New Datasets: GEOS5, MERRA HIPPO/ Ozone

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> Meteorological data set available for offline modeling

New data set available for model evaluation





GEOS5, MERRA

GEOS5: gridded output files from version 5 of the Goddard Earth Observing System Data Assimilation System (GEOS-5 DAS)

- GEOS5.1: 2004-Sep 2008, 6h
- GEOS5.2: Oct 2008 present

MERRA: Gridded output files from the Modern Era Retrospective-analysis for Research and Applications (MERRA) of the Goddard Earth Observing System Data Assimilation System (GEOS DAS), :

- 1979-present, 6h
- Original horizontal resolution: 0.5x0.6, 72lev vertical hybrid levels
- Interpolated horiz. resolutions: 1.9x2.5

interpolation is performed using a mass conserving interpolation by S.-J. Lin)





Variable (M74 / CEOS5)	Di	CAM-MZ4-NCEP		GEOS5	
Variable (WIZ4 / GEOSS)	m	name /units		name / units	
Zonal wind	3D	U	$m s^{-1}$	U	$m s^{-1}$
Meridional wind	3D	V	$m s^{-1}$	V	$m s^{-1}$
Temperature	3D	Т	Κ	Т	K
Surface temperature	2D	TS	Κ	TSKIN	K
Surface pressure	2D	PS	Ра	PS	Pa
Specific humidity (optional for MZ4)	3D	Q	kg kg ⁻¹	QV	kg kg ⁻¹
Land/Ocean/Sea Ice flag	2D	ORO		LWI	0=water, 1=land, 2=ice
Surface geopotential height	2D	PHIS	$m^2 s^{-2}$	PHIS	$m^2 s^{-2}$
Surface zonal (eastward) stress	2D	TAUX	$N m^{-2}$	TAUX	$N m^{-2}$
Surface meridional (northward)	2D	TAUY	$N m^{-2}$	TAUY	$N m^{-2}$
stress					
Surface heat flux /	2D	SHFLX	$W m^{-2}$	HFLUX	W m-2
Sensible heat flux					
Surface moisture flux /	2D	QFLX	$kg m^{-2} s^{-1}$	EVAP	$kg m^{-2} s^{-1}$
Evaporation from turbulence					
Solar flux at surface / Surface	2D	FSDS	$W m^{-2}$	SWGDWN	$W m^{-2}$
downward shortwave flux					
Snow height / Snow depth	2D	SNOWH	m	SNOMAS	$kg m^{-2}$
Soil moisture fraction	2D	SOILW	fraction		
Top soil layer wetness	2D			GWETTOP,	fraction
root zone soil wetness				GWETROOT	

ORO is calculated using the Landfrac from CAM and the TS (TS < 271.15 EQ ICE)





GEOS5, MERRA

- GEOS5.1 linear interpolation in space and time for surface values (as used in recent simulations)
- GEOS5.1 mass conserving interpolation





Comparison with ARCTAS Interpolation on the flight track using 3h output







Comparison of simulations using GEOS5 and GEOS5 (linear)

Ozone

O3 [mol/mol], 05May2008 12:00, Ion average





GEOS5, MERRA

CAMChem Simulation (prelim. results) using GEOS5 and MERRA compared to observations





Applications: Offline model simulations to support field campaigns

SF

GEOS5, MERRA

How to get those data?

- ESG: <u>http://www.earthsystemgrid.org</u> Under CCSM 4 Model Output
- Mass Store: /TILMES/GEOS5/05x06 /TILMES/GEOS5/19x25 /TILMES/MERRA/05x06 /TILMES/MERRA/19x25
- Glade Disc on bluefire:

/glade/proj3/cseg/data_tmp/





Available Datasets for Model Evaluation

- Model Chemistry Evaluation Program (MCEP) available at the Climate-Chemistry Working Group website
- HIPPO Aircraft Data
- New Ozone Climatology





HIPPO HIAPER Pole to Pole Observations



NESL

RAF Field project, PI: Prof. Steve Wofsy

NSF/NCAR GV



HIPPO_3 Mar/Apr 2010 (same track NB, SB)

HIPPO_4 Jun 2011 (NB track via E. Pacific)

HIPPO_5 Sep 2011 (NB track NB, SB)

