Basics of microphysics in weather and climate models

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1. Introduction

<u>"microphysics</u>" is the collection of micro-scale physical processes involved in the formation and evolution of cloud and precipitation particles.

- Condensation
- Evaporation
- Freezing
- Melting
- Collision-coalescence
- Breakup
- etc.

It's complicated!



There are two critical and distinct challenges:

- 1. <u>Inability to represent explicitly individual cloud particles and</u> relevant processes, even with massive advances in computing.
 - \rightarrow a small cloud (1 km³) can easily have 10¹⁷ droplets!
 - \rightarrow how to represent the cloud particle population?

2. <u>Fundamental uncertainty</u> of many physical processes at the scale of individual particles, especially for the ice-phase.

Even if we could explicitly model every cloud particle, there would still be critical process-level uncertainty!

Microphysics and clouds across scales



Scales of Atmospheric Motion

Morrison et al. (2020), JAMES

2. Basics of microphysics parameterization

Types of microphysics schemes:

- Bulk → one or a few <u>bulk</u> quantities are predicted (e.g., cloud mass mixing ratio)
- Bin → population is discretized into size or mass "<u>bins</u>" and one or a few quantities predicted in each bin
- Lagrangian → population is represented by a collection of "<u>super-particles</u>" that move in the flow



Morrison et al. (2020), JAMES

Bulk schemes remain the workhorses of *weather and climate models* because they are simple and cheap.

Many developments of bulk schemes over the past 40+ years:

- Inclusion of <u>ice microphysics</u>
- Prediction of additional bulk quantities besides mass, i.e., mass and number → <u>two-moment schemes</u>



In bulk schemes *usually* some functional form for the <u>particle size distribution</u> is assumed, e.g., *gamma*:

$$n(D) = N_0 D^{\mu} e^{-\lambda D}$$

The gamma distribution has 3 "free" parameters:



The predicted bulk quantities like *Q* are proportional to <u>integrals of the size distribution</u> (i.e., <u>moments</u>).

Nice thing about the gamma function is that the integrals are analytic! So we can invert these analytic integrals to solve for the size distribution parameters λ , μ , and/or N_0 .

Typical approach:

One-moment \rightarrow specify μ and N_0 , evolve λ from Q, μ , N_0 **Two-moment** \rightarrow specify μ , evolve λ and N_0 from Q, N, μ **Three-moment** \rightarrow evolve λ , N_0 , and μ from Q, N, Z

- **Q** = mass mixing ratio
- *N* = number mixing ratio
- **Z** = reflectivity factor (mixing ratio)



Work also starting in the 1950's-60's developed schemes that explicitly modeled drop size distributions using a fixed size/mass grid (e.g., Berry 1967; Kovetz and Olund 1969; Bleck 1970).



Growth/shrinkage rates of drops with size or mass of a given bin are calculated from theory or observations.

Example: diffusional growth of cloud droplets



Numerical methods are then needed to calculate how drops move between bins during growth. This has been a key challenge of bin schemes since their inception in the 1950's-60's. Much better numerical methods have been developed since the 1980's. Spectral broadening from <u>numerical diffusion</u> remains a problem, particularly from vertical advection.

Lagrangian particle-based microphysics

(e.g., Shima et al. 2009, Andrejczuk et al. 2010, Solch and Karcher 2010, Unterstrasser and Solch 2010, Riechelmann et al. 2012, Dziekan and Pawloska 2017, Grbaowski et al. 2018, Hoffman et al. 2018)

 Particle population represented by a sample of "super-particles" that follow trajectories within the modeled (e.g., LES) flow.



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- Particle population represented by a sample of "super-particles" that follow trajectories within the modeled (e.g., LES) flow.
- No spurious <u>numerical diffusion</u>!



Ice microphysics is particularly challenging because of the wide variety of particle shapes.

Traditional bulk approach:



← abrupt / unphysical conversions

Problems with pre-defined ice categories:

- **1. Real ice particles have complex shapes**
- 2. Conversion between categories is ad-hoc
- 3. Conversion leads to large, discrete changes in particle properties
- NOTE: Bin microphysics schemes have the identical problem

Observed crystals:



c/o Alexi Korolev

Recent shift from discrete ice <u>categories</u> to prediction of particle <u>properties</u> (density, shape, size, etc.)**.

