NOAA Weather Program Office
Air Quality Research and Forecasting

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Proposing Organization and Contact Information
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Letter of Intent for the AI-Based Emulation Model GOCART Aerosol Transport in the Unified Forecast System (UFS) to address Priority AQRF-7

- **i.** Redline Performance Solutions, LLC proposes to undertake a project to enhance performance of the Unified Forecast System (UFS) when implementing the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model to make it more efficient and effective to implement as part of the normal UFS workflow. Specifically, we will optimize the most computationally intensive tracer transport calculations, which in some instances can add 60% to the cost of the UFS. The optimization will be achieved by using a conservative model to emulate the aerosol transport based on Machine Learning (ML) and AI techniques.
- **ii.** RedLine Performance Solutions brings unique proficiencies in numerical weather prediction using the Unified Forecast System and has demonstrated subject matter expertise in performing on NOAA contracts that span many areas of research and development through each of RDHPCS, EPIC and EMC. Our expertise also extends to the operational weather forecasting applications and workflows implemented on WCOSS2 through our contracts in NCO.
- **iii.** Currently, GOCART's important forecast components are not included in the operational UFS due to computational limitations. Our proposed project will develop an AI-based emulator that significantly reduces the computational run-time of the UFS when GOCART-calculated aerosols are transported by the model, enabling its integration into NOAA's production workflows. As a result, it will enable NOAA to incorporate these crucial aerosol-related factors into both weather and air quality forecasts as part of the UFS workflow, improving forecast accuracy and runtime.

1. Proposal Title:
AI-Based Emulation for GOCART Aerosol Transport in the Unified Forecast System (UFS)

2. Principal Investigators (PIs) and Co-Investigators:

- **Lead PI**: Carolyn Pasti, RedLine Performance Solutions, LLC
- **Co-PI**: Dr. Daryl Kleist, NOAA/NWS/EMC
- **Co-Investigators**: University of Florida, Dr. Christine Angelini, Dr. Ron Flick

- **Consultants and SMEs**: RedLine Performance Solutions, Dr. Mark Potts, Innocent Souopgui, Steve Bongiovanni, David Huber

3. NOFO Competition:
RedLine is submitting this Letter of Intent to the NOAA competition under the **Air Quality Research & Forecasting (AQRF) Program**, addressing **Section 3** of NOAA's operational science improvement needs for air quality and weather forecasting. The project specifically aligns with **Priority AQRF-7** to **optimize chemistry processes** for increased computational efficiency through **AI/ML methods** including Deep Learning (Neural Networks), Transfer learning, and other conventional numerical methods, streamlining chemistry and aerosols computation in air quality forecasts so that they can be included in the operational forecast runtime window.

4. Planned Products/Outputs:

Our proposal includes:

- AI-based emulator to improve the computational efficiency of GOCART aerosol transport by the UFS dynamical core in order to meet operational timing requirements for running the global workflow.
- Framework and workflow for initial training and validation of AI model as well as for routine recalibration of model as new data becomes available.
- Open-source code repository for broad community use and development.
- Detailed performance reports showing the computational savings compared to the conventional PDE transport method.
- Verification/Validation metrics that provide confidence levels that the AI/ML emulator is accurate.

5. Planned Impacts/Benefits/Outcomes:

- **Enhanced computational efficiency**: The project will reduce the computational cost of running the GOCART model in the production UFS, allowing NOAA to include more detailed aerosol processes in its operational forecasts. Although we are in the process of quantifying the improvement at this point, typical AI models for similar PDE problems can see up to 10 times speed increase for that portion of the problem.
- **Improved air quality and weather forecasting**: The inclusion of GOCART transport will enhance the accuracy of forecasts related to aerosol concentrations, with the goal of benefiting air quality predictions.
- **Broader operational use**: The AI-based emulator is a candidate to be adapted for use in various NOAA models, supporting future infrastructure upgrades and scalability to other atmospheric composition models including fire, smoke, and dust.

6. Planned Methodology and Timelines:
The transport method used by FV3 solves partial differential equations (PDEs) to make predictions on a

cell-by-cell basis, constrained by both physical and numerical limits. Physical limits are enforced by the PDEs and the laws of conservation of mass and energy, while numerical constraints are grounded in well -known numerical constraints such as the CFL number.

To replicate this process efficiently, we will implement a hybrid approach incorporating several techniques:

- **Deep Learning (DL)** and **Hybrid Transfer Learning** for emulating the cell-by-cell behavior of the GOCART aerosol transport process.
- **Physics Informed Neural Networks (PINN)** to ensure that the physical constraints of mass and energy conservation are adhered to throughout the emulation.
- **Conventional numerical techniques** drawn directly from the existing FV3 tracer transport algorithm will be integrated into the AI model for additional accuracy.