~ 600 vertical profiles







HIPPO Aircraft Instrumentation

Harvard/Aerodyne - QCLS	CO ₂ , CH ₄ , CO, N ₂ O (1 Hz)
NCAR AO2	$O_2:N_2, CO_2 (1 Hz)$
Harvard OMS CO ₂	CO ₂ (1 Hz)
NOAA CSD O ₃	O ₃ (1 Hz)
NOAA GMD O ₃	O ₃ (1 Hz)
NCAR RAF CO	CO (1 Hz)
NOAA- UCATS, PANTHER GCs (1 per 70 – 200 s)	CO, CH ₄ , N ₂ O, CFCs, HCFCs, SF ₆ , CH ₃ Br, CH ₃ Cl, H ₂ , H ₂ O
Whole air sampling: NWAS (NOAA), AWAS (Miami), MEDUSA (NCAR/Scripps)	$O_2:N_2$, CO_2 , CH_4 , CO , N_2O , other GHGs, CO_2 isotopes, Ar/N_2 , COS, halocarbons, solvent gases, marine emission species, many more
Princeton/SWS VCSEL	H ₂ O (1 Hz)
NOAA SP2	Black Carbon (1 Hz)
MTP, wing stores, etc	T, P, winds, aerosols, cloud water
Simone Tilmes, Chemistry-Climat	e Working Group Meeting, 16. March 2011

Ozone Climatology (1995-2009)





WOUDC, Shadows, NOAA





Simone Tilmes, Chemistry-Climate Working Group Meeting, 16. March 2011

Tilmes et al., in preparation













NESI

HTAB Models



HTAB Models

S

800hPa







Questions?











Running CAMchem

- > Available Compsets
- Setup of the simulation
- Changes to the simulation
- Latest Developments





Compsets	Model (phys)/ radiation	Chemistry	Components / Meteorology
B_2000_TROP_MOZART (BMOZ) F_2000_TROP_MOZART (BMOZ) F_2000_CAMCHEM (FCHM)	CAM4, active CAM4, passive CAM4, passive	trop_mozart trop_mozart trop_mozart +	All active Prescr. ocn/ice, CLM dry dep Prescr. ocn/ice, CLM
		Neu wet dep	MEGAN VOC emis





Compsets	Model (phys)/ radiation	Chemistry	Components / Meteorology
B_2000_TROP_MOZART (BMOZ) F_2000_TROP_MOZART (BMOZ)	CAM4, active CAM4, passive	trop_mozart trop_mozart	All active Prescr. ocn/ice, CLM dry
F_2000_CAMCHEM (FCHM)	CAM4, passive	trop_mozart + Neu wet dep	Prescr. ocn/ice, CLM MEGAN VOC emis
F_SD_CAMCHEM (FSDCHM) F_SD_BAM (FSDBAM)	CAM4, passive	trop_mozart trop_bam	Prescr. ocn/ice, clm dry dep, offline: GEOS5 (56ley)
F_SD_WACCM_TSLT_GEOS5 (FSDWEG5)	CAM4, active	waccm_tslt	Prescr. ocn/ice, CLM MEGAN VOC emissions offline GEOS5 (88lev)





Compsets	Model (phys)/ radiation	Chemistry	Components / Meteorology
B_2000_TROP_MOZART (BMOZ) F_2000_TROP_MOZART (BMOZ)	CAM4, active CAM4, passive	trop_mozart trop_mozart	All active Prescr. ocn/ice, CLM dry
F_2000_CAMCHEM (FCHM)	CAM4, passive	trop_mozart + Neu wet dep	Prescr. ocn/ice, CLM MEGAN VOC emis
F_SD_CAMCHEM (FSDCHM) F_SD_BAM (FSDBAM)	CAM4, passive	trop_mozart trop_bam	Prescr. ocn/ice, clm dry dep, offline: GEOS5
F_SD_WACCM_TSLT_GEOS5 (FSDWEG5)	CAM4, active	waccm_tslt	Prescr. ocn/ice, CLM MEGAN VOC emissions offline GEOS5 (88lev)
B_2000_CN_CHEM (B2000CNCHM) B_1850_CN_CHEM (B1850CNCHM) F_1850_CN_CHEM (F1850CNCHM) B_1850-2000_CN_CHEM (B20TRCNCHM)	CAM4, active	super_fast_llnl	MEGAN VOC emis CLM dry dep, land nitrogen cycle
B_1850_CAM5 (B1850C5) B_1850- 2000_CAM5 (B20TRC5) E_1850_CAM5 (E1850C5) F_AMIP_CAM5 (FAMIPC5)	CAM5, active	MAM	
F_1850_CAM5 (F1850C5) F 2000_CAM5 (FG5) F 5 L	nate Working Group Meetin	g, 16. March 2011	NSF

Available Compsets

•/acd/fvitt/cesm/cesm1_0_beta12_chem (intern)

•svn co<u>https://svn-ccsm-</u>

models.cgd.ucar.edu/cesm1/exp_tags/cesm1_0_beta12_chem01





Setup of a Simulation

Run the model out of the box (using an existing Compset)