- Morrison and Grabowski (2008)
- P3 (Morrison and Milbrandt 2015, Milbrandt and Morrison 2016)
- ISHMAEL (Jensen et al. 2017; 2018)
- Tsai and Chen (2020)

**Particularly well suited for Lagrangian schemes (Shima et al. 2020)



3. Practical aspects

Simulations are often (very) sensitive to microphysics!



Horizontal cross sections of radar reflectivity at 1 km height from WRF squall line simulations using different bin schemes (left), bulk schemes (middle), and small random perturbations to initial θ (right).

Xue et al. (2017) *MWR* Morrison et al. (2020) *JAMES*

In WRF there are many scheme options**:



Some schemes are generally better than others, but no scheme is better for everything...

How to decide which to use?

Practical considerations:

- Type of application (research, NWP, climate, etc.)
- Computational cost
- Model resolution
- Cloud regime or case (e.g., shallow warm clouds, mixed-phase, etc.)

Some general guidelines

Depending on application, <u>computational cost</u> is often a limiting factor:

- Microphysics is expensive can be 50% or more of the total cost in run time
- Bin schemes about 10-100 times slower than bulk
- Multi-moment schemes more expensive than one-moment
- Cost difference in schemes largely reflects number of predicted variables → in WRF (depending on advection option) each extra predicted variable adds ~2% total run time
- There are some methods that can reduce cost of advection for multi-moment bulk schemes (Morrison et al. 2016) and bin (Gavze et al. 2020) that could be considered for WRF/MPAS.

For research \rightarrow typically want schemes with reasonable process level detail, .e.g. two-moment, but keeping in mind cost (~10-30% greater run time than one-moment).

Scheme type and complexity should be commensurate with cloud regime and model resolution, e.g.

- Obviously, clouds with ice require a scheme that can represent ice (i.e., not Kessler)
- Deep convection generally requires a scheme that can represent dense rimed ice (graupel or hail)
- Bin and Lagrangian schemes should only be used in models with high-enough resolution to explicitly represent cloud- or convective-scale dynamics

Future directions

- While increasing computer power will mean greater use of <u>bin</u> and especially <u>Lagrangian</u> schemes, <u>bulk</u> schemes will be a mainstay of weather and climate models into the foreseeable future.
- A move away from discrete ice categories toward prediction of particle properties.
- Greater use of Lagrangian schemes which provide an exciting avenue for cloud research that is still in infancy.
- Incorporation of rigorous statistical tools to understand scheme behavior and constrain better with observations and detailed process models (this includes ML)

(e.g., Morales et al. 2021; Morrison et al. 2020; van Lier-Walqui et al. 2020; Chiu et al. 2021; Seifert and Rasp 2020)

"Take home" points

- The parameterization of <u>microphysics</u> is an important component of atmospheric models, and it is uncertain.
- Different types of schemes have different ways of representing the particle size distribution: <u>bulk</u>, <u>bin</u>, <u>Lagrangian particle-based</u>
- Bulk schemes remain the workhorses of research and operational weather and climate modeling, though many advances have been made in bulk schemes over the decades.
- Practical choice of what scheme to use depends on application, computational cost, the cloud type being simulated, and model resolution.

Thank you!

Questions?

Funding for our microphysics work:



A pioneer of the field (1950's – 90's): *Edwin Kessler*



"I worked with a strong sense for interactions among processes... and in expectation that their study would be facilitated by simple means to portray microphysical processes..." - Kessler (1995)

Kessler Bulk One-Moment Warm-Rain Scheme (1969)



Predicted bulk microphysical quantities evolve in time and space from advection (via wind), microphysical processes, and sedimentation.



The microphysical process rates (e.g., drop evaporation or coalescence) depend on the <u>particle size distribution</u>.

Bin schemes have a significant advantage over bulk schemes because they evolve size distributions (have more degrees of freedom), but a challenge is numerical solving droplet growth.

In general, bin methods in Eulerian models suffer from <u>numerical diffusion</u> leading to acceleration of growth from small to large drops.



