

A Moment-based Polarimetric Radar Forward Operator for Rain **Microphysics** 2 Matthew R. Kumjian* and Charlotte P. Martinkus 3 Department of Meteorology and Atmospheric Science, The Pennsylvania State University, University Park, Pennsylvania, USA 5 Olivier P. Prat 6 North Carolina Institute for Climate Studies, North Carolina State University, Asheville, North 7 Carolina, USA 8 Scott Collis 9 Argonne National Laboratory, Chicago, Illinois, USA 10 Marcus van Lier-Walqui 11 Center for Climate Systems Research, Columbia University, and NASA Goddard Institute for 12 Space Studies, New York, New York, USA 13 Hugh C. Morrison 14 National Center for Atmospheric Research[†], Boulder, Colorado, USA Corresponding author address: Department of Meteorology and Atmospheric Science, The Pennsylvania State University, 513 Walker Building, University Park, PA 16802

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ABSTRACT

There is growing interest in combining microphysical models and polari-20 metric radar observations to improve our understanding of storms and pre-2 cipitation. Mapping model-predicted variables into the radar observational 22 space necessitates a forward operator, which requires assumptions that intro-23 duce uncertainties into model-observation comparisons. These include un-24 certainties arising from the microphysics scheme a priori assumptions of a 25 fixed drop size distribution (DSD) functional form, whereas natural DSDs 26 display far greater variability. To address this concern, this study presents a 27 moment-based polarimetric radar forward operator with no fundamental re-28 strictions on the DSD form by linking radar observables to integrated DSD 29 moments. The forward operator is built upon a dataset of > 200 million re-30 alistic DSDs from one-dimensional bin microphysical rain shaft simulations, 3. and surface disdrometer measurements from around the world. This allows 32 for a robust statistical assessment of forward operator uncertainty and quan-33 tification of the relationship between polarimetric radar observables and DSD 34 moments. Comparison of "truth" and forward-simulated vertical profiles of 35 the polarimetric radar variables are shown for bin simulations using a variety 36 of moment combinations. Higher-order moments (especially those optimized 37 for use with the polarimetric radar variables: the 6th and 9th) perform better 38 than the lower-order moments (0th and 3rd) typically predicted by many bulk 39 microphysics schemes. 40

41 **1. Introduction**

There is growing interest in combining numerical models and observations to further our un-42 derstanding of weather and climate. For microphysical comparisons, polarimetric Doppler radar 43 is a particularly attractive choice of observations, owing to the fact that these data can provide 44 several key pieces of information useful for characterizing bulk properties of precipitation, such as 45 hydrometeor sizes, shapes, concentrations, and motion (Kumjian 2013a). Radar data resolution is 46 also ideal because it can match or exceed the higher resolution of many mesoscale and storm-scale 47 model outputs (Keil et al. 2003). Radar data have been useful for a variety of purposes, including 48 for model evaluation (e.g., Hagos et al. 2014; Sinclair et al. 2016; Barnes and Houze 2016; John-49 son et al. 2016), data assimilation (e.g., Tong and Xue 2005; Jung et al. 2010b; Schenkman et al. 50 2011; Putnam et al. 2014), and gaining insights about precipitation microphysical processes (e.g., 51 Kumjian and Ryzhkov 2010, 2012; Dawson et al. 2014; Kumjian et al. 2014; Sulia and Kumjian 52 2017a,b). To make such comparisons within the variable space of observations, forward oper-53 ators must be used to convert model-predicted variables into quantities observed by some radar 54 platform. 55

Several polarimetric radar forward operators have been developed for use with bulk and bin 56 microphysics models (e.g., Pfeifer et al. 2008; Jung et al. 2008; Ryzhkov et al. 2011; Andrić et al. 57 2013). For bulk models, without exception the approach is to use model-predicted microphysical 58 quantities to construct a particle size distribution (PSD) for each hydrometeor type at each grid 59 box that matches the microphysics scheme's underlying assumptions about the PSD functional 60 form. Most often, the PSDs (including raindrop size distributions, or DSDs) are given by gamma 61 or normalized gamma functions (e.g., Willis 1984; Testud et al. 2001). The PSD is then discretized 62 into a series of particle size bins, whereupon electromagnetic scattering calculations are performed 63

(e.g., Ryzhkov et al. 2011). The hydrometeor scattering properties and PSD are then integrated to
 obtain the radar variables of interest at each grid box.

This approach has been successful in producing simulated fields of polarimetric radar variables 66 that reproduce basic observed signatures, particularly in convective storms (e.g., Jung et al. 2010a; 67 Ryzhkov et al. 2011, 2013a,b; Kumjian et al. 2012, 2014, 2015; Putnam et al. 2014, 2017; Dawson 68 et al. 2014; Johnson et al. 2016) and winter storms (e.g., Andrić et al. 2013; Sulia and Kumjian 69 2017a,b). However, these model-observation comparisons using forward operators often have 70 substantial uncertainties, the details of which usually are not assessed. One class of uncertainties 71 includes those associated with tunable parameters used or imposed by the forward operator to 72 characterize particle properties not explicitly predicted or diagnosed by the microphysics model; 73 for example, ice crystal shapes are treated using fixed maximum dimension-thickness relationships 74 in the forward operators of Ryzhkov et al. (2011) and Andrić et al. (2013). Other examples include 75 particle fall behaviors (i.e., particle orientation can strongly affect the simulated radar variables but 76 typically is not predicted or provided by microphysics schemes), and even the choice of electro-77 magnetic scattering calculations employed. An example of the latter is discussed by Schrom and 78 Kumjian (2018), who quantified large errors in simulated polarimetric radar variables when ho-79 mogeneous spheroids are used to approximate branched planar crystals like dendrites and stellars 80 in scattering calculations. 81

