Preview of Award 2209711 - Annual Project Report

Cover

Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Award or Other Identifying Number Assigned by Agency:	2209711
Project Title:	Frameworks: Large Scale Atmospheric Research Using an Integrated WRF Modeling, Visualization, and Verification Container Framework (I-WRF)
PD/PI Name:	Richard Knepper, Principal Investigator Sue E Haupt, Co-Principal Investigator Jared A Lee, Co-Principal Investigator Sara C Pryor, Co-Principal Investigator
Recipient Organization:	Cornell University
Project/Grant Period:	08/01/2022 - 07/31/2026
Reporting Period:	08/01/2023 - 07/31/2024
Submitting Official (if other than PD\PI):	N/A
Submission Date:	N/A
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	N/A

Accomplishments

*** What are the major goals of the project?**

The I-WRF project, part of the NSF Cyberinfrastructure for Sustained Scientific Innovation program, aims to establish a framework for application containers that streamline the deployment of the WRF numerical weather prediction model alongside the METplus validation tools across diverse computing resources, requiring minimal installation effort. This initiative will support three primary science use cases focused on assessing the combined impacts of environmental changes and climate variability on critical outcomes. Additionally, I-WRF seeks to broaden outreach efforts by simplifying demonstrations, training activities, and fostering interest among potential atmospheric scientists.

Major goals of the I-WRF project include:

- Develop an integrated, containerized framework for the Weather Research and Forecasting (WRF) model, incorporating a new multi-node WRF container, optimized Model Evaluation Tools (METplus) container, and visualization capabilities that enhance research productivity.
- Enable multi-node simulations capable of conducting research-grade applications over large spatial domains with high resolution.
- Simplify usability to broaden accessibility, enabling researchers from fields such as environmental engineering, transportation, civil engineering, air quality policy, agriculture, and urban planning to conduct their own modeling activities and interact conveniently with results.
- Establish a container framework where users do not need to individually configure and deploy components. Containers will encompass entire environments and necessary workflows for collaborative and complex tasks.
- Validate and test the integrated framework and container features on state-of-the-art parallel HPC and cloud platforms, focusing on scalable use cases like the impact of renewable energy evolution in a changing climate, land use effects on severe weather events, and the relationship between air quality and health outcomes.
- Utilize these containers as educational tools to introduce students to numerical atmospheric simulations and output evaluation through WRF and METplus tutorials and classroom materials.

• Promote awareness of the I-WRF project and its framework capabilities to empower a larger cohort of next-generation researchers with practical tools for atmospheric sciences research.

These goals collectively aim to advance the accessibility, usability, and educational impact of WRF and METplus tools, fostering broader engagement and innovation in atmospheric science research.

*** What was accomplished under these goals and objectives (you must provide information for at least one of the 4 categories below)?**

Major Activities: Below each objective is a summary of what was accomplished during PY2 of the 4-year project.

Specific Objectives: **Build an Integrated Multi-Node WRF and METplus Framework**

The collaborative effort between the Cornell University and NSF NCAR tech teams has successfully completed the initial development phase of the Integrated Weather Research and Forecasting model (I-WRF) framework (version 0.1.0). This framework enables simulations by integrating WRF and METplus verification containers, overcoming significant engineering challenges through seamless communication between native WRF outputs and MET tools via containerization. Efficiency was enhanced by streamlining container operations, removing redundant software components, testing preliminary visualization outputs, and determining the optimal storage solution for container images.

Using the 0.1.0 I-WRF framework containers and Docker engine runtime, we performed single-node Hurricane Matthew simulations across various platforms, including Jetstream2, Amazon Web Services (AWS), Cornell's Red Cloud, and a Windows Intel desktop. Hurricane Sandy simulations were conducted on Red Cloud and a Mac laptop. We chose Hurricane Matthew as an introductory case for testing the I-WRF components because it is the first test case in the WRF Online Tutorial, with input data readily available from that tutorial. Additionally, we executed the I-WRF containers on Derecho, a new supercomputer located at the NSF NCAR-Wyoming Supercomputing Center. Derecho's role is crucial in evaluating the scalability of I-WRF containers through storyline simulations of extreme meteorological events (Science Use Case 1). In the coming months, we will resolve remaining Message Passing Interface (MPI) issues to enable multi-node capability.

