UFS-R2O Progress & Year 3 Plan

Modeling Infrastructure Development Cross Cutting Team

6&7 December 2021

EMC, PSL, GSL, CSL, NSSL, ARL, NESDIS

Modeling Infrastructure - Description and Goal

The Modeling Infrastructure sub-project develops, tests, and supports core modeling capabilities required by the UFS Application Teams. The scope of work includes:

- Develop and support workflow(s) - GMU, EMC, DTC
- Develop and support inter-component coupling - NCAR/ESMF, EMC
- Develop and support intra-component coupling, such as physics-dynamics interface for the atmospheric model - GSL/DTC, NCAR/DTC

Modeling Infrastructure - Progress and status update

ESMF Development, Testing, Releases, and User Support

- Two major releases include performance optimizations, new hybrid threading options, improved interfaces for connecting DA systems, new exchange grid regridding options, and other features.
- In FY21, fielded over 60 user support requests from UFS community, including multiple NOAA labs and universities. User support provides critical technical guidance for users implementing coupled applications within the UFS.
- Improvements to ESMF testing infrastructure to automate testing of the library across a large number of compiler+MPI combinations and HPC platforms. Test results are collected nightly in a GitHub repository.
- Implemented automated testing of new ESMF development snapshots against the UFS.

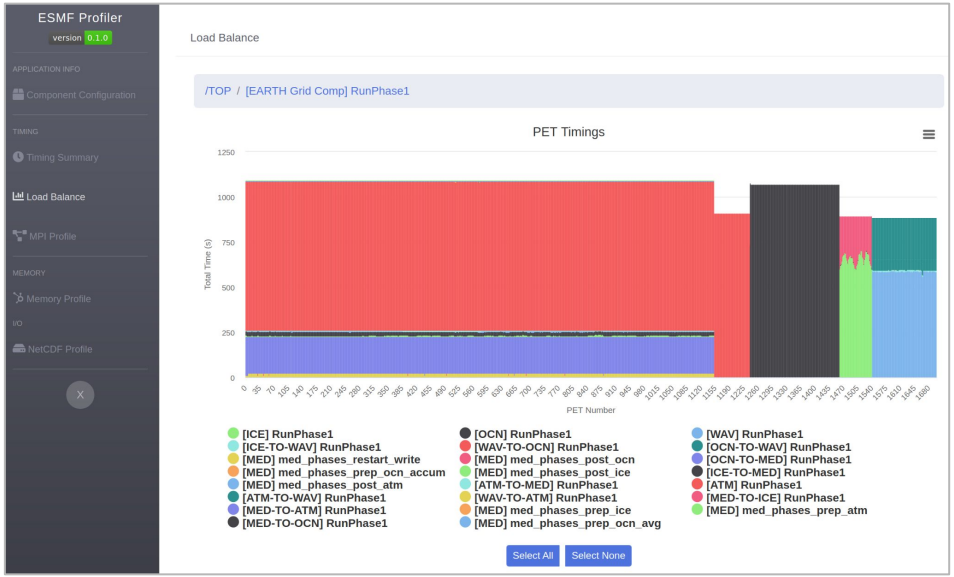
Community Mediator (CMEPS) Development

- CMEPS is a NUOPC-compliant coupler and has replaced the aging NEMS Mediator with a more flexible design and modular code structure. CMEPS has been validated through several of the “coupled model prototypes” (P5-P7).
- MOM6 and CICE6 NUOPC caps were “unified” and are being shared between NOAA/UFS and NCAR/CESM. Development on a unified WW3 cap has started.
- A new exchange grid option was added to CMEPS and an initial evaluation conducted. The exchange grid improves distribution of surface fluxes and handling of fractional surface cells.
- A simplified, readable, YAML-based specification of coupling field exchanges was implemented.

Modeling Infrastructure - Progress and status update

UFS Coupled Model Profiling and Optimization

- Conducted profiling of MRW/S2S application at C384 resolution. Identified load balanced configurations on Hera. WCOSS2 showed significant variability in performance across runs.
- Introduced the *esmf-profiler*, a web-based profiling tool for visualizing and assessing load balance of coupled models. Load balance plots can be generated and automatically posted online to facilitate collaborative optimization efforts.
- Began integrating **ESMF-managed threading** into the UFS. Preliminary results for the "prototype 7" coupled benchmark show that ESMF-managed threading allows tighter packing of model components on the HPC, *resulting in ~18% reduction in HPC resource utilization, while retaining the same model throughput*.



