

Addressing Uncertainty in Cloud Microphysics Using Radar Observations and Bayesian Methods

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ASR
Atmospheric
System Research

Motivation



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We cannot rely on computation power to resolve microphysical uncertainties

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- The study of how hydrometeors (some sort of watery thing in the atmosphere, e.g. cloud droplets, rain drops, snow, hail, graupel, etc.) form, grow, interact, precipitate.

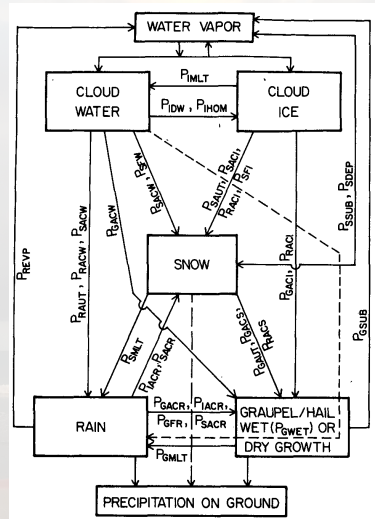
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Brief overview of microphysics 1/3

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Lin et al 1983

Brief overview of microphysics 2/3

Basic goal of microphysics

Estimate the model-grid scale response to *unknown* microscale interactions between individual hydrometeors (e.g. cloud droplets, rain drops, snow, hail, etc.)

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“Bulk” Microphysics

Model a complicated population of particle sizes via a statistical distribution (e.g. a gamma or exponential distribution), and evolve moments M_k of that distribution

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

Usually one or two moments are prognostic (typically M_3 and M_0 , sometimes M_6)

Brief overview of microphysics 3/3

Uncertain distributions, uncertain processes

Figure out how these moments evolve through the physical processes we expect, e.g. evaporation, collision-coalescence, drop breakup. Use (limited) empirical, laboratory, theoretical, ad hoc, evidence to calculate process rate formulae

$$\frac{dM_k}{dt} = F(M_1, M_2, \dots, M_n, RH, T, P, \text{turb})$$

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Fixed assumptions, unquantified errors

- The form of $N(D)$ is typically fixed (e.g. exponential or gamma distribution).
- the form of $dM_k/dt = F(\dots)$ is typically fixed

Does microphysics uncertainty matter?

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ZHU ET AL.: LAM INTERCOMPARISON OF TWP-ICE

D11

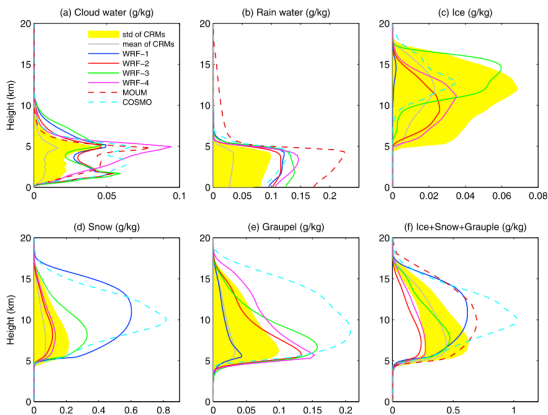
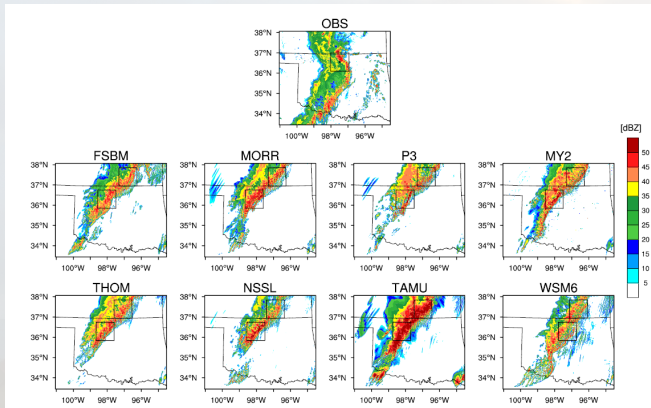


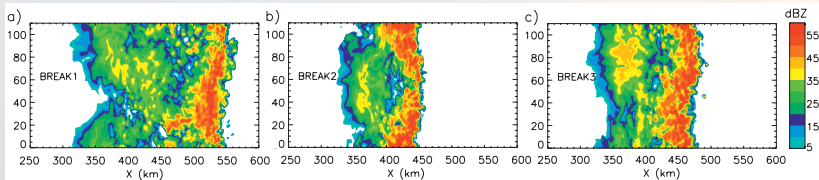
Figure 11. Vertical profiles of (a) cloud water, (b) rain water, (c) ice, (d) snow, (e) graupel, and (f) sum of solid phase hydrometeor mixing ratios over the pentagonal area averaged over the period from 12 UTC January 23 to 12 UTC January 24. The CRM results are from seven baseline runs over the same period. The standard deviations of CRM results are indicated by the yellow shades.

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courtesy of Jiwen Fan

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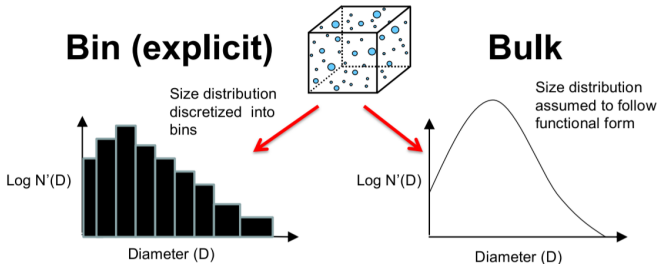


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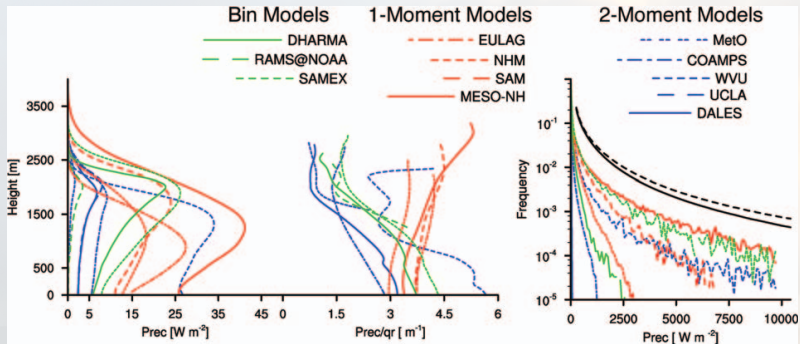
Does microphysics uncertainty matter?

Will “bin” schemes solve these problems?

Bin schemes resolve the size distribution, avoiding the approximation of an assumed size distribution form. However, process rates remain uncertain, and other issues arise (e.g. numerical diffusion)



Does microphysics uncertainty matter?



van Zanten et al 2011

Spread between bin schemes is at least as great as between bulk schemes!

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These are issues *across all existing microphysics schemes* (bin, bulk, Lagrangian, etc.)

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Bayes' theorem

$$P(\mathbf{x}|\mathbf{y}, M) = \frac{P(\mathbf{x}|M) \cdot P(\mathbf{y}|\mathbf{x}, M)}{P(\mathbf{y}|M)} \quad (1)$$

Bayesian Parameter Estimation

Fundamental question: what is the most probable set of parameter values, given the information (theoretical, empirical, expert guess, etc.) available? The combination of information can be . . .

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- $P(\mathbf{x}|M)$ – prior PDF of control parameters
- $P(\mathbf{y}|\mathbf{x}, M)$ – likelihood of observations given parameter values
- All probabilities are conditional on the choice of model M !

Markov chain Monte-Carlo (MCMC)

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The density of samples matches $P(\mathbf{x}|\mathbf{y}, M)$

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The Bottom Line:

MCMC methods are great for tricky (strongly nonlinear, multimodal, ill-posed) parameter estimation problems where model integration is relatively cheap. Even then, they require care and expert guidance (model/observation).

