APPENDIX A – Summary of physics parameterizations in CAM and WRF

CONTENTS

0) Common requirements for scientific functionality

In CAM, all physics packages must be able to record their net forcing on the output history files. This is necessary for diagnostic purposes. It follows that all packages must calculate a tendency, regardless of whether they use a forward or backward step internally. These requirements, which are enforced by the interface design, can be summarized:

- Physics packages must not change the model state.
- Physics packages must return tendencies for any model state variables that they wish to change.

The following set of requirements are not enforced by the interface, but must instead be enforced by the mathematical formulation and the algorithm design of each physics parameterization.

All column physics packages are required to conserve the vertical integral of:

- the mass of each constituent (including sources and sinks)
- momentum (including boundary forces)
- total energy (including boundary fluxes)
- dry static energy (including boundary fluxes and kinetic energy dissipation)

The interface design requires that each column physics package which produces a mass, momentum, or energy tendency must provide any boundary forces or fluxes associated with those tendencies so that the appropriate balance can be checked in the physics module.

In WRF physics also provides tendencies rather than updating state variables when it comes to PBL, radiation, cumulus parameterization, and sub-grid turbulence schemes. Thesetendencies are provided to the solver which advances the model by one time-step per call. However, there are two exceptions:

1. Land surface (which one may not be considering as part of the physics) that updates its own land state variables directly.
2. Microphysics is done as an adjustment at the end of the model step in the solver, and so also directly updates state variables. This is done to ensure saturation adjustment which is part of the microphysics is accurate.

Apart from microphysics, the physics is all added concurrently, so there is no other splitting for physics.The physics tendencies are kept constant during the three Runge-Kutta steps during which only dynamics and advection tendencies change on each step. The microphysics is applied only after the last RK step.

WRF has options to call physics less frequently than the model step, in which case the tendency is keptfixed between calls. This is mostly done for radiation, and possibly for cumulus parameterization, but is rarely, if ever, done for PBL/land physics, and cannot be done for microphysics.

Regarding conservation, WRF does not have a rigorous standard that is tested, but minimally expects that total water is conserved by physics processes, and accounting for rainfall.

1) Radiation- Dudhia, Conley

CAM and WRF require representations of the following from other parts of the code.

- Solar and Microwave background radiance (top boundary condition)
- Surface SW and LW albedo and emission (bottom boundary condition)
- Thermodynamic state of the atmosphere
- Atmospheric gaseous composition
- Condensed liquid water concentration and size distribution of droplets
- Condensed ice concentration and microphysical state
- Aerosol droplet concentration and microphysical state and composition

Mie theory is applied (offline) to the condensed liquid water and aerosol droplets to construct tables of optical properties. Typically each aerosol (or size-bin of aerosol) has a fixed size distribution. Consistent specification of size distribution, chemical composition, and microphysical state between transport, microphysics, and optical assumptions is an ongoing struggle, as is the simplification from real-world conditions (complex internally mixed aerosols) to model representations.

Ice optical properties are typically derived from specialized ice optical codes (e.g. MADA)

Simplified representations of optical properties are derived from line-by-line databases of gas optical properties (Hitran).

Current Capability:

WRF :

- LW: RRTM, CAMRT, GFDL(NCEP)
- SW: GFDL, CAMRT, Dudhia, Goddard

CAM:

- RRTMG from AER
- CAMRT customRadiative Transfer Code (Kiehl / Briegleb)

CAM/WRF Overlap:

Incompatible requirements:

Cloud Fraction specification in CAM leads to concept of subcolumns. While subcolumns can be useful for some of the coarser resolutions of WRF, subcolumn specifications based on cloud fraction are not used on typical WRF horizontal scales. CAM applies the subcolumns in a Monte-Carlo Independent Column Approximation (McICA).

McICA might be useful to both parameterizations for in-cloud variability.

CAM is often run for a much larger range of gas concentrations in paleo-climate simulations and for changes to greenhouse gas concentrations. Optical representations of gasses for WRF can typically be simplified. Typically, only H_2O and O_3 vary in a WRF simulation.

WRF is typically only run for vertical levels up to about 50mb. For climate simulations, better resolution of the stratosphere can be necessary for accurate estimation of top of atmosphere and tropopauseradiative forcing estimation.

WRF has representations of snow and graupel and rain.

In WRF-Chem, the MOSAIC aerosol parameterization is coupled with the Goddard shortwave radiation parameterization.

CAM-Chem uses the bulk aerosol module with a lower resolution of the size distributions of the aerosols.