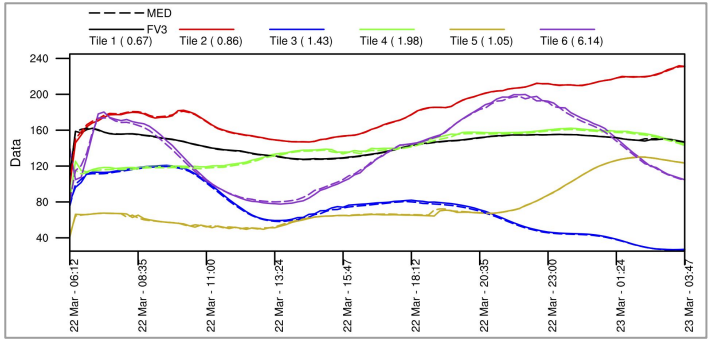
A *load balance* plot of the UFS MRW "prototype 7" configuration generated by the ESMF Profiler. Performance profiles can be pushed to GitHub to easily share results and collaborate on coupled model optimization efforts.

Modeling Infrastructure - Progress and status update

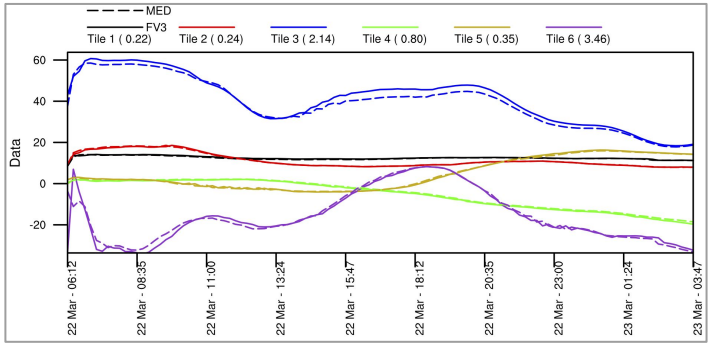
Exchange Grid in CMEPS for Surface Flux Computations

- The *exchange grid* was implemented as an option in the CMEPS Mediator to more consistently handle fractional surface cells (e.g., coastlines) and to better capture extremes in surface fluxes.
- ATM-OCN exchange grids are generated on the fly in CMEPS using *ESMF_XGridCreate()* by passing in the constituent grids/meshes.
- The exchange grid was validated in a configuration of CESM using an idealized tropical cyclone test.
- In the UFS, the ATM-OCN flux computation was moved to CMEPS with fluxes computed on the atmosphere grid to demonstrate that CMEPS can reproduce existing UFS ATM flux computations.

