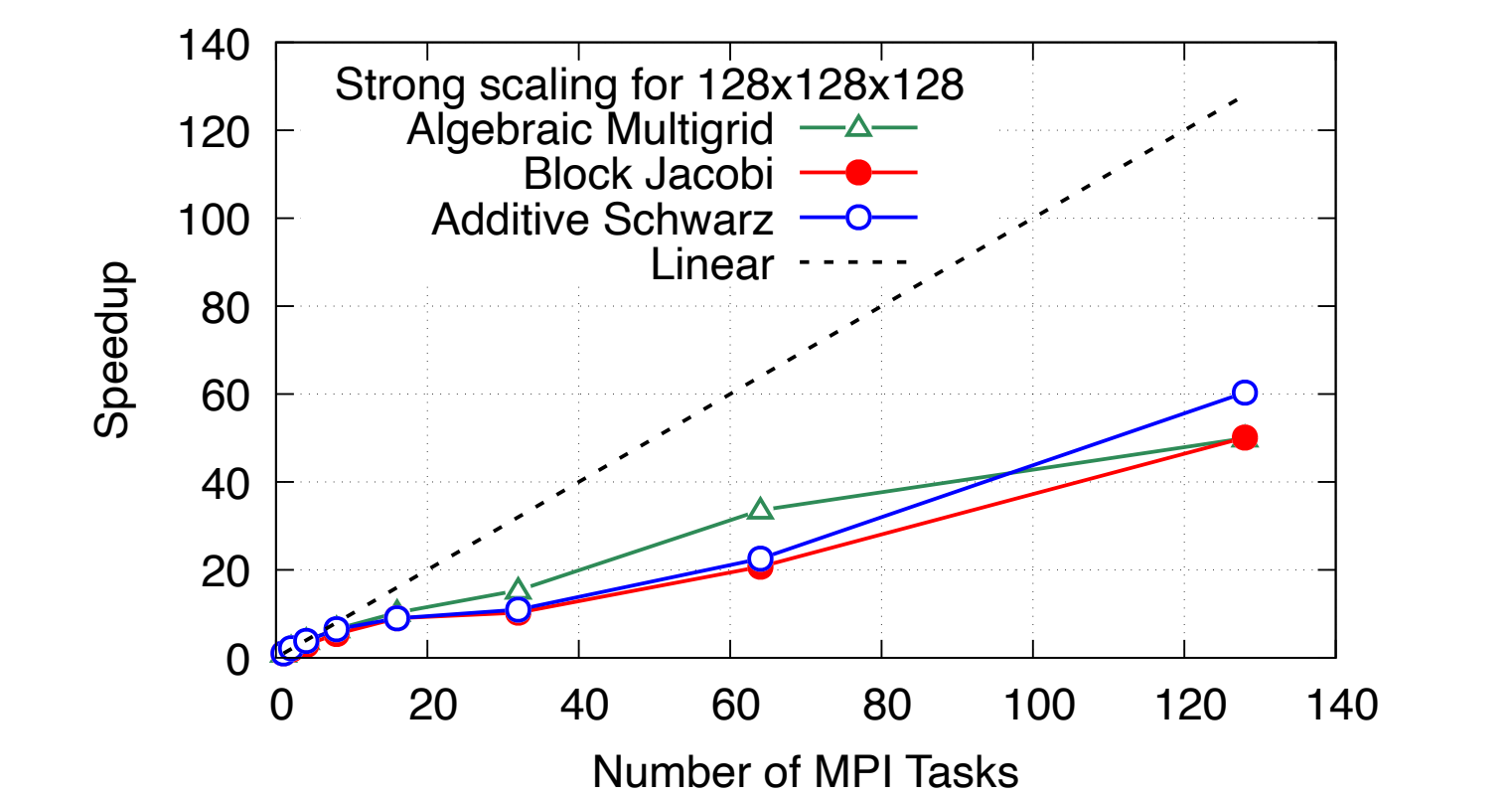
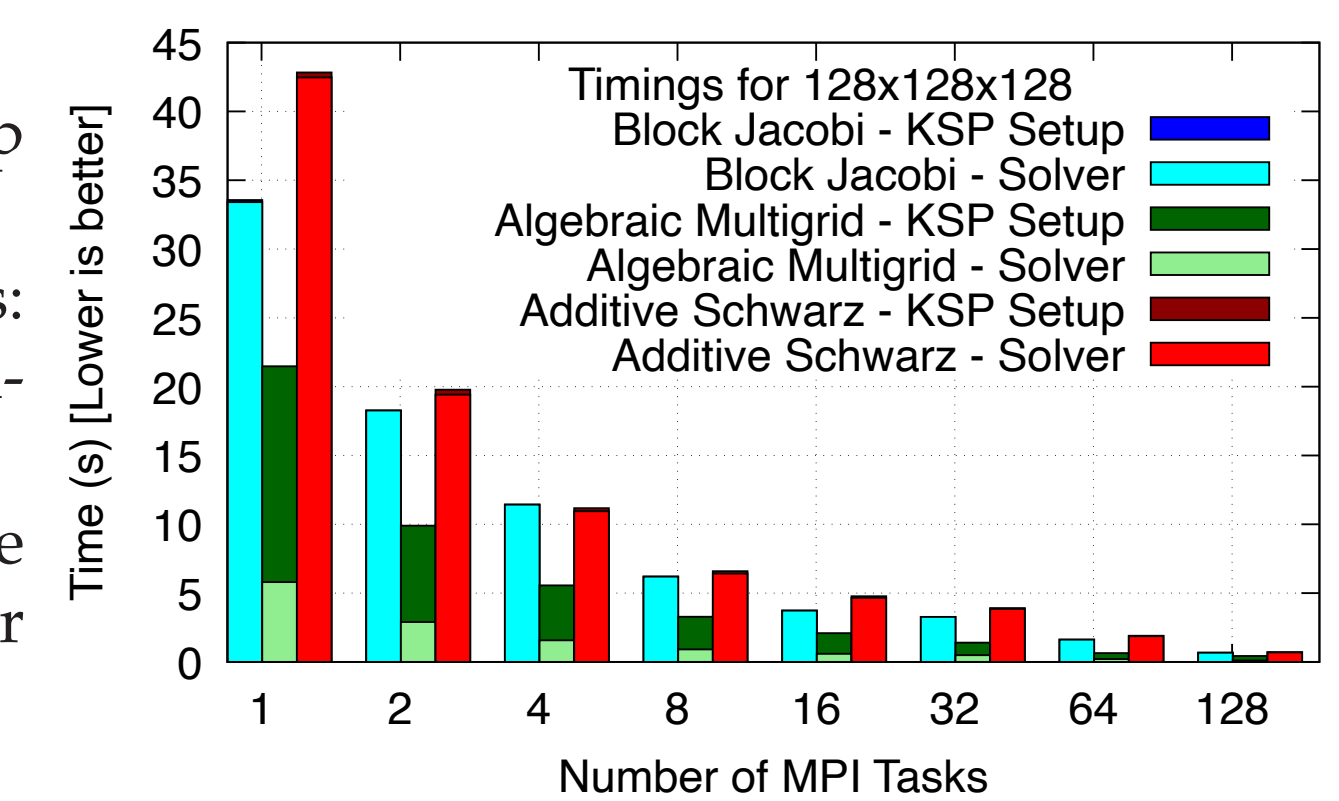
