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# Integrated modeling of aerosol, cloud, precipitation and land processes at satellite-resolved scales



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#### ABSTRACT

With support from NASA's Modeling and Analysis Program, we have recently developed the NASA Unified-Weather Research and Forecasting model (NU-WRF). NU-WRF is an observation-driven integrated modeling system that represents aerosol, cloud, precipitation and land processes at satelliteresolved scales. "Satellite-resolved" scales (roughly 1–25 km), bridge the continuum between local (microscale), regional (mesoscale) and global (synoptic) processes. NU-WRF is a superset of the National Center for Atmospheric Research (NCAR) Advanced Research WRF (ARW) dynamical core model, achieved by fully integrating the GSFC Land Information System (LIS, already coupled to WRF), the WRF/ Chem enabled version of the GOddard Chemistry Aerosols Radiation Transport (GOCART) model, the Goddard Satellite Data Simulation Unit (G-SDSU), and custom boundary/initial condition preprocessors into a single software release, with source code available by agreement with NASA/GSFC. Full coupling between aerosol, cloud, precipitation and land processes is critical for predicting local and regional water and energy cycles.

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#### Software availability

Name of software: NU-WRF Developers: NASA GSFC and affiliates

Contact address: Dr Toshihisa Matsui, NASA Goddard Space Flight

Center, Mail Code 612; Greenbelt, MD, 20171, USA.

Email: toshihisa.matsui-1@nasa.gov

Availability and Online Documentation: Restricted to US

Government and NASA collaborators via Software Usage Agreement; Manual available at: http://nuwrf.gsfc.nasa.gov/sites/default/files/docs/nuwrf\_userguide.pdf

Year first available: 2011

Hardware required: Intel/AMD (tested on Intel Xeon), IBM Power Software required: Linux (tested on SLES 11.1), other Unix variants Programming language: Fortran 90, C, C++, Bash, Tcsh, Python, Perl

Program size: 1.6G (source code)

#### 1. Introduction

The NASA Unified-Weather Research and Forecasting (NU-WRF) modeling system has been developed at NASA's Goddard Space Flight Center (GSFC), in collaboration with NASA's Marshall Space Flight Center (MSFC) and university partners, as an observationdriven integrated modeling system that represents aerosol, cloud, precipitation and land processes at satellite-resolved scales. We define "satellite-resolved" scales as being within a typical mesoscale atmospheric modeling grid (roughly 1–25 km), although this work is designed to bridge the continuum between local (microscale), regional (mesoscale) and global (synoptic) processes. We assert that representing the full coupling between aerosol, cloud, precipitation and land processes is critical for predicting local, regional, and global water and energy cycles associated with highimpact phenomena such as floods, hurricanes, mesoscale convective systems, droughts, and monsoon circulations. The philosophy of NU-WRF development is to provide a NASA-oriented superset of the community WRF model that unifies and incorporates NASA's unique experience and capabilities in validating, simulating and assimilating current earth science satellite observations into models to support observationally-based improvements of Earth system model components. NU-WRF is built upon the Advanced Research WRF (ARW; Skamarock et al., 2008) dynamical core model, with additional components that include the GSFC Land Information System (LIS; Kumar et al., 2006; Peters-Lidard et al., 2007), the WRF/Chem enabled version of the Goddard Chemistry Aerosols Radiation Transport (GOCART; Chin et al., 2000a, b) model, GSFC radiation and microphysics schemes including revised couplings to the aerosols (Tao et al., 2003; Lang et al., 2007, 2011; Shi et al., 2014), and the Goddard Satellite Data Simulator Unit (G-SDSU; Matsui et al., 2013, 2014). NU-WRF now provides the community (via a source code release process at NASA/GSFC) with an observation-driven regional Earth system modeling and assimilation system at satellite-resolved scales.

The following sections describe the coupling between atmospheric physics, land surface models and aerosol-chemistry models in NU-WRF, the interoperable features and adoption of Earth system modeling standards, and the application of NU-WRF in modeling coupled aerosol-cloud-and land surface processes.

#### 2. NU-WRF components

As shown in Fig. 1, NU-WRF consists of 6 main components: the ARW model, LIS, GOCART, GSFC radiation and microphysics schemes, and G-SDSU. Below we describe each of these components in more detail.

#### GEOS5, MERRA

Satellite Obs

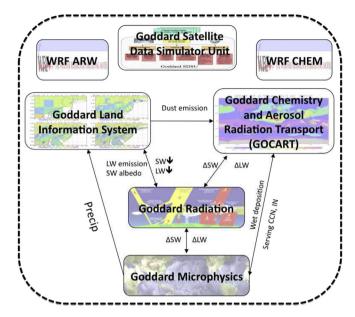


Fig. 1. A schematic representation of NU-WRF components and their interfaces.

#### 2.1. Advanced Research WRF (ARW) model

The ARW is a mesoscale/microscale modeling and assimilation system developed by the National Center for Atmospheric Research (NCAR) with National Oceanographic and Atmospheric Administration (NOAA) and Department of Defense (DoD) partners. First released in November 2000, the model incorporates advanced numerics and data assimilation techniques, a multiple relocatable nesting capability, and numerous physics packages from the operational and research communities. The ARW is designed for flexibility and easy portability to multiple computing environments, and has been used for a wide range of applications (e.g., simulations of thunderstorms, orographic precipitation, tropical cyclones, turbulence and gravity waves, large eddy simulations, air quality, regional climate, general circulation studies). NOAA and the Air Force Weather Agency (AFWA) have transitioned the ARW to operations, replacing the legacy Rapid Update Cycle and Pennsylvania State University/NCAR Mesoscale Model version 5 forecast models.

