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2 **Using an Arbitrary Moment Predictor to Investigate** 3 **the Optimal Choice of Prognostic Moments in Bulk** 4 **Cloud Microphysics Schemes**

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9

10 **Key Points:**

- 11 • A bin microphysics scheme is modified to act like a bulk microphysics
12 scheme.
- 13 • The new scheme can predict arbitrary combinations of two or three
14 moments of the hydrometeor size distribution.
- 15 • Box model tests show that standard configurations of two-moment
16 schemes perform poorly for predicting some microphysical processes.
17

18 **Abstract**

19 Most bulk cloud microphysics schemes predict up to three standard
20 properties of hydrometeor size distributions, namely, the mass mixing ratio,
21 number concentration, and reflectivity factor in order of increasing scheme
22 complexity. However, it is unclear whether this combination of properties is
23 optimal for obtaining the best simulation of clouds and precipitation in
24 models. In this study, a bin microphysics scheme has been modified to act
25 like a bulk microphysics scheme. The new scheme can predict an arbitrary
26 combination of two or three moments of the hydrometeor size distributions.
27 As a first test of the arbitrary moment predictor (AMP), box model
28 simulations of condensation, evaporation, and collision-coalescence are
29 conducted for a variety of initial cloud droplet distributions and for a variety
30 of configurations of AMP. The performance of AMP is assessed relative to the
31 bin scheme from which it was built. The results show that no double- or
32 triple-moment configuration of AMP can simultaneously minimize the error of
33 all cloud droplet distribution moments. In general, predicting low-order
34 moments helps to minimize errors in the cloud droplet number
35 concentration, but predicting high-order moments tends to minimize errors
36 in the cloud mass mixing ratio. The results have implications for which
37 moments should be predicted by bulk microphysics schemes for the cloud
38 droplet category.

39 **Plain Language Summary**

40 Countless cloud droplets with a variety of sizes exist in every cloud. Since
41 cloud models cannot keep track of every individual droplet, most models
42 instead predict quantities such as the total mass of cloud droplets and the
43 total number of cloud droplets inside a model grid box. The values of these
44 quantities dictate how fast clouds grow, how spatially extensive they are,
45 and how well they reflect sunlight. In this study we explore whether the
46 evolution of clouds could be improved if models instead predicted other
47 properties of the cloud droplets, such as total surface area of all droplets or
48 total diameter of all droplets. Our results show that improvements to current
49 cloud models are likely possible.

50 **1 Introduction**

51 With improvements in computational speed and memory, atmospheric
52 models are being designed with increasingly complex parameterizations to
53 represent physical processes and systems such as the land surface, ocean,
54 sub-grid turbulence, convection, and clouds. One of the more
55 computationally expensive parameterizations in many contemporary models
56 is the cloud microphysics parameterization. Traditionally, microphysics
57 parameterizations predicted only the total mass mixing ratio (proportional to
58 the 3rd moment of particle size distributions, or PSDs) of a limited number of
59 cloud hydrometeor categories (e.g. Kessler 1969; Lin et al. 1983). Such

60 schemes are known as single-moment schemes. It is becoming common for
61 weather and climate models to predict both the mass mixing ratio and
62 number concentration (0^{th} moment of PSDs) of each hydrometeor type (e.g.
63 Meyers et al., 1997; Morrison et al., 2005; Seifert & Beheng, 2006; Thompson
64 & Eidhammer, 2014). Although these double-moment schemes take longer
65 to run and can require more assumptions, most studies have found that the
66 increased complexity of the scheme leads to better predictions (Ekman,
67 2014; Igel et al., 2015 and references therein). Triple-moment schemes,
68 which predict an additional third property of the cloud particle size
69 distributions (Dawson et al., 2014; Milbrandt & Yau, 2005; Shipway & Hill,
70 2012), are currently primarily used for research applications and are not
71 nearly as prevalent as single- and double-moment schemes. Most, if not all,
72 triple-moment schemes have been designed to predict the radar reflectivity
73 factor (6^{th} moment of PSDs). A review of bulk microphysics schemes was
74 given recently by Khain et al. (2015). Finally, it should be noted that the
75 proportionality of the 3^{rd} moment to mass and 6^{th} moment to reflectivity
76 factor is only strictly valid for constant density spheres such as spherical
77 liquid drops. The proportionality does not hold for most ice hydrometeors.
78 Since the focus of this study will be on liquid, I will continue to use these
79 physical interpretations of the 3^{rd} and 6^{th} moments.

80

81 The choice to predict the 3^{rd} , 0^{th} , and 6^{th} moments in cloud microphysics
82 schemes has been made naturally. The 3^{rd} moment must be predicted in
83 order to absolutely conserve water mass in any model. Mass conservation is
84 a law of physics; however, no other such fundamental laws exist to guide our
85 choice of which additional moments to predict. The 0^{th} moment, or number
86 concentration, is an easy property to understand and formulate predictive
87 equations for. The earliest double-moment schemes provide little or no
88 justification for the choice to predict this property because it is such an
89 obvious one to make (Koenig and Murray 1976; Ziegler 1985). Perhaps the
90 best motivation is that number concentration is strongly associated with the
91 nucleation of new cloud droplets and ice crystals. Another motivation is that
92 the number concentration is conserved during condensation and provides a
93 constraint on the PSD during that process. Therefore, there are strong,
94 physically-based arguments to be made for predicting the 0^{th} moment.
95 Nonetheless, for other processes, such as collision-coalescence, it is not
96 obvious that the 0^{th} moment is logically a better quantity to predict than
97 another moment of the distribution since number is not conserved when
98 droplets collect one another. Finally, predicting the 6^{th} moment, or
99 reflectivity factor, in triple-moment schemes is convenient for contrasting
100 model output and radar observations, and for data assimilation, but is a
101 choice that is harder to motivate based on physical considerations.