Estimating Ice Microphysics Parameters

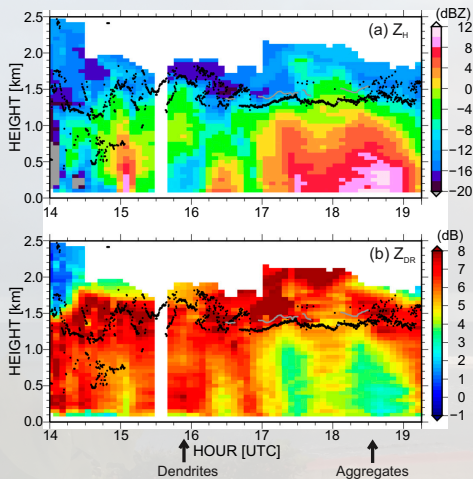


FIG. 7. Time-vs-height cross sections of the X-SAPR (a) Z_H and (b) Z_{DR} on 2 May 2013. Each profile represents the mean values of all points with elevation angles of 14° – 15° (165° – 166°) in 50-m height increments from three HRHI scans (azimuth angles of 7° , 52° , and 97°) every approximately 5 min. The horizontal gray lines and black dots respectively represent liquid-cloud top estimated from the KAZR Doppler spectrum width and cloud base observed by a ceilometer.

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Precipitating cold Arctic clouds (obs analysis: Oue et al JAMC 2016)

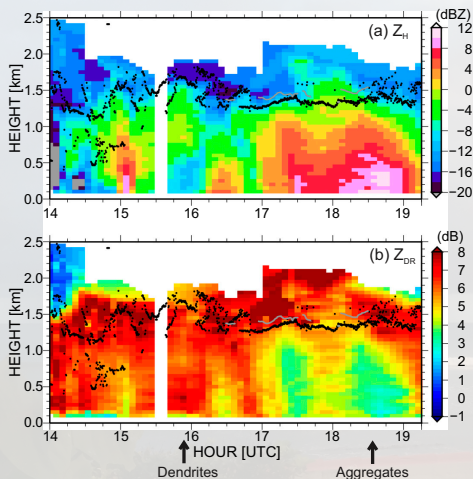


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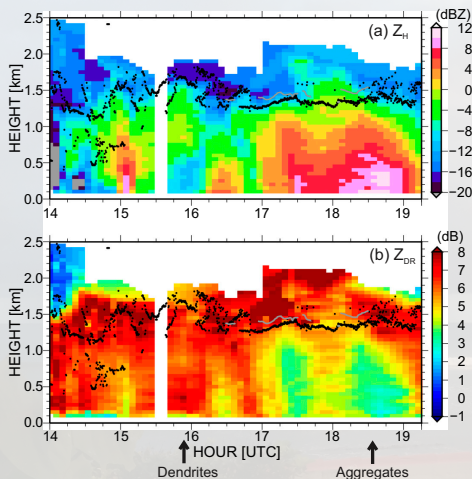


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Polarimetric radar observations show “microphysical fingerprints” of processes evolving hydrometeor properties

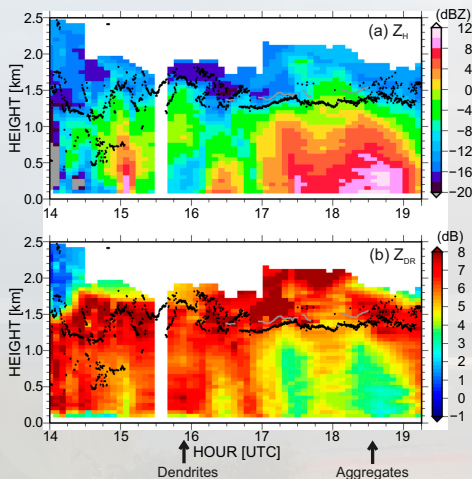


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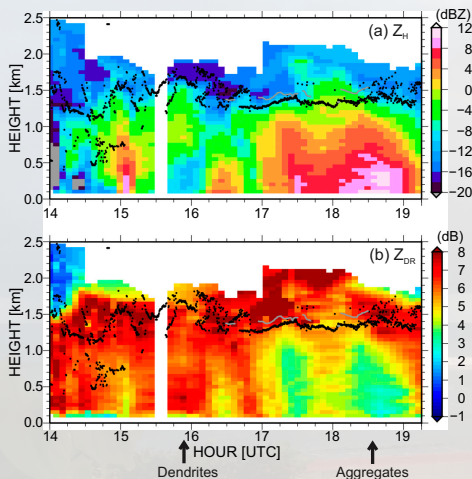


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Plan: Target processes in observations and use to constrain relevant model parameters

Estimating Ice Microphysics Parameters

Profiles drawn from timeseries, classified by (assumed) dominant growth process

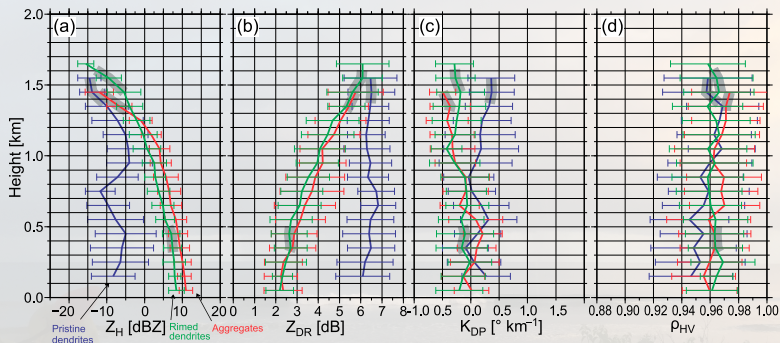
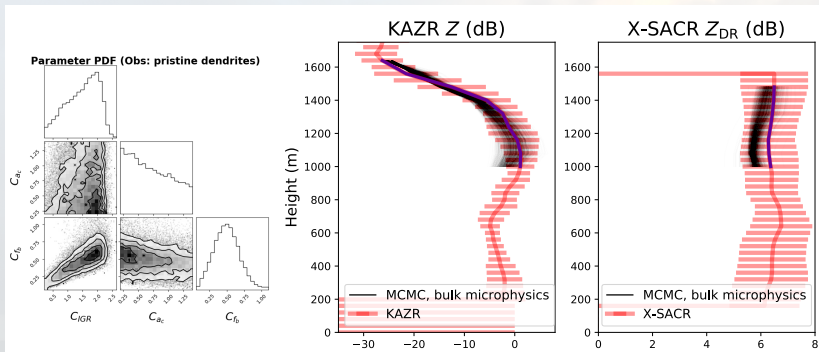
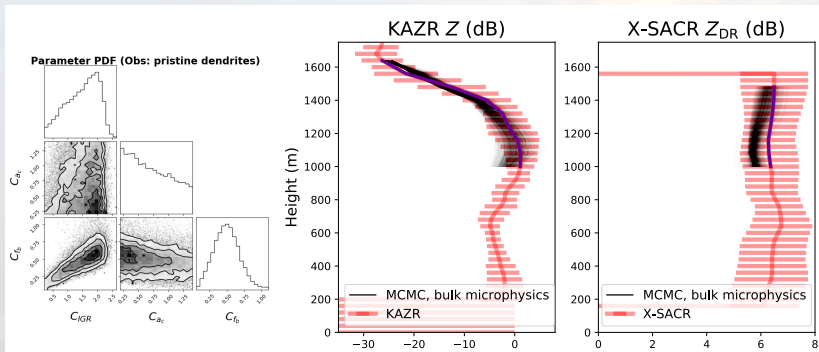


FIG. 17. Vertical profiles of averaged (a) Z_H , (b) Z_{DR} , (c) K_{DP} , and (d) ρ_{HV} from the X-SAPR HRHIs, during which the pristine dendrites (blue line), aggregates (red line), and rimed dendrites (green line) were observed at the ground. The averaging areas are presented in Figs. 6, 9, and 13. Averages were calculated in 100-m altitude increments from all values with elevation angles $<20^\circ$ or $>160^\circ$. The total number of samples in each profile exceeds 1900. Error bars represent standard deviations. Gray shading represents layers between ceilometer-measured cloud base and topmost liquid-cloud top.