WRF has been engineered to support different radiation parameterization. CAM has historically only supported on version.

Solar calendar for WRF supports both a CAM type calendar and a true calendar.

CAM is working toward including photolysis in it's computations. When photolysis is included, heating rates are no longer equal to flux divergence.

With smaller horizontal scales, the time step for WRF decreases. A rough estimate is that the timestep is 1 minute per km of resolution. This many calls to RRTMG may be too expensive, requiring a simplified computation for highly resolved computations.

WRF assumes an isothermal layer above 50mb.

Different assumptions for the microphysics of ice and water are assumed in WRF and CAM. This leads to different optical parameterizations.

WRF uses both orographic shading and slope effects. CAM does not.

<u>Towards 100K+ processors:</u>

In highly horizontally resolved simulations, three dimensionalradiative transfer may be necessary.

The large memory size of the optical parameters does not scale.

Radiative transfer computations inherently couple vertical levels, making vertical domain decomposition more difficult.

Implementation of an on-line size-integrated Mie computation or initialization-time size-integrated Mie computation could provide a significant increase in flexibility for microphysical representations of condensed species.

<u>Requirements for scientific functionality</u>:

Radiation parameterization should compute direct and diffuse

- Upward
- Doward

fluxes at

- Top of Atmosphere
- Top of Model
- Tropopause
- Surface

using the solar and surface boundary conditions.

An Independent Column Approximation should support both in-cell and in-cloud variability of clouds.

Heating rates should accurate for the composition specified.

Mie computations should be based on the microphysical assumptions elsewhere in the model. And they should be traceable to all external data and methods.

Gas optical parameterizations should be based on line-by-line databases.

Radiative forcing of gasses and aerosols should be comparable to line-by-line RT codes

<u>Metrics for evaluation:</u>

- Comparison with line-by-line RT models
- Each gas forcing should be compared with reference computations
- Aerosol forcings should be compared with AEROCOM
- Cloud forcing should be compared with satellite and ground observations

MB: Aerosol-Radiation Interactions

In WRF-Chem, aerosols can affect the radiation scheme. The MOSAIC aerosol parameterization is coupled with the Goddard shortwave radiation parameterization using aerosol optical depth, single scattering albedo, and asymmetry factor derived from MOSAIC particulates and Mie theory (Ghan et al., 2001b).

2) PBL - Dudhia, Large

Current Capability:

WRF :

- YSU
- MYJ (NCEP) prognostic TKE MY2.5
- Asymmetric Convective Model (ACM) Blackadar upward, local downward.

CAM:

- HotlslagBoville
- Modified Holtslag-Boville , imposing entrainment
- UW diagnostic TKE MY2.0
- Thin lowest layer (~20m) < canopy height

Both models have a variety of PBL schemes representing a range of methods.

CAM/WRF Overlap:

PBL eddies are sub-grid scale to all current CAM and WRF applications, and therefore the schemes need to represent the same processes in both models. Likewise there are similar needs as both models are applied in a range of environments, including extreme conditions from stable Antarctic to unstable ITCZ and deep dry mixing over the Sahara.

Both models need the same types of surface forcing functions e.g. bulk transfer schemes, and the same similarity ideas and stability functions.

Hurricane interaction is important in both models when run at comparable scales. This particularly relates to the treatment of surface fluxes over water in extreme wind conditions (e.g. the effects of waves and sea spray).

Ocean coupling for climate or regional climate has overlapping requirements in the PBL scheme, and needs an ability to take and provide fields for coupling, such as stresses and fluxes.

Cloud top strato-cumulus is a complicating factor affecting the performance of PBL schemes, and is a common problem in weather and climate models.

A goal would be for WRF and CAM to have the same suite of optional schemes, with resolution dependent parameters a possibility based on evaluation.

Incompatible requirements:

WRF in the future will be sometimes run at scales down to LES (~100 m grids), and if this is a need for ESM, sub-grid three-dimensional turbulence would need to take over the role of the PBL scheme (which are basically one-dimensional), as another option. WRF already has such an LES capability in simple form.

Hurricanes at cloud-resolving resolution are sensitive to formulations of sea-surface momentum and enthalpy fluxes at high winds, and so WRF has some options designed for such extremes that may not be needed for larger grid sizes.

Towards 100K+ processors:

PBL schemes are fundamentally easily balanced and scale well, because they are columnwise independent, typically not computationally intensive, and floating-point operation counts are not highly variable from one column to another.