While the tech team advances the framework, use case scientists are concurrently preparing their use cases for I-WRF testing. For example, the Land Use/Land Cover (LULC) team is studying the impact of urban land cover on hydrological events like severe thunderstorms that cause substantial economic losses. WRF simulations were conducted at 1-km grid spacing using ERA5 reanalyses and High-Resolution Rapid Refresh (HRRR) analyses for initial and lateral boundary conditions. The simulations were assessed for fidelity, and configurations were adjusted accordingly. The simulations were then perturbed to incorporate future projections of LULC. Detailed results of these simulations were published by I-WRF Postdoc Xin Zhou, et al. (Journal of Geophysical Research-Atmospheres, May 2024, https://doi.org/10.1029/2023JD039972). The configuration and input data from this study will be used for future I-WRF simulations.

An objective of this and other use cases is to compare simulations on native HPC systems and within containers on the same system, aiming to identify opportunities for container optimization. These cases will serve as exemplars for the research community.

Enhance NCAR Training

Documentation of the Hurricane Matthew container simulations on Jetstream2 and other platforms is complete, including the development and testing of user-friendly instructions for ease of use and reproducibility. These materials are set to become integral to future WRF tutorials and laptop training sessions conducted by NSF NCAR. Currently, about 50% of students encounter difficulties configuring machines for WRF training sessions. The introduction of turnkey I-WRF containers is expected to significantly reduce educational barriers, fostering increased student recruitment and addressing diversity gaps.

With these advancements, students will be able to initiate WRF simulations independently, without extensive support from cyberinfrastructure or teaching staff. This development will lower entry barriers for institutions with limited resources, broadening access to computational tools and knowledge, and empower students to accelerate their work autonomously.

Support Multi-Node Simulations

Efforts are ongoing to support large-scale, multi-node simulations with diverse inputs. Execution scripts have been developed for a LULC use case linked to a flagship project of the World Climate Research Programme. The next use case, focusing on climate change impacts on wind and solar resources, presents different computational challenges requiring higher core and node counts.

WRF containers will support multi-node integration during the summer of 2024, a significant advancement enabling scalable, container-based modeling. This breakthrough will facilitate faster application deployment, seamless data analysis, and visualization using containerized Python scripts. The platform's portability across desktop, cloud, and supercomputing environments enhances research flexibility and promotes community-driven container and scientific application development.

Facilitate Ease of Use to Enable a Wider Range of Researchers

To enhance accessibility, Cornell and NSF NCAR I-WRF developers are actively documenting progress on GitHub. This documentation, along with valuable lessons learned, form the basis of the I-WRF User Guide under development for the user community. Currently hosted on Read the Docs, managed through our GitHub repository, and linked from the I-WRF project website (https://i-wrf.org/), the guide provides detailed instructions for running version 0.1.0 on Jetstream2, Red Cloud, and a Windows desktop or laptop. Efforts are underway to provide guidance on deploying both current and future versions on HPC systems like Derecho.

The User Guide will include Apptainer documentation and consistent command-line instructions, as well as generic execution scripts for various use cases, such as LULC feedback to extreme weather, climate change impacts on renewable resources, and urban air quality. These adaptable templates will expediate application development by atmospheric scientists and research software engineers.

Increase Project Awareness and Community Guidance

To raise awareness of I-WRF container project achievements, challenges, and software engineering advancements, we presented at six conferences: the 2023 NSF Cyberinfrastructure for Sustained Scientific Innovation PI Meeting, 2024 American

Meteorological Society Annual Meeting, Spring 2024 Coalition for Academic Scientific Computation Meeting, 2024 Minority Serving-Cyberinfrastructure Consortium (MS-CC) Annual Meeting, 2024 Energy Systems Integration Group Forecasting & Markets Workshop, and the 2024 International Conference on Digital Government Research. For presentations and publications, visit https://i-wrf.org/about/publications.