- Create a new case called <case_name>:
 - CESM_ROOT = /acd/fvitt/cesm/cesm1_0_beta12_chem (intern)
 Go to your model directory CESM_ROOT, then cd scripts and invoke:
 - create_newcase -case \$HOME/<case_name> -res f19_f19 -compset \$COMPSET -mach bluefire (change 'bluefire' to your computer name)

f19_f19: data ocean (finite volume of the atmosphere); f19_g16: active ocean

- A new directory <case_name> is created in your <home_dir> (below, <case_dir> is <home_dir>/<case_name>)
- (Make changes to defaults)
- Configure the case, in <case_dir>: configure -case
- Build the model: ./*.build file
- Run the model: bsub < ./*.run (or ./*.submit) for bluefire
 - model output is in <run_dir>: /ptmp/<username>/<case_name>/run
 - namelist that was used for run in <run_dir>/atm_in
- Archiving:
 - short-term archiving in /ptmp/<username>/archive
 - long-term archiving on the mass store





Setup of a Simulation

Modification to the Simulation:

- env_conf.xml, env_build.xml, env_run.xml, env_case.xml, env_mach_pers.xml
- *.run to change run specific parameters (length per segment, account number)





Setup of a Simulation

Modification to the run (no changes to the model configuration):

• env_run.xml: change run specifications, run time, output, restart etc.,

- CONTINUE_RUN: needs to be set to TRUE to continue a run
- RESUBMIT: set value to the number of segments you want to run (value counts down during the simulation)
- REST_OPTION: will write out restart files in the frequency chosen
- REST_N: frequency of restart file output (0: no restart file)
- DOUT_L_MS: archiving to mss is not a default and needs to be set
- *.run to change run specific parameters (length per segment, account number)
- after these changes you can just resubmit the run





Changes to the Simulation

Modification to the namelist (f.ex. model output, emission, met field)

(http://www.cesm.ucar.edu/cgi-bin/eaton/namelist/nldef2html-pub)

- cp user_nl_cam to your <case_dir>,
- edit user_nl_cam in your <case_dir>
 - fincl ...
 - ncdata: initial condition file
 - met_data_file, met_data_path (meteorology)
 - bnd_topo (boundary conditions for offline model runs)
 - srf_emis_specifier (emissions)
 - srf_emis_type = 'CYCLICAL' ; srf_emis_cycle_yr = 2000
 - for SERIAL 'srf_emis_cycle_yr' this is not allowed
 - srf_emis_type = 'FIXED'; srf_emis_fixed_ymd = 20000101 for
 - &satellite_options_nl: sathist_fincl, sathist_hfilename_spec, sathist_track_infile
 - configure –cleannamelist to unlock env_conf.xml
 - configure –case in your <case_dir> (you do not need to rebuild the model)
 - run the model





Changes to the Simulation

Modification to your configuration: env_conf.xml

- edit env_conf.xml in your <case_dir>
 - RUN_STARTDATE: change start date of the simulation (including possible changes to the namelist)
 - CAM_CONFIG_OPTS:
 - change vertical levels (-offline_dyn –lev nn)
 - modify chemical mechanism (-usr_mech_infile)
- configure –cleannamelist to unlock env_conf.xml
- configure –case in your <case_dir> (you do not need to rebuild the model)
 run the model





Changes to the Simulation

Modification of your calendar option: GREGORIAN/ NO_LEAP

- edit env_run.xml
 - change CALENDAR value = "NO_LEAP" to "GREGORIAN" default for SD model runs is "GREGORIAN", else it is "NO_LEAP"
- edit env_build.xml in your <case_dir>
 - calendar option: set USE_ESMF_LIB to TRUE
 - invoke *.clean_build
 - build your model again: invoke *.build





Latest Developments

- Specified Dynamics Compets for CAM-chem/ WACCM
- History sampling along observation tracks
 - Satellite track (more than one dataset can be included)
 - Aircraft flight path
- Local time averaging history output (C. Bardeen)
- Other updates





History sampling along observation tracks

Tracking file determines sequence of coordinates and time

- Uses nearest model time: maximum deviation from observation time is +/- half the time step of the current model time
- Uses nearest lon/lat model coordinate to the observed values



Horizontal grid distributed across MPI tasks

History sampling along observation tracks

Tracking file determines sequence of coordinates and time

- Uses nearest model time: maximum deviation from observation time is +/- half the time step of the current model time
- Uses nearest lon/lat model coordinate to the observed values







Local Time Averaging

Namelist settings: avgflag_pertape = 'A','L' fincl2 = 'Q','T','PS' lcltod_start = 0,0 lcltod_stop = 0,7200





Updates

MOZART4 Chemistry: trop_mozart (103 species)

- Including HCN, $CH_3CH + C_2H_2$, HCOOH

Emissions in trop_mozart (thanks to Louisa Emmons)

- Anthropogenic: POET, with REAS over Asia (time-varying for 1997-2010; 1997 used for 1992-1996).
- Biomass burning: GFED-v2 1992-1996: avg of 1999-2007; 1997-2008: for each year/month; 2009-2010: FINN.
- Biogenic, soil, ocean, volcano: POET, GEIA, etc. as described in Emmons et al., 2010.

Improved Climatology for the Stratosphere (O₃, NOy, CH₄, CO) Time dependent 3D chemistry sources aircraft emissions





Questions?



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