Development of the Configurable ATmospheric Chemistry (CATChem) model and its application within the Unified Forecast System forming a unified UFS-Chem

Collaborative effort between NOAA ARL, NOAA CSL, NOAA GSL, and NCAR

Special Acknowledgments: Barry Baker (NOAA/ARL), Rebecca Schwantes (NOAA/CSL), Jian He (NOAA/CSL/CIRA), Jordan Schnell (NOAA/GSL/CIRA), Li Zhang(NOAA/GSL/CIRA), Zachary Moon(NOAA/ARL/ERT), Colin Harkins (NOAA/CSL/CIRA, Georg Grell (NOAA/GSL), Brian McDonald (NOAA/CSL)

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Current Structure of the UFS for Atmospheric Chemistry and Composition

Model	Chemistry Available	Application
RRFS – Smoke/Dust	Simplified Aerosols: Smoke + Dust tracers	Regional Wildfire Smoke Forecasts
UFS - Aerosols	Simplified Aerosols: GOCART	Global Weather Forecasts with aerosol feedbacks
Online CMAQ	Complex chemistry from CMAQ: Ozone and Aerosols	Regional Air Quality Forecasts
UFS-RAQMS	Simplified chemistry with data assimilation: Ozone and Aerosols	Global air quality forecasts

Problems:

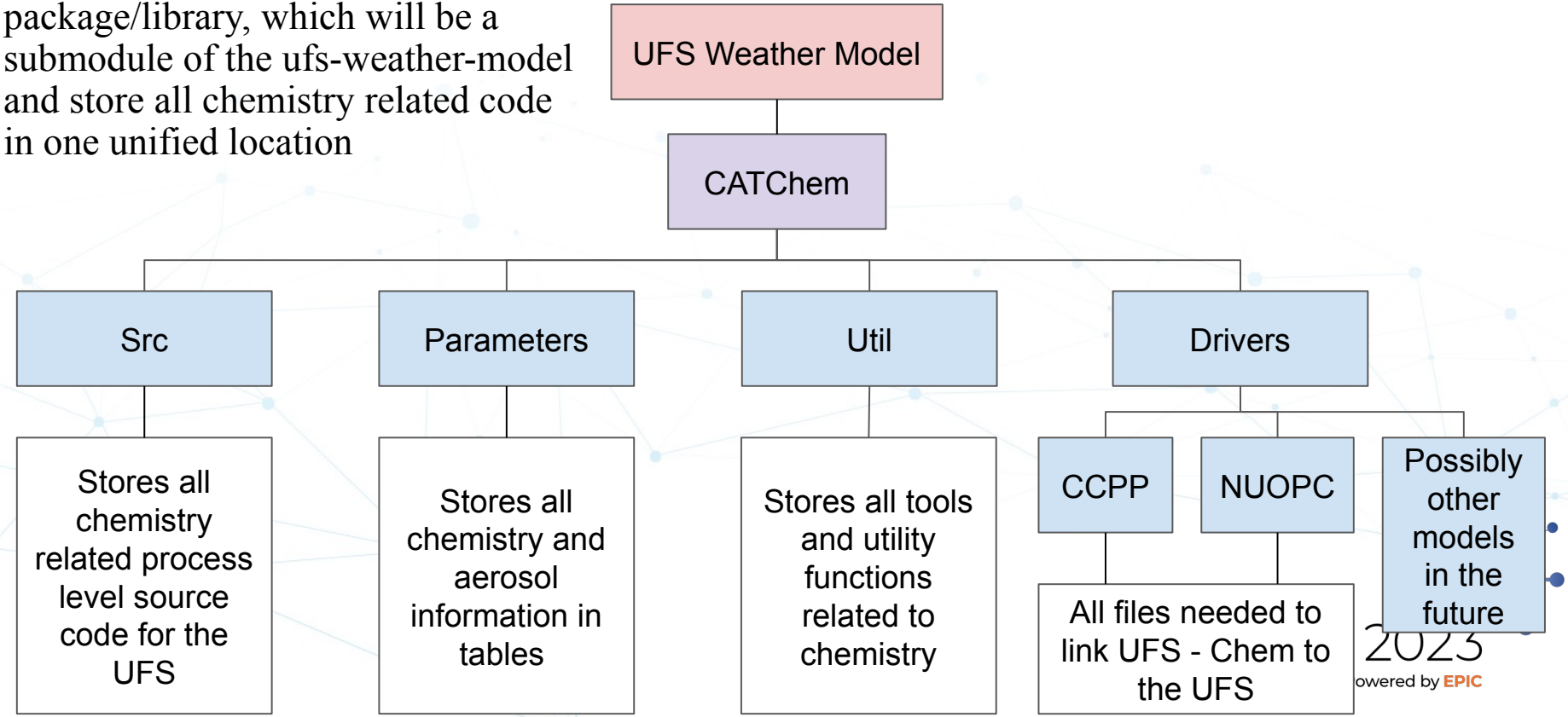
- Chemistry-related code is duplicated across the UFS, which is not unified and time intensive to maintain
- The reliance on multiple externally developed models also limits expertise within NOAA
- We would like to add research capabilities for atmospheric composition and chemistry, but it is unclear how to do this with chemistry divided across so many models/applications