102

103 From a statistical standpoint, Morrison et al. (2019) find that knowledge of
104 just the 0^{th} and 3^{rd} moments gives little constraint on higher order moments.
105 They suggest that predicting a combination of high and low moments such

106as is done by triple-moment schemes may be best for reducing uncertainty
107in the simulations of all moments. Therefore, there may be more uncertainty
108in which two moments ought to be predicted in a double-moment scheme
109than in which three moments ought to be predicted in a triple-moment
110scheme.

111

112There has been no systematic study to address the question of which
113moments to predict, which in retrospect, is somewhat surprising. Wacker and
114Lüpkes (2009) and Milbrandt and McTaggart-Cowan (2010) examined the
115problem for the case of sedimentation. Both studies find that the evolution of
116the moments in a precipitation shaft strongly depends on the predicted
117moments and the value of the shape parameter in the gamma probability
118distribution function. Predicting the 0th and 3rd moments yields the lowest
119average error of the 0th-7th moments only if the shape parameter is
120diagnosed based on current conditions. Predicting the 0th and 8th moment
121yields the lowest average error when the shape parameter is held constant
122(Milbrandt & McTaggart-Cowan, 2010), but unfortunately does not give mass
123conservation.

124

125Sedimentation is a relatively simple process to examine since it is essentially
126a moment advection problem. The difficulty in examining the dependency of
127additional processes on predicted moments lies in developing bulk scheme
128equations for each moment. Kogan and Belochitski (2012) developed
129equations for the 0th, 2nd, 3rd, 4th, and 6th moments for all major warm phase
130processes and Szyrmer et al. (2005) developed generic tendency equations
131for any moment for condensation and evaporation. In this study a different
132approach is taken. To avoid developing equations, a bin microphysics
133scheme is modified to behave like a bulk scheme. The modifications allow
134the bin scheme to be run as a “bulk-emulating” arbitrary moment predictor
135scheme. This arbitrary moment predictor scheme can be run with either a
136double- or triple-moment configuration and with any combination of
137moments predicted. By comparing its performance to the underlying bin
138scheme, the new scheme is used to make suggestions about the optimal
139choice of prognostic moments in bulk microphysics schemes for the cloud
140droplet category.

141

142The development of the new scheme is described in Section 2, simulations
143are described in Section 3, results for double-moment configurations are
144discussed in Section 4 and for triple-moment configurations in Section 5.

145 **2 Methods**

146 2.1 Overview

147The design of the Arbitrary Moment Predictor (AMP) microphysics scheme
148follows work first described in Igel and van den Heever (2017). Their work
149has been substantially expanded and the AMP scheme is described in detail

150 here for the first time. A similar methodology was also adopted by Paukert et
 151 al. (2019). A flow chart is shown in Figure 1 to illustrate the process for a
 152 single arbitrary hydrometeor category. The basic approach is to initialize a
 153 grid box with a binned distribution of hydrometeors for each hydrometeor
 154 species that conforms to a gamma probability distribution function (PDF)
 155 based on the current values of predicted moments of each species. Next, the
 156 bin microphysics routines are run using this binned gamma PDF. At the end
 157 of the call to the bin microphysics routines, a user-defined set of moments
 158 (i.e. the arbitrary moments) of the hydrometeor distributions are calculated.
 159 In a box model, these moments are used to find new parameters of the
 160 gamma PDF for each species at the beginning of the next time step. In a full
 161 physics model, these moments would be passed back to the main model for
 162 use in other routines such as advection. Currently AMP can be configured as
 163 a double- or triple-moment scheme by changing the number of moments
 164 that are calculated at the end of the microphysics routines. The number of
 165 moments is not required to be the same for each species, but the 3rd
 166 moment is always predicted. It would be trivial to also allow it to act like a
 167 single-moment scheme, but that has not been done. At this time, cloud
 168 droplets and raindrops are the only two hydrometeor species included in
 169 AMP.

170 2.2 Technical Description

171 In this section, the technical development of the AMP scheme is described.
 172 The particular bin microphysics scheme that is used in this study is the
 173 Hebrew University Spectral Bin Model (SBM) (Khain et al., 2004). In principle
 174 any bin scheme may be used.

175

176 Like in most bulk schemes, the number distribution in AMP is assumed to
 177 conform to a gamma PDF. This number distribution is defined here as

$$178 \quad n(D \vee N_0, \nu, D_n) = \frac{dN}{d \ln D} = \frac{N_0}{\Gamma(\nu)} \left(\frac{D}{D_n} \right)^\nu e^{-\frac{D}{D_n}}$$

179 (1)

180 where n is the probability size distribution of a hydrometeor category, N is
 181 the cumulative size distribution, D is the hydrometeor diameter, N_0 is the
 182 total number mixing ratio, ν is the shape parameter, and D_n is the scaling
 183 diameter (Walko et al. 1995). Note that (1) uses $dN/d \ln D$ rather than dN/dD .
 184 This choice is made for convenience because the SBM uses a mass-doubling
 185 set of bins. Since mass will always be conserved in AMP, and because the
 186 SBM solves for mass mixing ratio in each bin, it is useful to also define a
 187 mass distribution as

$$188 \quad r(D \vee r_0, \nu, D_n) = \frac{\pi}{6} \rho_w D^3 n(D) = \frac{r_0}{\Gamma(\nu+3)} \left(\frac{D}{D_n} \right)^{\nu+3} e^{-\frac{D}{D_n}}$$

189 (2)

190 where $r_0 = \frac{\pi}{6} \rho_w N_0 D_n^3 \frac{\Gamma(\nu+3)}{\Gamma(\nu)}$ is the mass mixing ratio for a hydrometeor

191 category and $m(D) = \frac{\pi}{6} \rho_w D^3$ is the mass of a single hydrometeor. Finally, the
 192 number distribution can be rewritten with r_0 rather than N_0 :

$$193 \quad n(D \vee r_0, \nu, D_n) = \frac{r_0}{m(D) \Gamma(\nu+3)} \left(\frac{D}{D_n} \right)^{\nu+3} e^{-\frac{D}{D_n}}$$