The ARW dynamical core uses an Arakawa-C horizontal grid; a dry, hydrostatic pressure-based terrain-following vertical coordinate (Laprise, 1992); time-split integration of flux-form, fully compressible non-hydrostatic equations using a 3rd-order Runge-Kutta scheme (Klemp et al., 2007); a choice of 2nd-to 6th-order advection schemes including positive-definite and monotonic selections; options for observational, gridded and spectral nudging; several choices for upper boundary absorption and Rayleigh damping; several variants of digital filter initialization; and numerous choices for land surface, surface layer, Planetary Boundary Layer (PBL), radiation, microphysics (single- and doublemoment), and cumulus (deep and shallow) parameterizations. The most recent ARW releases also include simple mixed-layer ocean and lake models. A plug-in library (WRF/Chem; ESRL, 2012) provides aerosol, gas-phase chemistry, photolysis, and dry deposition parameterizations. A companion data assimilation library (WRFDA, formerly WRF-Var; Barker et al., 2012) provides 3D Variational (3DVAR; Barker et al., 2004), hybrid Ensemble-3DVAR (Wang et al., 2008a, b), and 4DVAR (Huang et al., 2009) assimilation capabilities.

#### 2.2. Land information system (LIS)

LIS is a high-resolution land modeling and data assimilation system that integrates the use of advanced land surface models, high resolution satellite and observational data, data assimilation techniques, and high performance computing tools (Kumar et al., 2006). LIS has been coupled to the ARW, enabling: i) a coupled system to study land-atmosphere interactions, and ii) an uncoupled system to prepare initial conditions by multi-year "spinup" integrations and data assimilation techniques (Kumar et al., 2008b). The LIS infrastructure (http://lis.gsfc.nasa.gov; Peters-Lidard et al., 2007; Kumar et al., 2006) was originally developed to unify the capabilities of the 0.25-degree Global Land Data Assimilation System (GLDAS; Rodell et al., 2004) and the 0.125-degree North American Land Data Assimilation System (NLDAS; Mitchell et al., 2004) into a common software framework capable of running multiple Land Surface Models (LSMs) on points, regions or the globe at user-defined spatial resolutions typically ranging from  $2 \times 2.5^{\circ}$  down to 1 km. The 1-km capability of LIS allows it to take advantage of Earth Observing System (EOS)-era satellite observations, such as the Moderate Resolution Imaging Spectroradiometer (MODIS) products including snow covered area, leaf area index, green vegetation fraction (GVF), and surface temperature.

The land-atmosphere interface is a core coupling component of NU-WRF, and began as the LIS-WRF coupled modeling system described by Kumar et al. (2008a). The advantages of coupling LIS and WRF include the ability to spin-up land surface conditions using multiple input forcings (e.g., NLDAS, The Modern-Era Retrospective Analysis for Research and Applications-Land product. MERRA-Land (Reichle et al., 2011; Reichle, 2012)) on a common grid from which to initialize the regional model. The framework also supports flexible and high-resolution, satellite-based soil and vegetation representation [e.g., real-time MODIS GVF (Case et al., 2014) as produced by the NASA Short-term Prediction Research and Transition Center (SPoRT; Jedlovec, 2013)], additional choices of LSMs, and various LIS plug-in options such as land data assimilation (Kumar et al., 2008b), parameter estimation (Santanello et al., 2007, 2013a,b), and uncertainty analysis (Harrison et al., 2012). Higher-resolution initial land surface conditions have been shown to improve prediction of cumulus convection associated with heterogenous distributions of land-surface fluxes and mesoscale circulations (Pielke, 2001).

#### 2.3. GOCART

The GOCART model simulates major aerosol types, namely sulfate, dust, black carbon, organic carbon, and sea-salt, and precursor gas species (Chin et al., 2000a, b, 2002, 2004, 2009, 2014; Ginoux et al., 2001). Global-scale simulations of GOCART have been extensively evaluated with observations from field campaigns, ground-based networks, and satellites (e.g. Chin et al., 2000a,b, 2002, 2003, 2004, 2007, 2009, 2014; Ginoux et al., 2001, 2004; Kinne et al., 2003, 2006; Yu et al., 2004, 2006, 2008; Kim et al., 2013), and the physics modules have been widely used by many research groups and operational centers such as NASA/GSFC's Global Modeling and Assimilation Office (GMAO) and NCEP. The Goddard Earth Observing System Model, Version 5 (GEOS-5) coupled with GOCART has been used to generate aerosol forecasts for several NASA aircraft campaigns (e.g., Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ), and Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC<sup>4</sup>RS)). The GOCART aerosol modules have also been implemented into the community WRF/

Chem framework in a collaborative effort between GSFC and NOAA (e.g., Zhao et al., 2011).

As part of the NU-WRF development, the GOCART aerosol capability was moved to NU-WRF as an online aerosol module. The NU-WRF team has coupled GOCART with LIS such that LIS provides key information (e.g., soil moisture and soil porosity) that GOCART uses to calculate dust emissions. GOCART has also been coupled with the Goddard radiation and microphysics scheme to simulate the direct and indirect aerosol effects on energy budget, cloud, and precipitation (see the next section). Parameterization schemes to estimate biogenic secondary organic aerosols have been integrated from WRF/Chem into NU-WRF as well. In addition, several model utilities have been developed and modified to facilitate NU-WRF applications, including: 1) the GOCART2WRF module that was developed to use time varying global GOCART results as initial and boundary conditions for NU-WRF simulations, and 2) the PRE-P\_CHEM\_SOURCES module that was updated to incorporate pollutant emissions inventories from expanded sources with varying resolution and formats.