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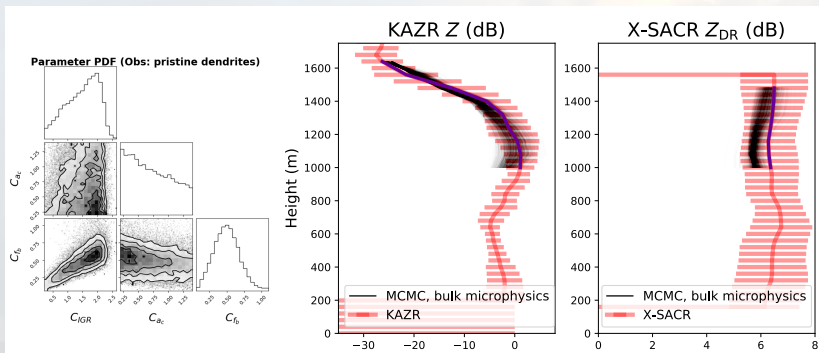


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Polarimetric and profiling radars provide constraint on (2 out of 3) ice growth parameters

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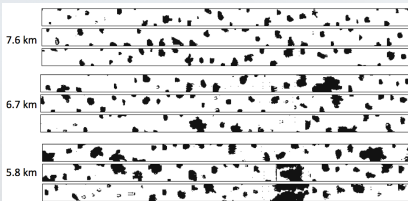


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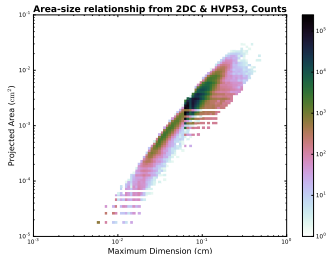
Covariance in the parameter PDFs indicates compensating effects of joint perturbation

More Ice Microphysics: Aggregation

In situ (2DC & HVPS)

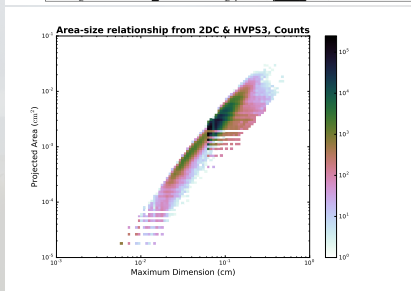
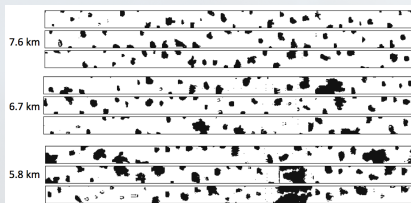


We seek to constrain ice sticking efficiency using observations from a trailing-stratiform MCS (May 20 2011 MC3E)



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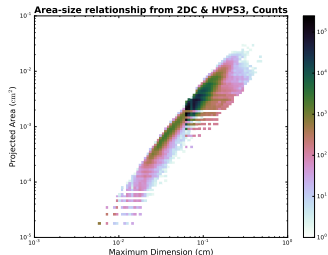
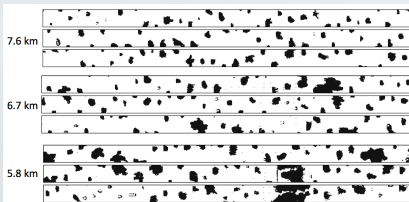


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Ann Fridlind, Andrew Ackerman, Christopher Williams, Greg McFarquhar, Wei Wu

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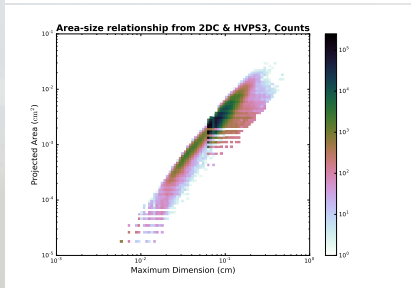
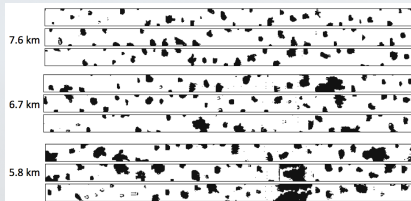


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In situ measurements provide some constraint on ice distribution and particle properties at the top of an aggregating ice column

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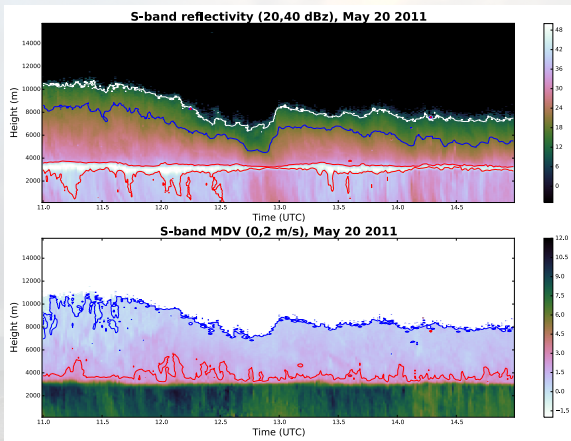
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There is uncertainty in this information that should qualify our aggregation estimates

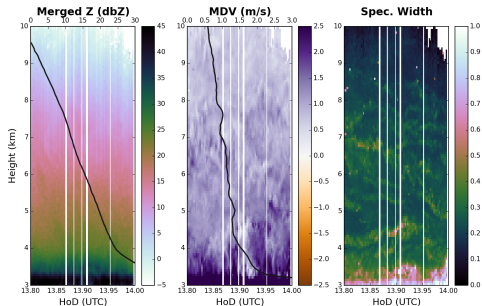
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Profiling radar mean Doppler velocity and reflectivity provide information on aggregation of particles (merged KAZR and NOAA S-band shown)



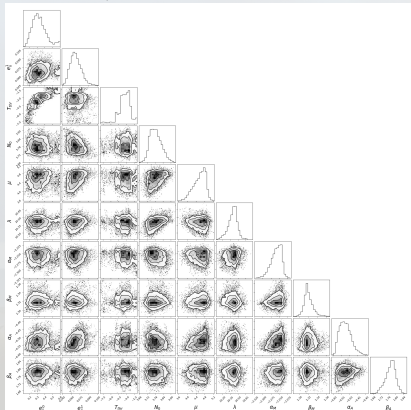
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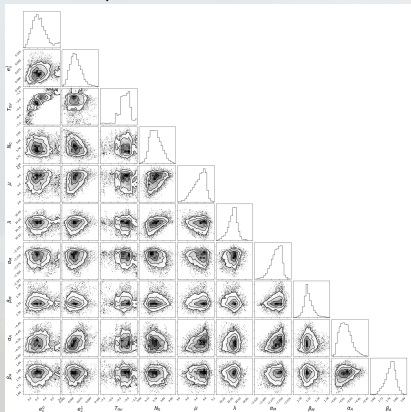
Sticking efficiency *and* ice property/PSD



Using a column model with bin microphysics, estimate ice sticking efficiency in the presence of uncertainty in particle size distribution and properties

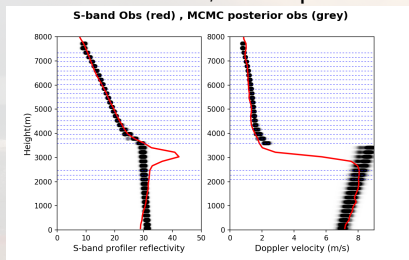
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Fwd-simulated Z, MDV profiles