Overall Unifying Goals

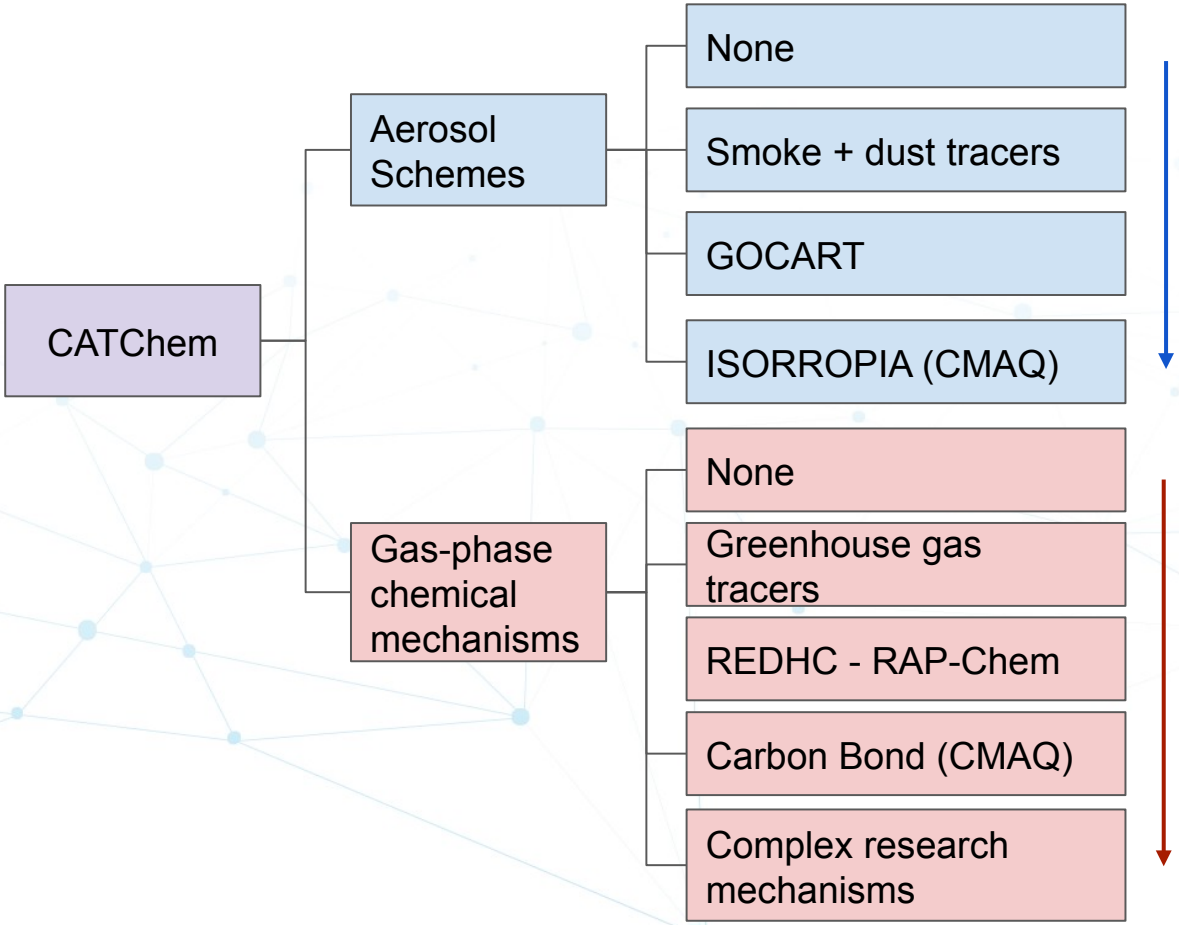
- Add, update, and advance chemical and aerosol processes in the operational forecasts in order to
  - Improve aerosol feedbacks in weather forecasts
  - Improve aerosols in wildfire smoke forecasts
  - Improve ozone and aerosols in air quality forecasts
- Add enhanced research capabilities including more complex chemistry, aerosol, and physics options in order to improve operational forecasts indirectly or on longer timescales by
  - Collaborating more with the research community
  - Advancing current understanding of air quality and atmospheric composition processes
- **Unite** together across all of NOAA and in the community to advocate for the importance of adding aerosols and chemistry for accurately representing processes in the operational forecast models
  - A simple aerosol scheme is needed in the UFS weather model
  - Smoke & dust tracers are needed for wildfire smoke operational forecasts
- **In order to accomplish these goals, we need to unify chemistry in the UFS (UFS-Chem)**
  - OAR laboratories use and develop UFS-Chem for research and R2O activities
  - EMC uses and develops UFS-Chem for operational forecasts and O2R activities
  - We jointly work together to advocate for the importance of including aerosols and chemistry within the UFS