#### 2.4. GSFC radiation and microphysics

In addition to coupling WRF with LIS and GOCART, NU-WRF unifies the WRF model with physical process improvements realized through Goddard's Cloud Resolving Model (CRM)-based microphysics and radiation packages.

The Goddard Microphysics scheme is the same as the one used in the Goddard Cumulus Ensemble (GCE) model and is mainly based on Lin et al. (1983), with additional processes from Rutledge and Hobbs (1984). The Goddard microphysical scheme is a two-class liquid and three-class ice scheme with four different options: 3ICE-graupel, 3ICE-hail, and 2ICE (only cloud ice and snow) and warm rain only (no ice). Details of the Goddard microphysical scheme can be found in Tao and Simpson (1993) and Tao et al. (2003). Recently, the Goddard microphysics scheme has been modified to reduce overestimated and unrealistic amounts of cloud water and graupel in the stratiform region (Lang et al., 2007, 2011).

The Goddard radiation schemes have been developed over the past two and a half decades at NASA for use in general circulation models (GCMs), regional models and CRMs (Chou and Suarez, 1999, Chou et al., 2001). A few recent improvements were made to the Goddard radiation package before it was added into WRF: (i) the short-wave radiation code was optimized for computational speed (improved by a factor of 2) by avoiding the cloud-overlapping scheme used in the global model; (ii) cloud microphysics assumption were made closely to that of the Goddard microphysics; and (iii) the aerosol direct effect on both long-wave and short-wave radiation has been accounted from the GOCART aerosols mass mixing ratio through consistent assumption of their sizes and chemical compositions.

The Goddard microphysics have provided improved precipitation forecasts (or simulations) from tropical and mid-latitude convection to high-latitude snow storms [e.g., a linear convective system in Oklahoma (International H<sub>2</sub>O project, IHOP-2002; Santanello et al., 2009), an Atlantic hurricane (Hurricane Katrina, 2005; Tao et al., 2011a), a Pacific Typhoon (Typhoon Morakot 2009; Tao et al., 2011b); high latitude snow events (Canadian CloudSat CALIPSO Validation Project, C3VP 2007; Shi et al., 2010), a mesoscale convective system in Africa (Shi et al., 2014) and MC3E (Tao et al., 2013a,b)].

#### 2.5. G-SDSU

The G-SDSU is an end-to-end multi-satellite simulator unit, which has been developed at NASA GSFC in collaboration with

several universities and other institutions (Masunaga et al., 2010, Matsui et al., 2013). The purpose of G-SDSU is to convert the NU-WRF geophysical parameter output into the satellite-observable signals. G-SDSU is composed of i) a model-output reading module, ii) a satellite orbit and scanning module, iii) optical modules, and iv) radiative transfer modules. The G-SDSU has six simulators at present, including a passive visible-IR simulator, a passive microwave simulator, broadband simulators, lidar simulators, and a radar simulator that support various NASA's operating satellite instruments. All simulators are hardwired with an integrated IO interface and driver with MPI libraries (Matsui et al., 2014), and radiative properties are integrated between active and passive sensors, which enables use of multi-sensor radiance and back-scatter signals.

The G-SDSU can compute satellite-observable radiances or backscattering signals from the model-simulated atmosphere profiles, surface boundary conditions, liquid/ice condensates profile, and aerosol profiles. It first computes appropriate optical properties at specific sensor-channel frequencies/wavelengths, and optical properties are spatially interpolated according to the satellite sensor-viewing geometry. Then, radiative transfer engine computations specify radiance/brightness temperature at model resolution, and the signals are convolved in the sensor field-of-view based on the antenna gain function (Matsui et al., 2013). These simulated radiances and backscattering can be directly compared with well-calibrated satellite direct observations instead of using the satellite-retrieved products. In this way, the G-SDSU bridges NU-WRF and satellite observation (and programs) through a radiance-based evaluation framework as shown in Fig. 1.

NU-WRF simulation outputs can be directly processed by the G-SDSU, which allows us to scrutinize the performance of the macro-

and microphysics in coupled aerosol-cloud-precipitation-land surface processes by analyzing discrepancies between modeled and satellite-observed radiances and backscattering. The combination of NU-WRF and G-SDSU then allows us to better understand NU-WRF physics biases as well as forecast skill (Matsui et al., 2014). The G-SDSU was also used as the official satellite simulator to support pre-launch algorithms of the Global Precipitation Measurement (GPM) mission (Matsui et al., 2013).

## 2.6. Support for WRF and WRF/Chem boundary and initial conditions

The community ARW includes a WRF Preprocessing System (WPS; see NCAR, 2012) and two additional programs (see ESRL, 2012) to preprocess meteorological and chemistry fields. NU-WRF adds additional programs to support new data sources. Fig. 2 summarizes the available (non data assimilation) preprocessors and their respective roles. The NU-WRF specific elements are described below.

The GEOS2WRF module is a collection of NASA-developed preprocessors for handling meteorological output from GEOS-5 (Molod et al. 2012) in HDF4, HDFEOS2, or netCDF format. A frontend program simply extracts user-specified variables from a GEOS-5 file and writes out in binary, while back-end programs are used as-needed to derive WRF input variables from available data, or to extrapolate to underground pressure levels. See Table 1 for a listing of current GEOS2WRF programs and their functions.