Requirements for scientific functionality:

- Accurate treatment of stable and unstable surface boundary layer.
- Conservation of energy and scalars.
- Provides exchange coefficients and surface air properties to land-surface scheme.
- Provides fluxes/stresses for potential coupled ocean scheme.
- Provides vertical mixing coefficients for chemistry applications.
- Receives fluxes from land/ocean surface scheme (conserves fluxes).

Metrics for evaluation:

Both models have to output diagnostics of 2m temp and humidity, and 10 m winds, as key products of the simulations. Similarly evaluation metrics of these models would depend on data from global observations of these quantities, and so overlap exists in the kind of data required to evaluate the PBL schemes in both models.

3) Convection - Neale, C. Liu, Richter

Convection represents one of the most crucial processes in climate and weather problems across multiple time and space scales. It has a role to play on the scale of kilometers over a few hours, in the case of extreme precipitation event forecasts all the way to global climate changes problems, in the case of climate sensitivity experiments. It is clear that no one convective parameterization will perform adequately in addressing all these weather and climate problems and as such an NCAR-ESM should maintain a suite of parameterizations able to tackle the whole range of scales. The NCAR-ESM framework should also demand adequate transport properties by convection for trace species away from the surface and into the upper atmosphere.

Current capabilities:

A number of convective parameterization schemes are used with WRF and CAM relevant at horizontal scales ranging from <10 to 100s of kilometers. The capability of different schemes varies between those representing deep and shallow convection separately (in CAM) and those representing all convective processes (in WRF). Schemes include the Grell, Kain-Fritsch & Betts-Miller schemes in WRF and the Zhang-McFarlane, Hack and University of Washington (UW) schemes in CAM. WRF currently maintains the ability to run without convective parameterization at horizontal scales of 4km or less.

CAM/WRF overlap:

The different horizontal resolution and integration configuration (forecast versus climate mode) between WRF and CAM currently precludes a significant amount of overlap. However, following the development of high resolution (50km) CAM and CCSM integrations and the incorporation of the CART-ARM Parameterization Testbed (CAPT) capability in CAM it is conceivable that simulations in a common simplified forecast (little or no data assimilation) could be performed. An intensive observation period e.g., IHOP over North America, could be analyzed with a significant amount of overlap between both model configurations. Given the same initialization, horizontal grid-size and the choice of convective parameterization in the two models a useful intercomparison could proceed. Opportunities for overlap may also continue with the Nested Regional Climate Model (NRCM) framework where downscaling methods from a courser CAM model grid run on global scales are use to force a regional WRF simulation on a finer grid.

Incompatible Requirements:

The most significant incompatibility between the two model configurations is the need to maintain energy balance within individual parameterization schemes for long climate CAM integrations of several hundreds of years. An incompatibility also exists between the cloud-cover assumptions between the two models. WRF assumes individual grid boxes can either be totally cloudy or cloud free. CAM currently assumes partial cloudiness in grid-boxes determined primarily by relative humidity. This represents challenges in estimating cloud-overlap primarily for radiative and microphysical processes, but the configuration will also be important to the formulation of convective processes.

Towards 100K+ processors:

Convection parameterization schemes have traditionally been a diagnostic calculation in atmospheric columns independent from their nearest neighbors. Maintaining this paradigm should allow good scaling with many processors. It is conceivable that future paradigms for convection may require communication with immediate neighbors (e.g. slant-wise convection in frontal zones), but this is unlikely to restrict scaling to the same extent as is likely with current dynamical cores on regular latitude-longitude grids.

Requirements for scientific functionality:

(generally for parameterized convection?)

- Energy conserving
- Enthalpy conserving
- The ability to transport chemical species (mass fluxes)
- The ability to represent convective downdrafts
- The ability to represent convective momentum transports
- Microphysical representation sufficient to determine cloud water (amount/phase/drop-size)

Metrics for evaluation:

Direct (convection alone - mostly)

- Vertical heating rates and profiles (compare with TRMM/CLOUDSAT)
- Cloud top heights
- Rainfall rates (compare with standard rainfall datasets, NAR)
- Rainfall frequency, duration

Indirect (coupling with other processes)

- The amplitude and phase of the diurnal cycle over land (compare with IOP data)
- The representation of mesoscale structures during warm season rainfall events land (IHOP)
- The representation of convectively coupled wave structures over tropical oceans (including the MJO)
- Hurricane structure, initiation, track and intensity
- The representation of summer monsoonal systems (onset, strength and duration)
- Standard forecast skill evaluations, particularly of precipitation (WRF, CAPT)
- Convectively generated gravity waves in the stratosphere (obs??, WACCM)
- Acceptable errors when used in data assimilation exercises (DART)