194 (3)

195

196 At the beginning of each call to AMP, the values of the parameter set r_0, ν, D_n
 197 for both cloud droplets and rain must be determined from the predicted
 198 moments. For double-moment configurations of AMP, r_0 and D_n are
 199 determined from the values of the predicted moments of each species and
 200 the value of ν is specified as a constant value. For triple-moment
 201 configurations, all three parameters, r_0, D_n , and ν are determined solely from
 202 the values of the predicted moments of each species. The procedure for
 203 determining the parameter values is described fully in the Appendix. In brief,
 204 binned distributions are inherently doubly truncated, which forces us to use
 205 iterative methods to find the parameter set that creates a binned gamma
 206 $n(D)$ with the appropriate moment values. The procedure is applied to each
 207 hydrometeor species separately. Note that as in standard bulk schemes, AMP
 208 splits the liquid hydrometeors into two categories: cloud droplets and
 209 raindrops. Specifically, drops with diameters of 80 μm or larger are
 210 considered rain drops.

211

212 It is important to mention that AMP is treated as an ideal bulk scheme. As
 213 such, it will not behave in the same way as any particular existing bulk
 214 scheme. Existing bulk schemes often take very different approaches to
 215 parameterizing some processes, most notably for example, collision-
 216 coalescence. Existing bulk schemes artificially separate this process into
 217 autoconversion and accretion, whereas bin schemes, and by extension AMP,
 218 makes no such artificial distinction. As such, this study cannot make any
 219 comments on the strengths or weaknesses of the parameterization of
 220 individual processes in existing bulk schemes. Rather, the idea here is to
 221 suppose that AMP is a perfect bulk scheme, that is, one with a perfect
 222 representation of process rates, and the only limitation in this otherwise
 223 perfect scheme is that distributions must conform to gamma PDFs. While
 224 existing bulk schemes do not have perfect parameterizations currently, it
 225 can be supposed that a perfect parameterization that does not rely on
 226 binned representations could be developed in the future. In this case, how
 227 well could this “perfect” bulk scheme do?

228

229 Inherently AMP assumes that the underlying bin scheme is perfect. This is
 230 the primary limitation of the study since problems with bin schemes are
 231 known to exist – for example, numerical diffusion across bins can lead to

232artificially wide distributions (see Morrison et al. (2018) for a recent summary
233of these problems). Regardless, they are built on the fundamental physical
234principles and equations that underly the three processes that are
235investigated in this study with a minimal number of simplifying assumptions.
236For this reason, bin schemes have been used as a benchmark against which
237to compare bulk schemes in many past studies (see Khain et al. 2015).
238Furthermore, developers of many bulk schemes have used bin schemes to
239parameterize individual processes, such as sedimentation, collision-
240coalescence, and droplet activation (Feingold et al., 1998; Morrison &
241Milbrandt, 2015; Saleeby & Cotton, 2004, 2008; Thompson & Eidhammer,
2422014; Thompson et al., 2008).

243

244In regards to the specific bin scheme being used in this study, the HUCM
245SBM, it is imperfect like any other bin scheme. It should be noted that the
246developers of this bin scheme have extensively studied the problem of
247artificial broadening and minimized it to the extent possible (Khain et al.,
2482004; Pinsky & Khain, 2002). Nonetheless, it is acknowledged that errors in
249the bin scheme associated with spectral broadening or any other source will
250impact the quantitative results of this study.

251 **3 Box Model Simulations**

252This paper describes initial tests that have been done using AMP to
253understand which (arbitrary) moments of the cloud droplet size distribution
254should be predicted to minimize the errors in distribution moments during
255condensation, evaporation, and collision-coalescence. Each process has
256been simulated in isolation in a 0-D box. A suite of 280 initial conditions are
257designed to span a reasonable phase space for initial cloud water content,
258cloud droplet concentration, and the cloud droplet size distribution shape
259parameter. Specifically, initial cloud water content ranges from 1 to 5 g/kg in
260increments of 1 g/kg, cloud droplet concentration is doubled from 100 to
2613200 mg^{-1} , and the shape parameter ranges from 1 to 15 in increments of 2.
262The ranges of cloud water content and cloud droplet concentration give
263initial mass mean cloud droplet diameters of 8.4 μm to 58 μm . 58 μm is
264typical of very large cloud droplets or small drizzle drops.

265

266Simulations with each initial condition were conducted with several
267configurations of AMP. Double-moment configurations predicting the 3rd and
2680th, 2nd, 4th, 6th, or 8th moments of the cloud droplet category were tested. The
269double-moment configurations will be designated as 2M-3X where X
270indicates the second predicted moment. For example, 2M-34 indicates the
271AMP configuration with the 3rd and 4th moments predicted. In all 2M tests, the
272shape parameter was held constant for the duration of the simulations. For
273triple-moment configurations, all combinations of two even-numbered
274moments plus the third moment were tested for the cloud droplet category.
275Triple-moment configurations will be denoted 3M-3XY where X is the first
276predicted moment and Y is the second.

277

278In 2M configurations, the 0th and 3rd moments of rain were always predicted;
279in 3M configurations, the 6th moment of rain was also predicted. Additional
280testing showed that the results were not highly sensitive to the configuration
281of the rain category (not shown). Although accretion of cloud droplets by rain
282is the dominant mechanism by which cloud is converted to rain, the
283insensitivity to the rain configuration in the collision-coalescence tests is
284consistent with the theoretical work of Seifert and Beheng (2001) who
285showed that accretion rates are primarily controlled by the total mass mixing
286ratios of cloud and rain.

287

288Simulations are also run with just the HUCM bin scheme without any use of
289gamma PDFs. These bin simulations will be used to evaluate the AMP
290simulations.