Unify Chemistry across the UFS through CATChem development

We propose to develop a chemistry package/library, which will be a submodule of the ufs-weather-model and store all chemistry related code in one unified location



Options to use gas & aerosol chemistry of varying complexity



UFS-Chem will be flexible and configurable where users can choose the aerosol scheme and the gas-phase chemical mechanism of the right complexity for their desired application or science question

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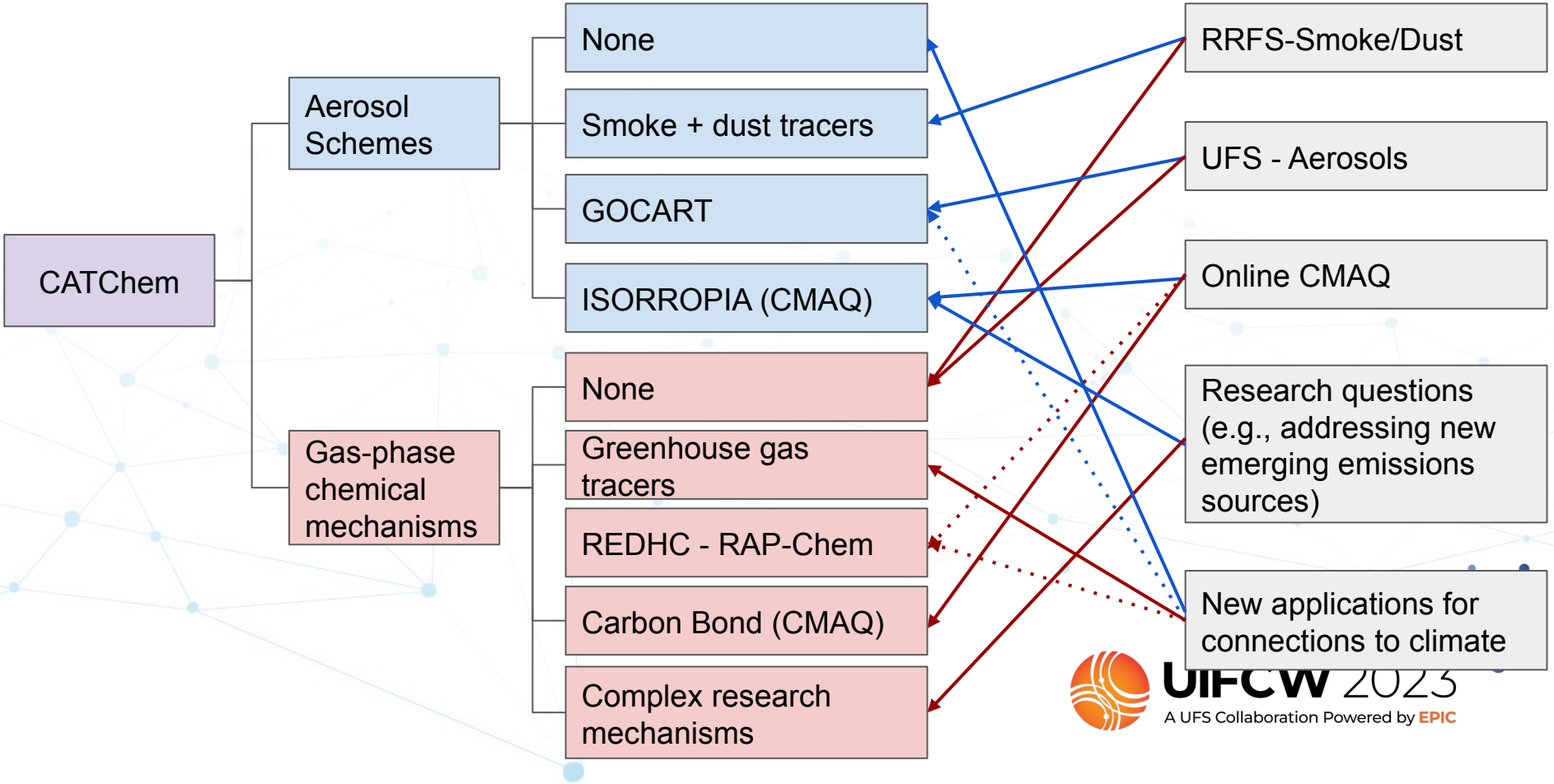
Options to use gas & aerosol chemistry of varying complexity