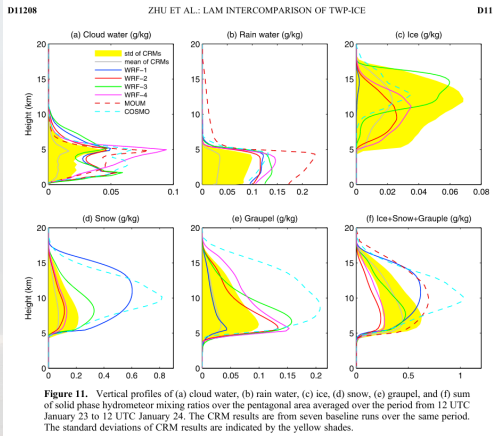


Still some critical outstanding issues

Perhaps the most substantial source of microphysical modeling uncertainty is **structural uncertainty**, e.g. DSD assumptions, process rate formulations

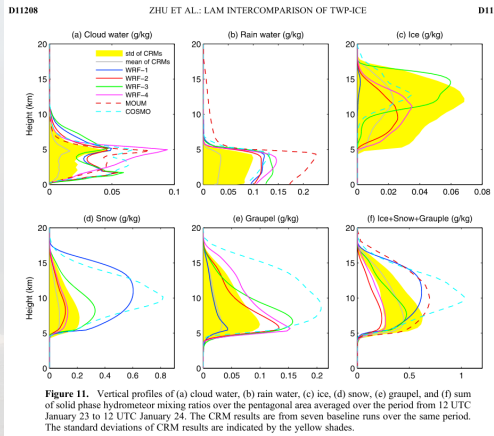
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Still some critical outstanding issues

Our uncertainty in microphysical processes should be thought of as a PDF existing in the space of all possible functions and all relevant microphysical variables/parameters and each current scheme is one point in this space



Progress in representing structural uncertainty

Typically, microphysical modelers have not considered systematic variations in microphysics scheme structure to constrain structural uncertainty — most tuning of parameters has been done ad hoc (i.e. not probabilistically)

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- SPPT: Stochastic Perturbed Physics Tendencies (less limited structural uncertainty)

The forecasting community has engineered an approach to addressing structural physics uncertainty. There may be benefits to engaging the microphysics community to robustly estimate parameteric and structural uncertainties using observations

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Structural complexity that can be added/subtracted as needed as required by comparison to observations

BOSS

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Hugh Morrison, Matthew Kumjian, Olivier Prat, Karly Reimel

BOSS vs. Traditional Microphysics Schemes

Traditional bulk schemes

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cloud DSD moments

$$M_k = \int D^k N(D) dD$$

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Microphysical processes rates are parameterized as power laws.

$$\frac{dM_{p1}}{dt} \approx F(T, p, q) \sum_j a_j (M_{p1}^{b_{1,j}} M_{p2}^{b_{2,j}} M_{p3}^{b_{3,j}} \dots)$$

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Structural Complexity in BOSS

Structural complexity can be added in two ways:

Prognostic variables

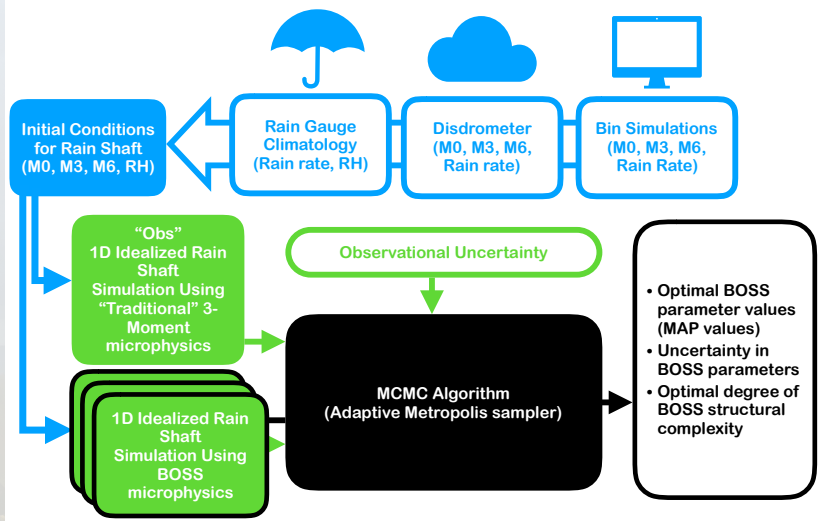
- BOSS can evolve any prognostic moments of the size distribution
- M3 (mixing ratio) is a typical choice because of mass conservation and invariance with coalescence/breakup
- Other moments can be chosen to maximize *information content of observations*

Power law terms

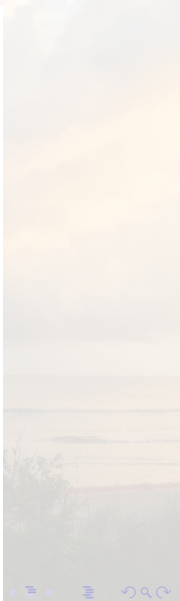
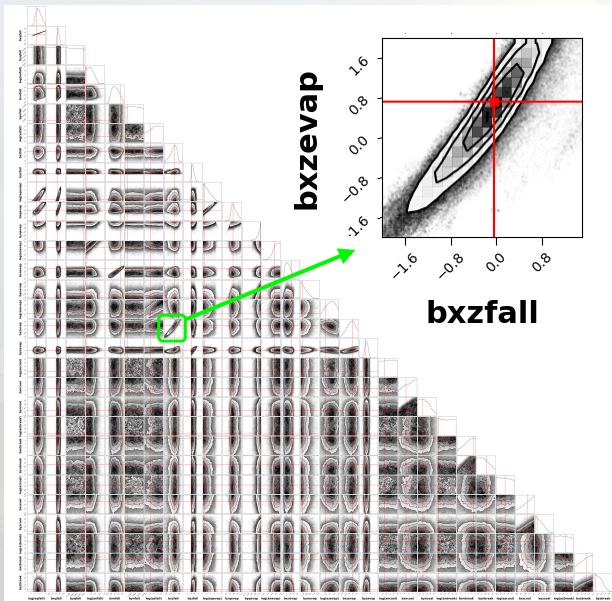
$$\frac{dM_{p1}}{dt} \approx F(T, p, q) \sum_j a_j (M_{p1}^{b_{1,j}} M_{p2}^{b_{2,j}} M_{p3}^{b_{3,j}} \dots)$$

- Can add power law terms to model more complex responses (i.e. $j=1,2,\dots$)
- Ideally, there should be a way to balance model accuracy *and* parsimony