291

292Both the condensation and evaporation tests were run with temperature of
293283 K and pressure of 1000 hPa. Evaporation tests used a relative humidity
294of 95% while condensation tests used a supersaturation of 0.5%. The
295temperature, pressure, and humidity of the box was held constant in time.
296Condensation tests were run for one minute. Such a short time was used
297since droplet distributions growing by condensation quickly become
298unrealistically narrow in the absence of distribution broadening mechanisms
299that occur naturally outside of box model simulations. Evaporation tests were
300run for thirty minutes to allow enough time for complete evaporation of the
301initial cloud water. Collision-coalescence tests were also run for thirty
302minutes; unsurprisingly, many initial conditions failed to produce
303precipitation in that time. All sets of initial conditions that did not produce
304rain with any AMP configuration or with the bin model were discarded.

305

306Although only two or three moments were predicted in each AMP simulation,
307values of all moments (0th – 9th) were diagnosed and written to the output
308after each time step by integrating over the final size distribution produced
309by the parameterization routines.

3104 Results Using AMP in Double-Moment Configurations

311Results for each process are analyzed similarly. A percent error was
312calculated for each moment in each simulation by comparing its value to
313that in the corresponding bin simulation. The bin simulations are considered
314truth for the purposes of comparison. Absolute values of the percent errors
315are used. For each diagnosed moment, there are 280 percent error values
316from the 280 initial conditions for each AMP configuration.

317 4.1 Condensation

318The 5th, 25th, 50th, 75th, and 95th percentiles of the 280 percent error values
319associated with the condensation simulations are shown in Figure 2 for the

3200th, 3rd, and 6th moments diagnosed after one minute of condensation. Most
 321impressively, the percent error of the 3rd moment (mass) is almost always
 3221% or less, regardless of the combination of moments predicted (Figure 2b).
 323Errors increase somewhat from 2M-30 to 2M-38, but ultimately all
 324configurations accurately predict the evolution of mass during condensation.
 325

326The cloud droplet number concentration (0th moment) should be conserved
 327during condensation since new particles are not generated by condensation.
 328Figure 2a shows that conservation of the 0th moment is only achieved by
 329explicitly predicting the 0th moment. Otherwise, there is about a 10-20%
 330median error after one minute of condensation regardless of the moments
 331predicted. This is quite a rapid increase in error that is approximately linear
 332in time; after five minutes, the median error is about 60-100% (not shown).
 333The most immediate concern may be that errors in the number
 334concentration would propagate to errors in the average cloud droplet
 335diameter. Figure 3a shows error distributions for the ratio of the 1st moment
 336to the 0th moment (mean diameter) and 3b shows error distributions for the
 337ratio of the 3rd moment to the 2nd moment (effective diameter). They show
 338that the median errors for these two quantities are not nearly so different
 339between 2M-30 and the other 2M configurations after one minute as they are
 340for the number concentration. For cloud droplet effective diameter, the
 341median errors are quite similar across all configurations (Fig. 3b) since it
 342does not rely on the prediction of number concentration. Therefore, while a
 343lack of conservation of the cloud droplet number concentration propagates
 344to an error in the mean diameter, this error is relatively small compared to
 345the original error in number concentration.

346

347Perhaps unsurprisingly, median errors in the 6th moment are minimized by
 348explicitly predicting the 6th moment (Fig. 2c). Nonetheless, apart from 2M-30,
 349all combinations of predicted moments have values of the 95th percentile
 350error of only about 20%. This result indicates that these configurations all
 351generally keep errors in cloud droplet reflectivity factor low. However, 2M-30
 352is the only configuration for which errors in the predicted cloud droplet
 353number concentration are low. Therefore, there is no AMP configuration
 354which allows us to simultaneously minimize the errors in all moments even
 355for a relatively simple physical process like condensation.

356 4.2 Evaporation

357The errors in the AMP simulations are evaluated as a function of time for
 358evaporation. Since the time for complete evaporation depends on the initial
 359conditions, the fraction of mass remaining in the bin simulation of each
 360simulation set is used as a proxy metric for time. Median percent errors are
 361shown as a function of this “time” in the top row and the median evolution of
 362the normalized moments are shown in the bottom row of Figure 4. The
 363moments have been normalized by their initial value.

364

365 Median errors are generally 20% or less for both the 0th and 3rd cloud droplet
366 moments regardless of the AMP configuration (Fig. 4a-b). Errors tend to be
367 larger toward the end of the simulation when most cloud mass has already
368 evaporated. So, while the percent errors are larger, the absolute errors are in
369 fact small.

370

371 Unlike for condensation, 2M-30 does not result in substantially lower errors in
372 the predicted cloud droplet number concentration compared to other
373 configurations (Fig. 4a). In fact, by the end of the evaporation process, 2M-30
374 has the highest errors of all configurations. Figure 4d indicates that the 2M-
375 30 simulations have the most variability in the evolution of the number
376 concentration and that these simulations tend to evaporate full droplets too
377 slowly. Similar behavior was seen by Igel and van den Heever (2017b).
378 Evaporation will naturally result in a size distribution with a non-zero number
379 of droplets in the smallest size bin, i.e. a truncated left distribution tail that is
380 difficult to capture with fixed size distribution functions. However, the
381 truncated left tail will be less prominent in distributions of higher moments,
382 and therefore it may be easier numerically to capture the evolution of the
383 distribution with these higher moments. To investigate this problem, the
384 binned distribution of cloud droplets at the end of the call to the bin
385 microphysics routines during each AMP simulation was written to a file. Each
386 distribution could then be compared to the idealized distribution that was
387 initialized at the start of the subsequent time step. When the 0th moment is
388 predicted with AMP, fitting a PDF to a truncated size distribution usually
389 results in a left tail that is too small. For example, in 70% (91%) of left-
390 truncated distributions after the first timestep, the number concentration in
391 the first bin of the re-initialized gamma distribution is $\geq 50\%$ ($\geq 10\%$) less
392 than the predicted number concentration in the first bin at the end of the
393 previous time step. If the bin scheme were to always produced perfect
394 gamma distributions, then these two values would always be equal. These
395 statistics indicate that undersized left tails are quite common in 2M-30
396 configurations of AMP during evaporation. An undersized left tail would cause
397 too few droplets to be evaporated during each time step as is observed in
398 Figure 4d.