The MERRA2WRF module is a separate NASA-written program customized to handle HDF4, HDFEOS2, or netCDF files containing MERRA reanalyses (Rienecker et al. 2011). The MERRA files are maintained by the Goddard Earth Sciences Data and Information Services Center (see <a href="http://disc.sci.gsfc.nasa.gov/daac-bin/">http://disc.sci.gsfc.nasa.gov/daac-bin/</a>

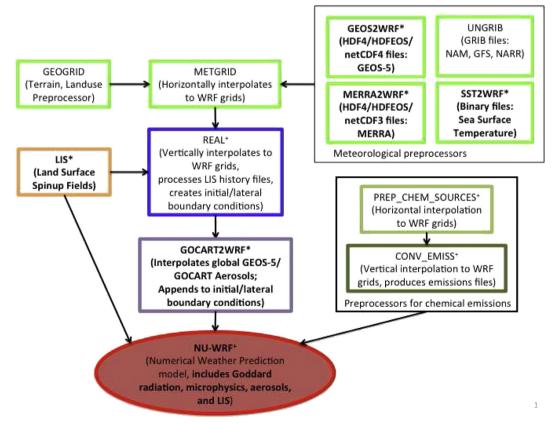


Fig. 2. NU-WRF preprocessing steps (excluding data assimilation). (\*) indicates NASA-written components, while (+) indicates components modified to add new features.

**Table 1** Summary of GEOS2WRF programs.

Program	Description
GEOS2WPS	Opens GEOS-5 file, extracts user-specified variables, and writes out in WPS binary format.
CREATEHGT	Derives 3D geopotential height on GEOS-5 grid from temperature, specific humidity, and terrain height.
CREATELANDSEA	Derives land-sea mask from ocean and lake fractions.
CREATEPRESSURE	Derives 3D pressure on GEOS-5 grid from pressure thicknesses.
CREATERH	Derives relative humidity from temperature, specific humidity, pressure.
CREATESOILHGT	Derives terrain height from surface geopotential.
EXTRAPISOBARIC	Extrapolates to underground isobaric levels.

DataHoldings.pl). MERRA2WRF processes MERRA files specifically (see Table 2), and is easier to use than the more generic GEOS2WRF.

The SST2WRF module is a NASA-developed program that processes 12 different sea surface temperature (SST) products produced by Remote Sensing Systems (see Table 3). These products are derived from microwave IR, Tropical Rainfall Measuring Mission Microwave Imager (TMI), and/or Advanced Microwave Scanning Radiometer for Earth Observing System (AMSR-E) satellite observations, and may be superior to SST fields normally included in NWP output (e.g., GFS, NAM).

The NASA-developed GOCART2WRF module provides aerosol initial and lateral boundary conditions for NU-WRF by processing GEOS-5 GOCART netCDF4 files. GOCART2WRF extracts chemical and aerosol variables, horizontally and vertically interpolates them to the WRF grid, and calculates lateral boundary tendencies. These data are inserted into WRF netCDF input files that already contain required meteorological fields.

The PREP CHEM SOURCES module is a community program for horizontally interpolating emission data to the WRF grid (see ESRL, 2012). We modified this program to add support for Global Fire Emissions Data Version 3 (GFEDV3; Van der Werf et al. 2010); new GMI climatological chemistry fields required by GOCART; and use of the same map projection software employed by the WRF Preprocessing System.

The CONV EMISS module is a community program that vertically interpolates the output from PREP CHEM SOURCES to the WRF grid, and creates the emissions files read in by WRF (see ESRL, 2012). We modified this program to support the new GMI climatological fields, and to improve the interpolation to WRF model levels.

Returning to Fig. 2, all users continue to run the WPS GEOGRID program to process terrain and other terrestrial data. Users with GRIB or GRIB2 data continue to use the WPS UNGRIB program to extract fields, and use the WPS CALC ECMWF P and HEIGHT UKMO preprocessors as needed to derive missing fields. Users with GEOS-5, MERRA, or SST data use GEOS2WRF, MERRA2WRF, and SST2WRF, respectively. All users continue to run the standard WPS

**Table 2**Summary of GES DISC MERRA files processed by MERRA2WRF.

File Type	Variable Descriptions
const_2d_asm_Nx	Longitude, latitude, surface geopotential, lake and ocean fractions
inst6_3d_ana_Nv	Longitude, latitude, synoptic hour, nominal pressure, surface pressure, pressure thickness, temperature, horizontal winds, specific humidity
inst6_3d_ana_Np	Longitude, latitude, synoptic hour, sea level pressure
tavg1_2d_slv_Nx	Longitude, latitude, synoptic hour, 10-m horizontal winds, 2-m temperature and specific humidity, skin temperature
tavg1_2d_ocn_Nx	Longitude, latitude, synoptic hour, sea ice fraction

**Table 3**Summary of Remote Sensing System products supported by SST2WRF. Each product has three variants: real-time, algorithm version 1, and algorithm version 2. Version 2 is considered to be the highest quality.

Instruments	Resolution	Valid time
Microwave IR	9-km global	1200 UTC
TMI and AMSR-E	25-km global	0800 LT
TMI	25-km global	0800 LT
AMSR-E	25-km global	0800 LT

"METGRID" program and "REAL" program to interpolate to the WRF grid. Finally, GOCART2WRF, PREP CHEM SOURCES, and CONV EMISS are only needed when running NU-WRF with chemistry and aerosol physics.

#### 2.7. Support for LIS land surface parameters and initial conditions

In addition to providing support for alternative WRF and WRF/ Chem boundary and initial conditions in NU-WRF, significant effort has gone into providing support for LIS land surface parameters and initial conditions. When initializing an NU-WRF run with LIS, the WRF Preprocessing System (WPS, including GEOGRID, UNGRIB, and METGRID) are run as normal. A LISCONFIG utility is used to customize the LIS preprocessor (LDT) and LIS configuration files so that the LIS domain matches WRF (grid dimensions, resolution, map projection, etc.). After running LDT and LIS, the WPS "REAL" program reads in a summary netCDF file containing LIS landmask, landcover, soiltype, elevation, annual max and min GVF, snow cover, snow depth, snow liquid water equivalent, canopy water, average surface temperature, instantaneous and monthly albedo, max snow albedo, deep soil temperature, daily real-time SPoRT-MODIS GVF and monthly climatological GVF, soil layer temperatures, soil layer liquid moisture, soil layer total moisture, relative soil moisture, land use fractions, and the names of the land use and soil type classification systems.