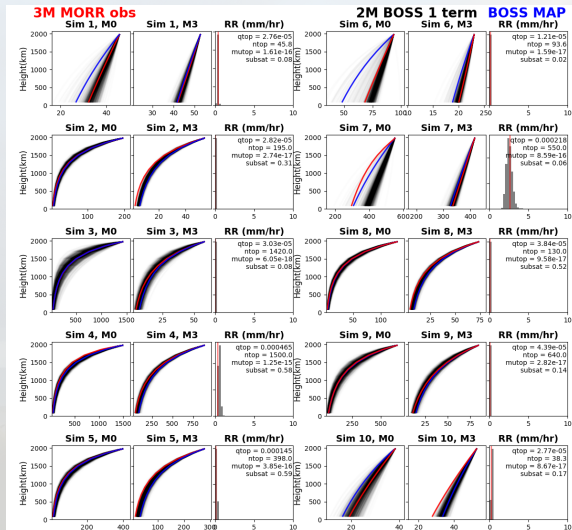
BOSS Experimental Design



BOSS Results: Parameter PDF

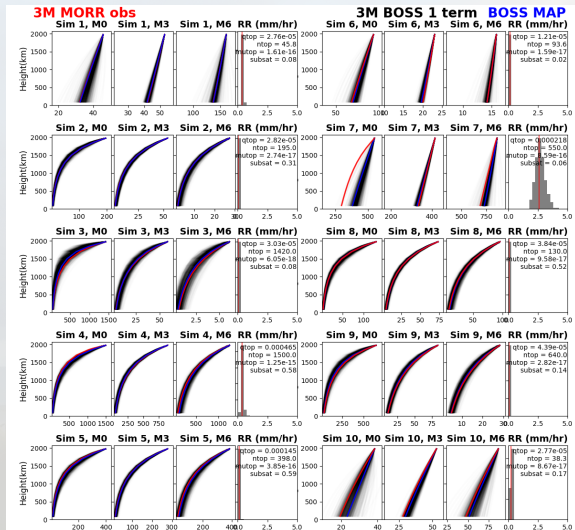


BOSS Results



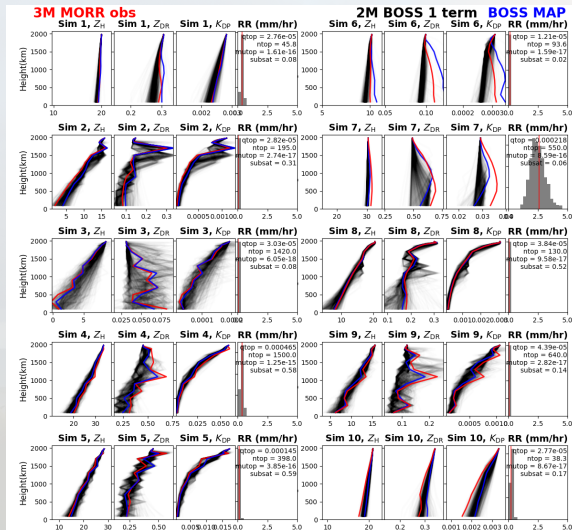
2-moment BOSS
(M0, M3)
constrained by "obs"
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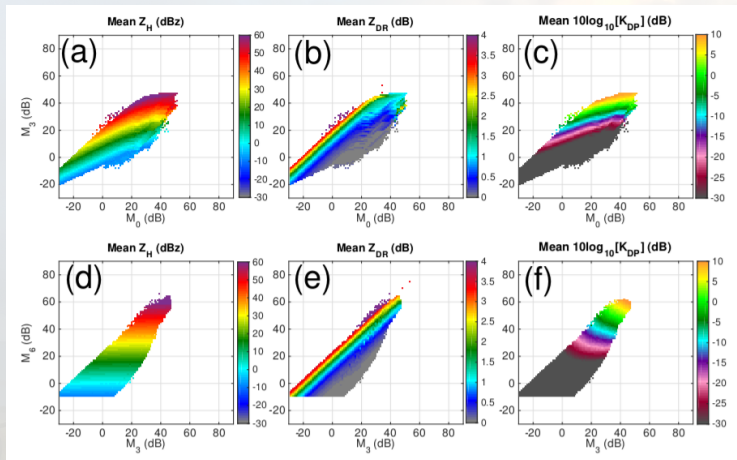
3-moment BOSS (M0, M3, M6) constrained by "obs" of M0, M3, M6 from 3-MORR

BOSS Results



2-moment BOSS
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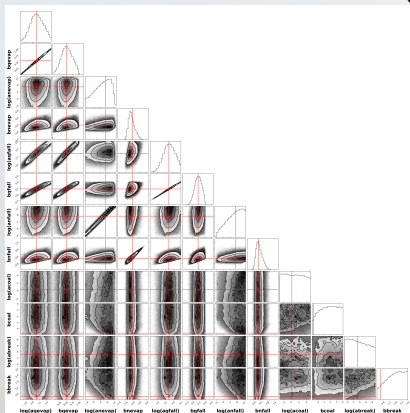
Moment-based Polarimetric Radar Fwd. Op.



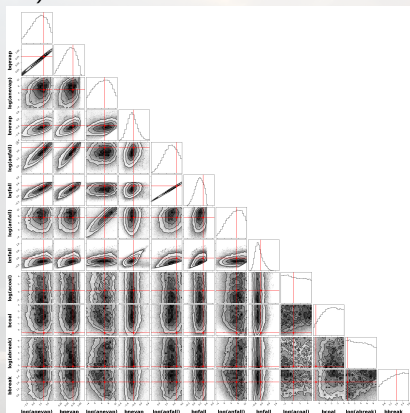
Kumjian et al, (in preparation)

Ideal constraint vs. radar constraint

Parameter PDF for 2-moment (M0M3) version of BOSS



Constraint by idealized “obs” of prognostic moments (M0,M3)



Constraint by forward-simulated profiles of Z_H , Z_{DR} , and K_{DP}

BOSS Conclusions

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There is still need for a systematic (i.e. probabilistic) quantification of structural uncertainty in BOSS

A Retrieval example

Problem:

- Retrieve cloud and rain properties using vertically-pointing radar Doppler spectrum

Addressing Structural Error:

A Retrieval example

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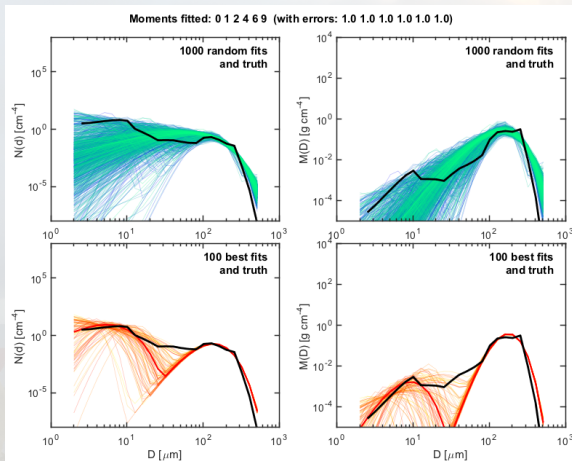
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- Analyze errors associated with doing this fit *in the space of the observable quantities*

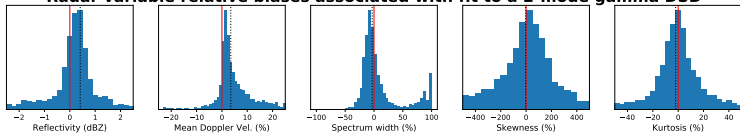
Cloud Property Retrieval using Radar



Cloud Property Retrieval using Radar

Distribution of radar variable errors associated with the assumption of a 2-mode gamma in our retrieval

Radar variable relative biases associated with fit to a 2-mode gamma DSD



The end

A new approach to microphysics

We hope that others will share our enthusiasm and optimism for a statistical approach to addressing uncertainties in microphysics parameterization schemes!

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Thanks for listening!