Another class of uncertainties in model-observation comparison arises only when comparing to the observations themselves, originating from structural errors associated with the accuracy of approximations explicitly made in the formulation of the microphysics schemes. For example, most bulk microphysics parameterization schemes assume a functional form for the PSD, typically one that facilitates analytic integration (like the gamma PSD mentioned above). This leads to a unique mapping between model-predicted variables (e.g., total number concentration, total mass content)

and radar observational quantities. Real PSDs, however, have much greater variability (i.e., not 88 all PSDs have shapes well defined by the simple analytic PSDs assumed in most bulk schemes), 89 leading to a greater number of degrees of freedom than bulk schemes are able to represent. In 90 other words, although there is a unique mapping between PSD moments and radar variables for 91 most bulk microphysics schemes, no such relationship exists in nature¹ (with the exception of a 92 nearly unique mapping between the sixth moment of the raindrop size distribution and radar re-93 flectivity). This necessitates a treatment that accounts for this model deficiency in order to make 94 valid comparisons between radar variables resulting from real and simulated PSDs. 95

This paper circumvents the problem of imposed PSD shape by creating a moment-based forward 96 operator: one that does not assume any PSD functional form. The moment-based forward operator 97 developed herein is flexible and can be used with a variety of bulk microphysics schemes: it 98 directly connects the polarimetric radar variables to integrated PSD moments, regardless of the 99 underlying PSD functional form assumed in such schemes. For example, traditional two-moment 100 bulk microphysics schemes predict mixing ratios for mass (proportional to the third moment) 101 and total number (the zeroth moment). Inputs from such a scheme for the forward operator are 102 values of the zeroth and third moments at each model grid point, with no assumptions about 103 the underlying PSD shape. Note that the moment-based approach is *necessary* in order to use 104 instrument forward operators with bulk microphysics schemes that do not assume an underlying 105 functional PSD form (e.g., Chen and Liu 2004; Szyrmer et al. 2005; Laroche et al. 2005; Kogan 106 and Belochitski 2012). For most current bulk microphysics schemes that do use a fixed PSD 107 functional form, our moment-based forward operator also provides an estimate of uncertainty 108 owing to natural PSD variability not accounted for in these schemes. Such a framework is also 109

¹Note that these uncertainties are also relevant to the calculation of microphysical process rates; however, this is beyond the scope of the current study and will be addressed in future work.

¹¹⁰ used to find the optimal combinations of moments that minimize uncertainty in mapping to the ¹¹¹ radar variables. This can help guide the choice of prognostic variables in bulk schemes such that ¹¹² they are optimized for use in conjunction with radar observations.

Our study is the first step towards this moment-based approach, using the simplest framework: 113 rain (liquid-only) microphysics. Unlike the uncertainties and complexities associated with snow 114 crystals described above, raindrop shapes are relatively well understood (e.g., Pruppacher and Pit-115 ter 1971; Beard 1976; Beard and Chuang 1987; Brandes et al. 2005; Thurai et al. 2009), as are their 116 electromagnetic scattering properties at weather radar wavelengths (e.g., Bringi and Chandrasekar 117 2001; Ryzhkov et al. 2011). Additionally, dual-polarization radar variables are known to provide 118 information – at least qualitatively – on rain microphysical processes such as evaporation (Li and 119 Srivastava 2001; Kumjian and Ryzhkov 2010; Xie et al. 2016), size sorting (Kumjian and Ryzhkov 120 2012), and collision-coalescence-breakup (Kumjian and Prat 2014). In developing this moment-121 based forward operator, we also present the relationships between integrated DSD moments and 122 the polarimetric radar variables, and quantify the uncertainty associated with DSD shape in terms 123 of the polarimetric radar variables for broader use. 124

The next section outlines the methods used in this study. Section 3 describes how to identify the optimal prognostic moments for use with polarimetric radar data. The forward operator is developed in section 4. Section 5 shows example tests using a simulated rain shaft. The paper closes with a discussion and summary of the main conclusions in section 6.

129 **2. Methods**

DSDs are the key to linking microphysical model output to radar data because they are used to compute the bulk physical quantities of interest predicted by the model, typically total number and mass mixing ratios, as well as the radar variables, such as equivalent reflectivity factor at ¹³³ horizontal polarization (Z_H), differential reflectivity (Z_{DR}), and specific differential phase (K_{DP}). ¹³⁴ For a review of these dual-polarization radar variables, see Kumjian (2013a,b) and Kumjian (2018) ¹³⁵ and references therein.

The first step towards developing the forward operator is to create a database of DSDs. A large population of DSDs is desired because the forward operator should be able to handle any realistic precipitation situation. DSDs from both state-of-the-art bin model simulations and ground-based disdrometers are used (described below). The simulations allow for DSDs from a wide portion of the parameter space, representative of a diverse set of precipitation regimes, whereas the disdrometer data include DSDs from several different geographic regions.

