processes, this project enables NASA scientists to derive more precise insights from PACE observations, enhancing the reliability of Earth science data and reinforcing NASA's mission to address global environmental challenges.

Alignment with NASA STMD: STMD focuses on developing transformative technologies that enable and improve space missions [17]. This project aligns with STMD's emphasis on *advancing AI and ML technologies for space applications*. By leveraging state-of-the-art DL techniques, this work contributes to the growing field of AI-driven remote sensing, paving the way for broader applications in satellite data processing and interpretation. Moreover, the proposed methods, which emphasize rapid and accurate data retrieval, could be adapted for other Earth-observing and space missions, offering a scalable framework for future NASA AOS missions.

1.5 IMPLEMENTATION STRATEGY AND MILESTONE SCHEDULE

1.5.1 OBJECTIVE 1: NEW DL MODELS FOR SATELLITE DATA RETRIEVAL

In **Objective 1**, the main task is to develop ***new*** DL models to replace the time-consuming calculation in the conventional data retrieval algorithm, e.g., MAPP [3]. Specifically, the data retrieval starts with initial estimates of aerosol and ocean parameters. Then, we iteratively find the solution via minimizing a cost function, defined as:

$$\begin{aligned}\chi^2(\mathbf{x}) &= \Phi(\mathbf{x})_{data} + \Phi(\mathbf{x})_{prior} \\ &= \frac{1}{2}(f(\mathbf{x}) - \mathbf{y})^T \mathbf{S}_\epsilon^{-1}(f(\mathbf{x}) - \mathbf{y}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1}(\mathbf{x} - \mathbf{x}_a), \qquad (1)\end{aligned}$$

where $\mathbf{x}$ is the vector containing aerosol and ocean parameters; $\mathbf{y}$ is the sensor measurement vector; f is the forward function that maps state vector $\mathbf{x}$ into sensor measurements $\mathbf{y}$; $\mathbf{x}_a$ is the priori state estimate; $\mathbf{S}_\epsilon$ and $\mathbf{S}_a$ are tuning matrices to adjust the weights of latest sensor measurements and historical parameter estimates, respectively. The iteration stops when the difference between $f(\mathbf{x})$ and $\mathbf{y}$ is within a pre-defined error limit.

In MAPP [3], the forward function f was VRT calculation, which is a time-consuming process. ***Our goal*** in Objective 1 is to develop DL models to replace the VRT. Thus, the input for the DL model will be state vector **x,** and the output will be sensor measurements **y.** Then, we can follow the conventional MAPP steps to minimize Eqn. 1 to iteratively refine the state vector $\mathbf{x}$ to get the aerosol and ocean properties.

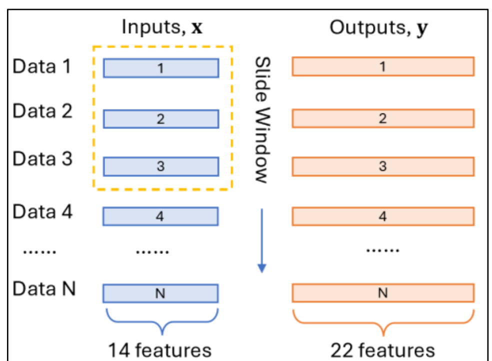

Figure 4. The training dataset. A Slide Window is applied on the input vectors to provide context information to DL models

Training Data Processing: The dataset used to train the proposed DL models was obtained during our prior work and provided by the NASA collaborator of this project. As shown in **Figure 4**, this dataset can be viewed as a table, where each row represents an individual data instance, and columns consist of input and output vectors. The input vector contains a collection of aerosol and ocean parameters, represented by 14 features, and the output vector comprises raw satellite measurements, represented by 22 features. The output was generated from pre-run VRT calculations. The total size of the training data is ***2 million***, and the size of the testing dataset (with the same input/output configuration as the training dataset) is ***200K***. We applied the ***Slide Window*** to the dataset to include multiple data instances. This allows the DL models to leverage contextual input information when generating output predictions. The sliding window scans the entire dataset by shifting over the data instances sequentially. The size of sliding window is a tuning parameter, which can be determined based on prediction results on the testing dataset.

Design of New DL Models: In this project, we will develop two new DL models, including ***CNN*** and ***RNN***. As presented in **Figure 5**, proposed CNN is designed to generate the output vector **y** based on multiple input vectors **x** within the ***slide window***. The CNN model begins with an input layer that accepts the structured slide window sequence data as a matrix. This input is then passed through multiple convolutional and max pooling layers. Each convolutional layer extracts increasingly abstract patterns, while the pooling layers provide efficient dimensionality reduction and prevent overfitting. The output of the final pooling layer is flattened into a one-dimensional vector and passed to fully connected layers, which interpret the extracted features and map them to the final output vector.