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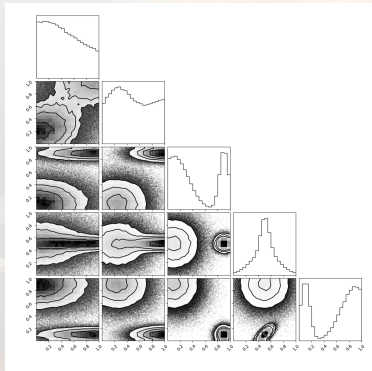
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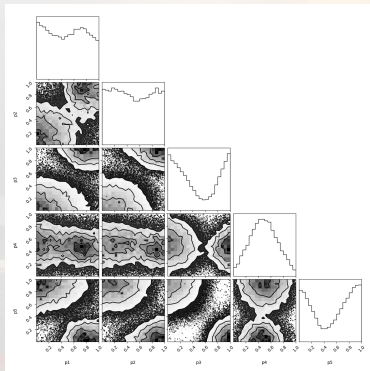


about 500,000 samples

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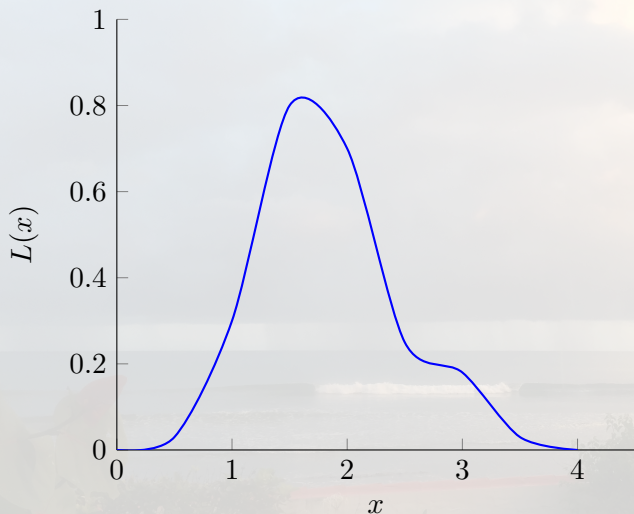
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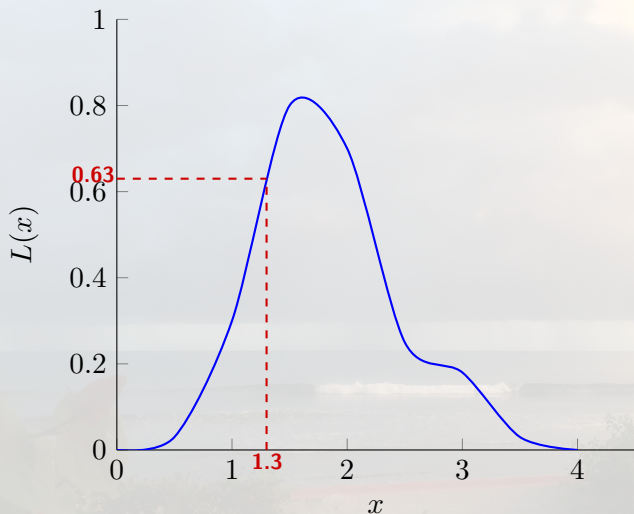
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This method will be applied to determine if the PDF of parameters in the NASA GISS ModelE GCM is multimodal, i.e. has multiple valid solutions that may exhibit different climate sensitivities (PI: Greg Elsaesser)

Markov chain example - the Metropolis sampler



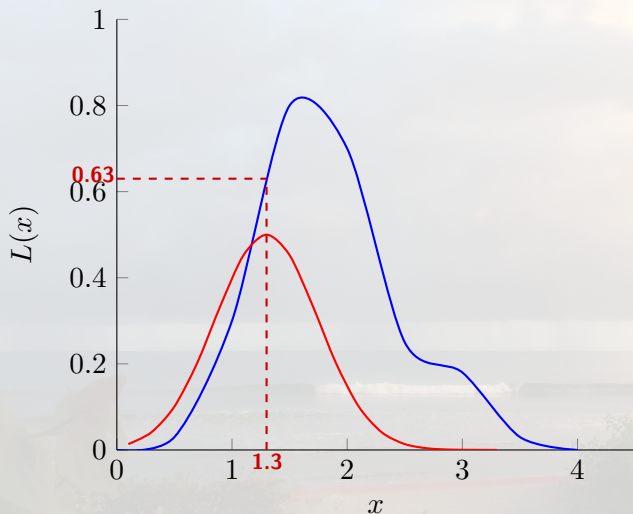
Markov chain example - the Metropolis sampler



Markov Chain

i	$x(i)$
1	1.3

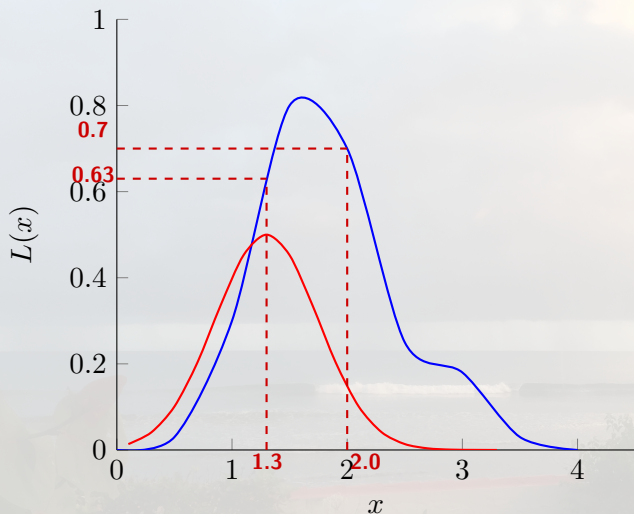
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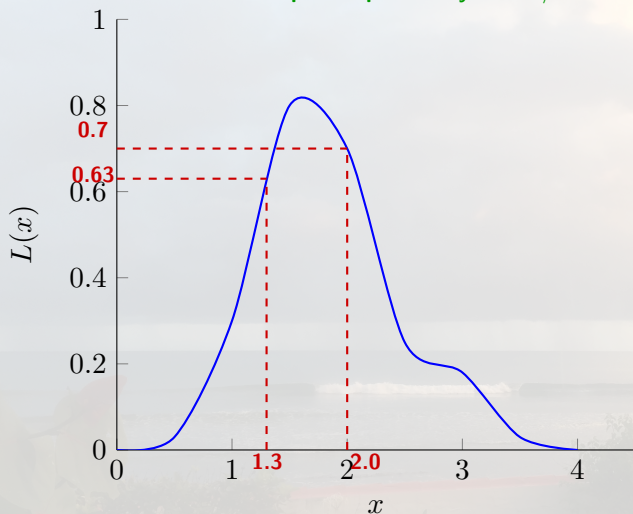


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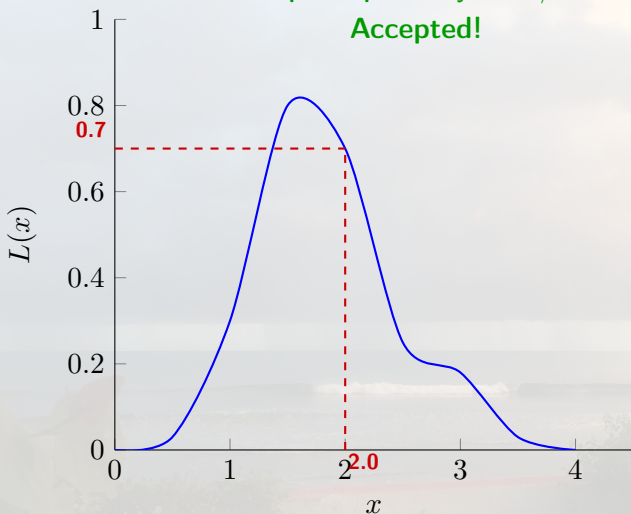
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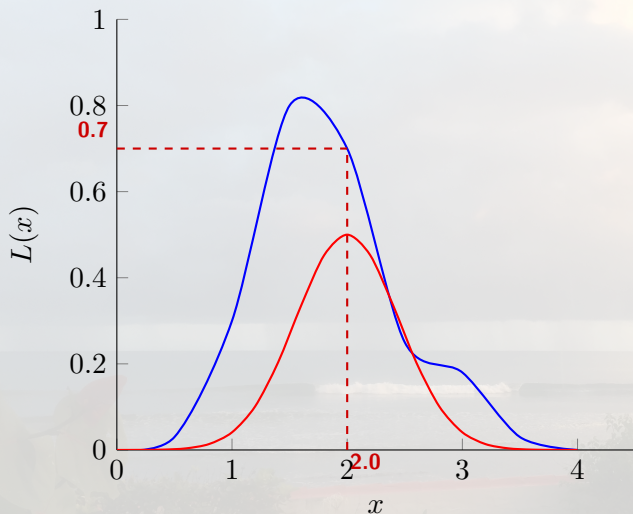
Accepted!