These engagements have expanded potential use cases and fostered new collaborations. For instance, following the MS-CC presentation, we met with Rae Quadara, Assistant Director of the MS-CC Climate Science Program, to explore synergies between I-WRF and MS-CC initiatives. MS-CC aims to enhance the use of cyberinfrastructure in climate science research at Historically Black Colleges and Universities (HBCUs) and Tribal Colleges and Universities (TCUs). We plan to pilot our Hurricane Matthew I-WRF tutorial with HBCU/TCU students during an MS-CC workshop to gather feedback on its effectiveness.

Significant Results:

Key outcomes or Other achievements:

*** What opportunities for training and professional development has the project provided?**

How-To Documentation & Training

I-WRF containers and corresponding documentation are publicly accessible via the project website (https://i-wrf.org/), the NCAR/i-wrf GitHub site (https://github.com/NCAR/i-wrf), and the ncar/iwrf Docker Hub container registry (https://hub.docker.com/r/ncar/iwrf/tags).

For detailed instructions on running Hurricane Matthew simulations using I-WRF version 0.1.0 on platforms like Jetstream2, please refer to the how-to documentation for Jetstream2 available at https://i-wrf.readthedocs.io/en/latest/Users_Guide/matthewjetstream.html#matthewjetstream.

The Cornell team is creating execution scripts that enable the containers to operate on targeted execution environments, along with testing and integration suites that will optimize the application containers for training tutorials.

The NSF NCAR team will provide long-term sustainable support for compiling and configuring the containers, as well as post-processing scripts that facilitate seamless data transfer between containers without modification.

Knowledge Sharing & Professional Development

Expertise was shared between NSF NCAR and Cornell, as well as among use case scientists, during our I-WRF PI meetings. Similarly, knowledge exchange occurred between subject matter experts and engineers on the tech teams during our I-WRF Tech Team meetings. PI and Tech Team meetings were held monthly to ensure consistent cross-training and knowledge dissemination. Our GitHub repository serves as an effective tool for tracking development issues and facilitating timely communications and issue resolution. In-depth discussions between meetings were conducted to address specific technology implementation challenges and share lessons learned.

Additionally, an undergraduate student and a postdoctoral fellow participated in the project’s software engineering activities and meetings, enhancing their technical and professional development skills in research methodologies, scientific writing, and communications.

*** Have the results been disseminated to communities of interest? If so, please provide details.**

Scientific Meetings, Publications, and Conferences

PI Rich Knepper presented “I-WRF: Containerized Framework for Weather Modeling, Verification, and Visualization” at the Minority Serving-Cyberinfrastructure Consortium Annual Meeting, held May 29-31, 2024, in Washington, DC. This presentation was also delivered at the International Conference on Digital Government Research, hosted by National Taiwan University from June 11-14, 2024. Additionally, Knepper provided an I-WRF Update at the Spring Coalition for Academic Scientific Computation Meeting held March 12-14, 2024 in Arlington, VA, and presented a scientific poster on “Large Scale Atmospheric Research Using an Integrated WRF Modeling, Visualization, and Verification Framework” at the NSF Cyberinfrastructure for Sustained Scientific Innovation PI Meeting, held September 26-27, 2023 in Houston, Texas.

Co-PIs Jared A. Lee and Sara C. Pryor also delivered presentations. Lee presented the “Status of Climate Change Projections on Wind & Solar Resources” at the Energy Systems Integration Group (ESIG) Forecasting & Markets Workshop on June 13, 2024, in Salt Lake City, Utah. Pryor presented “CSSI: Frameworks: Large Scale Atmospheric Research Using an Integrated WRF Modeling, Visualization, and Verification Framework (I-WRF)” at the 104th Annual Meeting of the American Meteorological Society, held from January 28 to February 1, 2024, in Baltimore, MD.

I-WRF Postdoctoral Fellow Xin Zhou served as lead author on a publication in the Journal of Geophysical Research–Atmospheres titled “Urban Effect on Precipitation and Deep Convective Systems over Dallas-Fort Worth,” published May 14, 2024.

Additionally, the I-WRF project was featured at Cornell’s SC Conference exhibit, held November 12-17, 2023, in Denver, CO. It was also part of a scientific poster presented at a Cornell Emerging Tech Dialogues event held May 29, 2024, on the Ithaca, NY campus.