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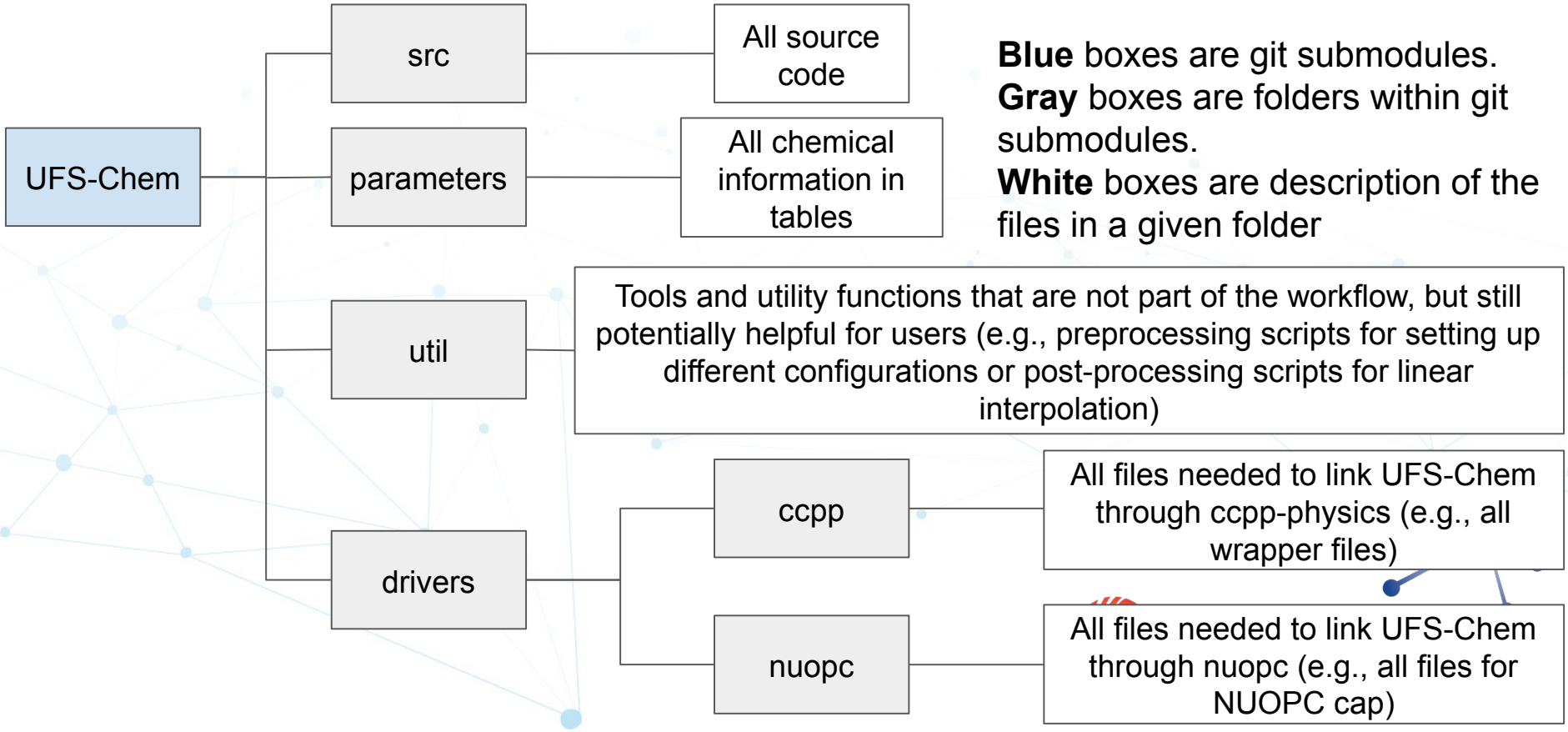