4) Clouds / cloud microphysics - Morrison, Gettelman

Current Capability:

Currently, a bulk 2-moment 4-class microphysics scheme is available in CAM/CCSM. This scheme also includes cloud-aerosol interaction for warm (liquid) clouds. We will soon have cloud-aerosol interactions for ice in CAM (hopefully for CAM4). Several microphysics schemes are available in WRF, including 1-moment and 2-moment schemes. Cloud-aerosol interaction is included in the Lin et al. microphysics package as part of WRF-CHEM. We are currently working to extend cloud-aerosol interactions to the Morrison et al. two-moment scheme in WRF.

CAM/WRF overlap:

Treatment of several microphysical processes is similar between the WRF and CAM microphysics schemes, for example, collection of cloud water, autoconversion, evaporation of rain and snow, etc.

Incompatible requirements:

There are several important differences between the CAM and WRF microphysics.

- Cloud fraction is not considered in the WRF microphysics, but there is fractional cloudiness in CAM. This also impacts the bulk condensation/evaporation of cloud water which is based on saturation adjustment in both CAM and WRF.
- Assumption of homogeneous cloud/thermodynamic fields in the WRF microphysics. This follows on from (a). WRF assumes uniform properties in a column. Sub-grid distribution of cloud water is considered in CAM. This has critical implications for precipitation development because of its strong non-linearity with cloud water amount. We are currently doing further testing to determine the impact of other sub-grid distributions (e.g., rain) in the CAM microphysics.
- Ice deposition/sublimation is currently treated using saturation adjustment in CAM, in WRF it is treated explicitly using the grid-scale ice supersaturation derived from the predicted thermodynamic fields. Note that in CAM, we plan to address this issue in the near future to allow ice supersaturation and explicit calculation of vapor deposition.
- Precipitation is treated diagnostically in CAM, and prognostically in WRF. Diagnostic precipitation is used in CAM due to the relatively long (20-30 minute) time step (see below).
- WRF microphysics schemes typically include dense precipitation ice (graupel and/or hail), this is neglected in the current CAM microphysics.
- There are additional numerical considerations in CAM due to the long time step. Currently this is dealt with by sub-stepping the precipitation microphysics. These issues are not addressed in the WRF microphysics.

Toward 100K processors:

We do not foresee any problems with scaling these parameterizations to many 1000's of processors. Microphysics is a column process and does not need knowledge of adjacent columns.

<u>Requirements for scientific functionality:</u>

- Short Term Forecast Accuracy - Microphysics schemes should produce the correct distribution of precipitation and surface pressure in a short term forecast. This is particularly true (and is an end in itself), for NWP applications. However, short term accuracy can also be a necessary but not sufficient condition for getting the right solution to climate problems 'for the right reasons'. It is the essence of the 'seamless prediction' of climate. Deviations from short term forecast accuracy can be used to improve parameterizations.Note that this implies the availability of a data assimilation system. [We are assuming that this is treated elsewhere in the ESM discussion].
- Representing extreme events - Closely related to (a) for NWP. Schemes should reproduce infrequent but extreme events well (the tail of the PDF). For climate purposes this implies getting the climatological probabilities of extreme events correct. This is important on almost all prediction time scales (short, medium, seasonal, long term). Impacts of weather and climate are mostly dependent on extreme events, such as hurricanes, extreme precipitation events, droughts (extremely long periods without precipitation).
- Cloud-Aerosol Interaction Aerosols may significantly affect the water budget and evolution in clouds by modifying cloud properties. The most important implications of this are changes to cloud radiative properties (climate: CAM) and changes to precipitation (weather:WRF). It will be highly desirable for both climate and weather applications to include cloud-aerosol interaction. This is currently evolving in both CAM and WRF. The modification of precipitation and radiation may have substantially altered surface climate in the recent past, and may do so in the future. [See aerosol section as well].
- Cloud Radiative Forcing of Climate - Cloud radiative forcing is the largest atmospheric uncertainty in estimating future anthropogenic climate change. Cloud Forcing also has strong local and regional effects. Understanding how cloud radiative forcing is sensitive to microphysics is a key goal. Moving across scales with this forcing (see below) is a test of the robustness of the system.
- Benchmarking across scales - Ideally, microphysical formulations in GCMs should be scale independent. In practice, because they are often driven by small scale processes (upward motions in cloudy regions only), the grid scale does matter. The goal is to be able to use detailed and coarse parameterizations at different scales to test convergence. Developing a framework where it is easy to add and test a parameteization would allow testing for convergence, and testing across scales. Moving between time and space scales is good way of testing answers. Examples of doing this are through a sub-column generator that can drive WRF microphysics in CAM for example, or even test convective parameterizations against embedded cloud model results. [This is relevant for convection too].