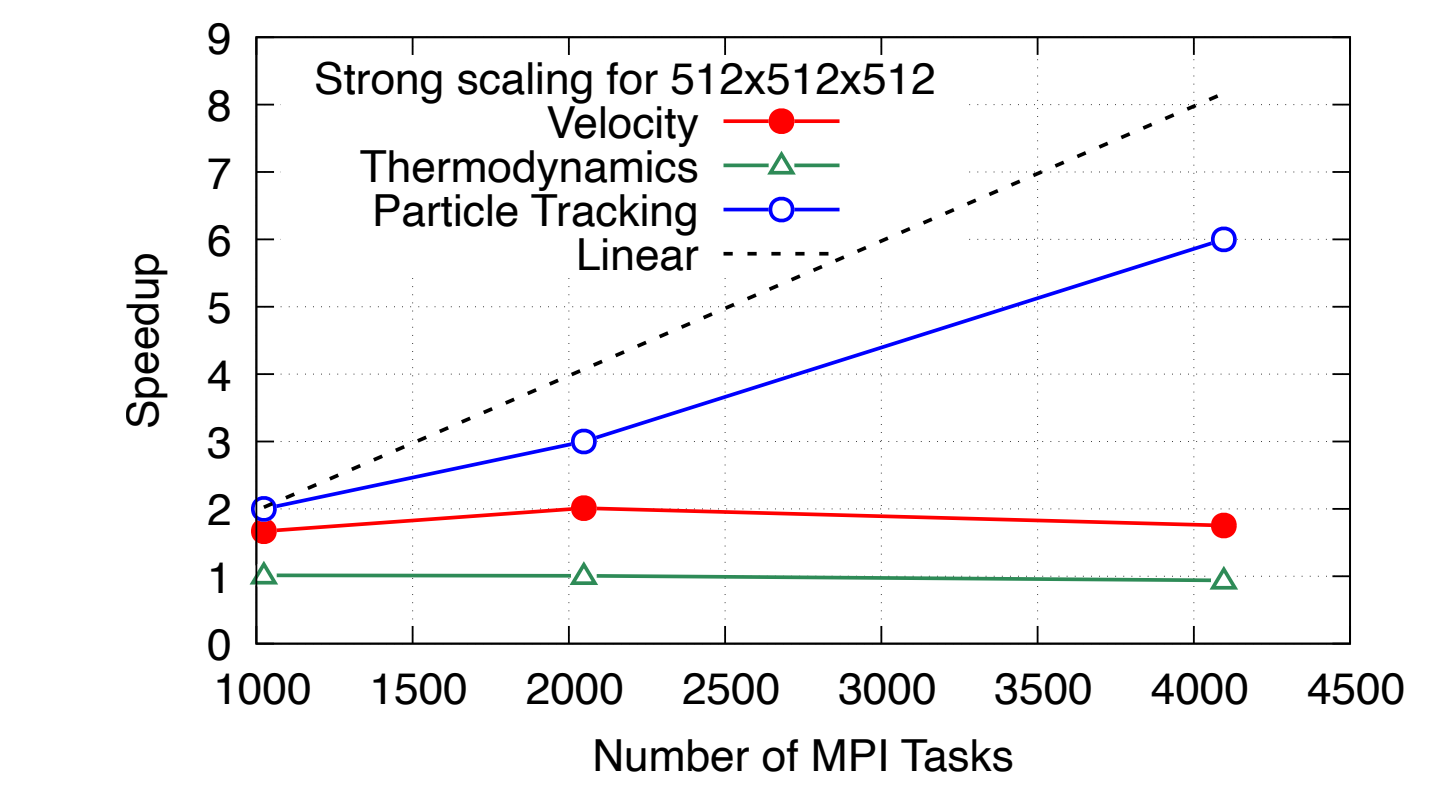