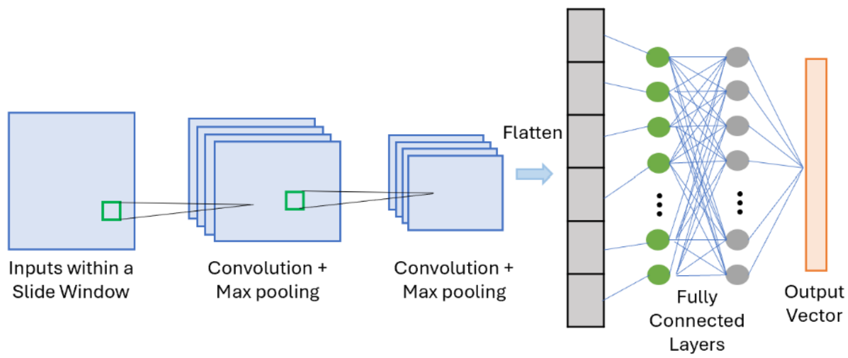

Figure 5. The proposed CNN architecture for the satellite data retrieval.

In the proposed CNN model architecture, we will determine the optimal model parameters via evaluating the model on the testing dataset. Tuning parameters include the number of hidden layers and the number of nodes on one layer. These experimental trials will also provide insights to other researchers in choosing the optimal model structure for satellite data retrieval.

The proposed RNN structure is presented in **Figure 6**. The core unit is the Long Short-Term Memory (LSTM) cell, which was designed to capture temporal dependencies in time series data [18]. The RNN model begins with an input layer that processes sequences of input vectors within the slide window. These sequences are passed through multiple LSTM layers, which use memory cells to effectively retain long-term dependencies and extract temporal patterns from the data. To reduce overfitting, dropout layers are incorporated, randomly deactivating certain neurons during training. The output from the LSTM layers is then passed to a fully connected layer, which combines the extracted features to predict the target output vector.

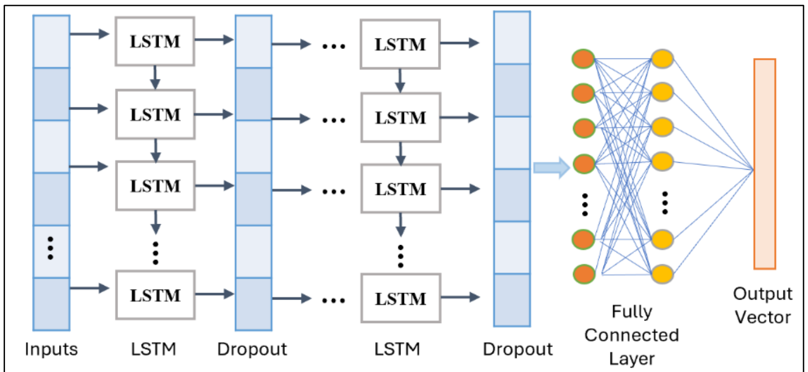

Figure 6. The proposed RNN architecture for satellite data retrieval.

Like the CNN model, we will obtain optimal model parameter values based on experimental trials on the testing dataset. These model parameters include the number of LSTM layers, the number of nodes on one layer, and the size of slide window.

1.5.2 OBJECTIVE 2: INNOVATIVE DL TRAINING ALGORITHM

In **Objective 2**, the ***main task*** is to train the proposed DL Models to learn the satellite data retrieval. We will incorporate with 2 DL training algorithms, including ***supervised learning*** and ***deep reinforcement learning***, while the first one trains DL models with given input/output pairs, the second one focuses on training DL models via trial-and-error experiences, to let DL models learn the input/output mapping automatically.

Training DL Models with Supervised Learning: The core of supervised learning is to let the DL model learn the input/output mapping relationship with provided input/output data [19, 20]. In this project, given the training data provided by the NASA collaborator has already included input/output pairs, supervised learning is ideal for training the proposed DL models. Within the supervised learning framework, the DL models will be trained to estimate the output values $\hat{\mathbf{y}}$ and be compared with the ground truth values $\mathbf{y}$ (provided in the training dataset). Then, the objective function, e.g., the mean square error (MSE), will be calculated to measure the model prediction accuracy, via:

$$MSE = \frac{1}{N}(\hat{\mathbf{y}} - \mathbf{y})^2,$$

where N is the number of input-output pairs in the training dataset. The ***training goal*** is to update DL model parameters to minimize the MSE.