ATM vs. CMEPS Latent Heat Flux

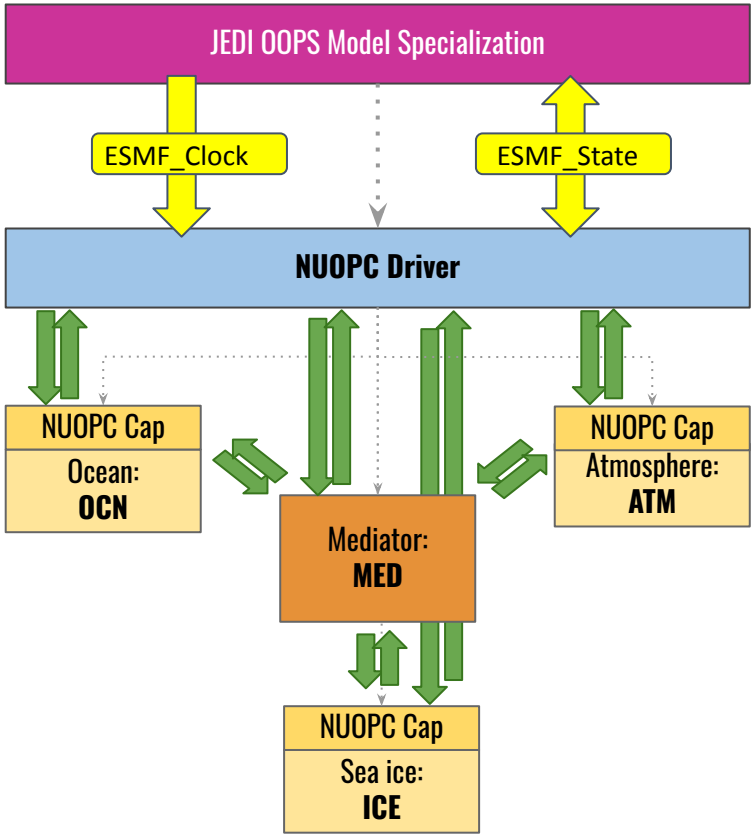


ATM vs. CMEPS Sensible Heat Flux



Comparison of atm-ocn surface fluxes computed inside CMEPS against the same fluxes computed inside the UFS ATM. In both cases, fluxes are computed on the atmosphere grid. Close correspondence indicates that CMEPS can closely reproduce the fluxes. A later step will move the flux computation to the exchange grid. *Images courtesy U. Turuncoglu/NCAR/ESMF.*

Modeling Infrastructure - Progress and status update



JEDI Connection to UFS Unified Driver

- The UFS Unified Driver provides a single interface for JEDI to control UFS forecasts, in both uncoupled and coupled configurations.
- The *fv3jedi* layer was updated to connect to the UFS Unified Driver. The build system was updated to build UFS and JEDI into a single executable.
- Initial work was with the atmosphere-only configuration. 2D and 3D atmosphere fields can now be sent to JEDI through ESMF states to enable in-core model estimate of observations.
- All OOPS layer model interface tests pass, except for the “reforecast” test because the UFS atmosphere cannot yet be “hot” restarted in memory by resetting the state.

CCPP Development, Capabilities, Releases

- Included in UFS Weather Model and used in the development of GFS, GEFS, RRFS, HAFS
- On track for transition to UFS operations in 2023
- New multi-institutional CCPP Physics Code Mgmt team addressing repositories and review/commit process
- New schemes (e.g., GSL drag suite), active development of existing ones
- Rules and dictionary of Standard Names established for facilitate distributed development
- Ongoing collaboration with NCAR on development of the next-gen CCPP Framework and its adoption in UFS
- Two public releases (v4.1.0 in Oct 2020 and v5.0.0 in March 2021) with documentation, online tutorial, support
- Single-column model included in release and support and being extensively employed in UFS community

Modeling Infrastructure - Progress and status update

Workflow Coordination

- We have defined the problem
  - Broad consensus that the multitude of independently developed workflows across the UFS applications are resulting in confusion and duplication of effort, and that this is a problem that needs to be solved
- We have defined a path forward
  - We have defined and documented the requirements for a Unified Workflow System through extensive engagement with the UFS community (workshops, reports, Slack, tag-ups, regular meetings…)
  - Slides on Unified Workflow Framework
- We have engaged with our partners
  - We have created a core workflow team that includes participation and input from EMC leadership, multiple application developers, university researchers, and other UFS stakeholders
- We have engaged with EPIC
  - Workflow development efforts through EPIC and UFS Workflow Project are now formally aligned

HAFS Workflow

- Exercised regression tests, began transferring documentation to readthedocs, and worked on support for Thompson microphysics.

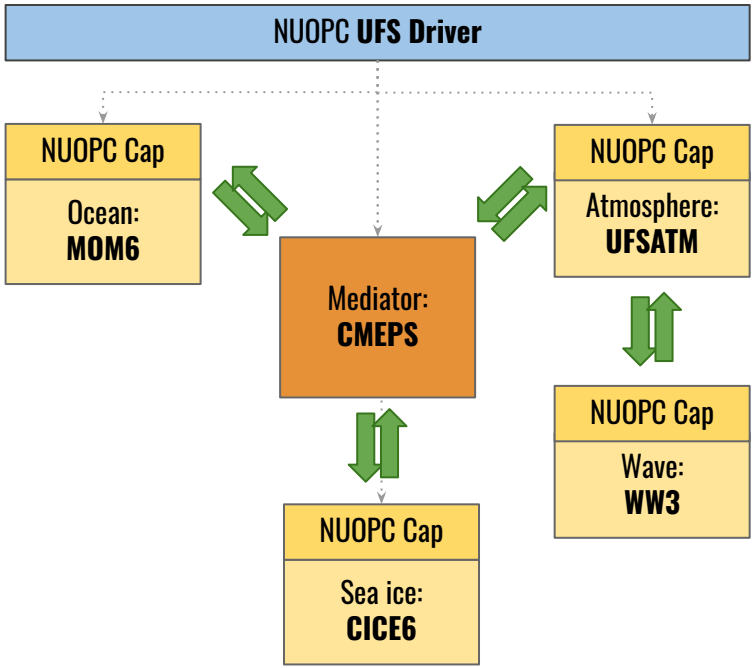
Modeling Infrastructure - Major Accomplishments

Community Mediator (CMEPS) in UFS MRW/S2S and HAFS

CMEPS was integrated into the UFS as the coupler component for the MRW and HAFS applications and has been validated through a series of coupled model prototypes (UFSATM-MOM6-CICE6-WW3) and through HAFS real time experiments and regression tests. Coupled model components can be selectively turned on/off to support a wide range of UFS configurations.