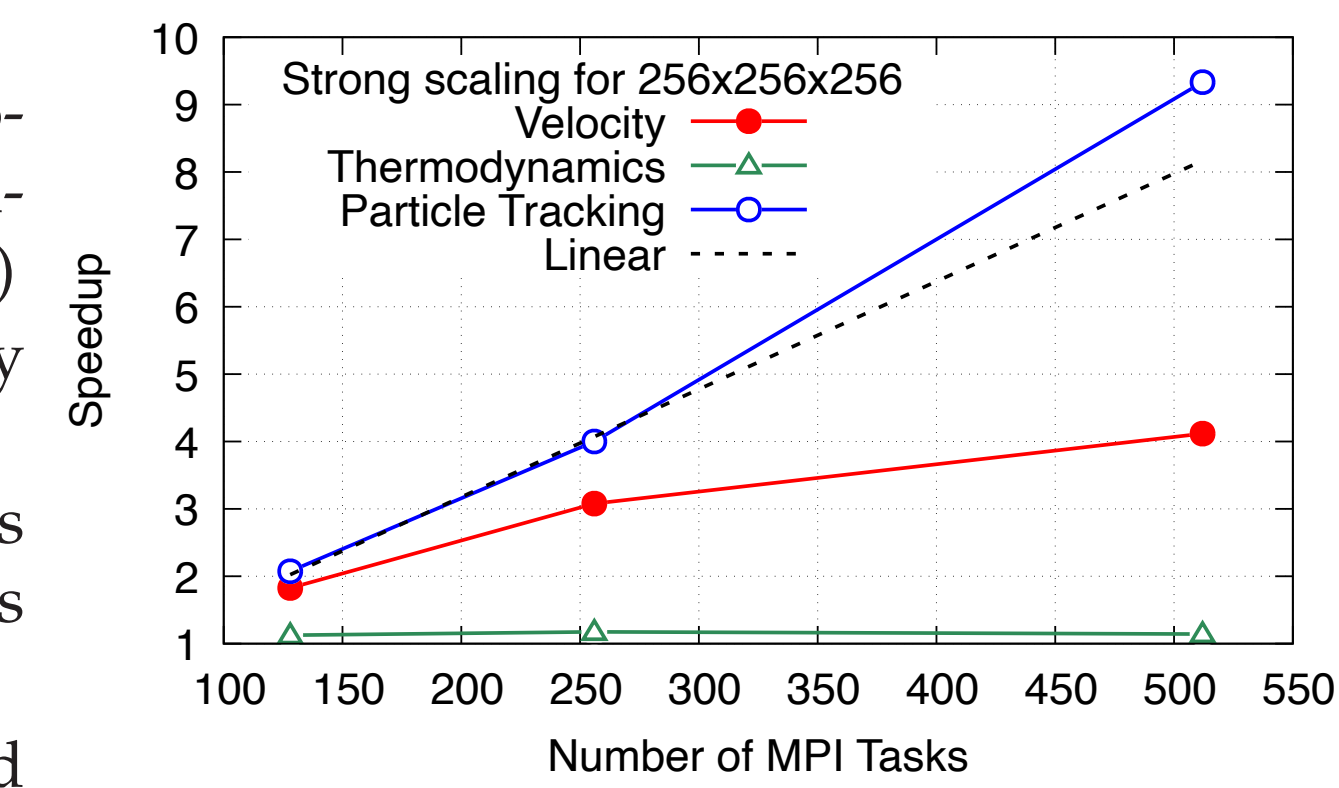
- Fourier Neural Operator (FNO) method to define fast surrogate models for dynamical systems