The dataset will be briefly described here; details are provided in Morrison et al. (2018). Dis-142 drometer data from the U.S. Department of Energy (DOE) Atmospheric Radiation Measurement 143 (ARM) program Climate Research Facility are used (Ackerman and Stokes 2003; Mather and 144 Voyles 2013). These include samples from model RD80 Joss-Waldvogel impact disdrometers 145 (e.g., Joss and Waldvogel 1967) and two-dimensional video disdrometers (2DVD; e.g., Tokay 146 et al. 2001; Kruger and Krajewski 2002). The data come from geographically diverse regions, 147 including ARM permanent sites in the U.S. Southern Great Plains, Tropical Western Pacific, and 148 Eastern North Atlantic (Mather and Voyles 2013; Sisterson et al. 2016; Long et al. 2016, respec-149 tively), as well as field campaigns in the Indian Ocean (Yoneyama et al. 2013; Gottschalck et al. 150 2013), and Finland (see Miller et al. 2016; Petäjä et al. 2016). These data cover all months and 151 seasons, including stratiform, convective, continental, and maritime regimes. Data quality control 152 and filtering procedures are described in Morrison et al. (2018). After these procedures, 671303 153 disdrometer DSD samples remain (a sample is a 30- or 60-second average). 154

The simulations used herein employ the one-dimensional spectral bin microphysical model of Prat and Barros (2007) and Prat et al. (2012), following the setup used by Kumjian and Prat

(2014). DSD evolution is explicitly predicted for one hour in a one-dimensional, 3-km tall rain 157 shaft with 10-m vertical grid spacing. The model is initialized with a prescribed DSD at the top of 158 the domain. At the first time step, the raindrops (which are discretized into 40 size bins) begin to 159 fall and the DSD then freely evolves under the influence of microphysical processes. The model 160 considers interactions among raindrops including drop coalescence, collisional and aerodynamic 161 breakup, and sedimentation. Overall, the model performs well, consistently able to reproduce 162 realistic DSDs as compared to radar and disdrometers (Prat et al. 2008; Prat and Barros 2009; 163 Kumjian and Prat 2014). One potential bias exists for very heavy rainfall (> 100 mm hr⁻¹), in 164 which an overly aggressive drop breakup formulation may result in an underestimate of median 165 drop size (Kumjian and Prat 2014). A total of 10742 simulations were performed, covering a wide 166 range of initial conditions, including rainfall intensity, mean drop size, DSD shape, etc. (details 167 can be found in Morrison et al. 2018). To populate the DSD dataset, DSDs are taken at every model 168 height and output time (every 1 minute). Doing so allows us to obtain samples of transient and non-169 steady-state DSDs from processes such as size sorting that are not well captured in disdrometer 170 data, but are readily observed in dual-polarization radar observations (e.g., Kumjian and Ryzhkov 171 2012). The bin simulations produced 184180279 DSDs. Thus, the combined dataset is strongly 172 dominated by the bin simulations owing to their availability. 173

Many of the model-predicted physical quantities of interest are proportional to specific moments of the DSD:

$$M_k \equiv \int_{D_{\min}}^{D_{\max}} N(D) D^k dD \tag{1}$$

where M_k is the k^{th} moment of the DSD, integrated from the minimum drop size D_{\min} to maximum drop size D_{\max} , and N(D) is the DSD (number concentration of drops with diameters in the size range D to D+dD). For example, the zeroth moment (M_0) of the DSD is the raindrop total number ¹⁷⁹ concentration, whereas the third (M_3) is proportional to the total raindrop mass content. For each ¹⁸⁰ DSD in the dataset, the integer moments k = [0, 10] were computed using eqn (1). Because the ¹⁸¹ moment values may span several orders of magnitude, we convert them to decibels (dB) using

$$M_k[d\mathbf{B}] = 10 \times \log_{10} \left(\frac{M_k \left[\mathrm{mm}^k \ \mathrm{m}^{-3} \right]}{1 \ \mathrm{mm}^k \ \mathrm{m}^{-3}} \right)$$
(2)

Note that the units depend on moment order k. The moment values will be expressed in dB for the 182 remainder of the paper. In the current paper, we relate the polarimetric radar variables computed 183 from observed and simulated DSDs to their respective moments. The moments themselves dis-184 play natural covariability that lends itself to scaling relationships and a general DSD normalization 185 method discussed in further detail in Morrison et al. (2018). All calculations are performed at S 186 band (\sim 11-cm wavelength), assuming liquid drops at 20 °C and are valid for low radar antenna 187 elevation angles ($< 10^{\circ}$). The raindrop shapes are taken as a function of size following Bran-188 des et al. (2005). The T-matrix method (Mishchenko 2000) is used to compute the forward and 189 backward scattering amplitudes, from which the radar variables are calculated following Ryzhkov 190 et al. (2011). This is the same method employed by Kumjian and Prat (2014) and numerous other 191 studies. 192

As mentioned in the introduction, we have not explored the effect of other sources of uncer-193 tainty such as choice of drop shape model, liquid water temperatures, and distribution of canting 194 angles – we have focused solely on the uncertainty associated with the mapping between model-195 predicted quantities (integrated DSD moments) and polarimetric radar variables that is related to 196 natural DSD variability. Uncertainty not estimated here can be easily added in subsequent work 197 by summation of variances, assuming no correlation between different error terms. Thurai et al. 198 (2007) showed that, at S band, the discrepancies in Z_H and K_{DP} arising from different choices of 199 raindrop shape models and liquid water temperature are negligible, whereas Z_{DR} differences could 200

²⁰¹ be up to 0.1 - 0.2 dB in magnitude for a small subset of DSDs characterized by large median drop ²⁰² sizes. For most of the DSD parameter space considered by our forward operator, then, we expect ²⁰³ the added uncertainty arising from these choices to be smaller than the spread in Z_{DR} values arising ²⁰⁴ owing to natural variability.