399

400 The 2M-32 configuration seems to best predict the cloud mass evolution for
401 the first half of evaporation while the other configurations perform similarly
402 (Figure 4b). For the reflectivity factor, predicting higher moments clearly
403 leads to reductions in the median error (Figure 4c). Interestingly, for
404 evaporation, the error in the 6th moment is minimized by predicting the 8th
405 moment during the latter half of evaporation, and not by predicting the 6th
406 moment. For evaporation, it is clearly seen that predicting a moment does
407 not necessarily lead to the best simulation of that moment - predicting the
408 0th moment does not minimize errors in the number concentration and
409 predicting the 6th moment does not always minimize errors in the reflectivity
410 factor. Lower errors for reflectivity factor with 2M-36 rather than 2M-30 are in

411 agreement with the results of Szyrmer et al. (2005) who examined steady-
412 state evaporation in a rain shaft model.

413 4.3 Collision-Coalescence

414 The results of the collision-coalescence tests are shown in Figure 5 in the
415 same way as for evaporation in Figure 4. Recall that although tests are only
416 run for the configuration and initial conditions of the cloud droplet category,
417 the rain category is active in all collision-coalescence simulations. Therefore,
418 total liquid mass is constant during all simulations.

419

420 Errors in the cloud droplet reflectivity factor are about the same for each
421 AMP cloud droplet configuration (Figure 5c). However, the errors for the
422 cloud droplet number concentration (Figure 5a) and mass mixing ratio
423 (Figure 5b) are distinctly different for each AMP configuration. Errors in the
424 cloud droplet number concentration increase whereas errors in the cloud
425 droplet mass mixing ratio decrease as higher moments are predicted. The
426 magnitude of errors varies substantially among the AMP configurations;
427 median errors in the mass mixing ratio are 10% or less during the entire
428 evolution of the cloud droplet distribution for 2M-38 whereas they approach
429 100% at the end of the process for 2M-30 (Figure 5b). This result suggests
430 that the evolution of cloud mass during the collision-coalescence process
431 could potentially be substantially improved in current bulk schemes by
432 predicting a higher moment. The cost though is that the evolution of the
433 cloud droplet number concentration would deteriorate. Of the three
434 processes examined, collision-coalescence provides the clearest example of
435 how no single AMP configuration minimizes the errors of all cloud droplet
436 moments simultaneously.

437

438 Collision-coalescence errors also clearly illustrate some shortcomings of
439 assuming a gamma PDF for the cloud droplet size distribution. Nearly all AMP
440 simulations convert cloud mass to rain too slowly (Fig. 5e). Since AMP and
441 the bin scheme both use the same parameterization for collision-
442 coalescence, this slowness must be due to the use of an assumed size
443 distribution function. The failure of all AMP configurations to produce rain
444 quickly enough likely arises because the initiation of rain from a collection of
445 cloud droplets depends crucially on the production of a small number of
446 larger droplets that reside in the right tail of the cloud droplet size
447 distribution. Any microphysics scheme must be able to “remember” that
448 these larger droplets exist since they are the ones that will collect the most
449 additional cloud droplets in subsequent time steps and first grow to rain drop
450 sizes. When low moments of the distribution are predicted, Figure 6 shows
451 that AMP indeed fails to retain the largest cloud droplets with an assumed
452 gamma PDF in 90% or more of simulations when at the same time the
453 corresponding bin simulations show that rain production has begun. As a
454 result, these AMP configurations produce rain much too slowly (Fig. 5e). AMP
455 is much more likely to remember the few-but-important large cloud droplets

456if high moments of the cloud droplet distribution are predicted since higher
457moments give more weight to these larger droplets. Figure 6 shows that this
458is the case although a large majority of simulations in 2M-36 and 2M-38 still
459underestimate the right tail of the cloud droplet distribution during the
460earliest stages of rain production in the bin simulations. Interestingly, 2M-36
461and 2M-38 convert cloud water to rain too slowly even though the calculated
4626th moment tends to be too large (Fig. 5f). This result seems to illustrate just
463how difficult it is for a bulk scheme to replicate the behavior of a bin scheme
464even when the process parameterization is identical.
465

466 4.4 Discussion

467It is impossible to take the results for all three microphysical processes and
468determine which is the “best” combination of moments to predict for the
469cloud droplet distribution. First, doing so will require running 3D simulations
470of warm phase clouds which is beyond the scope of this paper but is planned
471for future work. Second, the answer to this question seems likely to be
472application specific. For example, one combination of moments may be best
473for predicting liquid water path, while another is best for predicting cloud
474albedo.
475

476Nonetheless, some synthesis of the preceding tests is desirable. To do so,
477the median time-averaged absolute normalized errors of the 0th - 6th
478moments of the cloud droplet distributions in the AMP simulations have been
479calculated for each AMP configuration and for each process. These errors are
480additionally averaged over all processes (colored lines in Figure 7) and
481across the 0th to 3rd moments (black line) and 0th to 6th moments (gray line).
482The normalization is done with respect to the initial values of each moment
483in each simulation and all processes are given equal weight in the average.
484These summary quantities are similar to the one used by Milbrandt and
485McTaggart-Cowen (2010).
486

487Figure 7 clearly shows that the process-ensemble errors in the 0th to 2nd
488moments of the cloud droplet distribution are minimized for 2M-32 or 2M-34
489whereas errors in all higher order moments are minimized in 2M-36 or 2M-
49038. The inability of 2M configurations to simultaneously simulate low and
491high moments well was also found by Szyrmer et al. (2005). Unsurprisingly
492then, the average error in all cloud distribution moments (both 0th-3rd and 0th-
493- 6th) is minimized by predicting a middling moment (Figure 7). Predicting the
4943rd and 4th moments or 3rd and 6th moments seem optimal. Morrison et al
495(2019) speculated that this may be the case based on their analysis of the
496relationships between moments of rain drop size distributions.