- [1] Z. Gao *et al.* Investigation of turbulent entrainment-mixing processes with a new particle-resolved direct numerical simulation model. *J. Geophys. Res. Atmos.*, 123(4):2194–2214, 2018.
- [2] www.petsc.org
- [3] Z. Li *et al.* Fourier neural operator for parametric partial differential equations, 2021. <https://arxiv.org/abs/2010.08895>

CPU PROFILES AND SCALING

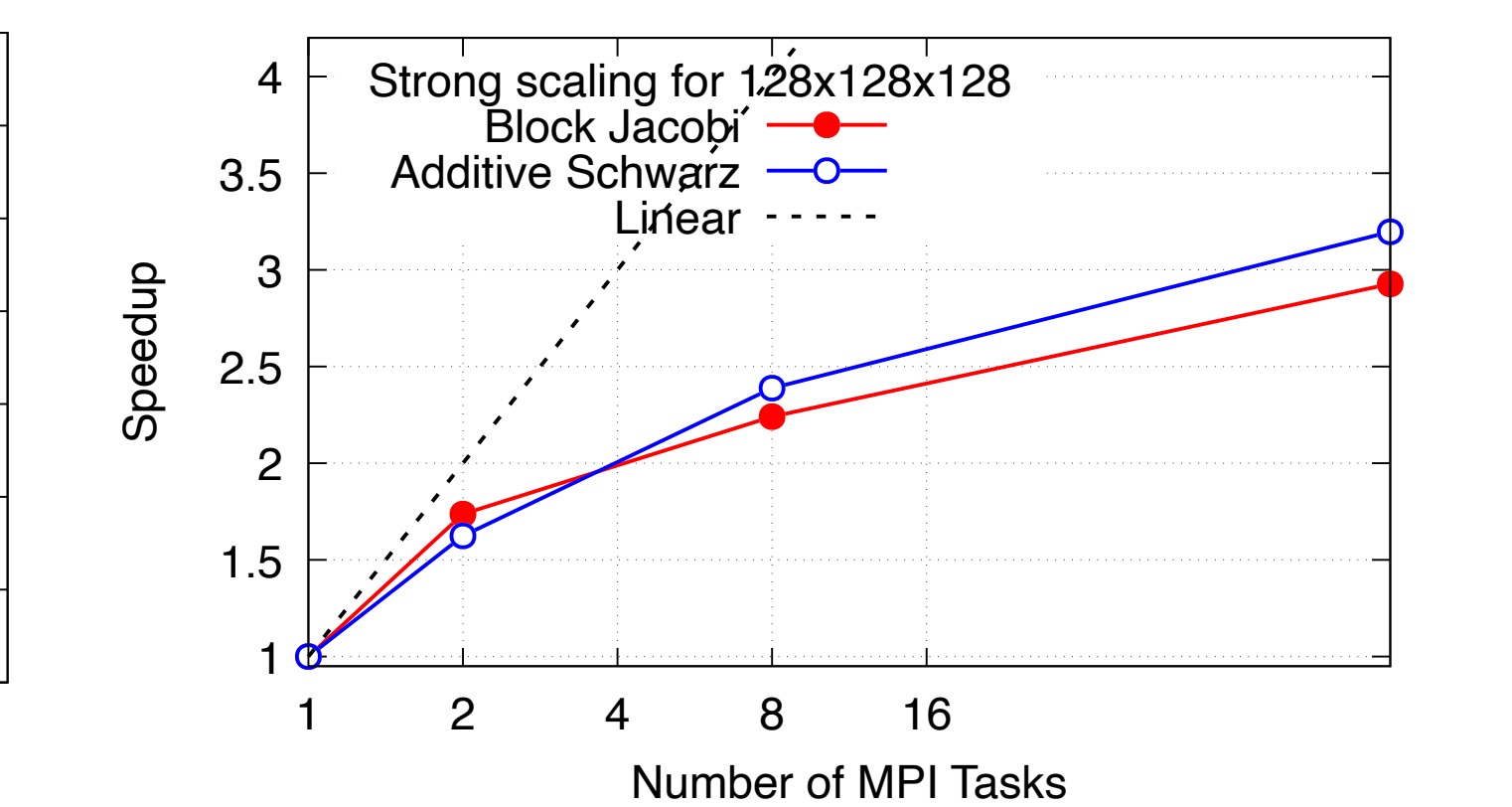