For more information on these and other outreach activities, please visit https://i-wrf.org/about/publications. Additional outreach efforts include news releases such as “Knepper presents advances in weather modeling technology at the International Conference on Digital Government Research” (available at https://i-wrf.org/about/DSCO%20I-WRF%20News.pdf) and an “Introduction to I-WRF Containers” YouTube video.

*** What do you plan to do during the next reporting period to accomplish the goals?**

The primary objective for the upcoming project year is the release of incremental versions of I-WRF. These releases aim to advance scientific research by incorporating feedback from researchers and cyberinfrastructure professionals to enhance the performance of the I-WRF container framework. Insights gained will guide NSF NCAR and Cornell development teams in prioritizing features that deliver maximum value to atmospheric science researchers, incorporating best practices for configuring and deploying the containers. This effort will facilitate more efficient utilization of advanced high performance computing (HPC) and cloud computing resources supported by the NSF, as well as expand the use of WRF on local computational resources, including desktops and laptops.

Our specific focus will be on improving user experience by providing easily adaptable templates for early career scientists, graduate students, and newcomers to atmospheric research, thereby expanding the talent pool. Additionally, enhancements to the WRF Docker Hub image will allow users to supply their own files for building, aimed at lowering adoption barriers and fostering a larger community of users. Further improvements in ease of use will enable a broader range of researchers in fields such as environmental engineering, transportation, civil engineering, air quality policy, agriculture, and urban planning to conduct their own modeling activities and interact conveniently with the results.

I-WRF version 0.2.0 will focus on initial deployment of visualization containers supporting the Hurricane Matthew test case. The visualization container will house Python scripts (and the Python environments required to run them) to generate plots of the WRF model output and the validation output from METplus that were produced by the WRF and METplus containers, respectively.

Version 0.3.0 will include an option to run the end-to-end I-WRF container system for the LULC use case that was described previously. The addition of a second use case to the release will also necessitate some abstraction of the run scripts and configuration options from what is available in the v0.2.0 release, to maintain a system that is as turnkey and easy-to-use as possible.

Version 0.4.0 will enable significant applications, including the study of climate change impacts on wind and solar energy production (Science Use Case 2: Sara C. Pryor, Sue Ellen Haupt & Jared A. Lee). The computational demands of such simulations are substantial but manageable within the multi-node I-WRF containers. Our objective is to analyze variations in the frequency and intensity of regional wind and solar production patterns, including droughts and periods of high production. We will employ the WRF-Solar-Wind model with a 4-km grid spacing across the contiguous United States (CONUS) to downscale MPI climate simulations from 2015–2024, validating the first 9–10 years using the METplus container. These findings are expected to enhance understanding of climate impacts on renewable energy resources, providing crucial insights for grid system planners.

Version 0.5.0, to be completed in PY4, will explore other use cases to test the scalability of I-WRF, such as Land Use/Land Cover research and containerizing WRF-Chem. WRF coupled with Chemistry (WRF-Chem) has not yet been containerized and has a relatively limited user base, partly due to the added complexity in workflow related to initializing chemical species and preparing emission files. Our goal is to integrate tools that streamline the WRF-Chem workflow and overcome bottlenecks. These simulations will be computationally intensive, particularly with the chemistry component doubling the computational load, and will present technical challenges requiring complex input and validation of data streams. Significant advancements in visualization tools beyond current capabilities will be necessary.

An essential goal of using WRF-Chem within a container framework is to quantify how climate change may counteract improvements in air quality resulting from emission control measures, potentially leading to more severe periods of degraded air quality in the Northeast corridor. By the time we complete this version, we will be done with our major new development deliverables, at which time this will become version 1.0.0.

All upcoming versions of I-WRF releases will undergo testing and validation on the Derecho supercomputer and other parallel HPC and cloud platforms. We aim to enhance our containerized systems to closely adhere to HPC center best practices and recommended container security measures. Unnecessary software elements used during development will be reduced. Furthermore, we will evaluate the best approach for assessing the correct operation of newly created containers, such as integrating GitHub code version control with GitHub Actions' automated test system pipeline.

On the educational forefront, we plan to use I-WRF containers to introduce students to numerical atmospheric simulations. We plan to feature these containers prominently in WRF and MET tutorials at NSF NCAR. We will collaborate closely with NSF NCAR instructors to integrate these containers into workshop curricula. Furthermore, we will inform other institutions, including Metropolitan State University in Denver, Central Michigan University, and others, about their availability.