Lagrangian particle-based microphysics

- Can represent stochastic nature of the "stochastic" collection equation → the impact of "lucky drops" on rain formation
- Easy and computationally efficient to add "attributes", i.e., chemical/physical properties of particles
- Allows straightforward coupling with sub-grid scale fluctuations (i.e., velocity, supersaturation) (Abade et al. 2018; Hoffman et al. 2018; Chandrakar et al. 2021)



Lagrangian particle-based microphysics provides an exciting path forward, but there are important <u>challenges</u>...

- Lots of "super-particles" are needed to get good statistics, rule of thumb is a few hundred per grid cell (though there are approaches to reduce the cost, e.g. Grabowski et al. 2018)
- Fundamental process and parameter uncertainties remain:
 - collision-coalescence and drop breakup
 - ice nucleation
 - vapor growth of ice
 - riming
 - aggregation
 - ice particle habit, density, fallspeed

Bin schemes are confined to research modeling because:

- Computational cost
- Require fine model grid resolution to resolve cloud dynamics

However <u>bin</u> schemes are widely used to test and develop <u>bulk</u> microphysics schemes.



Khairoutdinov and Kogan (2000), MWR

How can the *size distribution parameters* be related to the *predicted bulk quantities* like mass mixing ratio *q*?

Gamma size distribution (*D* is a measure of particle size, often diameter):

$$n(D) = N_0 D^{\mu} e^{-\lambda D} \qquad (1)$$

Mass of a single cloud or rain drop as function of D (ρ_w is density of liquid water):

$$m = \frac{\pi}{6} \rho_w D^3 \tag{2}$$

Relating the size distribution to the predicted *q*:

$$q = \int_0^\infty mn(D)dD \qquad (3)$$

Combining (1), (2), and (3) and rearranging terms:

$$q = \int_0^\infty \frac{\pi}{6} \rho_w N_0 D^{3+\mu} e^{-\lambda D} dD \qquad (4)$$

In <u>one-moment</u> bulk schemes that <u>only</u> predict q, we can specify N_0 and μ and (4) can be analytically integrated to obtain an expression for λ :

$$\lambda = \left[\frac{\pi \rho_w N_0 \Gamma(\mu+4)}{6q}\right]^{\frac{1}{\mu+4}}$$
(5)

where Γ is the Euler gamma function.

In *two-moment* bulk schemes that predict *q* and number mixing ratio *N*, we can relate *N* to the size distribution as (for gamma):

$$N = \int_0^\infty n(D) dD = \int_0^\infty N_0 D^{\mu} e^{-\lambda D} dD = \frac{N_0 \Gamma(\mu + 1)}{\lambda^{\mu + 1}}$$
(6)

We can then specify μ and combine (5) and (6) to obtain expressions for λ and N_0 :

$$\lambda = \left[\frac{\pi \rho_w N \Gamma(\mu+4)}{6q \Gamma(\mu+1)}\right]^{\frac{1}{3}}$$
(7)

$$N_0 = \frac{N}{\Gamma(\mu+1)} \left[\frac{\pi \rho_w N \Gamma(\mu+4)}{6q \Gamma(\mu+1)} \right]^{\frac{\mu+1}{3}}$$
(8)

In *three-moment* bulk schemes that predict *q*, *N*, and reflectivity factor *Z*, we can relate *Z* to the size distribution as (for gamma):

$$Z = \int_0^\infty D^6 n(D) dD = \int_0^\infty N_0 D^{\mu+6} e^{-\lambda D} dD = \frac{N_0 \Gamma(\mu+7)}{\lambda^{\mu+7}}$$
(9)

We can then solve for all three gamma distribution parameters μ , λ , N_0 from the predicted q, N, Z. This leads to a cubic polynomial equation for μ as a function of NZ/q^2 .

In general we can relate the predicted quantities to size distribution *moments*, where the *k*th order moment is defined as

$$M_{k} = \int_{0}^{\infty} D^{k} n(D) dD = \int_{0}^{\infty} N_{0} D^{\mu+k} e^{-\lambda D} dD = \frac{N_{0} \Gamma(\mu+k+1)}{\lambda^{\mu+k+1}}$$
(10)

In this case,
$$N = M_0$$
, $q = \frac{\pi}{6} \rho_w M_3$, and $Z = M_6$.