4975 Results Using AMP in Triple-Moment Configurations

498 Simulations with AMP in triple-moment configurations were also conducted
 499 as described in Section 3. Median time-averaged absolute normalized errors
 500 of the number, mass, and reflectivity factor of the cloud droplet distribution
 501 like those in Figure 7 are shown in Figures 8-11 for each process and for all
 502 processes averaged together. While a lot of information is contained in each
 503 figure, I will focus on the 'x's and 'o's in each panel which indicate the
 504 configurations with the highest and lowest errors, respectively, for each
 505 moment.

506

507 Overall, the results for the 3M tests are qualitatively similar to the 2M tests.
 508 Cloud mass is well predicted during condensation regardless of the
 509 combination of predicted moments (Fig. 8). Droplet number concentration
 510 during condensation is only conserved if the 0th moment is predicted (Fig. 8a-
 511d), and cloud reflectivity factor errors are usually low if the 6th or 8th moment
 512 is predicted (right half of Fig. 8). Overall, errors during condensation are
 513 minimized in the 3M-304 and 3M-306 configurations (Fig. 8b-c). 3M-306 is
 514 the typical combination of moments predicted by triple-moment bulk
 515 schemes. Errors are maximized in the 3M-368 configuration.

516

517 Errors for cloud mass in AMP during evaporation are generally low for all 3M
 518 configurations (Fig. 9). Errors in the droplet number concentration are
 519 highest when the 0th moment is actually predicted (Fig. 9a-d) whereas errors
 520 in number are minimized when combinations of higher order moments are
 521 predicted (Fig. 9h). Again, this unusual result may stem from large
 522 departures of size distributions from the assumed gamma PDF shape. As it
 523 turns out, all moments have their highest error when the 0th moment is
 524 predicted - 3M-308 for lower order moments (Fig. 9d) or 3M-302 for higher
 525 order moments (Fig. 9a). Errors in reflectivity factor also remain lowest when
 526 combinations of higher order moments are predicted (Fig. 9h-j). These
 527 results taken together mean that errors overall are minimized in 3M-346 (Fig.
 528 9h).

529

530 Again, the errors during collision-coalescence in 3M configurations of AMP
 531 mirror behaviors of 2M configurations. Errors in the number concentration
 532 are strongly reduced in 3M configurations when the 0th moment is predicted
 533 regardless of which other moment is also predicted (Fig. 10a-d). 2M-30
 534 results in lower errors than any 3M configuration that doesn't include the 0th
 535 moment (not shown). This result serves to emphasize the importance of
 536 predicting the 0th moment of the cloud droplet size distribution during
 537 collision-coalescence in order to minimize errors in the evolution of the
 538 number concentration. On the other hand, errors in the higher order
 539 moments (4th-6th) are lowest in 3M-368 when errors in lower order moments
 540 (0th-2nd) are maximized (Fig. 10j). Errors in both the cloud droplet number
 541 and mass concentrations are lowest in 3M-308 (Fig. 10d). Although this

542 configuration also has the highest errors for the 5th and 6th moments, errors
 543 in the 5th and 6th moments are generally similar regardless of the AMP
 544 configuration and so the overall errors are minimized for 3M-308 again.
 545

546 Overall, errors in 0th-3rd moments of the cloud droplet size distribution are
 547 each minimized in a different configuration (3M-302, 3M-304, 3M-306, and
 548 3M-328, respectively; Fig. 11a-c, g), and errors in the 4th-6th moments are all
 549 minimized in a fifth configuration (3M-368; Fig. 11j). Like for the 2M cloud
 550 droplet configurations, no single 3M configuration minimizes the error in all
 551 moments simultaneously. Likewise, errors in each of the three processes are
 552 minimized by predicting a different combination of moments – 3M-304/3M-
 553 306 for condensation, 3M-346 for evaporation, and 3M-308 for collision-
 554 coalescence (Fig. 9b-c, Fig. 9h, Fig. 10d). Evaporation stands out as the only
 555 process for which errors were minimized when the predicted integer
 556 moments are all close. For the other two processes, the optimal
 557 configuration includes both high and low order moments. This result agrees
 558 with Morrison et al. (2019) as discussed in the introduction.
 559

560 The preceding paragraph identifies seven configurations as “best” for
 561 predicting the cloud droplet category depending on the evaluation used. This
 562 result serves to highlight that it is impossible to design a bulk scheme that
 563 can perform well under all circumstances. When all errors for the 0th-3rd
 564 moments are averaged together, 3M-304 emerges as the configuration with
 565 the lowest error (Fig. 11b), whereas when the 0th-6th moments are averaged
 566 together it is 3M-306 (Fig. 11c), although the difference in error between 3M-
 567 304 and 3M-306 is slight for both averages. While this error metric is by no
 568 means perfect, this result is an encouraging one since existing triple-moment
 569 schemes typically predict the 0th, 3rd, and 6th moments.

570 **5 Conclusions**

571 In this study, a flexible “bulk-emulating”, arbitrary moment predictor
 572 microphysics scheme has been developed by modifying a bin microphysics
 573 scheme. Moments of the size distribution are calculated at the end of one
 574 microphysical time step, used to find parameters of the gamma PDF, and
 575 used to initialize a binned distribution at the start of the next microphysical
 576 time step. Therefore, the arbitrary moment predictor and bin schemes have
 577 identical process parameterizations, but different representations of the
 578 hydrometeor size distributions. There are two motivations for developing this
 579 scheme. First, it allows an “apples-to-apples” comparison of bulk and bin
 580 schemes and gives us a way to understand the consequences of assuming a
 581 gamma PDF in bulk schemes. Second, the arbitrary moment predictor
 582 scheme can predict any combination of distribution moments. This
 583 capability allows us to investigate which combinations of predicted moments
 584 minimize the errors of a bulk scheme. As far as the author is aware, these
 585 are novel capabilities for a cloud microphysics scheme.