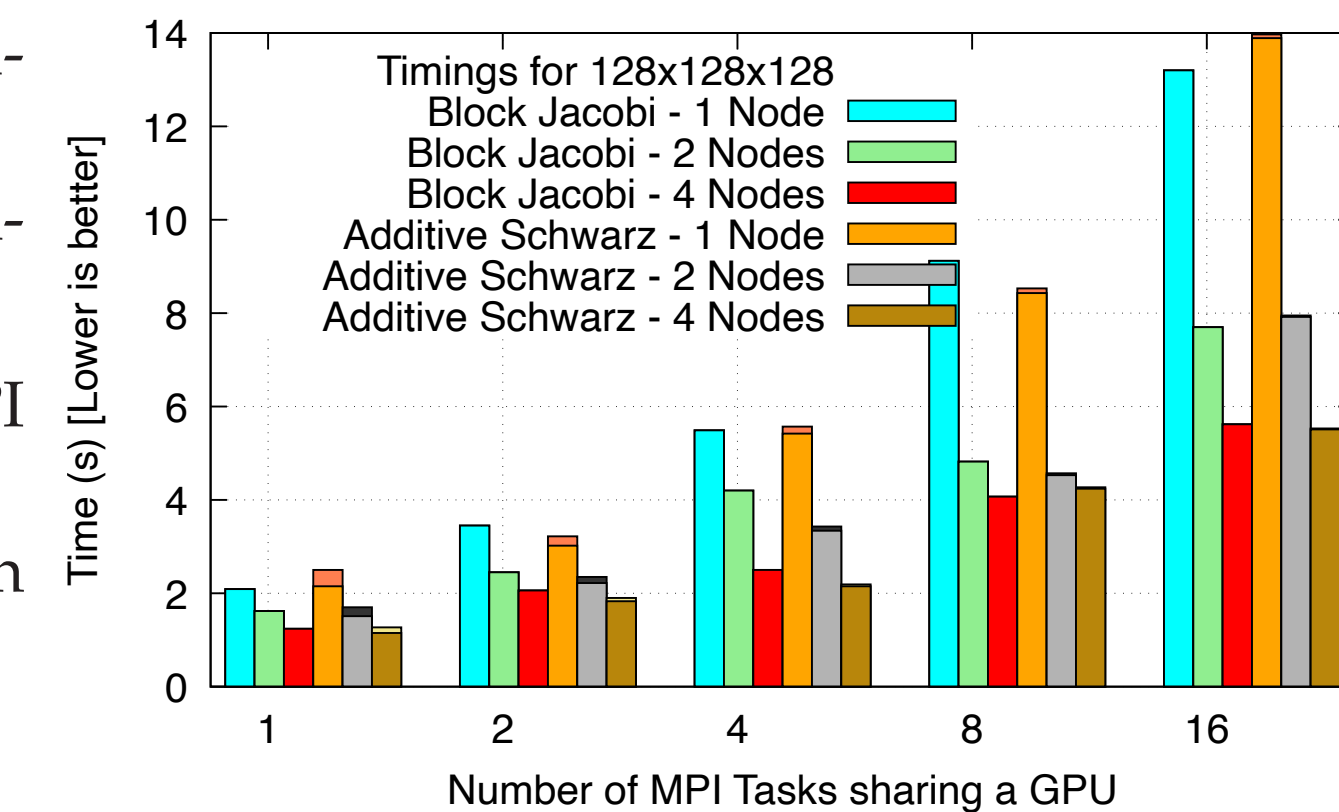
- Strong scaling behavior of various components on NERSC Perlmutter (2 AMD Milans per node, with HPE Slingshot 11 NIC)
- Particle tracing solver scales reasonably well up to 32 nodes (4096 MPI tasks)
- Thermodynamical field's solver shows poor strong scaling (related CUDA ports are being developed)
- Navier-Stokes solver for velocity field shows sub-linear scaling