Basic Requirements imply:

- Mass conservation - For climate application, one of the main requirements is strict energy and water mass conservation. Both the CAM and WRF 2-moment microphysics schemes described above apply strict conservation criteria so this should not be an issue. Advection of condensed species must also conserve mass and energy (moist static energy).
- Treatments of Precipitation - High-resolution NWP (and climate) applications will require rather sophisticated treatment of precipitation. This may include prognostic treatment of precipitation (due to importance of horizontal transport over fine scales) as well as inclusion of dense ice (graupel and/or hail). There is no theoretical or practical reason that prognostic precipitation could not also be used at lower resolution - diagnostic precipitation has traditionally been used because it is computationally cheaper than the prognostic treatment. Sub-steping and/or sub-columns are one way to deal with this.
- Sub-grid processes - Fractional cloudiness as well as consideration of sub-grid distributions of cloud water/ice/precip are viewed as being strongly desirable for lower resolution simulations. There is no reason that fractional cloudiness and sub-grid distributions could not be considered for high-resolution as well, although this has not traditionally been the case since they models have typically been used to simulate cloud systems that are well-resolved. However, recent work has begun to address these issues in the context of high-resolution models such as MMF, since they may be critical for representing climatically-important cloud types such as shallow cumulus even in cloud models with fairly high resolution (1-5 km).

We view consideration of these issues as very important not only at low resolution, but potentially at high resolution (1-5km) as well. Of course, the actual parameterizations of cloud fraction and sub-grid distributions will vary significantly with resolution. Note that these issues are also relevant to radiation scheme and cloud-aerosol interaction. One possible solution is to employ sub-columns to treat cloud fraction/sub-grid distributions. The key issue is the necessity of using numerical techniques that allow a robust solution with fewer than of 4-5 subcolumns; otherwise the treatment is impractical due to its inefficiency. We are currently exploring such techniques in the context of CAM physics. A framework that allows seamless testing of various approaches at all scales is desirable (e.g.: Embedding a cloud model in a 25-100km resolution climate integration, or embedding a large eddy simulation in a cloud resolving 1-4km weather integration).

Metrics for evaluation:

Different metrics have generally been applied in evaluating microphysics schemes in either climate or NWP application. For climate application, impact on cloud radiative forcing is the key, thus for CAM we have focused on evaluation of cloud properties that determine the radiative forcing: liquid and ice water paths and particle sizes. In NWP, surface precipitation and surface pressure field are the key metrics, more detailed aspects such as radar reflecitvity structure, cold pool intensity, etc. have also been used as metrics. Any microphysics scheme in ESM should be evaluated using both broad categories of metrics. There is a wide range of existing case study data for evaluation and a rich history of use of such datasets (e.g., GCSS). Global datasets derived from satellite are also critical, although there is considerable uncertainty in important retrieval quantities (e.g., water paths and droplet sizes). Long-term observing sites (e.g, ARM, Cloudnet) will be critical for any statistical model evaluation. With most data sets, reformatting model physical states into diagnostics which resemble observations is the most useful (e.g.: using simple or complex satellite 'simulators' embedded into models).

In addition, new techniques from data assimilation are starting to be used even for climate model evaluation. These techniques use minimization of short term forecast errors to try to objectively determine the best model state, and then apply it to a given test case. It is highly desirable to be able to use this capability in CAM as well as in WRF in the future.

5) Aerosols, aerosol-cloud, aerosol-chemistry interactions – Rasch, Barth, Gettelman

Both WRF and CAM have multiple formulations for aerosols.

WRF-Chem has two aerosol schemes.

- Modal Aerosol Dynamics model for Europe (MADE – predicts number and mass) (Ackermann et al., 1998; Binkowski and Shankar, 1995) includes secondary organic aerosols (Schell et al., 2001). Multi-component, internal mixtures are represented.
- Model for Simulating Aerosol Interactions and Chemistry (MOSAIC) (Zaveri et al., 2005a, b; 2008) is a sectional (4 bins or 8 bins) approach, but does not include SOA. Each bin is internally mixed; different bins are externally mixed. Multi-component aerosols are represented.