**Note: these specific equations only apply for spherical (isometric) particles. In general, one needs to relate m to D in order to derive closed set of equations (typically by assuming the form $m = aD^b$, in which case simple analytic derivations can still be done.
Calculation of the microphysical process term requires knowledge of how an individual drop is affected by processes, or how new drops are created or destroyed:

$$S_{\chi} = \frac{d\chi}{dt} \propto \frac{dM_k}{dt} = \int_0^\infty \left(\frac{dD}{dt} k D^{k-1} n(D) + D^k \frac{\partial n(D)}{\partial t}\right) dD \tag{11}$$

Example, rain drop condensation (neglecting ventilation):

$$\frac{dD}{dt} = \frac{4G(T,p)S}{D} , \frac{\partial n(D)}{\partial t} = 0$$
 (12)

Combining (10) - (12):

$$\frac{dM_k}{dt} = \int_0^\infty 4G(T, p) SkD^{k-2} n(D) dD = 4G(T, p) SkM_{k-2}$$
(13)

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In general, the process rate for a given moment depends on other moments, so microphysics parameterization represents a closure problem.

Equations for $\frac{dD}{dt}$ and $\frac{\partial n(D)}{\partial t}$ sometimes derived from theory or lab observations, but often heuristics. Generally large uncertainty, especially for ice-phase processes.

In most bulk schemes, closure is provided by assuming a size distribution functional form, like gamma. With λ , N_0 , and μ known (calculated or specified), then we can obtain any moment from (8).

Closure does <u>not</u> *require* an explicit functional form for the size distribution. Size distribution moments can also be statistically related to one another. Only a few bulk schemes use this approach (Szyrmer et al. 2005; Morrison et al. 2020).

Closure in <u>bin</u> and <u>Lagrangian particle-based</u> schemes is provided by *explicitly evolving* the size distribution.

Liquid Phase

"Warm rain" coalescence process:

 \rightarrow 2-moment, 2-category bulk schemes model this process well



Still important uncertainties for liquid at the process level, e.g. turbulent mixing/growth processes that broaden cloud drop size distributions, drop breakup...



The simulation of ice-containing cloud systems is often <u>very sensitive</u> to how ice is partitioned among categories



Morrison and Milbrandt (2011), MWR

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Recent shift (in parameterization of ice phase):

Representation by fixed hydrometeor <u>categories</u> to Prediction of hydrometeor <u>properties</u>

- Predicted rime/axis ratio (bin scheme) Hashino and Tropoli (2007)
- Predicted rime fraction Morrison and Grabowski (2008), Lin and Colle (2011) (diagnostic F_r)
- Predicted crystal axis ratio and density Harrington et al. (2013), Jensen et al. (2017)

• Predicted Particle Properties (P3) - Morrison and Milbrandt (2015)

New Bulk Microphysics Scheme:

Predicted Particle Properties (P3)

NEW CONCEPT

"free" ice category – predicted properties, thus freely evolving type

VS.

"pre-defined" ice category – traditional; prescribed properties
 (e.g. "ice", "snow", "graupel", etc.)

Compared to traditional schemes (for ice phase), P3:

- avoids some necessary evils (ad-hoc category conversion, fixed properties)
- is better linked to observations
- is more computationally efficient

Morrison and Milbrandt (2015), JAS- Part 1Morrison et al. (2015), JAS- Part 2Milbrandt and Morrison (2016), JAS- Part 3

A given (free) category can represent any type of ice-phase hydrometeor

Prognostic Variables:

Q_{dep} – deposition ice mass mixing ratio	[kg kg⁻¹]
Q _{rim} – rime ice mass mixing ratio	[kg kg ⁻¹]
N_{tot} – total ice number mixing ratio	[# kg ⁻¹]
B _{rim} – rime ice volume mixing ratio	[m ³ kg ⁻¹]

Predicted Properties:

F_{rim} – rime mass fraction, $F_{rim} = Q_{rim} / (Q_{rim} + Q_{dep})$	[]
$\boldsymbol{\rho}_{\textit{rim}}$ – rime density, $\rho_{\textit{rim}}$ = $Q_{\textit{rim}}$ / $B_{\textit{rim}}$	[kg m ⁻³]
$m{D}_{m{m}}$ – mean-mass diameter, $m{D}_m \propto m{Q}_{tot}$ / $m{N}_{tot}$	[m]
V_m – mass-weighted fall speed, $V_m = f(D_m, \rho_{rim}, F_{rim})$	[m s ⁻¹]
etc.	