Pending the success of piloting the I-WRF Hurricane Matthew tutorial with the Climate Science Program of the Minority Serving-Cyberinfrastructure Consortium, we plan to incorporate this tutorial into future MS-CC workshops. These workshops are designed to engage students from Historically Black Colleges and Universities (HBCUs) and Tribal Colleges and Universities (TCUs).

The Cornell and NSF NCAR project teams will actively respond to calls for participation from major conferences such as the American Meteorological Society, American Geophysical Union, Energy Systems conferences, and Cyberinfrastructure conferences like the Practice and Experience in Advanced Research Computing (PEARC) and Supercomputing Conferences (SC).

Use case scientists will pursue publications in leading journals in the Atmospheric Sciences and related fields. Additionally, we plan to present the impact of I-WRF tutorials on HBCUs and TCUs at the 2025 Minority Serving-Cyberinfrastructure Consortium Annual Meeting in Washington, DC.

The technical plan for our next project year will be reviewed during an upcoming I-WRF Advisory Board meeting and advice will be solicited on implementation and strategies to further increase project awareness and impact.

All capabilities will continue to be documented and publicly available in the I-WRF User Guide accessible from both the I-WRF GitHub site and the I-WRF website. Docker Hub will be updated with new I-WRF container images.

Products

Books

Book Chapters

Inventions

Journals or Juried Conference Papers
View all journal publications currently available in the NSF Public Access Repository for this award.

The results in the NSF Public Access Repository will include a comprehensive listing of all journal publications recorded to date that are associated with this award.

Zhou, Xin and Letson, Fred and Crippa, Paola and Pryor, Sara C. (2024). Urban Effect on Precipitation and Deep Convective Systems Over Dallas-Fort Worth. *Journal of Geophysical Research: Atmospheres*. 129 (10) . Status = Added in NSF-PAR

Federal Government's License = Acknowledged. (Completed by Knepper, Richard on 07/29/2024) Full text Citation details

Richard Knepper, Sara C. Pryor, Bennett Wineholt, Melissa Bukovsky, and Jared Lee. 2023. The I-WRF Framework: Containerized Weather Modeling, Validation, and Verification. In Practice and Experience in Advanced Research Computing 2023. ACM, New York, NY, USA,. Status = PUBLISHED.

Licenses

Other Conference Presentations / Papers
Richard Knepper (2023). *CSSI: Frameworks: Large Scale Atmospheric Research Using an Integrated WRF Modeling, Visualization, and Verification Framework (I-WRF)*. 2023 NSF CSSI PI Meeting. Houston, TX. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Richard Knepper (2024). *I-WRF Update*. Spring 2024 Coalition for Academic Scientific Computation Meeting. Arlington, VA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Richard Knepper (2024). *I-WRF: Containerized Framework for Weather Modeling, Verification, and Visualization*. 2024 International Conference on Digital Government Research. Taipei, Taiwan. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Richard Knepper (2024). *I-WRF: Containerized Framework for Weather Modeling, Verification, and Visualization*. 2024 Minority Serving-Cyberinfrastructure Consortium Annual Meeting. Washington, DC. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Rich Knepper, Sara C. Pryor, Xin Zhou, Jared A. Lee, Sue Ellen Haupt (2024). *I-WRF: Containerized WRF, MET, and METplus for Portability, Scaling, and Outreach*. 104th Annual Meeting of the American Meteorological Society. Baltimore, MD. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Jared A. Lee (2024). *Status of Climate Change Projections on Wind & Solar Resources*. 2024 Energy Systems Integration Group Forecasting & Markets Workshop. Salt Lake City, UT. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Other Products
Audio or Video Products *I-WRF Framework: Containerized Weather Modeling, Validation, and Verification (YouTube) – a brief introduction to I-WRF and Hurricane Matthew demo: https://www.youtube.com/watch?v=UUSa1iRJ8wg*