CDEPS "data models" can replace active components to support hierarchical model development, isolation of coupling feedbacks and integration of forcing datasets into the UFS.

Use of the CMEPS has led to substantial collaboration among model developers at NOAA EMC and NCAR, including efforts to unify the MOM6, CICE6, and WW3 NUOPC "caps." This has led to more robust code and helped to identify bugs.



UFS MRW Coupled Model Configuration

Modeling Infrastructure - Major Accomplishments

ESMF Release 8.1 (March 2021)

- **Improved internal mesh representation**, based on the MOAB library. Faster grid/mesh creation and regridding. Reduced memory footprint. This is a long term infrastructure change and not all mesh-based operations are yet supported with MOAB.
- ESMF-managed threading. Allows for **flexible hybrid threading of model components**, including independently setting threading levels of each model component. Improves HPC utilization.
- Detailed NUOPC internal **performance profiling**
- Refinements to external NUOPC interface to support **connection of coupled forecast models to data assimilation systems** (e.g., JEDI)

Details of ESMF 8.1 release

ESMF Release 8.2 (October 2021)

- NUOPC coupled model run sequences were improved to support **conditional execution of model component phases** based on alarms
- The **exchange grid** was expanded to support additional regridding methods, including bilinear and higher order patch regridding, which are especially relevant for mapping vector fields to the exchange grid.
- Robustness of ESMF-managed threading was improved by addressing a number of issues that came up in application testing of ESMF's **hybrid threading capabilities.**

Details of the ESMF 8.2 release

CCPP Framework

- Support for blocked data structures. This allowed removal of GFS derived data types from the physical parameterizations, making them easier to understand and more interoperable
- Replacement of hard-coded/imported physics constants with host model variables in several schemes for further compliance with standards
- New "active" attribute in variable metadata that tells CCPP whether a variable is active (i.e. allocated/initialized by the host and available for use by the physics), which allowed us to phase out the incomplete support for optional arguments in the CCPP framework and metadata
- Enhanced capabilities that aid debugging efforts
    - Comparison of actual array dimensions to those specified in the metadata
    - Stricter checking of units
- Improvements of the build system and integration in the UFS

CCPP Physics - Currently Supported Suites

Type	Operational	Developmental			
Suite Name	**GFS_v15p2**	**GFS_v16beta**	**csawmg***	**GSD_v1***	**RRFS_v1alpha**
Host	**MRW v1, SCM**	**MRW v1, SCM**	**SCM**	**SCM**	**SRW v1,SCM**
Microphysics	GFDL	GFDL	**M-G3**	**Thompson**	**Thompson**
PBL	K-EDMF	**TKE EDMF**	K-EDMF	**saMYNN**	**saMYNN**
Surface Layer	GFS	GFS	GFS	GFS	MYNN
Deep Cu	SAS	saSAS	**Chikira-Sugiyama**	**Grell-Freitas**	N/A
Shallow Cu	SAS	saSAS	saSAS	**MYNN and GF**	**MYNN**
Radiation	RRTMG	RRTMG	RRTMG	RRTMG	RRTMG
Grav Wave Drag	uGWP	uGWP	uGWP	uGWP	uGWP
Land Surface	Noah	Noah	Noah	**RUC**	**Noah-MP**
Ozone	NRL 2015	NRL 2015	NRL 2015	NRL 2015	NRL 2015
H2O	NRL	NRL	NRL	NRL	NRL

Modeling Infrastructure - Major Challenges

- Substantial effort has been required to maintain a stable JEDI-UFS system (when the two are linked as a single executable) as both UFS and JEDI are fast moving repositories. There is a lack of regression tests for the combined JEDI-UFS, such that the code breaks frequently if either system is updated. There has been a recent effort to provide the JEDI core team with a UFS container that could be used for CI testing.

- Without sustained effort to build, test, and integrate toolsets under the Unified Workflow Framework, we will not be able to unify the UFS workflows. This requires buy-in across the UFS community.