586

587The arbitrary moment predictor microphysics scheme was run in several
588configurations of the cloud droplet category for many different initial
589conditions in a box model. Three processes were investigated –
590condensation, evaporation, and collision-coalescence. The evolution of the
591number concentration, mass mixing ratio, and reflectivity factor of the cloud
592droplet size distribution were compared to their evolution using a pure bin
593scheme with the same initial conditions. Based on these simulations, the
594following conclusions are drawn:

- 595 • No 2M or 3M cloud droplet configuration can simultaneously minimize
596 the error of all cloud droplet distribution moments. This result is in
597 agreement with the results of Szyrmer et al. (2005) and Milbrandt and
598 McTaggart-Cowan (2010) for precipitating hydrometeors.
- 599 • Predicting a moment may or may not minimize the error of that
600 moment. During condensation the error in the number concentration
601 and reflectivity factor was minimized when the 0th moment and 6th
602 moment were predicted, respectively in both 2M and 3M
603 configurations. During evaporation, errors in the number concentration
604 were instead maximized when the 0th moment was predicted.
- 605 • Errors during collision-coalescence were higher than those for
606 condensation and evaporation. Nearly all arbitrary moment predictor
607 simulations produced rain too slowly. This result points to a
608 fundamental limitation of assuming gamma PDFs.
- 609 • Double-moment bulk schemes predicting the 3rd and 4th or 3rd and 6th
610 moments of the cloud droplet size distribution may have the potential
611 to perform better than those predicting the standard combination of
612 the 3rd and 0th moments.
- 613 • Current triple-moment bulk schemes may already be predicting the
614 optimal combination of cloud droplet size distribution moments.
615

616The last two conclusion points need to be confirmed by running AMP in a 3D
617model with all processes occurring simultaneously. Implementation of AMP in
618a 3D model will be done in the future to further investigate and substantiate
619these results. The current results will serve as a basis for interpreting the
620results obtained in a 3D model.

621

622Finally, it is important to frame the conclusions drawn above. The
623suggestions made by AMP are very general and only apply strictly to what
624may be thought of as the ideal bulk scheme. Existing bulk schemes behave
625in non-ideal ways. Therefore, in practice, real-world bulk schemes may not
626actually perform best when predicting the moments suggested above.
627Rather, what our results show is that an ideal bulk scheme with physical
628parameterizations as good as those in the bin scheme will behave best with
629the predicted moments above. As we continue to improve bulk schemes
630with better physics, the results should become ever more relevant.

631

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 637 will be deposited upon acceptance of the manuscript.)

638 Appendix

639 Here the procedure for determining the parameter values for $n(D)$ at the
 640 start of the microphysics routines is described. The variable first, second,
 641 and third predicted moments will be referred to as the Ist, IInd and IIIrd
 642 predicted moments, respectively. Note, for example, that the IInd predicted
 643 moment is not necessarily the 2nd moment of a PSD. The IInd predicted
 644 moment instead is the second predicted moment and can take on any value
 645 (i.e. it is arbitrary) except for the 3rd. In standard bulk microphysics
 646 schemes, the Ist predicted moment is the 3rd moment and the IInd predicted
 647 moment is the 0th moment.

648

649 To start, it is important to point out that there are two sets of moments in
 650 the AMP scheme. The first is the set of moments *predicted* by the bin
 651 scheme, ${}^p M_j$. The subscript j is the moment number. For example, ${}^p M_3$ is the
 652 Ist predicted moment and ${}^p M_0$ is the IInd predicted moment in standard
 653 double-moment bulk schemes. At the start of the microphysics routines, the
 654 predicted moments are used to find parameters of $n(D)$. Once $n(D)$ is known,
 655 any moment of $n(D)$, not just the Ist, IInd and IIIrd moments, may be calculated.
 656 This brings us to the second set of moments, which are those moments
 657 *diagnosed* from $n(D)$ and denoted by ${}^d M_j$. The goal at the start of each call to
 658 the microphysics routines is to find a set of parameters r_0, ν, D_n of $n(D)$ such
 659 that ${}^p M_j = {}^d M_j$ for each hydrometeor type. At the end of each call to the
 660 microphysics routines, the values of ${}^p M_j$ are updated by calculating the
 661 corresponding values of ${}^d M_j$.

662

663 Moments of a continuous distribution are calculated by integrating $n(D)$
 664 multiplied by a power of D over all diameters from 0 to ∞ . In the model, the
 665 distribution is discretized which requires us to know the discrete value of
 666 $\ln D$, also known as the bin width (w). For the case of mass-doubling bins, w
 667 = $\ln(2)/3$ for all bins. The moments ${}^d M_j$ are then calculated as

$$668 \quad {}^d M_j = \sum_{i=1}^{nbins} n(D_i) D_i^j w$$

669 (A1)

670

671 To solve for the parameter set, we first recognize that r_0 is independent of D_n
 672 and ν and that all moments are directly proportional to r_0 . This means that

673 we can initially choose an arbitrary, temporary value of r_0 that we will call
 674 r_{0temp} for use in calculating dM_j for all j . In that case ${}^dM_j/{}^pM_j$ is a constant for
 675 all values of j . Specifically,

$$676 \quad \frac{{}^dM_j}{{}^pM_j} = \frac{r_{0temp}}{r_0}$$

677 (A2)

678

679 Once D_n and ν are calculated, r_0 can be solved for analytically using Eq. A2
 680 and then values of dM_j can be recalculated with the updated (true) value of
 681 r_0 such that ${}^pM_j = {}^dM_j$.