Other Publications

Patent Applications

Technologies or Techniques
The I-WRF project team developed the following technologies and techniques: • I-WRF Version 0.1.0 • Running I-WRF on Jetstream2 with Hurricane Matthew Data: https://i-wrf.readthedocs.io/en/latest/Users_Guide/

matthewjetstream.html#matthewjetstream • Running I-WRF on Red Cloud with Hurricane Matthew Data: https://i-wrf--60.org.readthedocs.build/en/60/Users_Guide/matthewredcloud.html#matthewredcloud • Running I-WRF on Windows (Intel CPU) with Hurricane Matthew Data: https://i-wrf--60.org.readthedocs.build/en/60/Users_Guide/matthewwindows.html#matthewwindows

Thesis/Dissertations

Websites or Other Internet Sites
NCAR/i-wrf github
https://github.com/NCAR/i-wrf

“NCAR/i-wrf” is the I-WRF GitHub repository under development.

ncar/iwrf dockerhub
https://hub.docker.com/r/ncar/iwrf/tags

“ncar/iwrf” is the Docker Hub where I-WRF images are stored.

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Knepper, Richard	PD/PI	1
Haupt, Sue	Co PD/PI	1
Lee, Jared	Co PD/PI	2
Pryor, Sara	Co PD/PI	1

Full details of individuals who have worked on the project:

Richard Knepper
Email: rich.knepper@cornell.edu
Most Senior Project Role: PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: Programmatic oversight of the I-WRF project ensuring deliverables outlined in the proposal are met on schedule.

Funding Support: No funding support from other projects used for this award.

Change in active other support: No

International Collaboration: No
International Travel: No

Sue E Haupt
Email: haupt@ucar.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: Oversees all science use cases and is co-developer of the Renewable Energy use case.

Funding Support: No funding support from other projects used for this award.

Change in active other support: No

International Collaboration: No
International Travel: No

Jared A Lee
Email: jaredlee@ucar.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 2

Contribution to the Project: Coordinates the operations of the NCAR technical team and is the general project manager for WRF development.

Funding Support: No funding support from other projects used for this award.

Change in active other support: No

International Collaboration: No
International Travel: No

Sara C Pryor
Email: sp2279@cornell.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: Scientific guidance, management of a post-doctoral researchers, and interface with the WRF user community among researchers to provide information about the I-WRF Framework for adopters.

Funding Support: No funding support from other projects used for this award.

Change in active other support: No

International Collaboration: No
International Travel: No

What other organizations have been involved as partners?
Nothing to report.

Were other collaborators or contacts involved? If so, please provide details.
Nothing to report

Impacts

What is the impact on the development of the principal discipline(s) of the project?

The project team is actively developing, testing, and implementing an integrated multi-container framework for the WRF model. This initiative marks a significant milestone by enabling multi-node containerized simulations equipped with verification and visualization capabilities. This advancement aims to streamline the utilization of WRF for atmospheric researchers, democratizing access across various platforms—from desktops to cloud infrastructures and supercomputers.

The urgency for enhanced climate simulations is underscored by global events like the UN Climate Change Conference and the NSF Engineering Visioning Alliance on The Role of Engineering in Addressing Climate Change. These forums highlight the critical need for comprehensive simulations of future climate scenarios to bolster climate resilience within the U.S. economy. Our project addresses these imperatives through focused science case studies and importantly, it empowers a broader community of researchers to conduct diverse simulations. This broader engagement is essential for delivering actionable insights to stakeholders, exploring uncertainties, and driving fundamental advancements in climate science.

What is the impact on other disciplines?

I-WRF's integrated capabilities and user-friendly design will empower researchers across diverse fields to independently conduct modeling activities and seamlessly interact with their findings. By employing a containerized framework, the system lowers the barriers for early career scientists in various disciplines, facilitating easier adoption of numerical simulations and evaluation processes. This accessibility eliminates the prerequisite of Linux expertise previously needed to engage with the WRF system tutorials, thus democratizing access for new users to explore its capabilities.

Furthermore, the standardized software environments facilitate reproducible results, fostering collaboration among distributed domain experts and minimizing variability in outcomes due to different computing architectures. Ultimately, these containerized systems promote excellence in science and engineering across disciplines while enhancing inclusivity by enabling a broader spectrum of individuals to participate in simulations using the WRF model and METplus verification system.

What is the impact on the development of human resources?