Figures 1-3 show the joint histograms of M_0 through M_{10} versus the polarimetric radar variables 205 using all DSDs in the dataset. These figures reveal the relationships between polarimetric radar 206 variables and moments of different order k. As expected, some moments exhibit much clearer 207 relationships with the radar variables than others. For example, Z_H is nearly perfectly described by 208 M_6 , whereas the dependence on M_0 is rather weak (Fig. 1). This is expected given that M_6 defines 209 the radar reflectivity factor for spherical liquid drops with diameters small compared to the radar 210 wavelength; at S band, most drops are safely considered electromagnetically small. That is to say, 211 the Rayleigh approximation holds for all but the largest raindrops, where minor deviations from a 212 linear $Z_H - M_6$ relationship arise. K_{DP} (Fig. 3) appears closely related to M_4 and M_5 as suggested 213 in previous studies (e.g., Sachidananda and Zrnić 1986; Bringi and Chandrasekar 2001; Lee et al. 214 2004; Maki et al. 2005). This is in sharp contrast to Z_{DR} , which has more tenuous relationships 215 with the moments, with higher-order moments displaying only slightly stronger relationships to 216 Z_{DR} (Fig. 2). In part, these weak relationships are because Z_{DR} does not depend on raindrop 217 concentration, whereas Z_H and K_{DP} do. 218

These joint histograms have implications for which prognostic moments offer the greatest utility for linking model output with the polarimetric radar variables. M_0 , for example, has a broad distribution for all three radar variables compared to higher-order moments. This implies a wide range of M_0 values can produce the same Z_H , Z_{DR} , or K_{DP} values. As such, M_0 has limited utility in informing Z_H , Z_{DR} , or K_{DP} compared to higher-order moments. From the perspective of model validation as well as data assimilation, the best prognostic DSD moments are likely to be those most directly informed by observed radar quantities; in that context, the standard choice of M_0 and M_3 in bulk microphysics schemes is unfortunate, as these moments are only weakly related to radar variables. This motivates the following question: which combination of moments offer the greatest information content (i.e., least spread in the joint histograms) for the radar variables? The next section addresses this question.

3. Identifying Optimal Predicted Moments for Polarimetric Radar Measurements

Though bulk microphysics schemes typically predict M_0 and M_3 , the S-band radar variables are strongly related to higher moments in part because the back- and forward-scattering cross sections are proportional to D^6 for particles with diameters small compared to the radar wavelength. This leads to challenges in comparing radar observations with microphysical model output. Here we assess which pair of moments (i.e., for a two-moment scheme) minimizes the variability in Z_H , Z_{DR} , and K_{DP} for a collection of realistic DSDs, and thus would offer the most information content on those radar variables if prognosed.

We first discretize the pair of moments M_k and M_j into 1-dB × 1-dB bins. Within each bin, the 238 Z_H , Z_{DR} , or K_{DP} values from the DSD dataset are collected. For example, in Fig. 4a, an arbitrary 239 bin is selected, within which M_0 values range between 30-31 dB and M_3 values between 32-33240 dB. Within this bin, there are $\sim 2.2 \times 10^5$ DSDs, with the bulk of their corresponding Z_H values 241 ranging from 35 to 46 dBz (Fig. 4b). We can quantify the spread of Z_H values within each pixel 242 by calculating the standard deviation. However, before computing the standard deviation of Z_H 243 values, the evident linear trends (in logarithmic space) must be removed. Otherwise, variability 244 within this bin will be a result of the linear trend, as opposed to the variability *about* this linear 245 trend. Thus, for each 1-dB \times 1-dB bin, linear trends in Z_H with M_0 and M_3 across this bin are 246

removed. The standard deviation is then computed, resulting in a 2-dimensional map of detrended standard deviation σ_{Z_H} spanning the range of moment values (not shown).

To objectively quantify variability in prognostic moment pairs, we define a variable ξ :

$$\xi \equiv \sum_{m}^{M} \sum_{n}^{N} \sigma_{X} \left[M_{k}^{(m)}, M_{j}^{(n)} \right] \times P \left[M_{k}^{(m)}, M_{j}^{(n)} \right]$$
(3)

where *M* and *N* are the number of bins for discretized moments M_k and M_j , respectively; σ_X is the standard deviation of the detrended polarimetric radar variable *X* for the *m*th bin of M_k and *n*th bin of M_j , and *P* is the joint normalized probability distribution function (PDF) of moments M_k and M_j in bins *m* and *n*, respectively. Physically, ξ represents the PDF-weighted spread in a given radar variable for a given pair of moments (M_k , M_j). Note that K_{DP} is expressed in dB for these calculations to facilitate comparison with Z_H and Z_{DR} .