682

683 For complete gamma PDFs, equations exist to solve analytically for D_n and ν .
 684 However, binned distributions inherently represent doubly-truncated
 685 distributions that span from the smallest bin's diameter to the largest bin's
 686 diameter. Analytical solutions for D_n and ν do not exist for truncated,
 687 incomplete gamma PDFs. To solve for these two parameters, we instead use
 688 iterative routines to minimize the error of dM_j compared to pM_j . Values of dM_j
 689 can be calculated at any point during the iterative procedure from the
 690 current guesses of the parameter values. The goal is to ensure that at the
 691 end of the iterative procedure that Eq. A2 is satisfied.

692

693 From Eq. A2 we can write

$$694 \quad \frac{{}^pM_{II}}{{}^pM_3} = \frac{{}^dM_{II}}{{}^dM_3} \quad \text{and} \quad \frac{{}^pM_{III}}{{}^pM_3} = \frac{{}^dM_{III}}{{}^dM_3}$$

695 or

$$696 \quad 1 - \frac{{}^pM_{II}}{{}^pM_3} \frac{{}^dM_3}{{}^dM_{II}} = 0 \quad \text{and} \quad 1 - \frac{{}^pM_{III}}{{}^pM_3} \frac{{}^dM_3}{{}^dM_{III}} = 0$$

697 (A3)

698 if the correct values of D_n and ν have been determined. If the correct values
 699 of D_n and ν have not been determined, then the left-hand sides of (A3) can
 700 be evaluated to quantify the error associated with the current values of D_n
 701 and ν . The Fortran Minpack hybrd1.f routines are used to iteratively
 702 minimize the absolute value of the LHSs of Eq. A3. The performance of this
 703 routine (and all iterative solvers) depends crucially on the first guess for the
 704 parameters. To determine a first guess, we use either the values of the
 705 parameters from the previous timestep, or we use look-up tables. The look-

706 up tables are functions of $\frac{{}^pM_{II}}{{}^pM_3}$ and $\frac{{}^pM_{III}}{{}^pM_3}$. Once D_n and ν have been

707 determined, Eq. A2 is used with pM_3 to solve for r_0 . These lookup tables were
 708 constructed in MATLAB by systematically creating binned distributions with 4

709 million combinations of D_n and ν , calculating values of $\frac{pM_{II}}{pM_3}$ and $\frac{pM_{III}}{pM_3}$, and
 710 inverting the data to make D_n and ν functions of $\frac{pM_{II}}{pM_3}$ and $\frac{pM_{III}}{pM_3}$ in the tables.

711

712 It is possible to predict values of pM_j for which no solution exists in both the
 713 double- and triple-moment configurations. In this case we ensure that
 714 $pM_3 = dM_3$, and additionally if possible that $pM_{II} = dM_{II}$ in the triple-moment
 715 configurations. Therefore, mass is always conserved by AMP. In this case,
 716 values of pM_j are updated by finding the change in the initial and final values
 717 of dM_j and adding it to pM_j .

718

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827

828 **Figure Captions**

829

830 **Figure 1.** A flow chart depicting the steps taken in AMP to predict moments
831 of one hydrometeor species.

832 **Figure 2.** Box and whisker plots of the percent errors of the AMP simulations
833 relative to the BIN simulations after one minute of condensation for the a)
834 0th, b) 3rd, and c) 6th moments of the cloud droplet distributions. Boxes show
835 the 25th, 50th, and 75th percentiles of the error distributions, and whiskers
836 show the 5th and 95th percentiles. See the text for more details.

837 **Figure 3.** Like Figure 2 except for (a) cloud droplet mean diameter and (b)
838 cloud droplet effective diameter.

839 **Figure 4.** Evolution of the median percent error (a-c) and median
840 normalized moment values (d-f) during evaporation for the (a, d) 0th, (b, e)
841 3rd, and (c, f) 6th moments of the cloud droplet size distribution. 25th and 75th
842 percentile values are shown intermittently. In (d-f), the median evolution of
843 the bin simulations is shown by the black dashed line. Note that the x-axes in
844 all panels are defined such that the black dashed line in (e) is straight.

845 **Figure 5.** As in Figure 4 except for the collision-coalescence tests.

846 **Figure 6.** Fraction of 2M AMP simulations in each configuration that have
847 too few droplets in the largest cloud droplet bin (the right tail of the cloud
848 droplet size distribution) when the distribution is initialized as a gamma PDF
849 at the start of a time step compared to the explicit size distribution from
850 which the moments are calculated at the end of the previous time step. The
851 fractions are shown as a function of the time in the corresponding bin
852 simulations at which a given fraction of the cloud mass remains unconverted
853 to rain water (as in Figure 5).

854 **Figure 7.** Median across 2M AMP simulations (average of all three
855 processes) in each configuration of the time-averaged absolute normalized
856 error of the 0th through 6th moments of the cloud droplet size distribution.
857 The black and gray lines show the mean average absolute error of the 0th-3rd
858 moments and 0th-6th moments, respectively. Circles indicate the
859 configuration with the lowest average error for each line.

860 **Figure 8.** Median across all AMP condensation simulations in each 3M
861 configuration of the time-averaged absolute normalized error of the 0th
862 through 6th moments of the cloud droplet size distribution. The light and dark
863 orange bars show the mean average absolute error of the 0th-3rd moments
864 and 0th-6th moments, respectively. 'x's and 'o's indicate the configuration
865 with the highest and lowest average error, respectively, for each set of bars
866 with the same color. Errors in (a-d) for the 0th moment are not shown and are
867 generally about 10⁻¹⁰.

868 **Figure 9.** As in Figure 8 except for the evaporation simulations.

869 **Figure 10.** As in Figure 8 except for the collision-coalescence simulations.

870 **Figure 11.** As in Figure 8 except for the average across all process
871 simulations.