Training DL Models with Deep Reinforcement Learning: Deep Reinforcement Learning has gained attention recently, due to its ability to enable models to learn optimal behaviors through trial and error, interacting with a dynamic environment to achieve specific objectives [21]. This method leverages a reward system where actions taken by the DL model result in rewards or penalties based on their effectiveness. It is particularly effective in situations *where the desired output or correct answer is not explicitly known, allowing the model to explore and discover strategies that yield the best outcomes*.

Under the deep reinforcement learning framework, the ***core*** is to define a reward function that encourages the DL model to produce the desired output. In our task, the data retrieval objective is to minimize the ***objective function*** specified in **Eqn.** 1. Thus, the goal of the DL model is to generate optimal values to minimize the objective function. We can define the reward function as $-\chi^2(\mathbf{x})$ since the DL model aims to maximize the reward function in the training process. **Figure 7** presents the data flow for the proposed deep reinforcement learning algorithm. The training process starts with feeding input vectors (within the slide window) to the DL model to calculate the output vector $\mathbf{y}$. Then, the output vector will be fed into **Eqn.** 1 to compute the objective function, i.e., $\chi^2(\mathbf{x})$. Then, we update the parameters in DL models to maximize $-\chi^2(\mathbf{x})$. In this process, $-\chi^2(\mathbf{x})$ is defined as the reward function. This strategy enables the DL models to adaptively improve their performance to accurately predict aerosol and ocean parameters from satellite data. Compared to

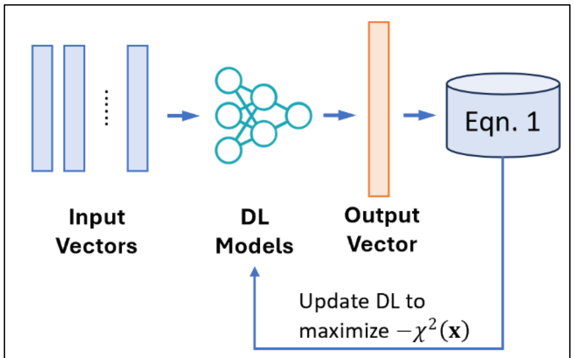

Figure 7. The data flow for the proposed deep reinforcement learning training algorithm

the supervised learning, this training algorithm ***does not need ground truth values***, which eliminates the need of pre-running VRT calculations to generate ground truth values.

Computational Hardware: The training of the proposed DL models can be completed at the PI's lab, which is equipped with a workstation for training DL models. The workstation is equipped with Intel Core 13th i9 CPU, Nvidia RTX 3090 GPU, and 64 GB RAM. For training a 4-layer DL Model with 2 million training data pairs, the training time is approximately 2 hours.

DL Model Evaluation: After training, we will evaluate the performance of the proposed DL models with PACE satellite data. Specifically, the NASA expert, Dr. Stamnes, will provide the PI with the real-world PACE observation data. Then, the PI will pre-process it to fit the designed DL models. We will use the DL model results on the 200K testing dataset to direct the selection of optimal models, then, we will conduct the data retrieval process to extract aerosol and ocean parameters from raw sensor observations. We will also conduct a comparative analysis of the DL models against conventional data retrieval algorithms. The ***key metrics*** for this comparison will include estimation accuracy, query time, and calculation complexity.

1.5.3 MEASURABLE OUTCOMES, TIMELINE, AND KEY MILESTONES

Measurable Outcomes: The expected outcomes of this project include several key deliverables that are presented on the table below:

Project Outcomes	Evaluation Criterion
O1: The development of DL-based models for satellite data retrieval.	The developed model should reach high prediction accuracy (>**95%**) in the testing dataset.
O2: The design and implementation of DL training algorithm.	The training time for using the proposed training algorithm will be recorded and compared.
O3: Peer-reviewed publications, co-authored by PI and NASA expert	The number of published peer-reviewed paper > **1**
O4: Presentations of project findings at relevant conferences	The number of presentations at research conferences and research seminars > **1**
O5: Submissions of future federal proposals	The number of submitted federal proposals > **3**

A detailed paper and proposal development plan is presented in Section 1.8.

Timeline and Key Milestones: The table below presents the proposed project timeline (12 months), where key ***milestones*** and ***project outcomes*** are identified after each research objective.

Objectives	**Tasks**	**2025**		**2026**					
		Q4		Q1		Q2		Q4	
1	Training Data Preparation and Processing								
	Design Convolutional Neural Networks								
	Design Recurrent Neural Networks								
Milestone 1: Obtain Two DL Models for Sensor Data Retrieval						**O1**			
2	Supervise Learning Training Algorithm Design								
	Deep Reinforcement Leraning Training Algorithm Design								
	DL Model Training and Evaluation								
Milestone 2: Trained DL Models Achieves High Prediction Accuracy (>95%								**O2**	
Paper Writing and Report to NASA						**Q4**			**Q5**