The PDF weighting ensures that contributions from rare or outlier pixels are commensurate with 256 their occurrence. However, the PDF generated by the bin simulations and disdrometer data is arbi-257 trary (based on availability of disdrometer data and locations, choice of bin simulation parameter 258 space, etc.) and thus may inadvertently introduce biases if used as is. Instead, a climatology of 259 observed rainfall rates from 5-minute ground-based rain gauges (see Morrison et al. 2018) is used 260 to subsample the DSD dataset. This provides a dataset of 2×10^5 DSDs that has approximately 261 equal contributions from the disdrometer and bin simulations and that reflects the climatological 262 distribution of rainfall rates in the U.S. as measured from ground-based gauges. 263

The resulting ξ maps are shown in Figure 5. One can see that ξ is minimized for different pairs of moments for Z_H , Z_{DR} , and K_{DP} . This is expected, given that each variable has different dependencies on the DSD. For example, given that Z_H is nearly equal to M_6 at S band, most combinations of M_6 and another moment provide the lowest ξ values (Fig. 5a). In contrast, (M_5 , M_9) produces the lowest ξ for Z_{DR} (Fig. 5b). Also note the large ξ values for moment order less than or

equal to M_3 , which reveals large variability in the radar variables for the moments traditionally pre-269 dicted by bulk microphysics schemes. To identify the moment pair that minimizes variability for 270 all three variables, $\xi(Z_H)$, $\xi(Z_{DR})$, and $\xi(K_{DP})$ were normalized by their respective mean values 271 and summed together (Fig. 5d). The moment pair that yielded the minimum variability² and thus 272 is determined to be the optimum moment pair for informing models with dual-polarization radar 273 observations was found to be (M_6, M_9) . For the remainder of the paper, we will show traditional 274 prognosed moments (M_0, M_3) and the ones indicated by this analysis (M_6, M_9) . Additionally, given 275 the practical consideration of predicting M_3 in bulk microphysics schemes (as it is proportional to 276 total mass), (M_3, M_6) will be shown as well. Unlike M_0, M_3 , and M_6, M_9 has no conventional 277 physical meaning³ other than the ninth moment of the DSD. 278

4. The Moment-based Forward Operator

The moment-based forward operator is built using the full (combined) dataset rather than the 280 subsampled one. This is because we desire the forward operator to cover the maximum possible 281 spread of moment values, even if these values are rare in nature. We take a lookup table approach 282 to the forward operator: linear interpolation (in logarithmic moment space) of the binned (M_i, M_k) 283 values is used as a function of the input moment values. Then, the corresponding mean values (in 284 each $1-dB \times 1-dB$ pixel) of Z_H , Z_{DR} , and K_{DP} are found. For example, the two-moment version 285 of the forward operator takes as inputs a given moment pair (M_i, M_k) from, say, output from a two-286 moment bulk microphysics scheme that predicts M_i and M_k . The mean value for each polarimetric 287 radar variable in the corresponding bin is assigned. Sensitivity tests (not shown) suggested 1-dB 288

²Note: this is somewhat sensitive to how the ξ for each variable are summed. Different weightings may be applied as needed. For example, if less confidence is placed on comparing Z_{DR} to observations owing to calibration issues, or on K_{DP} owing to difficulties in its estimation because of

noisy total differential phase (Φ_{DP}) fields, one could weight the summation away from one of the variables in favor of the other two.

³If normalized by M_6 , then M_9 could be considered the "reflectivity-weighted mass" of the distribution.

 \times 1-dB moment bins were an adequate balance between attaining sufficiently high resolution in 289 the M_i - M_k parameter space and keeping the look-up tables manageable in size for our purposes 290 herein. Note that the forward operator may be easily updated as more DSD data become available 291 (e.g., from ongoing and future field campaigns), or with additional bin model simulations, etc., 292 and can be generated at higher resolutions if needed in future work. A graphical depiction of three 293 versions of the two-moment operator is shown in Fig. 6. The three versions use the $(M_0, M_3), (M_3, M_3)$ 294 M_6), and (M_6, M_9) moment pairs, respectively, for the polarimetric radar variables Z_H , Z_{DR} , and 295 K_{DP} . These versions of the forward operator would be used with schemes that predict M_0 and M_3 296 (most existing two-moment bulk microphysics schemes), M_3 and M_6 , and M_6 and M_9 , respectively. 297 The (M_0, M_3) operator (Fig. 6a-c) is based on the moments typically predicted in double-moment 298 bulk microphysics schemes, where M_0 is the total number concentration of drops and M_3 is pro-299 portional to the total mass per unit volume of the drops. This version of the forward operator may 300 be used with many commonly used two-moment bulk microphysics schemes, with the inputs sim-301 ply being the predicted M_0 and M_3 at each model grid point. For the same M_0 , we see an increase 302 in Z_H , Z_{DR} , and K_{DP} as M_3 increases. This makes sense physically: as M_3 (mass) of the drops in-303 creases for a fixed number concentration, the drops must be increasing in size. A different pattern 304 emerges for the (M_3, M_6) operator (Fig. 6d-f). Because M_6 is almost identically Z_H at S band, 305 there is little change in Z_H for increasing M_3 when M_6 is held fixed. For a given M_3 , increasing 306 M_6 leads to larger Z_H , Z_{DR} , and K_{DP} . The (M_6, M_9) operator (Fig. 6g-i) is similar to the (M_3, M_6) 307 operator, though a given value of the radar variables generally is spread over fewer of the 1-dB by 308 1-dB moment bins owing to less natural variability in the (M_6, M_9) moment pair (see Morrison 309 et al. 2018). 310