CAM has two basic ways of representing aerosols:

- A bulk aerosol module (BAM). This package has a long history of use in MATCH and CAM, with additional functionality (e.g. Nitrate aerosols) available when the reactive photochemistry package originating from MOZART and available from CAM-CHEM is enabled. Its default configuration contains a representation for the following aerosol types as external mixtures: sulfate, soot, organic carbon, 4 sizes of dust, and 4 sizes of sea salt. Additional species (e.g. variants tagged by origin, or photochemical pathway) are relatively easily added. The current formulation requires about 16 extra variables to carry these aerosol types.
- A modal representation developed by Steve Ghan, Xiaohong Liu. This package is under development. It shares some components with the BAM (e.g. some of the sources like dust, and sea salt, and production mechanisms are based upon the same code). It treats aerosols as internal mixtures and predicts mass and number for each "mode". This formulation is currently much more expensive than the BAM. The "benchmark" formulation requires approximately 50 additional species. Simpler formulations are in development that are much cheaper.

There are a few additional aerosol species (e.g. volcanic stratospheric aerosols, PSCs, etc) that are occasionally employed in CAM and WACCM, but these are not as thoroughly vetted as those in the two previous categories.

<u>Commonalities:</u>

The CAM bulk formulations can be considered to be either a simplified "modal" formulation (only mass is predicted but standard deviation is prescribed) or a sectional framework (bin sized is fixed). The more complex modal representations include very similar formulations to WRF.

It is likely that many aspects of the aerosol formulations themselves could be treated similarly in the two model frameworks (e.g. emissions, chemical transformation, condensation, deposition, coagulation, etc), and similar species are of interest in the two groups (e.g. sulfate, nitrate, dust, etc)

However, virtually all aspects of aerosols associated with clouds, and features that are subgridscale (e.g. vertical velocities) with respect to a “global” or “large scale” model will differ.

Aerosol-Cloud Interactions

Aerosol-cloud interactions (aerosol-liquid) are represented in WRF through coupling of the MOSAIC aerosol scheme with the Lin et al. microphysics parameterization (Gustafson et al., 2007) that includes prognostic treatments of cloud droplet number and activated (cloud-phase) aerosol species, aerosol activation and re-suspension (Ghan et al., 2001a), bulk cloud chemistry (Fahey and Pandis, 2001), and in-cloud and below-cloud wet removal of particulates and trace gases (Easter et al., 2004). Coupling with the 2-moment cloud microphysics scheme (Morrison et al., 2005) is underway. These schemes require that the simulations be advanced from one time step to the next on timescales of seconds or minutes. Each grid volume is assumed to be uniformly cloudy or cloud free.

CAM uses a drop activation formulation following Abdul-Razzak and Ghan (xxx), coupled to the cloud microphysical formulation of Morrison and Gettelman (yyy, zzz). Aerosol activation in the bulk formulation is still based on an assumed size distribution and a single mode (mass) for the aerosol species. Model cells are assumed inhomogeneous, with subgridscale features assumed for water vapor, cloud condensates, vertical velocities, fraction of column occupied by rain, etc. CAM typically runs at resolutions exceeding 50km, with time steps of order 15 minutes many important processes are “subgridscale”. The most notable issues involve clouds, critical for many aspects of aerosol production and loss. For example the vertical velocities responsible for cloud drop activation, and the up-and downdrafts where processes like drop activation, vertical transport, and scavenging take place are sub-grid-scale.

These issues mean that many critical processes for aerosols, and aerosol-cloud interactions are “subgridscale” and thus require explicit dependence upon the “subgridscale parameterizations of the model”, e.g. stratiform and convective cloud parameterizations, radiation, scavenging, etc. The formulations for aerosol transport, scavenging, cloud overlap, etc require an explicit connection with other components of the climate model.

WRF currently has no way of treating subgridscale features, so it is unlikely that its representation for these processes are adequate when run with coarse spatial resolution The treatment is expected to be much simpler in a model in which grid volumes are either “cloudy” or “cloud free”, and vertical velocities are resolved explicitly in each model cell.

Because the formulation for the cloud microphysics itself is likely to be very different for a global model vs a regional/cloud resolving model, it is likely that the aqueous chemistry, drop activiation, and scavenging formulations will require different implementations (e.g they wont share much code) although the chemical mechanisms, and physical assumptions could be identical.