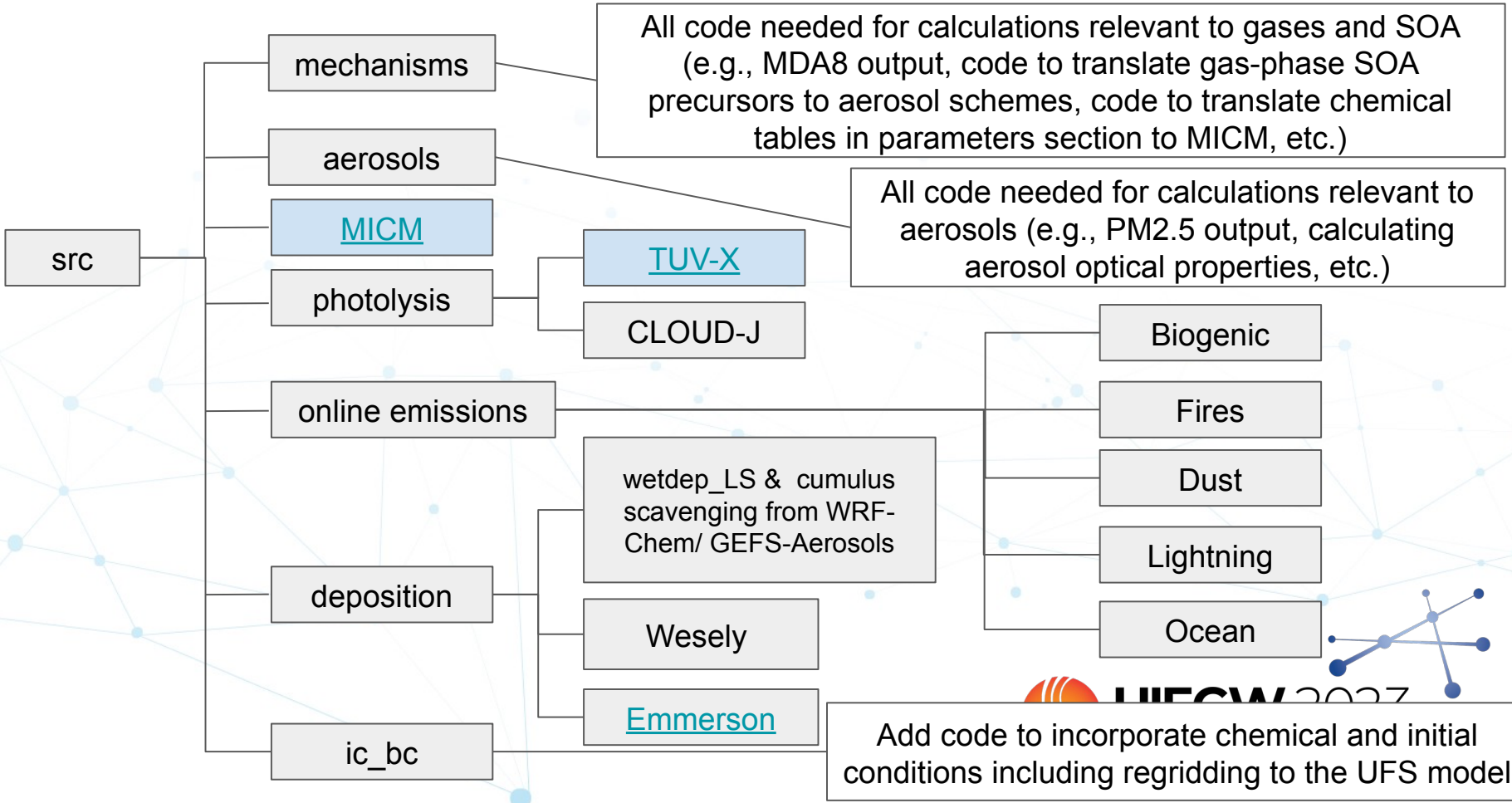
UFS-Chem Detailed Planned Structure