Recall that each $1-dB \times 1-dB$ pixel on these maps contains numerous DSDs and thus a distribution of polarimetric radar variable values within it. A novel feature of our moment-based

forward operator is that it facilitates estimating the uncertainty associated with a moment-based 313 approximation of natural DSDs. To compute such uncertainty, the standard deviation, skewness, 314 and kurtosis are computed using the detrended data to characterize the distributions of intrinsic 315 Z_H , Z_{DR} , and K_{DP} variability within each pixel. Figure 7 shows standard deviation of each radar 316 variable distribution within each pixel, for the three forward operators shown in Fig. 6. Comparing 317 the (M_0, M_3) operator (top row) with the (M_3, M_6) and (M_6, M_9) in the rows below, a large reduc-318 tion in the standard deviation of Z_H is evident, which follows naturally from the fact that (M_3, M_6) 319 and (M_6, M_9) both utilize M_6 . There is also a reduction in the standard deviation of Z_{DR} and K_{DP} 320 evident when moving from the top to bottom rows. Skewness magnitude (Fig. 8) and kurtosis (not 321 shown) are also substantially higher for (M_0, M_3) , compared with the other moment-pair choices. 322 High skewness magnitude and kurtosis imply that the uncertainty within these regions is non-323 Gaussian. Such non-Gaussianity poses problems for optimal estimation and Kalman-filter based 324 techniques that typically assume model linearity and Gaussian error statistics, with few exceptions 325 (e.g., Hodyss 2011; Amezcua and Leeuwen 2014; Bishop 2016). 326

5. Examples Using Simulated Rainshafts

To test the effectiveness of the forward operator, example rainshafts from the 1-D bin simulations are used. Radar variables are calculated at each minute directly from the bin model DSDs, which are considered "truth" for these tests. We also compute the moments from these DSDs, which serve as the inputs to the forward operator. The radar variables produced by the forward operator are compared to the truth (bin simulation) values computed directly from the DSD itself. This simulation is independent from the ones used to construct the DSD database.

Figure 9 shows vertical profiles of Z_H , Z_{DR} , and K_{DP} for a bin simulation initialized with a normalized gamma DSD aloft with rainfall rate R = 36.7 mm hr⁻¹. The "truth" profiles are shown

in blue lines, whereas the (M_6, M_9) forward operator profiles are in gray, with ± 1 standard devi-336 ation shown as horizontal bars on the forward-simulated profiles every 10 grid points. Each row 337 represents a different output time in the simulation. Each profile shows the evolution of the rain 338 shaft as raindrops fall towards the surface. At early times, size sorting of drops (e.g., Kumjian and 339 Ryzhkov 2012; Kumjian and Prat 2014) is evident by the rapidly increasing Z_{DR} and decreasing 340 Z_H and $K_{\rm DP}$ values at the bottom edge of the rain shaft. This provides a good test for the forward 341 operator given the somewhat exotic DSDs compared to later times when the profiles change little 342 in height. 343

The forward operator-retrieved Z_H profile nearly perfectly matches the "truth" profiles at each 344 time, which is unsurprising given that M_6 is one of the moments used to inform the forward sim-345 ulator. Additionally, the standard deviation is very small at all heights, as indicated by negligibly 346 small error bars. Thus, not only does the forward operator correctly diagnose Z_H , but it also cor-347 rectly suggests high confidence in the diagnosis. In contrast to Z_H , Z_{DR} and K_{DP} provide a more 348 difficult challenge for the forward operator given their weaker relationships to DSD moments (cf. 349 Figs. 2 and 3). Nonetheless, the forward operator does a satisfactory job at accurately diagnosing 350 the evolving Z_{DR} and K_{DP} profiles: relative error magnitudes (defined as the difference between the 351 "truth" and forward operator curves) generally are less than 0.5%, 5%, and 10% for Z_H , Z_{DR} , and 352 $K_{\rm DP}$, respectively. The relatively larger error magnitudes for $K_{\rm DP}$ are a result of using higher-order 353 moments (recall that M_4 and M_5 are the most closely related to K_{DP}). Additionally, the diagnosed 354 profiles are almost always within the ± 1 standard deviation bars. For times when the "truth" lies 355 outside the ± 1 standard deviation bars, the diagnosed Z_{DR} and K_{DP} values are still well within 356 typical theoretical radar measurement errors of $\sim 0.1-0.2$ dB for Z_{DR} and $\sim 0.1-0.2$ deg km⁻¹ for 357 K_{DP} (Melnikov 2004). Thus, the (M_6, M_9) forward operator performs well for the evolving rain 358 shaft. 359

Figure 10 compares the performances of three different versions of the forward operator: (M_0, M_0) 360 M_3) (Fig. 10a-c), a commonly used pair of prognostic moments for two-moment bulk micro-361 physics parameterization schemes, (M_3, M_6) (Fig. 10d-f), and (M_6, M_9) (Fig. 10g-i). This example 362 uses the same initial DSD aloft as in Fig. 9, with the output time t = 10 minutes shown. It is clear 363 that the (M_3, M_6) and (M_6, M_9) versions are both more accurate and have less predicted spread 364 $(\pm 1 \text{ standard deviation})$ than the (M_0, M_3) version, an expected result given the higher moment 365 orders used. In contrast, the less accurate (M_0, M_3) version of the forward operator has relatively 366 larger error bars, indicating that the forward operator correctly assesses lower confidence when 367 it is less accurate. This is a novel feature of the moment-based forward operator presented here. 368 That the "truth" profiles fall outside the forward operator ± 1 standard deviation bars illustrates the 369 low-information content of M_0 and M_3 for the polarimetric radar variables, and is not unexpected, 370 given that approximately 32% of all forward-simulated values will fall outside these bounds, as-371 suming Gaussian error statistics. Furthermore, in the case of (M_0, M_3) , Fig. 8 suggests that the 372 standard deviation may not well-characterize errors given strong deviations from Gaussianity. 373