Practical differences between the WRF and CAM formulations:

CAM can be run with aerosols employed in a “predictive” mode where the species evolve consistently with the meteorology, or in a “prescribed” mode where the species are read in from archives from earlier runs.

The aerosols can be allowed to influence the meteorology (e.g. through the cloud microphysics, and radiative transfer), or can be treated as “passive” scalars, that is, they are updated every time step either according to the evolution equations or interpolation and time, but are not “felt” as forcing terms in the model evolution. Phil sometimes refers to these modes as “active” and “passive” modes, but other nomenclature have evolved.

One can combine the two modes, so that some of the aerosol species are treated as “prescribed” species, and some are “predicted”. The radiative transfer codes, and the drop activation formulations do not need to recognize the difference between prescribed and predicted aerosols. The model has the capability of carrying two or more “versions” of an aerosol type (e.g. there can be a “predicted sulfate”, a “European sulfate”, and a “prescribed sulfate”), although the radiative transfer scheme in the end will only see one sulfate (which may be a combination of these).

There are a few components to aerosols physics where code might be shared. Ones that come to mind are source functions (e.g. dust mobilization codes), radiative transfer (once a column is divided into sub-columns through an “independent column approximation” (ICA)).

Towards 100K processors:

It is unclear how these formulations will scale to 100K processors.

Aerosol physics and chemistry should scale well since it is isolated to a grid point. The transport of an additional 20-50 species will add some burden to the transport component of any model. The subcolumn generator and separate treatment of radiative transfer, scavenging, and aqueous chemistry within each subcolumn will also require assessments of their implications on model performance in a global model, and this is another place where global and small scale model formulations are likely to differ.

It would be easy to “double” the number of species carried in the global model to treat separately “in-cloud” and “out-of-cloud” flavors of each of these species. This approach has been viewed as desirable from the global modelers, but we have not yet been willing to pay the computational price for using it.

Requirements for scientific functionality:

- Conservation of mass for transport processes

- Consistency in transporting both number and mass of aerosols – cannot have number when there is no mass of aerosol, for example.

Metrics for evaluation:

Scalars with known properties to verify above requirements

Observational datasets (e.g. MIRAGE field campaign) to evaluate model.

Again, this should scale fine: except to the extent that complex aerosol packages add lots of tracers and this puts additional demands on advection schemes. There also exist the issues of adding large lookup tables to the code for chemistry schemes and how to deal with low memory architectures.

6) Chemistry - Lamarque, Barth

Current Capability:

WRF-Chem: RADM2, RACM, and CBMZ chemical mechanisms. A kinetic preprocessor (KPP) has recently been installed so that additional mechanisms (the MOZART chemistry is soon to be implemented) can easily be included. The KPP solver is the Rosenbrock type solver. Photolysis rates are calculated using troposphere ultraviolet (TUV) radiation code, fast TUV, or fast-j method. Biogenic emissions are calculated using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) or from two other methods. Anthropogenic emissions are specified by the user before running the model. Dry deposition is coupled with the soil/vegetation scheme. Wet deposition is also included.

CAM-Chem: Tropospheric chemistry is implemented (MOZART and reduced mechanisms) with bulk aerosols. CAM-Chem uses MOZART preprocessor (Rosenbrock type implicit solvers). Photolysis rates are from lookup tables and adjusted to local gridpoint conditions (e.g. cloudiness). Photolysis rates can also be calculated from fast TUV. CAM-Chem includes interactive dry deposition and biogenic emissions with the CLM. Oceanic emissions are part of POP. Wet deposition of soluble species is also included.

Overlap:

Chemistry mechanisms are similar, emissions preprocessing, fast TUV, biogenic emissions scheme is similar.

Incompatible Requirements:

Currently the coding of the preprocessor is very different between models. Will need to choose one or re-write.

Chemistry in an urban (or forest canopy) may be very different than on the regional to global scale. Some parameterizations may need to be different at fine scales where clouds are resolved (e.g. the production of NOx from lightning, wet deposition, and even the PBL) and large scales.

Towards 100K processors:

Chemistry should scale well since it is isolated to a grid point. However, there may be issues with calculating photolysis rates (need to know cloudiness above and below as well as aerosols). It may be best to include photolysis rate calculation in radiation module.