This overall structure is similar to how the land model is configured and coupled to the UFS.

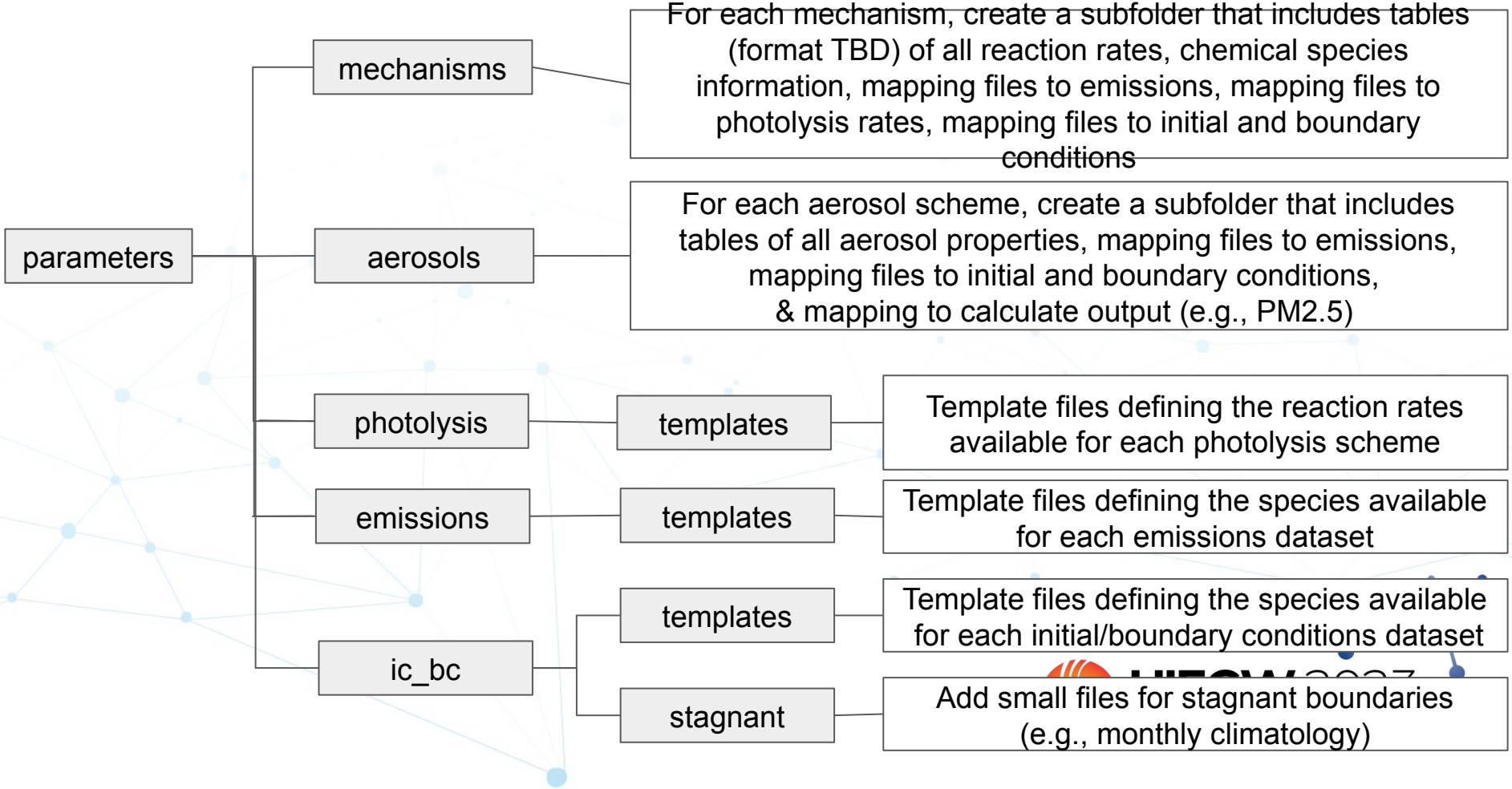
Blue boxes are git submodules.
Gray boxes are folders within git submodules.
White boxes are description of the files in a given folder