- PETSc's CUDA implementation can help address this
- Investigating impact of preconditioners: block Jacobi, algebraic multigrid, additive Schwarz
- Preliminary studies show additive Schwarz may improve scaling behavior (conducted on BNL-IC)

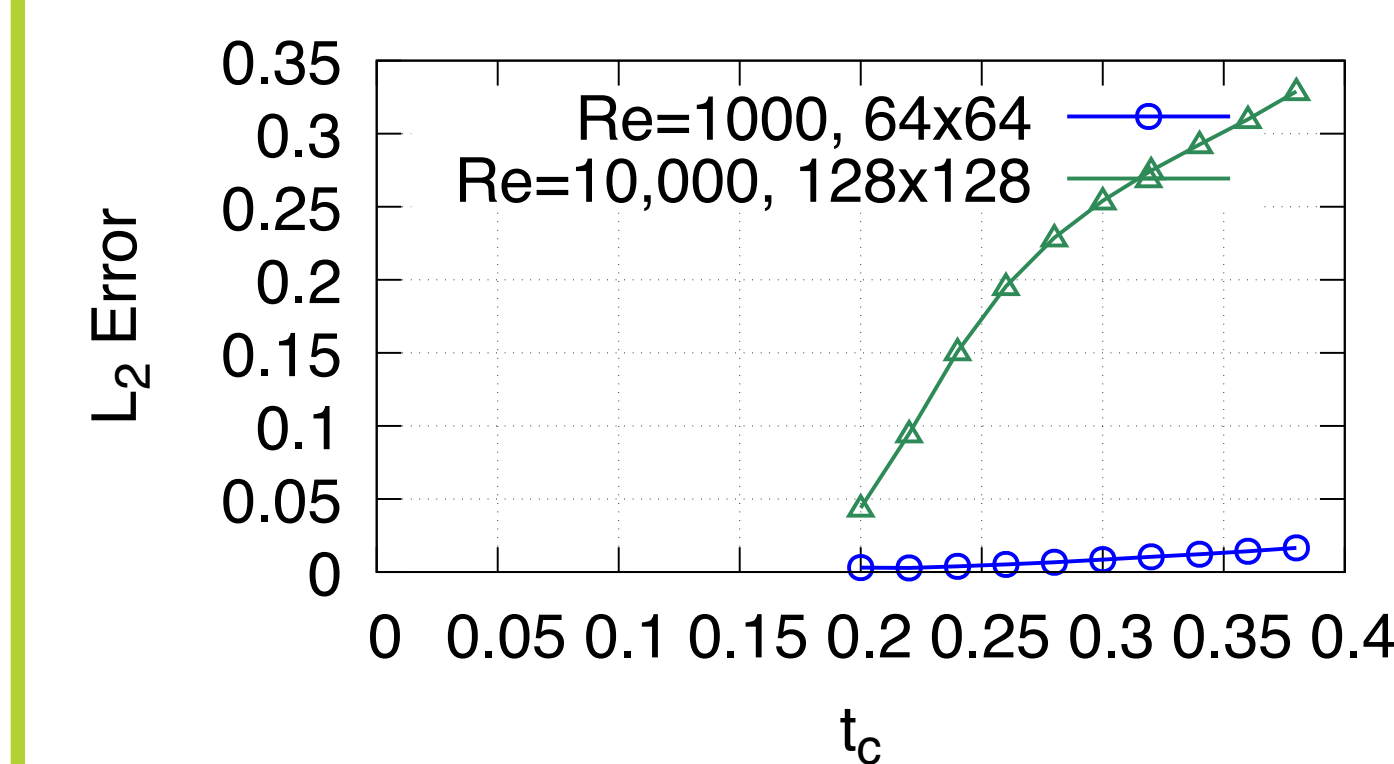


GPU EXPERIMENTS: NAVIER-STOKES SOLVER

- Comparison of two preconditioners' scaling for PETSc's CUDA implementation
- Conducted on BNL-IC; each node is connected to two Nvidia Pascal P100 GPUs
 - Best performance when each MPI task has its own GPU
 - Additive Schwarz scales better than Block Jacobi
- Multigrid preconditioner to be tested