Markov Chain

i	$x(i)$
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2	2.0



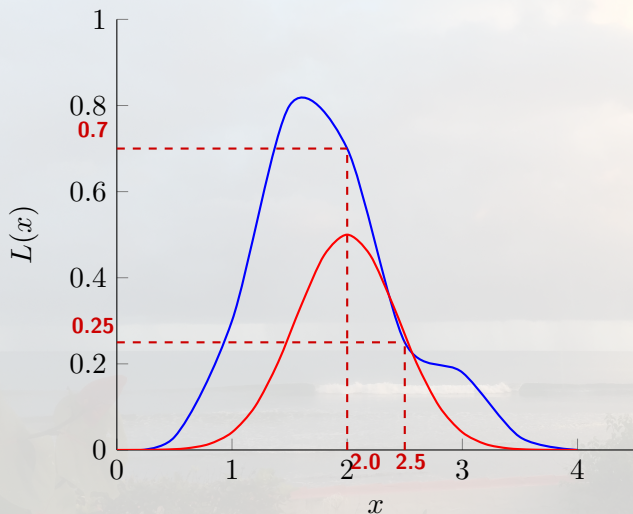
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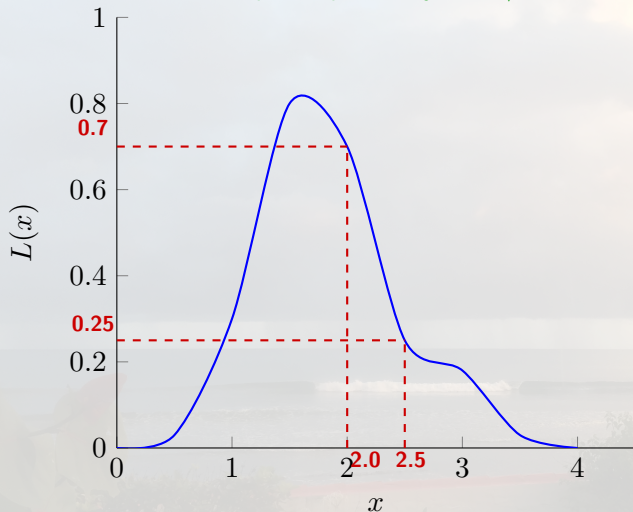


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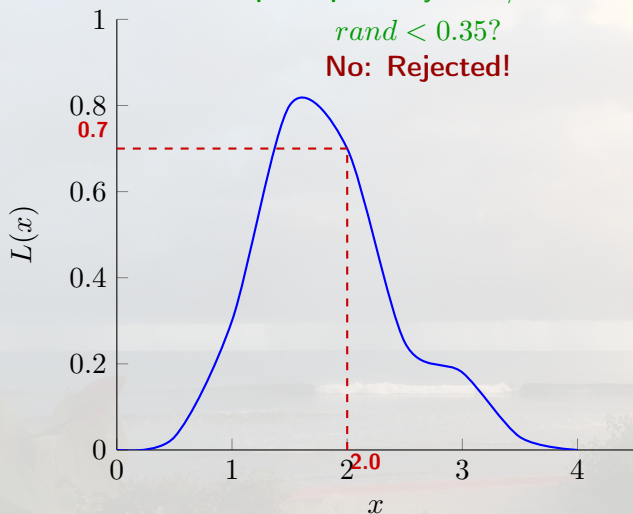
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$rand < 0.35?$

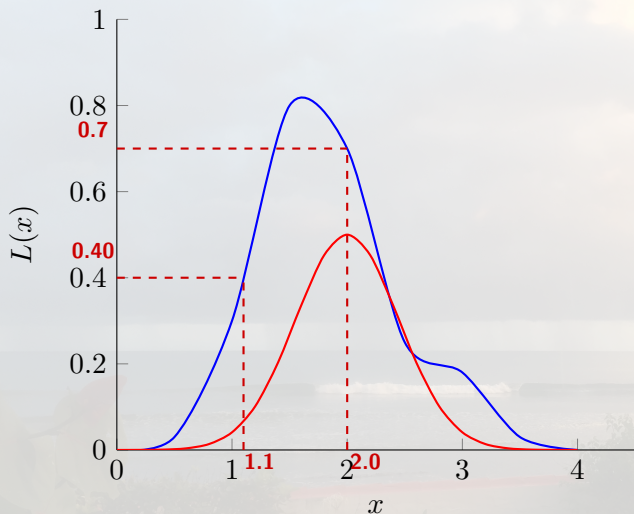
No: Rejected!



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Markov chain example - the Metropolis sampler



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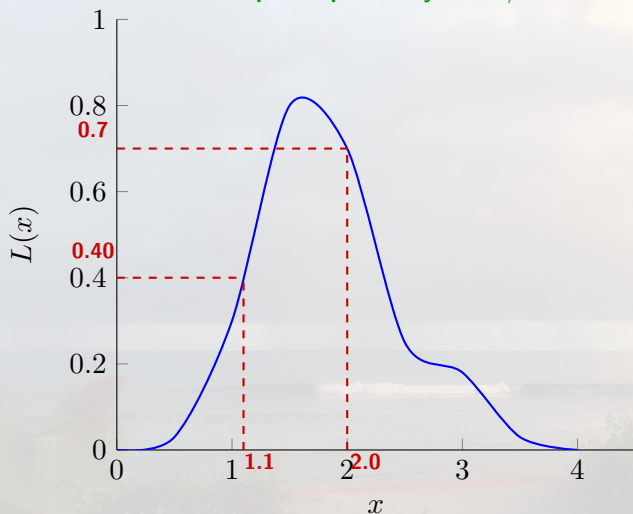
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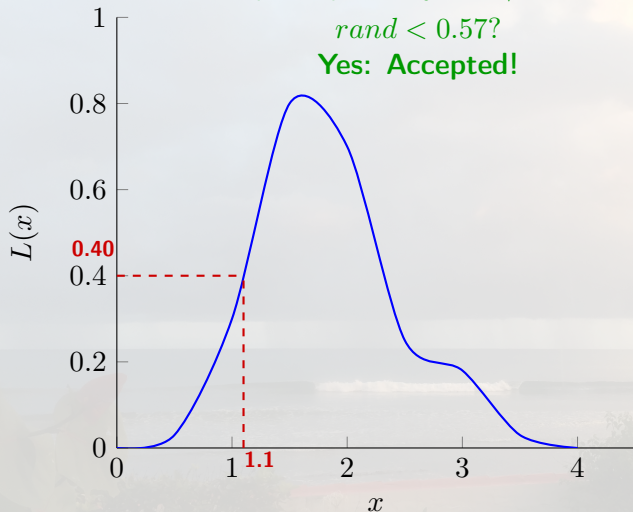
Markov Chain

i	x(i)
1	1.3
2	2.0
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4	1.1

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$rand < 0.57?$

Yes: Accepted!



What is the likelihood?

$$P(\mathbf{x}|\mathbf{y}) = \frac{P(\mathbf{x}) \cdot P(\mathbf{y}|\mathbf{x})}{P(\mathbf{y})} \quad (3)$$

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$\mathbf{f}(\mathbf{x})$ is result of propagating the control parameters \mathbf{x} through the forward model f .

\mathbf{y} is the (true) observational vector.

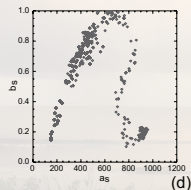
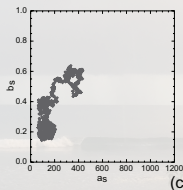
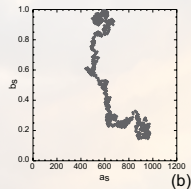
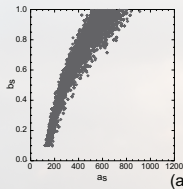
\mathbf{C} is the observation error covariance matrix.