Figure 11 shows another example; this time, the simulation is initialized with a normalized 374 gamma DSD aloft with much lower rainfall rate ($\sim 0.3 \text{ mm hr}^{-1}$), again one that was not included 375 in the initial dataset. As with the previous example, we see a marked improvement of the forward 376 operator performance going from (M_0, M_3) (Fig. 11a-c) to (M_3, M_6) (Fig. 11d-f) and again to 377 (M_6, M_9) (Fig. 11g-i). Once again, the ± 1 standard deviation bars reflect the increasing forward 378 simulator uncertainty with decreasing accuracy, particularly evident in the (M_0, M_3) version of 379 the operator. The (M_3, M_6) operator works well for Z_H and K_{DP} , but has slight positive bias for 380 Z_{DR} . However, the discrepancy is $\leq 0.1 - 0.2$ dB, which is well within observation error. The 381 superior performance of the (M_6, M_9) operators in both examples suggests it is robust for use in 382 both light and heavier rainfall rates. These results show that using a bulk microphysics scheme 383

that predicts M_3 and M_6 (and/or M_9) instead of M_0 and M_3 is better for use of dual-polarization 384 radar data as a constraint or for data assimilation. Note that including M_3 as a prognostic variable 385 is important for conserving mass in models, so not predicting it may be problematic in practice. 386 Thus, we advocate for models to use M_3 and M_6 as prognostic variables for two-moment schemes, 387 or M_3 , M_6 , and M_9 as prognostic variables for three-moment schemes. For two-moment bulk 388 microphysics schemes that predict M_0 and M_3 , dual-polarization radar data may still be used, just 389 with considerably larger errors and greater uncertainty in the mapping between model-predicted 390 quantities and the observed radar quantities. Whereas our forward operator attempts to quantify 391 this uncertainty, existing forward operators use the model-assumed DSD shape (which forces a 392 unique mapping between the predicted variables and radar variables that does not exist in nature) 393 and does not quantify uncertainties associated with this assumption. 394

In principle, the approach outlined above can be extended to any number of moments and any 395 radar variable with an accurate DSD-based forward operator. We have tested a three-moment 396 version of the forward operator using M_0 , M_3 , and M_6 , the most common prognosed moments for 397 existing three-moment schemes (e.g., Milbrandt and Yau 2005). The results showed only minimal 398 improvement over (M_3, M_6) and (M_6, M_9) owing to the low-information content of M_0 for radar 399 variables (cf. Figs. 1-3). Higher-order moments (e.g., M₃, M₆, M₉) may be more useful with 400 polarimetric radar variables and are attractive from a microphysical modeling perspective because 401 M_3 (mass) is a prognostic variable, as discussed above. Although some microphysical process 402 rates are strongly dependent on lower-order moments, using the three-moment combination (M_3, M_3) 403 M_6, M_9) allows for diagnosing lower-order moments quite well (Morrison et al. 2018) and thus is 404 not a significant concern. 405

6. Discussion and Summary

⁴⁰⁷ A large dataset of disdrometer-estimated and bin-model-simulated DSDs was constructed to ⁴⁰⁸ quantify the relationships between different integrated moments and the S-band polarimetric radar ⁴⁰⁹ variables, determine the uncertainty of those radar variables for a given pair of DSD moment ⁴¹⁰ values, and develop a moment-based polarimetric radar forward operator. This dataset comprises ⁴¹¹ 671 303 DSDs estimated from Joss-Waldvogel and 2D-video disdrometers at U.S. Department of ⁴¹² Energy sites around the world, as well as 184 180 279 DSDs simulated using a one-dimensional ⁴¹³ bin microphysical model that explicitly treats raindrop collisional processes.

The data reveal a strong relationship between the sixth moment of the DSD (M_6) and radar 414 reflectivity factor at horizontal polarization Z_H , as expected: for spherical liquid droplets with di-415 ameters small compared to the radar wavelength, the reflectivity factor is exactly equal to M_6 . The 416 specific differential phase K_{DP} was most closely related to M_4 and M_5 , as reported in some previ-417 ous studies (e.g., Sachidananda and Zrnić 1986; Bringi and Chandrasekar 2001; Lee et al. 2004; 418 Maki et al. 2005). In contrast, differential reflectivity Z_{DR} showed no strong relationship with any 419 of the DSD moments, but tended to have slightly reduced spread for higher-order moments. Future 420 work will explore additional observations and their relationships to DSD moments, such as mean 421 Doppler velocity from vertically pointing radar, lidar backscatter, etc. 422

The dataset was subsampled to 2×10^5 DSDs based on a climatology of observed rainfall in the U.S. (Morrison et al. 2018) to determine the expected natural variability of the radar variables for a given pair of moment values. The pair of moments minimizing this variability is M_6 and M_9 . Choosing these optimal moments is a way of recasting DSD variability such that natural variability is minimized in each (M_j, M_k) pixel. In contrast, moments predicted by most bulk microphysical parameterization schemes $(M_0$ and $M_3)$ revealed much greater variability for the polarimetric radar variables. This implies that, when comparing rain microphysical models and polarimetric radar observations, predicting higher-order moments (as opposed to or in addition to M_0 and M_3) could significantly improve the information content obtained from the radar variables.