WPS REAL reallocates the soil layers (for temperature and moisture) to match the levels provided by LIS. The metadata about these levels is also updated before writing to netCDF. For LIS land points, REAL uses surface parameters from LIS as the default and reconciles them with data generated from the WPS. Otherwise, REAL copies the LIS variables to the WRF arrays (WPS data is overwritten). Any "sea ice" from the WPS data processed by WPS is reset to zero.

For open water points (defined by LIS), most "land" variables are set to appropriate default values (e.g., zero greenness, zero snow, "water" land use, WRF defaults for albedo) However, elevation from WPS is retained since LIS doesn't provide it for water points. Snow albedo is set either to 0.75 or 0.08 depending on if sea ice (from WPS) is greater than 50%. For sea ice and small inland lakes, we utilize the algorithms in REAL.

#### 3. NU-WRF coupling design

A key attribute of NU-WRF is improved simulation of atmospheric processes via coupling of appropriate physics parameterizations and satellite observations. The coupling implementation strategy follows three main goals: (1) satisfy the scientific requirements discussed above; (2) maintain computational performance; and (3) avoid unnecessary code changes to ease future merges from the community WRF.

Although Kumar et al. (2008a) coupled LIS and WRF using ESMF, this coupling design did not fully support two-way nesting. Due to the design of the WRF software framework, adding support for multiple (nested) grids using ESMF-based coupling would require

significant modifications to the WRF I/O libraries to pass coupling data as an ESMF import or export state. We found this approach impractical, as it would complicate future merges with community WRF updates. Instead, we elected to implement a tight coupling approach where an adapter layer wraps LIS and presents it as a WRF framework component. ESMF is still used within LIS itself to manage LIS's sub-components (LSMs, domains, etc.), while in WRF we leverage a data structure (called the grid structure) to share variables between components. This approach requires identical LIS and WRF grids during computation, as well as identical processor layouts and domain decomposition, due to the lack of an explicit coupler that does such translations.

This implementation captures several direct physical effects:

- LIS receives WRF surface meteorological variables such as nearsurface temperature, winds, specific humidity, downward solar and infrared radiation flux, and precipitation. In return, LIS provides land surface parameters and variables such as porosity, soil layer temperatures and moisture, and turbulent fluxes of temperature, momentum, and moisture; these are copied to the WRF grid data structure.
- The GOCART dust parameterization (inside of WRF/Chem) receives LIS porosity via the grid data structure, and uses this information to calculate dust emissions.
- GOCART aerosols are passed via the grid data structure to the Goddard radiation scheme, and are used to calculate spectrum optical depths, single scattering albedos, and asymmetry factors in order to account for aerosol direct effect.
- GOCART aerosols are also passed via the grid data structure to the Goddard microphysics scheme, and are used in calculating cloud condensation nuclei and ice nuclei concentrations that affect activation of cloud droplets and ice particles in order to account for aerosol indirect effect.
- The WRF/Chem (Model of Emissions of Gases and Aerosols from Nature) MEGAN2 biogenic emission scheme (Guenther et al., 2006) has been modified to convert a portion of volatile organic compound emissions into secondary organic aerosols that are passed to the GOCART module.

All four NASA parameterization codes (aerosols, land surface, microphysics, and radiation) are sensitive to the state of the atmosphere (thermodynamics and dynamics); therefore all four will be affected by changes in that state due to altered radiative heating and flux (from the GOCART/Goddard radiation coupling), altered land surface processes (from the LIS/WRF coupling), and/or altered diabatic heating and precipitation processes and aerosol wet deposition (from GOCART/Goddard microphysics coupling) (Fig. 1). Indirect coupling also applies to the MEGAN2 parameterization, as biogenic emissions are partially a function of near-surface meteorological forcing (air temperature, downward solar radiation, etc.). Finally, changes in GOCART aerosol processes due to altered dust emissions (from the LIS/GOCART coupling) or altered biogenic emissions (from MEGAN2) will subsequently affect the Goddard microphysics and radiation calculations.

Since G-SDSU has its own I/O and parallel data decomposition, and since the G-SDSU products are purely diagnostic (no dynamic feedback to the WRF core), we found it unnecessary to couple with WRF as either an ESMF component or as a subroutine. Consequently we chose the WRF NetCDF file format as a one-way coupling mechanism from NU-WRF to G-SDSU in an off-line manner.

#### 4. NU-WRF repository management

The NU-WRF project uses the Subversion revision control system (SVN; see http://subversion.apache.org) to manage the

software. The repository trunk stores the main development path of NU-WRF, including the NWP model proper, LIS, G-SDSU, and various pre- and post-processors. Automated regression tests are performed from the trunk: checkouts and compilations occur nightly, and model runs for a number of use cases are performed weekly. As key milestones are reached, snapshots of the trunk are tagged and become releases (developmental, beta, or official).

When a new version of community software becomes available, we import it into SVN as a special vendor branch. An experimental branch is then forked from the trunk, and a 3-way merge is performed using SVN to absorb vendor changes and automatically detect conflicts with NASA changes. After conflicts are resolved and binaries are built, the use cases are reprocessed with the latest code and the weekly regression tests are performed. If all tests pass, the experimental branch is then merged back into the trunk.