Modeling Infrastructure - Work Plan for Year 3

- ESMF Year 3 Priorities
  - ESMF core infrastructure development, including releases, testing, porting, documentation, and user support.
  - Advance the CMEPS exchange grid to include additional surface flux computations beyond bulk atm-ocn fluxes. Develop approaches to consistently manage surface fluxes across coupled components and interaction with CCPP physics.
  - Address gaps in ESMF/NUOPC infrastructure to support operations needed for in-core coupled DA w/ JEDI: implement an in-memory “checkpointing” feature in ESMF/NUOPC that stores internal model state (physics and dynamics) and allows for resetting a model to a prior state at runtime
  - Optimization and load balancing of MRW/S2S and HAFS at operational configurations and resolutions in preparation for implementations in FY23/24. Leverage detailed performance profiles collected under under year 2 to determine and address sources of inefficiency.

Modeling Infrastructure - Work Plan for Year 3

- CCPP Year 3 Priorities
  - Code management and releases/community support for CCPP Framework, Physics, and Single-Column Model (SCM)
  - Requirements gathering and community visioning for future development of CCPP Framework
  - Continuous synchronization and unification of the CCPP Framework between UFS and NCAR, as per the NOAA/NCAR MoA.
  - Ability to compile the CCPP library in either single or double precision to explore improvements in computational performance.

Modeling Infrastructure - Work Plan for Year 3

- Workflow Year 3 Priorities
  - Advance development of Unified Workflow Framework development
    - Participate in development, testing and evaluation of emerging tool sets
    - Coordinate with Application teams to integrate these into their workflow configurations as appropriate to slowly transition the application workflows to a unified solution set
  - HAFS-specific
    - Maintain HAFS scripts and workflow by conducting regression and consistency checks, as applicable
    - Continue to update HAFS workflow documentation for developers
    - Possibly re-program part of this effort to unified workflow (pending discussion with App leads and DTC)

Modeling Infrastructure - Compute Requirements

Infrastructure development activities typically use lower resolution versions of the model and do not require long forecast jobs. Therefore only modest HPC is needed in general.

Profiling and optimization efforts require runs on a large number of nodes, but only for short forecasts.

Hera and Orion are the most critical systems. In-kind HPC can be provided on Cheyenne for development of jointly developed software, such as ESMF/NUOPC and CMEPS/CDEPS.

Modeling Infrastructure - Anticipated in kind effort

- ESMF is supported by a multi-agency core team with funded staff from NOAA, NRL, NASA, and NCAR. The majority of the core team is at NCAR/CGD.
- FY21 JTTI project “Advancing Land Modeling Infrastructure in the UFS for Hierarchical Model Development” is a related effort to implement a NUOPC-compliant NoahMP land model, and will enable coupling of other LSMs into the UFS. This project will ensure new land modeling capabilities are coordinated with MRW/SRW/HAFS model development.
- The CCPP Physics is developed by many community contributors, including EMC, JCSDA, PSL, GSL, GFDL, AER, NRL, AOML, NSSL, etc.
- The next-gen CCPP Framework is being developed primarily by NCAR
- The CCPP SCM has received strong infusion of capabilities and new cases deriving from an ongoing Hurricane Supplemental Project

Modeling Infrastructure - Risks

No major risks were identified.

Modeling Infrastructure - Summary & Closing Remarks

Under the first 1.5 years of the R2O project, substantial progress has been made in developing and testing highly complex coupled modeling system.

- The CMEPS Mediator was integrated and provides a flexible “hub-and-spoke” coupled model architecture. This has facilitated use of a single, unified codebase for multiple UFS applications.
- Preliminary results of new ESMF-managed threading capabilities demonstrate higher HPC resource utilization in the UFS coupled model, which is critically needed in light of the overall HPC shortfall.
- The ESMF exchange grid option in CMEPS can potentially provide a more consistent way of handling surface fluxes across the atmosphere--ocean/ice/land interface. Work with the MRW/S2S application team is needed to define an overall plan for computing and compositing surface fluxes across all components.
- CCPP is now an integral part of the UFS Weather Model and used in the development of GFS, GEFS, RRFS, HAFS. It is on track for transition to UFS operations in 2023.
- Two public releases of CCPP including documentation, training, and user support. Development of new physics schemes and suites.
- Unified Workflow requirements have been defined and approved by multiple stakeholders. Development plan has been coordinated and aligned with EPIC.