MACHINE LEARNING WITH NEURAL OPERATORS

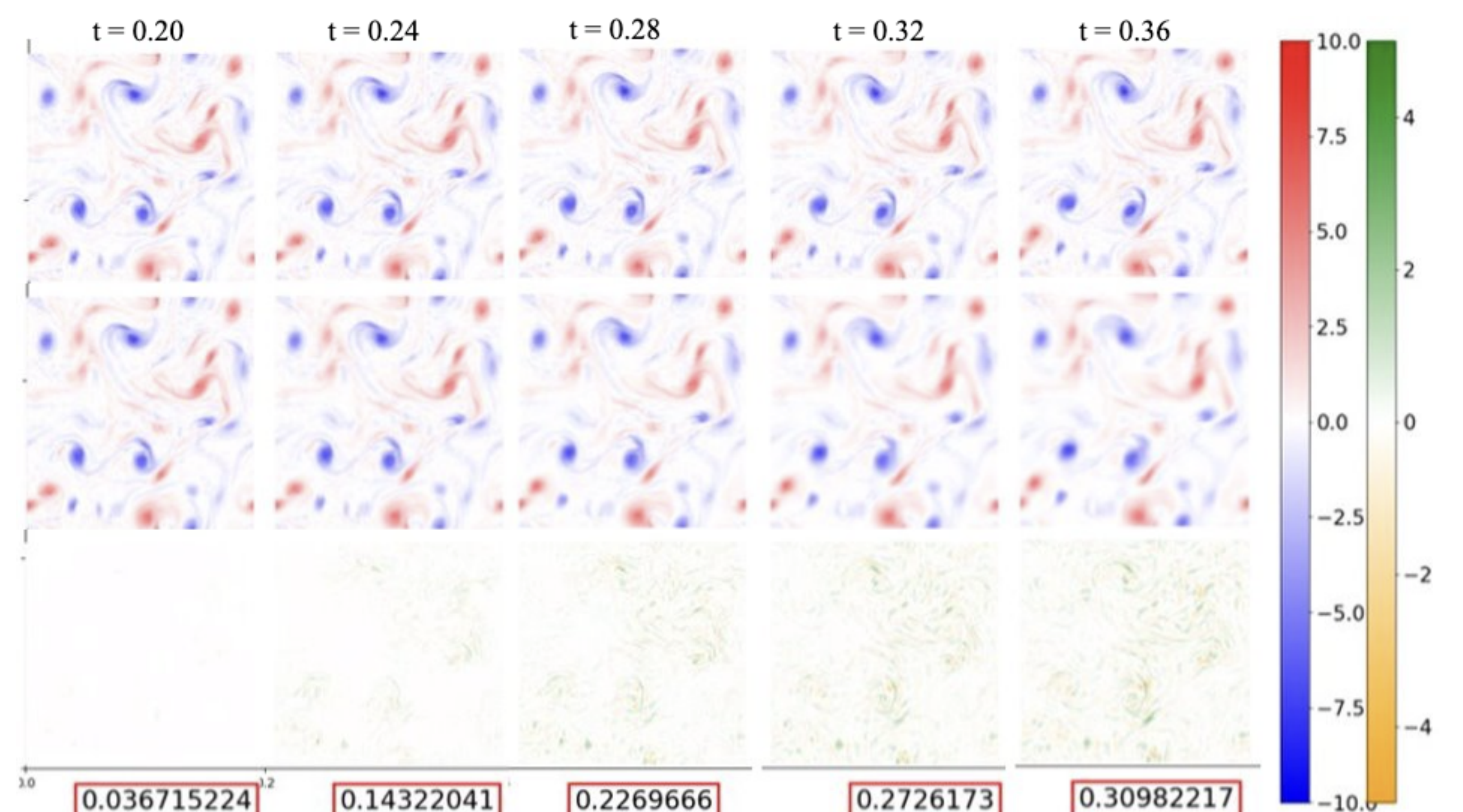


- Data set: 5000 (4000 train, 1000 test) simulations of 2D turbulence with different initial conditions.
- Simulations sampled for vorticity field over 0.4 convection times (t_c) in steps of $0.02t_c$ (total 20 snapshots; 10 inputs and 10 outputs).
- Plot illustrates accumulation in errors as time progresses.

- Image shows vorticity field of one sample: expected (top), FNO's prediction (center), difference (bottom).

[4] M. Atif, *et al.* Towards Accelerating Particle-Resolved Direct Numerical Simulation with Neural Operators. Submitted to CoDA 2023 Proceedings.

[5] T. Zhang, *et al.* Digital Twin of PR-DNS: Accelerating Dynamical Fields with Neural Operators in Particle-Resolved Direct Numerical Simulation. Authorea. July 09, 2023. DOI: 10.22541/es-soar.16889862.29246354/v1



ONGOING & FUTURE RESEARCH

- Optimizing node-level performance, identifying scalability bottlenecks, and porting compute-intensive kernels to GPUs using CUDA
- Incorporating aerosol interactions into the PR-DNS model
- Identify other components that could be potentially replaced with ML models, investigate their performance and errors
- CUDA MPS for GPU resource sharing among MPI tasks
- Portable GPU implementations via OpenMP's target offload model

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