To ease compilation, NU-WRF uses a unified build system written in the bash scripting language. These scripts allow the user to easily specify targets, and automatically check and resolve library dependencies between packages. The bash scripts interface with the native compilation systems for each package (e.g., simple Makefile for GEOS2WRF, a customized Perl script and special environment variables for WRF); this reduces the steps and details the user must handle. However, users must still specify paths to third-party libraries (netCDF, HDF4, etc.) and may need to modify the build system if porting to a new computer system or switching compilers.

#### 5. Computational performance

To demonstrate the computational costs of running NU-WRF, we ran the model using a 200  $\times$  200  $\times$  61 4-km resolution grid for a severe weather case (0000 UTC 10 April-0000 UTC 11 April 2009 over the southeastern U.S.). In all runs the model used an 8s time step with Goddard microphysics and radiation, the Grell-3 cumulus parameterization (Grell and Devenyi, 2002), the Mellor-Yamada-Janjic PBL scheme (Janjic, 2002), the Noah land surface model (Ek et al., 2003), and initial and lateral boundary conditions from the National Weather Service North American Mesoscale model. We varied the number of computer processors, the use of LIS-WRF coupling, and the use of GOCART coupled with the microphysics and radiation. All runs were conducted on the NASA GSFC Discover supercomputer, using 12-core nodes with Intel 2.8 GHz Xeon Westmere processors and interconnected with DDR InfiniBand fabric. NU-WRF was compiled using Intel 12.1 Fortran and C compilers and run using Intel MPI 4.0.1.

Fig. 3 shows a comparison of the execution times as a function of processor number. Significant reductions in execution time — nearly linear in log-space — are achieved by using up to 192 processors. Compared to the basic NU-WRF run (similar to the community WRF), the LIS coupling adds approximately 6%—10% overhead. Using the GOCART aerosol physics adds a 77%—80% overhead compared to the basic NU-WRF. Finally, using GOCART and LIS together adds 79%—90% more wallclock time.

#### 6. Model testing and verification

As described above, each individual component of NU-WRF (e.g., LIS, GOCART, WRF) had been extensively evaluated and tested, with resulting publications, prior to incorporation into NU-WRF. Therefore, our model testing strategy focused on two aspects: testing the software to enable two-way coupling between components, and testing the entire system using a case study approach.

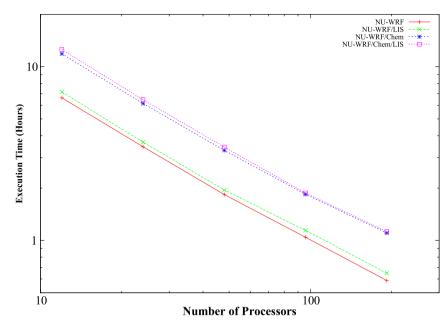


Fig. 3. Computational scaling of NU-WRF system comparing runs with and without LIS coupling and chemistry for a domain of 200 x 200 x 61 grid points at 4-km resolution

#### 6.1. Two-way coupled tests

As shown in Fig. 1 and discussed in Section 3, the major couplings between components include the LIS-WRF coupling, LIS-GOCART, GOCART-radiation, GOCART-microphysics, and microphysics—radiation couplings. For each pair, we simply verified that the required input and output variables, accounting for units and direction conventions, were passed between these modules. Once all of these coupling tests were passed, we proceeded to the system tests using case studies.

#### 6.2. System tests using case studies

As shown in Table 4, we defined 10 "use cases" for use as system tests to evaluate the scientific credibility of the NU-WRF system. As discussed in Laniak et al. (2013) model evaluation should include the attributes of transparency, refutability, and uncertainty quantification. In our case, we support transparency by making every use case available to the entire team through a shared use case repository. To address refutability, we discuss several science results in the next section resulting from hypotheses that the NU-WRF system simulates observed atmospheric states better than the default WRF model (e.g., Zaitchik et al., 2013; Shi et al., 2014). We did not undertake formal uncertainty quantification, although some work along those lines is ongoing through the LIS Uncertainty Estimation subsystem (e.g., Harrison et al., 2012; Santanello et al.,

2013a). These cases were all the subject of previous work using the standard WRF model, so the system tests focused on ensuring that the model behavior was better than and/or comparable to previous results. These tests were executed in the NU-WRF default configuration, which typically involved 1 km grid spacing, 64 vertical levels, the MYJ PBL scheme, the LIS/Noah LSM, Goddard microphysics and radiation schemes, and GOCART as needed.

#### 7. Science results

In this section we present some examples of the scientific studies and simulations enabled by NU-WRF. As discussed previously, the primary motivation for NU-WRF is to support integrated modeling of aerosol, cloud, precipitation and land processes at satellite-resolved scales. Science questions related to these processes include:

- What are the critical feedbacks in the coupled land—atmosphere system?
- 2. How sensitive is tropospheric chemistry to land surface processes and parameters?
- 3. What are the magnitudes of aerosol direct and indirect effects on radiation and microphysical processes?

Below, we highlight studies that have addressed these science questions related to land—atmosphere feedbacks that maintain

**Table 4** NU-WRF use cases used for system tests.

Case Name	Date(s)	Components tested
California snow C3VP lake effect snow Real-time NSSL, SE US tornado/large hail outbreak Real-time NSSL, Central US Tornado outbreak Southern Great Plains extended drought Very dry/mostly clear sky with deep PBL growth	00Z 30 December 2005–00Z 1 January 2006 12Z 19 January 2007–00Z 23 January 2007 00Z 10 April 2009–12Z 11 April 2009 00Z 28 March 2007–12Z 29 March 2007 00Z 1 April 2006–00Z 1 August 2006 00Z 14 July 2006–00Z 15 July 2006	Land-Radiation-Microphysics Land-Radiation-Microphysics Land-Radiation-Microphysics Land-Radiation-Microphysics Land-Radiation-Microphysics Land-Radiation-Microphysics
GOCART WRF/Chem test case  Hurricane Wilma Typhoon Morakot	00Z 1 January 2006–00Z 2 January 2006  00Z 18 October 2005–00Z 25 October 2005  00Z 7 August 2009–00Z 11 August 2009	All (Land—Radiation—Microphysics— GOCART) All All

drought, land-PBL-chemistry interactions, and the role of dust and aerosols in radiation and microphysics. Finally, we also discuss results from the use of satellite simulators for model evaluation.