UFS-Chem Detailed Planned Structure: Src Folder

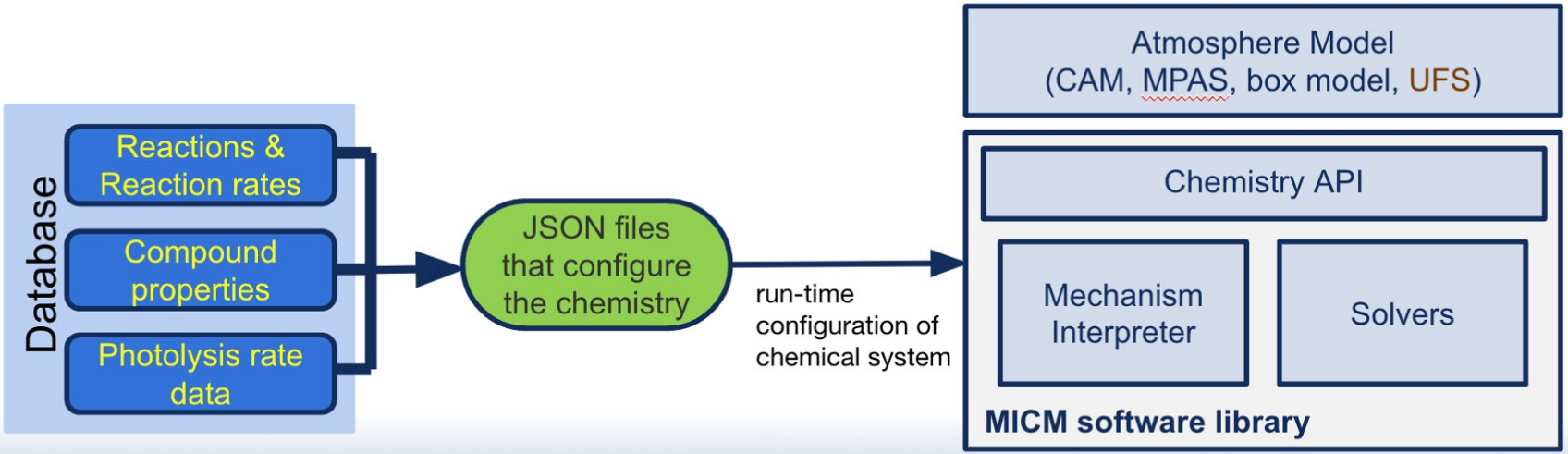


UFS-Chem Detailed Planned Structure: Parameters Folder

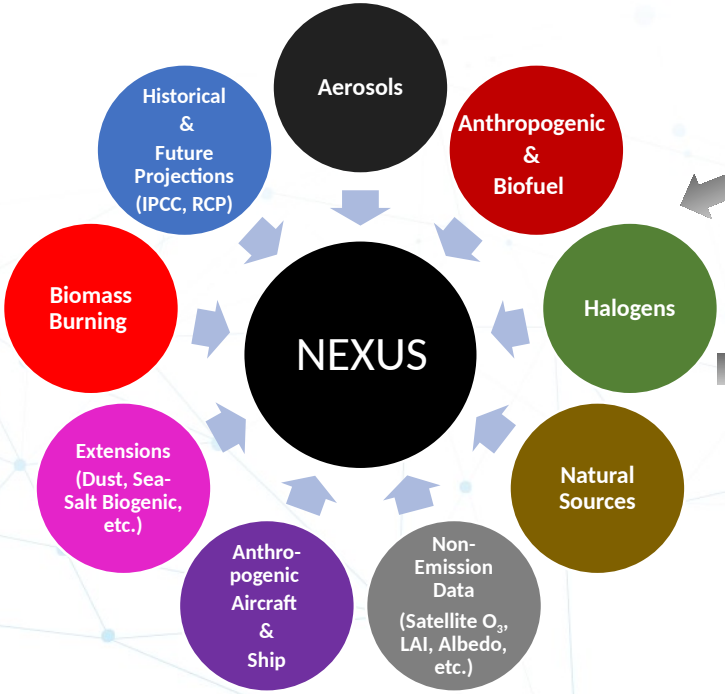


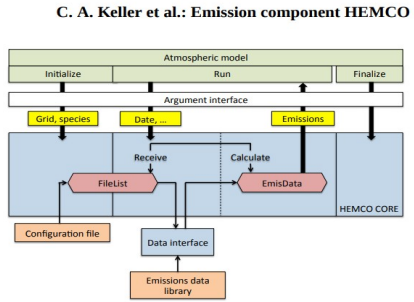
Model Independent Chemistry Module (MICM)

- Use MICM, which is a component of the MUlti-Scale Infrastructure for Chemistry and Aerosols (MUSICA), led by NCAR (https://github.com/NCAR/micm)
- By collaborating with NCAR on MICM development, chemistry developments from the research community incorporated into MICM will be efficiently linked to both NOAA and NCAR models.



NOAA Emissions and eXchange Unified System (NEXUS)





Emissions Processing System for NOAA's UFS Atmospheric Composition Models

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Goals of CATChem in the UFS

- Initial code repository is created, https://github.com/ufs-community/catchem
- Simplify maintenance and increase efficiency in code development
  - Reduction of libraries (e.g., MAPL and related libraries)
- Unify atmospheric composition & chemistry modeling in the UFS by creating a flexible system that can be used for a variety of applications
  - All chemistry related code is stored in one location
  - Enhance collaborations between OAR laboratories for research
  - Enhance collaborations between EMC and OAR to advance R2O and O2R activities
  - Reduces costs for transitioning research advances to operations
  - Engage the research community in development by positioning the UFS as a state-of-the-art modeling system for simulating atmospheric composition across regional to global scales
- Unify emission processing with NEXUS across applications
  - https://github.com/noaa-oar-arl/nexus
- Continue to develop MELODIES MONET - unifies model evaluation activities
  - https://github.com/noaa-csl/melodies-monet
  - https://github.com/noaa-oar-arl/monetio
  - https://github.com/noaa-oar-arl/monet