Requirements for scientific functionality:

- Conservation of species mass for transport processes
- Conservation of total species in multiple phases

- Chemistry solver needs to be accurate (conserve moles) and fast
- Flexibility in allowing for different chemical mechanisms, emissions, removal processes, photolysis representations, interaction with clouds (wet deposition and indirect effects)

Metrics for evaluation:

Scalars with known properties (e.g. inert, soluble and inert) to verify above requirements

Field campaigns (e.g. MIRAGE) are great testbeds for tropospheric chemistry.

7) Subgrid-scale dynamics not in PBL (Gravity Waves) - Richter

Gravity waves with horizontal wavelengths between 10 and 1000 km are not resolved in current global circulation models and hence need to be parameterized. Parameterization of gravity waves becomes increasingly important with altitude. In the troposphere, a parameterization of stationary orographically generated gravity waves is sufficient, whereas above the tropopause a broad spectrum of waves from various sources must be included. In the stratosphere momentum deposition from gravity waves is comparable to that from planetary waves. In the mesosphere and lower thermosphere gravity waves are the main sources of momentum deposition.

Current Capability:

Standard CAM includes an orographic gravity wave parameterization of McFarlane (1987). Upward extended CAM, WACCM, also includes the Lindzen (1981) gravity wave propagation scheme for non-stationary gravity waves. In the past, the Lindzenprameterization has been used with an arbitrarily specified gravity wave source spectrum. Recently, WACCM is moving towards GW source parameterizations including the following known gravity wave sources:

Convection: Beres et al (2004) scheme

Fronts: Modified Charron and Manzini (2002) scheme

CAM/WRF Overlap:

WRF does not need a GW parameterization as GWs are resolved if the model is run at a resolution of the order of 1 km, hence there is no overlap. WRF is a model that can be used to constrain the gravity wave parameterizations in CAM/WACCM.

Incompatible Requirements:

Current gravity wave source parameterizations are developed for models with grid sizes of 0(100km). These will need to be adapted if the model resolution is finer, and parts of the gravity wave spectrum are resolved.

Towards 100K processors**:**

At the moment gravity wave prameterizations are column based and hence there are no issues with going to 100K processors. Starting this summer WACCM will begin testing a lagrangian GW parameterization (to propagate GWs in space and time). This parameterization will require communication between columns, but at the moment the scalability of this parameterization is unknown.

Requirements for scientific functionality:

Momentum Conservation.

Metrics for Evaluation:

At the moment, there are no observations that can verify the gravity wave parameterization on the global scale. GW parameterizations are typically tuned to obtain a reasonable climatology of the middle and upper atmosphere. Important aspects of the climatology are: summer mesopause temperature (correct temp and height), strength of the stratospheric jets, correct variability in NH Winter, existence of the ozone hole, distribution of water vapor.

8) Processes specific to the upper-atmosphere - H. Liu, Marsh

Current capability:

The Whole Atmosphere Community Climate Model (WACCM), which is a version of CAM extended to the upper atmosphere, currently includes the following non-standard physics and chemistry modules: a version of the MOZART chemical solver with ionosphericchemistry , very short wavelength radiation (soft x-rays, EUV), particle precipitation in the aurora, ion-drag, joule heating, LTE and non-LTE IR cooling, and a parameterized electric and geomagnetic fields.Radiative transfer has also been modified to account for the conversion of photon energy to chemical potential energy as well as heat, i.e. absorbed solar energy is not necessarily thermalized locally, but can go into breaking chemical bonds.

An extended version of the model (up to ~500km) also includes major species diffusion and species dependent Cp, R, and mean molecular weight.

CAM/WRF Overlap:

None of the physics included in the WACCM extensions to CAM have been incorporated into WRF.

Incompatible requirements:

It may be difficult to implement species dependent Cp, R, and mean molecular weight into WRF.

Towards 100K processors:

All current physics modules operate on vertical columns, and so scale relatively well, and pose no significant problems. However, processes that may be included in future versions that operate along magnetic field lines (e.g. ion/electron transport due to Lorentz force) could require significant communication between adjacent columns, and so may not scale well.

Requirements for scientific functionality:

ESM should have the capability to be coupled to a plasmasphere/magnetosphere model for simulation of space weather events. The dynamical solver should be able to maintain sufficient accuracy during the very strong dynamical forcing during these events.

Future studies may require consideration of the variation of gravity with altitude, and or the shape of the Earth (or planet).

Metrics for evaluation:

Comparison of neutral winds, temperatures, and composition from extensive databases of satellite and ground based upper atmosphere observations. Comparison with focused observation campaigns, and particular space weather event (may require assimilation of observed dynamics in the lower atmosphere).

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