Practical issues with MCMC: Proposal issues 1

Poorly tuned proposal distribution can cause problems. Also, bad choice of start position can be problematic.

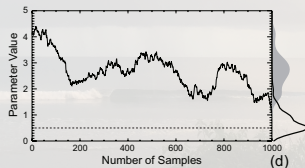
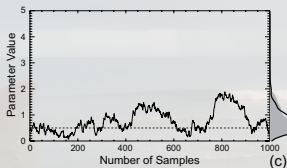
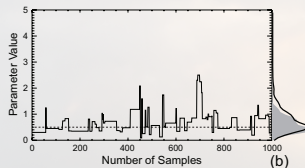
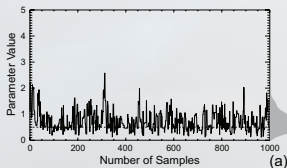
- A: Good proposal variance
- B: Proposal variance small, started far from large PDF values
- C: same as B, started within region of large PDF values
- D: Same as B, adaptive proposal variance

Figures from Posselt [2012]



Practical issues with MCMC: Proposal issues 2

Time series of chain can show problematic autocorrelation due to poorly chosen proposal and/or non-convergent sample.



Figures from Posselt [2012]

Practical issues with MCMC: Proposal issues 3

How does one construct a good proposal?

How does one avoid bad start position?

- Prior knowledge
- Run many chains with random start positions
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How does one construct a good proposal?

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- “Burn-in” phase where proposal is actively tuned

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- Run many chains with random start positions
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Practical issues with MCMC: Proposal issues 3

How does one construct a good proposal?

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- “Burn-in” phase where proposal is actively tuned
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Practical issues with MCMC: Proposal issues 3

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- Delayed Rejection (2nd proposal after 1st)

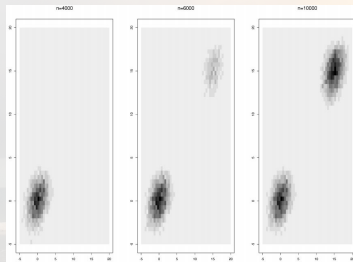
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Practical issues with MCMC: Assessing convergence 1

When do we stop our chain? How do we tell if we've converged to the target PDF?

- If the target distribution is known, compare
- Assess convergence of running statistical moments
- Kolmogorov-Smirnov test on chain sub-samples
- R-statistic – Gelman et al. [1996]
- *Caveat:* beware of 'pseudo-convergence'!



Practical issues with MCMC: Assessing convergence 2

R-Statistic – Gelman et al. [1996]

General idea:

- Run many chains
- Compute variance within each chain (W)
- Compute mean of each chain
- Compare mean of within-chain variances with variance of all chain means (B)

$$\hat{v}ar^+(\mathbf{x}|\mathbf{y}) = \frac{n-1}{n}W + \frac{1}{n}B \quad (6)$$

$$\hat{R} = \sqrt{\frac{\hat{v}ar^+(\mathbf{x}|\mathbf{y})}{W}} \quad (7)$$

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- Require many model integrations
- Often do not parallelize well
- For more info see:
 - Tarantola [2005]
 - MacKay [2005]
 - Robert and Casella

Simulated Annealing 1

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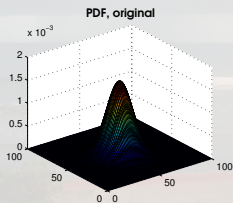
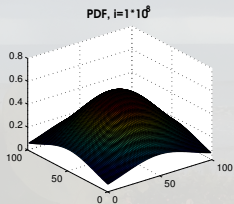
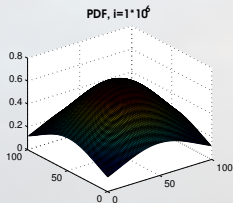
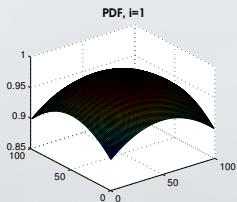
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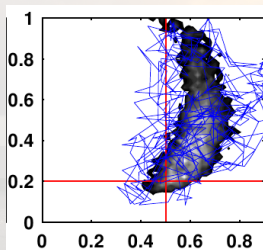
$$P_{SA} = P^{\frac{1}{T}}$$

$$T_i = \frac{200}{\log(i + 1)}$$

Simulated Annealing 2



Simulated annealing used to pre-sample before running Metropolis MCMC:



Gibbs Sampling

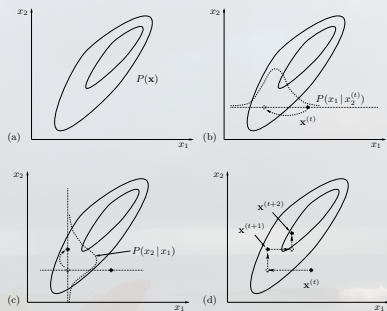


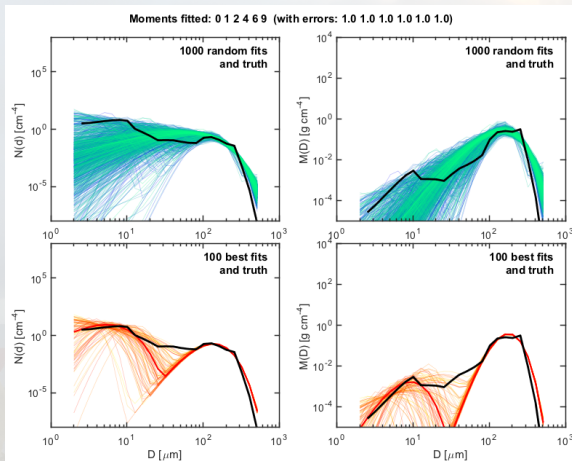
Figure from MacKay [2005]

- What if you can sample from the conditional distribution?
- Take turns sampling from conditionals of each dimension
- Acceptance ratio = 1 (always!)
- Freely available software (BUGS) - Bayesian inference Using Gibbs Sampling

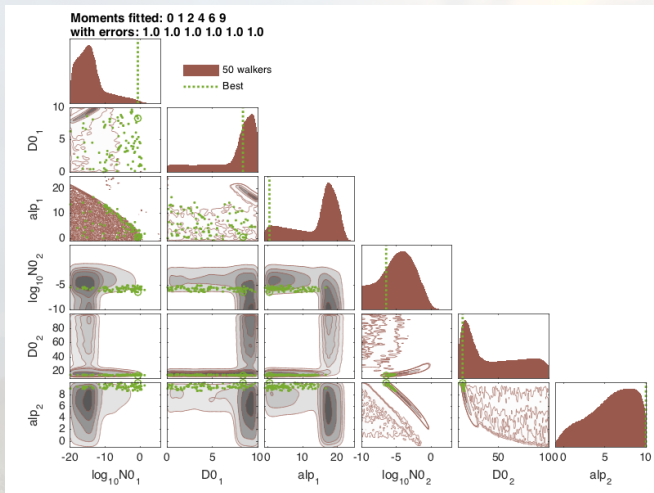
Other Monte Carlo topics

- Hamiltonian (hybrid) MCMC and No U-Turn Sampler
- Affine-invariant MCMC (The MCMC Hammer)
- Importance sampling
- Slice sampler
- Perfect sampler
- Nested (& multimodal nested sampling)
- MC methods for model comparison (estimation of 'evidence')
- Particle filter
- Ensemble Kalman Filter

Cloud Property Retrieval using Radar



Cloud Property Retrieval using Radar



References I

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- D. J. C. MacKay. *Information Theory, Inference, and Learning Algorithms*. Cambridge University Press, Cambridge, UK, 7.2 edition, 2005.
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