#### 7.1. Land-atmosphere interactions and drought

Building on the work of Santanello et al. (2009), NU-WRF has been implemented as a testbed for land—atmosphere interaction and coupling (LoCo) studies given its unique land surface and Planetary Boundary Layer (PBL) scheme options, allowing for the processes and feedbacks generated by different LSM-PBL couplings to be evaluated and contrasted (Santanello et al., 2011). The unique flexibility and coupling between LIS and WRF have been employed to show that dry regimes are more sensitive to the land surface physics than wet regimes, and to evaluate how particular LSM and PBL schemes perform during flood and drought conditions (Santanello et al., 2013b).

Previous studies with LIS-WRF coupling have shown the impact of land surface spinup on coupled prediction. Initialization of the land surface using LIS was used to improve sea-breeze circulation and 2-m temperature forecasts over Florida (Case et al., 2008). Additionally, a measureable impact of the soil moisture state was demonstrated on the coupled near-surface, PBL, and warm-season precipitation predictions in NU-WRF over the Southeastern U.S., resulting in improvement over that using a default land initialization in WRF (Case et al., 2011). Likewise, the LoCo methodology has been used to quantify the impact of LSM calibration on coupled forecasts, and to show that predictions can be improved by combining mesoscale observations with the optimization subsystem within LIS (Santanello et al., 2013a).

Studies of prolonged drought have demonstrated that NU-WRF is an appropriate tool for extended climate-scale simulations and seasonal prediction, including feedbacks between soil moisture anomalies, land surface conditions, and atmospheric response (Zaitchik et al., 2013). As part of this work, a simple soil moisture-albedo feedback was implemented into the Noah LSM, and it was found that both the soil moisture/humidity and soil moisture/albedo feedbacks were required in order to produce the observed precipitation anomaly during a drought period in the U.S. Southern Great Plains. More recently, Kumar et al. (2014) have shown that soil moisture and snow assimilation in LIS can have impacts on drought monitoring. This work suggests that assimilation of soil moisture and snow can substantially impact drought forecasts as well.

#### 7.2. Land-chemistry interactions

NU-WRF also allows for coupled interactions between the land. PBL, and chemistry to be quantified at the process-level. The coupled model has been applied to study the impact of vegetation classification on PBL development and air quality (e.g. ozone) (Z. Tao et al., 2013a,b). It was found that NASA's MODIS Land Use Land Cover (LULC) dataset estimates a doubling of urban area relative to the standard WRF USGS dataset circa 1993 (115,600 vs. 42,400 km<sup>2</sup>). A weeklong simulation reveals that this increased urban area results in over 1 K warmer temperatures and more than 100 m deeper Planetary Boundary Layers (PBLs) on average as compared to simulations using the standard US Geological Survey (USGS) LULC data. As a result, the average surface NO<sub>2</sub> concentration decreases by 13% while 8-hour-average ozone concentration increases by 3%. Overall, increased urban LULC tends to produce lower surface NO<sub>2</sub> concentrations due to deeper PBLs but generates more frequent high surface ozone events as a result of higher temperatures.

#### 7.3. *Dust*—aerosol—microphysics—radiation interactions

Aerosols affect the Earth's radiation balance and precipitation process directly and indirectly through direct radiative heating as well as indirect cloud microphysics-macrophysics modulation via the activation of Cloud Condensation Nuclei (CCN) and Ice Nuclei (IN). Shi et al. (2014) conducted a study of aerosol-microphysics-radiation coupling, including Goddard microphysics and radiation schemes within NU-WRF. Fully coupled NU-WRF simulations were conducted for simulating various aerosols and a mesoscale convective system (MCS) that passed through the Niamey, Niger area on 6–7 August 2006 during an African Monsoon Multi-disciplinary Analysis (AMMA) special observing period. The NU-WRF simulation shows that aerosol indirect effect tends to slightly reduce total rainfall regardless of the aerosol direct effect. Results also showed the aerosol direct effect, mainly due to mineral dust, had the largest impact near cloud tops just above 200 hPa where short-wave heating increased by about 0.8 K day<sup>-1</sup>; the weakest long-wave cooling was at around 250 hPa. Large concentrations of aerosol-induced CCN and IN tend to increase total amounts of all hydrometeor mass concentrations, because of reduced precipitation process. The aerosol direct effect acts to reduce precipitating cloud particles (rain, snow and graupel) in the middle and lower cloud layers while increasing the nonprecipitating particles (ice) in the cirrus anvil. When the aerosol direct effect was activated, regardless of the indirect effect, the onset of MCS precipitation was delayed about 2 h. Overall, for this particular environment, model set-up and physics configuration, the effect of aerosol radiative heating due to mineral dust overwhelmed the effect of the aerosols on microphysics in terms of timing of surface precipitation.