The team aims to nurture students and early career researchers by immersing them in both the technologies and research challenges involved. This initiative supports the cultivation of new scholars and technologists through training programs offered at NSF NCAR and partner institutions, alongside outreach activities within professional networks. Additionally, upon release of I-WRF v0.3.0/v0.4.0, we will pursue hosting short courses at the American Meteorological Society (AMS) Annual Meetings. These efforts will empower a greater number of emerging researchers in atmospheric science and promote best practices in compilation, configuration, and cyberinfrastructure deployment.

The project is supporting postdoctoral fellows, while also encouraging participation from Cornell's Masters of Engineering students and undergraduate students.

What was the impact on teaching and educational experiences?

NSF NCAR tutorials will utilize I-WRF containers to enhance the training of a wider range of graduate students and early career researchers in the atmospheric sciences, thereby bolstering the science and engineering (S&E) workforce. The team also intends to draw from previous collaborations and establish direct partnerships with institutions like Metropolitan State University of Denver (MSU Denver), Central Michigan University (CMU), and others to integrate the I-WRF containerized modeling system into their course curricula.

To further extend educational opportunities, we will develop and maintain an on-demand I-WRF Virtual Workshop aimed at democratizing learning access, particularly for institutions with limited resources.

What is the impact on physical resources that form infrastructure?

The I-WRF project focuses on enhancing the portability of the Weather Research and Forecasting (WRF) model across diverse cyberinfrastructures, including desktops, cloud platforms, and High Performance Computing (HPC) resources. Utilizing pre-compiled and tested Docker images, students can streamline setup times on desktops and small-scale cloud deployments. For researchers, productivity gains on HPC and cloud platforms will be achieved through tailored implementations for launching WRF jobs across different clusters and cloud providers.

To achieve this, we plan to adopt Python as the primary invocation layer, leveraging the Signac framework to generate submission scripts for Slurm or PBS schedulers on HPC systems. For cloud resources, we will employ Terraform Python CDKTF for resource provisioning scripts, while local desktop execution will utilize the Docker Engine Python interface, docker-py.

Our primary focus includes HPC environments supporting Apptainer containers and CPU-based cloud systems and desktops compatible with Docker container runtimes. This strategy aligns with current capabilities of WRF MPI Fortran code compilation, which is optimized for CPU architectures. While our approach ensures efficient performance through optimized library availability and minimal runtime overhead, it acknowledges potential limitations in supporting specialized hardware or constrained container environments.

What is the impact on institutional resources that form infrastructure?

Enhancing the portability of WRF containers expands institutional options for running WRF simulations. With improved training, institutions can reduce the resources required to support researchers using WRF. This advancement enables researchers to initiate multi-node WRF simulations independently, reducing reliance on institutional staff. The flexible containerized workflow allows researchers to leverage a wide range of cyberinfrastructure (CI) resources, including HPC systems and cloud environments, with minimal demands on CI providers.

What is the impact on information resources that form infrastructure?

I-WRF use case scripts, build files, and related materials will be distributed alongside sample data and storage configurations.

What is the impact on technology transfer?

Since the technologies developed in this project are open source, there is no need for technology transfer licensing, patent applications, or similar processes.

What is the impact on society beyond science and technology?

The I-WRF project aims to advance significant research that directly affects the daily lives of U.S. citizens, agriculture, energy production, and public health. It will achieve this by facilitating the execution of extensive simulations and by enhancing accessibility to computational methods in atmospheric research for a broader spectrum of students. Key studies will examine the societal impacts of climate variability and extreme weather events, assess the influence of climate change on wind and solar energy resources, and investigate how shifts in atmospheric dynamics and emissions related to global climate change might potentially reverse recent gains in air quality and the reduction of health risks.

What percentage of the award's budget was spent in a foreign country?
Nothing to report.

Changes/Problems

Changes in approach and reason for change
Nothing to report.

Actual or Anticipated problems or delays and actions or plans to resolve them
Nothing to report.

Changes that have a significant impact on expenditures
Nothing to report.

Significant changes in use or care of human subjects
Nothing to report.

Significant changes in use or care of vertebrate animals
Nothing to report.

Significant changes in use or care of biohazards
Nothing to report.

Change in primary performance site location

Nothing to report.