The approach will be implemented in three main steps:

6.1 Emulate the cell-by-cell model behavior using DL, focusing on narrow and computationally intensive areas where AI can achieve the greatest performance gains.

6.2 Apply location-invariant model refinement using Transfer Learning to generalize the model across different grid cells, ensuring robustness across the forecast area.

6.3 Integrate the final physical and numerical constraints using PINNs and conventional techniques, ensuring that the resultant model outputs are accurate and conform to both physical laws and numerical boundaries.

This stepwise approach enables the use of ML in targeted areas to improve performance while maintaining the physical fidelity of the overall transport model. Testing and validation will be conducted using NOAA datasets, and the final model will be integrated into the UFS for operational use.

The project timeline is as follows:

Critical Tasks and Phases *		
Start Date	End Date	Task
06/01/2025	11/15/2025	Install UFS and Generate full training data set
10/01/2025	11/30/2025	ML tools data assimilation
10/01/2025	06/15/2025	Iteratively develop AI model for emulation and validate output data
06/15/2026	08/15/2025	Verification of emulator
08/15/2026	09/30/2025	Final Report and commit to UFS repository

7. Proposed Starting and Ending Readiness Levels (RLs):

- **Starting RL**: RL 5 (Initial validation using NOAA datasets)
    - RedLine Performance Solutions has invested R&D in AI/ML efforts toward the goals of this project independently since May of 2023 and has already created a generalized UFS workflow with modifications for isolating the aerosol transport components. This extra code has two distinct purposes: 1) it allows us to extract the inputs (wind speed, pressure, constituent concentrations, drag coefficients, etc.) and outputs (constituent concentrations) of the PDE transport solver for training and validating the AI model and 2) provides an injection point in the UFS workflow for integrating the AI model into production as we reach that level.
    - Redline currently has UFS built and running on the University of Florida (UFL) "Hipergator" GPU based supercomputer, and will update UFS to the latest level at the start of the project in 2025.
    - Initial UFS runs including aerosols have been successfully completed on UFL Hipergator. These runs have been used to quantify the baseline compute and storage requirements for the data acquisition phase of this project and the resultant baseline data for training and validation currently resides there.
    - The AI training framework is under development and is currently able to map the input and training data for integrating into the final AI training process.
- **Ending RL**: RL 8 (Integration into UFS)
- **Use of NOAA Testbeds**: Generation of training data and development of the AI model will be performed on either NOAA RDHPCS resources or University of Florida HPC Hipergator system. If NOAA RDHPCS resources can be used, it will reduce the cost of the proposal as the purchase of computational resources from UFL will not be required.
- **NOAA Transition Plan**: This project currently does not have an official transition plan, but will follow the guidelines to collaborate with EPIC and work with EMC to promote the AI emulator. We plan to submit pull requests (PR's) to the appropriate repositories and add regression tests to the UFS-WM to ensure that the capability continues to be tested and recalibrated.

8. Potential Operational, Commercial, or Other End-User Collaborators or Adopter(s):

RedLine Performance Solutions will be collaborating with EPIC and incorporating the Aerosol Transport AI Emulator into the UFS repository upon the emulator's development, validation, and approval. We will follow the NWS NCO Operational Implementation Standards for WCOSS for smooth integration into operations by EMC. Since the emulator will be integrated into the UFS repository, it will be available to any organization that would like to use it. Potential collaborators and adopters include the following:

- NOAA's Environmental Modeling Center (EMC)
- National Weather Service (NWS) Central Operations (integrated into NWP)
- NOAA's Air Resources Laboratory (ARL)
- Commercial air quality and environmental monitoring providers.

9. Simple Budget Table:

Using UFL Compute Resources	Compute	Labor
Year 1	150K*	200K
Year 2	0	200K

*Compute resource dollars for entire project are allocated to year 1.

Total Project Cost using UFL Hipergator is $550K

Using NOAA RDHPCS Resources	Compute	Labor
Year 1	0	200K
Year 2	0	200K

Total Project Cost using NOAA RDHPCS is $400K

To minimize the cost of the project, we propose a combination of a graduate student and a post-doc candidate to be hired through the University of Florida.

Potential Future Benefits and Enhancements:

Replacing the current aerosol transport algorithm with an AI/ML model will significantly reduce the cost of the calculation which will allow aerosols and eventually smoke, dust, and fire to be added to the regular operational forecast suite, resulting in markedly better forecasts of air quality for customers.

The AI/ML model will be trained using global data, but will be extensible to regional forecasts as well, which will allow its inclusion in RRFS forecasts and result in faster turnaround for model refresh.

While neither of these features/benefits are part of this project, they are natural outflow of the work proposed here.