Diagnostic Particle Types:

Based on the predicted properties (rather than pre-defined)

P3 SCHEME – Determining $m(D) = \alpha D^{\beta}$ for regions of *D*: Similar for A(D); V(D) calculated from *m* and *A*...

Conceptual model of particle growth following Heymsfield (1982):





etc.

Morrison et al. (2015), JAS

The classical parameterization problem: *Microphysics and clouds across scales*



Scales of Atmospheric Motion

Parameterization of hydrometeor population: "traditional parameterization problem" *Even at its "native" scale, there are large <u>uncertainties</u> in our understanding of microphysics!*

- Incomplete theory with significant knowledge gaps
 → no benchmark model
- Fundamentally different from radiation (line-by-line models) or fluid dynamics/turbulence (Navier-Stokes). Perhaps more similar to land surface, hydrology, etc.

The hierarchy of microphysics schemes, and an analogy to gas dynamics...



c/o Shin-Ichiro Shima

Parcel results

- Idealized setup allows comparison to Lagrangian *numerical benchmark solutions*
- Various mass grids and condensational growth methods tested



Simplified P3 implemented in CAM5



What we want in advection schemes (for clouds/precip):

- Positive definite for mass (needed for water conservation), or even better monotonic, but <u>not</u> as critical for *non-mass* microphysical variables
- Preserves initial linear relationships between advected quantities
- Accurate
- Efficient

There are trade-offs!



1D analytic test cases

Mean error as a function of Courant number

Issues with advection and microphysics...

- The traditional approach is to advect each cloud/precipitation prognostic variable independently.
- Potential problems:
- Slow
- Derived quantities (e.g., ratios) may not be monotonic even if each scalar is advected using a monotonic scheme

New method: Scaled Flux Vector Transport

Morrison et al. (2016, MWR)

Scales mass mixing ratio fluxes to advect "secondary" microphysical scalars:

- 1) Mass mixing ratio (Q) quantities are advected using the unmodified scheme
- 2) "Secondary" non-mass scalars (*N*, *Z*, *V*, etc.) then advected by scaling of *Q* fluxes using higher-order linear weighting

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- 2) "Secondary" non-mass scalars (*N*, *Z*, *V*, etc.) then advected by scaling of *Q* fluxes using higher-order linear weighting

Retains features of applying unmodified scheme to ALL scalars, but at a reduced cost..

 \rightarrow Accurate (for analytic test cases), <u>fast</u>, and preserves initial linear relationships



WRF 2D squall line test

WRF-PD (5th order horizontal 3rd order vertical)

WRF-PD w/ SFVT

11% reduction in total model run time

Morrison et al. (2016), MWR

 The <u>efficiency</u> of SFVT increases as the number of secondary scalars increases relative to the number of mass variables.

• Thus SFVT works well with P3 because there are 3 secondary variables for each "free" ice category.

 It is particularly well-suited for <u>bin schemes</u> using the total bulk mass as the "lead" variables and the individual bin masses/numbers as the secondary scalars.

P3-like modifications to CAM5

- Modification of Morrison-Gettelman version 2 (MG2) scheme to combine "*cloud ice*" and "*snow*" in a single ice category and use physical representations of masssize (m-D) and projected area-size (A-D) relationships.
- Allows consistent linkages between fallspeed and effective radius (both depending on m-D and A-D), and removes the need for cloud ice to snow autoconversion.
- Two methods for specifying m-D and A-D:

- *P3:* constant m-D and A-D parameters, follows original P3 except representation of rimed ice is neglected

- *EM16:* varying m-D and A-D parameters from Erfani and Mitchell (2016) Eidhammer et al. (2017), *J. Climate*