A forward operator was developed to relate integrated DSD moments to polarimetric radar vari-432 ables. The operator provides the mean value of Z_H , Z_{DR} , and K_{DP} for a given pair of moment 433 values as inputs, as well as the uncertainty in the radar variables caused by natural DSD vari-434 ability (i.e., the detrended standard deviation in Z_H , Z_{DR} , and K_{DR} within a M_i - M_k bin), and 435 information about the distribution of radar variable values (i.e., the skewness and kurtosis). Us-436 ing one-dimensional rainshafts as a benchmark, several different versions of two-moment forward 437 operators were tested: (M_0, M_3) , (M_3, M_6) , and (M_6, M_9) . The (M_6, M_9) version performed well 438 for different rainshafts of varying rainfall rate, including more exotic DSDs arising from size sort-439 ing early in the rainshaft evolution. In contrast, the forward operators with lower moment orders 440 performed worse. The forward operator also correctly predicted its uncertainty, with greater vari-441 ability indicated for the less accurate versions. This is a novel aspect of the operator developed 442 herein. 443

The optimal moments for informing on the dual-polarization radar variables are of higher order 444 than bulk microphysics schemes typically prognose. Though such high moments individually 445 may not provide much of a constraint for lower-order moments needed for such schemes, they 446 can still reduce the uncertainty considerably when used in combination (i.e., multiple prognostic 447 moments) and/or in combination with lower-order moments (Morrison et al. 2018). In other words, 448 if attempting to diagnose the kth moment M_k , reference moment M_{k+n} always provides a better 449 estimate than reference moment M_{k-n} for all n. Further, Morrison et al. (2018) show that a three-450 moment normalization using M_3 , M_6 , and M_9 will result in only ~21% of the variability in M_0 451 compared to not using the DSD normalization. Thus, use of such higher-order moments in bulk 452

⁴⁵³ microphysics schemes may not be detrimental, and indeed could be beneficial when combined ⁴⁵⁴ with lower-order moments typically prognosed (like M_3).

The moment-based forward operator developed herein is necessary for coupling radar observa-455 tions with bulk microphysics schemes that do not assume a DSD functional form (e.g., Chen and 456 Liu 2004; Szyrmer et al. 2005; Laroche et al. 2005; Kogan and Belochitski 2012). Other forward 457 operators reliant on a discretized DSD would require assuming an explicit DSD functional form, 458 imposing structural error into the mapping between model output and radar observations. The 459 approach herein strives to minimize and quantify this type of uncertainty, such that the majority of 460 the remaining uncertainty contained in the forward operator arises owing to DSD natural variabil-461 ity, and is explicitly estimated. Ultimately, this type of approach should lead to improved mapping 462 of model output to the radar observational parameter space with a better characterization of un-463 certainty. For traditional bulk microphysics schemes, use of the moment-based operator described 464 here may prevent errors associated with overconfidently comparing approximate bulk schemes to 465 observations associated with more complex, realistic DSDs. 466

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	 Fig. 2. Fig. 3. Fig. 4. Fig. 5. Fig. 6. Fig. 7. Fig. 8. Fig. 9. Fig. 10. Fig. 11. 	 Fig. 2. Joint histograms of moments M_k and Z_{DR}, for k from 0 to 10 inclusive, all in dB. Color shading indicates the base-10 logarithm of count, according to scale	 Fig. 2. Joint histograms of moments M_k and Z_{DR}, for k from 0 to 10 inclusive, all in dB. Color shading indicates the base-10 logarithm of count, according to scale



FIG. 1. Joint histograms of moments M_k and Z_H , for k from 0 to 10 inclusive, all in dB. Color shading indicates the base-10 logarithm of count, according to scale.



FIG. 2. Joint histograms of moments M_k and Z_{DR} , for k from 0 to 10 inclusive, all in dB. Color shading indicates the base-10 logarithm of count, according to scale.



FIG. 3. Joint histograms of moments M_k and K_{DP} , for k from 0 to 10, inclusive, in dB and deg km⁻¹, respectively. Color shading indicates the base-10 logarithm of count, according to scale.



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FIG. 5. (a) $\xi(Z_H)$ (dB), (b) $\xi(Z_{DR})$ (dB), (c) $\xi(K_{DP})$ (dB), and (d) sum of ξ (dB) for the subsampled dataset as a function of moment orders *j* and *k*. Larger values indicate more variability for that moment combination. White values indicate no values. Note that these matrices are symmetric.



⁶⁹² FIG. 6. Graphical representation of different two-moment forward operators. Top row (a-c) is the M_0, M_3 ⁶⁹³ forward operator, middle row (d-f) is M_3, M_6 , and bottom row (g-i) is M_6, M_9 . Left column is Z_H , middle column ⁶⁹⁴ is Z_{DR} , right column is K_{DP} .



⁶⁹⁵ FIG. 7. As in Fig. 6, but here the standard deviation of the distribution of radar variable values within each ⁶⁹⁶ pixel is shown.



FIG. 8. As in Fig. 7, but here the skewness of the distribution of radar variable values within each pixel is shown.



⁶⁹⁷ FIG. 9. Example output of forward operator compared to "truth" from bin model (blue). M_6 - M_9 forward ⁶⁹⁸ operator shown (gray), with error bars indicating ±1 standard deviation. The model is initialized with a gamma ⁶⁹⁹ DSD aloft with 36.7 mm hr⁻¹ rainfall rate, with rows corresponding to output times 1, 5, and 30 minutes.



FIG. 10. Comparison of different versions of two-moment forward operators for the simulation shown in Fig. 9, but for an output time 10 minutes. Each row now corresponds to different operator: M_0 - M_3 , M_3 - M_6 , and M_6 - M_9 . columns are Z_H , Z_{DR} , and K_{DP} .



FIG. 11. As in Fig. 10, but for a simulation initialized with a gamma DSD with rainfall rate of 0.3 mm hr⁻¹. Each row now corresponds to a different operator: M_0 - M_3 , M_3 - M_6 , and M_6 - M_9 . columns are Z_H , Z_{DR} , and K_{DP} .