#### 7.4. Integrated model evaluation through satellite simulators

Earth system modeling has become more complex, and its evaluation using satellite data has also become more difficult due to model and data diversity. Matsui et al. (2014) demonstrated multisatellite, multi-sensor radiance-based evaluation methods for NU-WRF simulations. A case study was conducted over West Africa using NU-WRF (Shi et al., 2014) to simulate coupled aerosol-cloudprecipitation-land surface processes on the storm-resolving scale. NU-WRF simulated geophysical parameters were then converted to the satellite-observable raw radiance and backscatter from the A-Train Constellation satellites (Aqua MODIS, Aqua Advanced Microwave Scanning Radiometer - Earth Observing System (AMSR-E), CloudSat Cloud Profiling Radar (CPR), Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP)) and the geostationary Meteosat Second Generation satellite (MSG-1) Spinning Enhanced Visible and Infrared Imager (SEVIRI) under the consistent physical assumptions provided by G-SDSU, described above. This unique multi-sensor, radiance-based evaluation method revealed NU-WRF forecast and model physics biases through the spatial and statistical interpretation of various satellite raw radiances: infrared (IR) brightness temperature (Tb) for surface skin temperature and cloud-top temperature, microwave Tb for precipitation, ice and surface flooding, and radar and lidar backscatter for aerosol-cloud profiling. Although this unique radiance-based evaluation relies on the understanding of radiance and backscatter characteristics at different wavelengths and different sensor platforms, it allows more complete assessment of Earth system modeling without relying on the assumptions of remote sensing retrievals.

As shown in Matsui et al., 2014, unique information is available from satellites that is not only useful in sparsely observed regions, but also for providing a simultaneous measurement of coupled

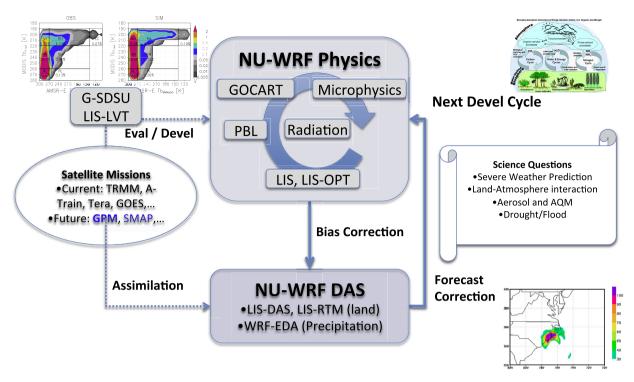


Fig. 4. Schematic NU-WRF components, including the developing NU-WRF Data Assimilation System (DAS), illustrating how the DAS and G-SDSU will provide feedback to the physics by characterizing errors.

processes. For example, combined Aqua microwave and infrared brightness temperatures allow joint diagnosis of fractions of raining and nonraining, low, middle and high clouds, and illustrated that the NU-WRF system severely overestimates nonraining high clouds and underestimates nonraining low clouds in a particular case study. This detailed diagnostic information then allows microphysics developers to better isolate physics issues, and thereby improve the modeling system.

#### 8. Summary and future directions

NU-WRF is a superset of the community WRF and features enhanced physics coupling and optimal use of satellite data to support advanced regional Earth system modeling. Various assets of GSFC including LIS, Goddard radiation and microphysics packages and coupling, and GOCART components are under active development. Enhancements in progress include i) upgrading microphysics in to a new 4ICE (cloud ice, snow, graupel, and hail) microphysics scheme to seamlessly simulate tropical and midlatitude systems without arbitrary changes in the scheme (Lang et al., 2014); ii) development of high-resolution dynamic dust erosion/emission sources; iii) development of irrigation modeling closely following Ozdogan et al. (2010) and Evans and Zaitchik (2008); iv) further optimizing the computational speed of the Goddard radiation scheme; and v) updating the land surface models in LIS to include the Noah land surface model with multiparameterization options (Noah-MP; Niu et al., 2011; Yang et al., 2011) as well as the latest version (4.0) of the NCAR Community Land Model (CLM; Lawrence et al., 2011; Oleson et al., 2010). These physics, computational, and database updates will enhance the science capability of the NU-WRF system, and will eventually contribute to the community WRF as well (as was the case already for Goddard radiation).

More importantly, we emphasize on-going development of an advanced high-resolution satellite data assimilation system that takes advantage of various new satellite data. On the land surface

side, we will build on the ensemble land data assimilation capabilities in LIS (LIS-DA) to incorporate satellite-based land surface products such as albedo, irrigated area, soil moisture, snow, and surface temperature. New land surface model physics with prognostic phenology schemes, photosynthesis-based canopy conductance and prognostic water table variables (e.g., Noah-MP and CLM), will support assimilation of additional satellite datasets such as Leaf Area Index (LAI) and terrestrial water storage. On the atmospheric side, we will build on the recently developed Maximum Likelihood Ensemble Filter (MLEF)-based WRF Ensemble Data Assimilation System (WRF-EDA) system to ingest information from in situ and satellite observations including cloud-precipitationaffected satellite-observed radiances. This WRF-EDA system has been shown to produce dynamically downscaled precipitation products with performance that is equal or superior to the WRF-GSI. In this manner, NU-WRF will continuously support upcoming satellite missions with the goal to improve model physics and prediction (Fig. 4): the Global Precipitation Measurement (GPM: just launched in February 2014), Joint Polar Satellite System (JPSS, launched 2013), Soil Moisture Active Passive (SMAP, planned 2014), and Geostationary Operational Environmental Satellite-R (GOES-R, 2015) missions. The use of satellite data to improve models in a research setting is an area ripe with opportunity, yet still in its infancy, despite the widespread use of data assimilation in operational numerical weather prediction. In contrast, the NU-WRF philosophy is to "learn" from the satellite data through the use of satellite simulators as an evaluation tool, and through combined optimization and data assimilation capabilities. In so doing, we maximize the return on the investment for NASA's satellite programs.

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