Model Parameter Estimation Using Nonlinear Ensemble Algorithms

Derek J. Posselt[1] and Craig H. Bishop[2]

[1]JIFRESSE, University of California, Los Angeles, CA
[2]Naval Research Laboratory, Monterey, CA

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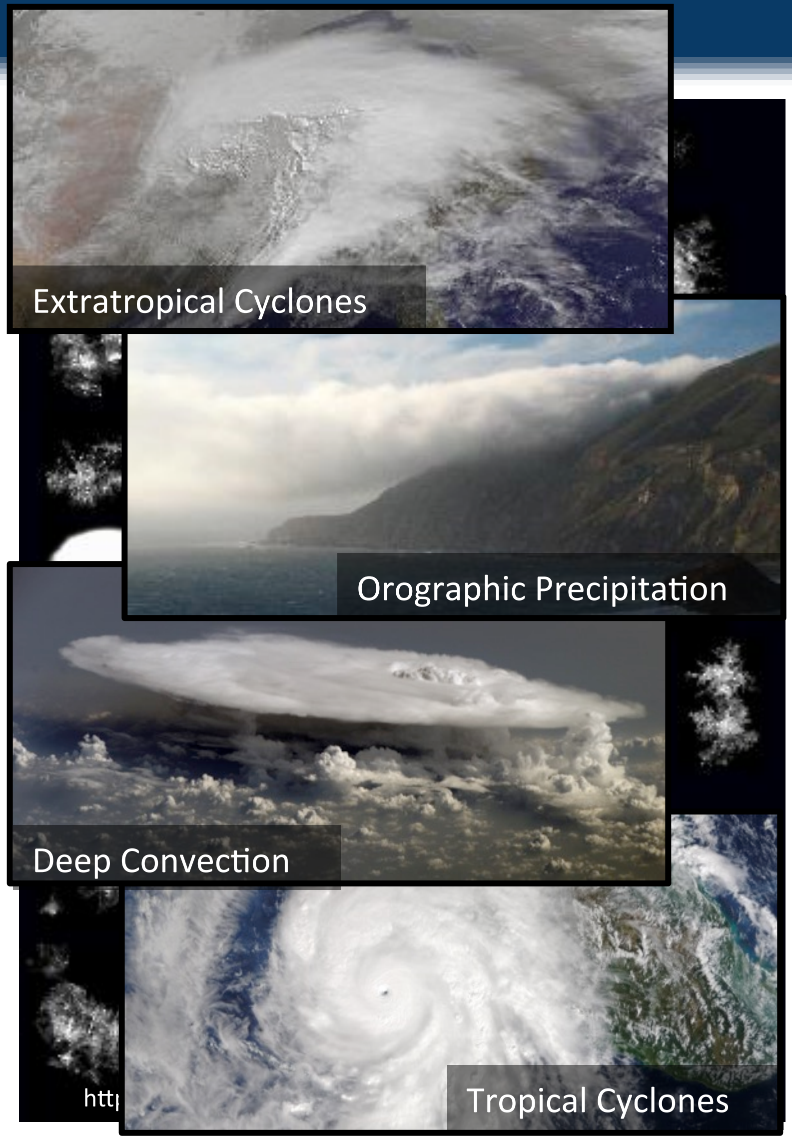
Parameter Estimation and Model Uncertainty

- Simplified processes lead to uncertainty in models
- Quantify uncertainty in model parameterizations:
  - Estimate model error and produce larger range of ensemble realizations
  - Tune models, and provide guidance for model improvement
  - Examine physical characteristics of system (as viewed through the lens of an imperfect model)
- **Challenges:**
  - **Nonlinearity (non-monotonicity) in parameter-output functional relationship**
  - **Parameters and model outputs bounded at zero (e.g., precipitation rate)**
  - **Regional and state dependence of optimal parameter values and parameter PDFs**



Data Assimilation: Probabilistic Evaluation of Model Uncertainty

1. Which parameters contribute most to model uncertainty?
2. (How) do parameter uncertainties change with model dimensionality?
3. How well do ensemble DA algorithms reproduce the Bayesian posterior distribution?

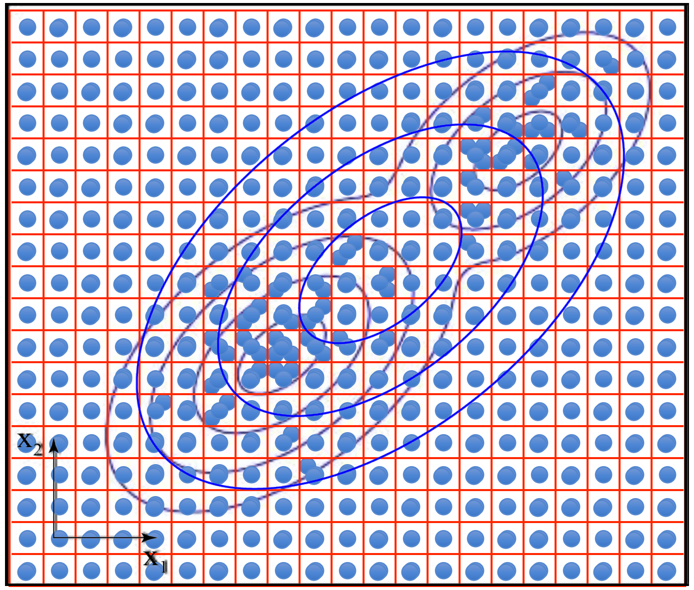
Represent the influence of parameters $\mathbf{x}$ on output of model $F(\mathbf{x}) = \mathbf{y}$

- Compute joint PDF of the parameter set for given observations. **No assumed form of the probability distribution**
- Obtain a measure of the influence of parameters on model state
- Evaluate ensemble filter algorithms

$$p(\mathbf{x} \mid \mathbf{y}) \propto p(\mathbf{y} \mid \mathbf{x})\, p(\mathbf{x})$$

Bayesian Parameter Estimation

Goal: estimate $p(\mathbf{x}|\mathbf{y})$ given $p(\mathbf{y}|\mathbf{x})$ and $p(\mathbf{x})$



Options:

- Assume a form for each distribution (e.g., Gaussian)
- Compute by brute force
- Random sample (Monte Carlo)
- Construct a Markov chain that samples $p(\mathbf{x}|\mathbf{y})$

Markov chain Monte Carlo:

- Produces a sample of $p(\mathbf{x}|\mathbf{y})$
- Avoids states that provide a poor fit to observations (low likelihood $p(\mathbf{y}|\mathbf{x})$)
- Flexible probability distributions (no need for Gaussian assumption)

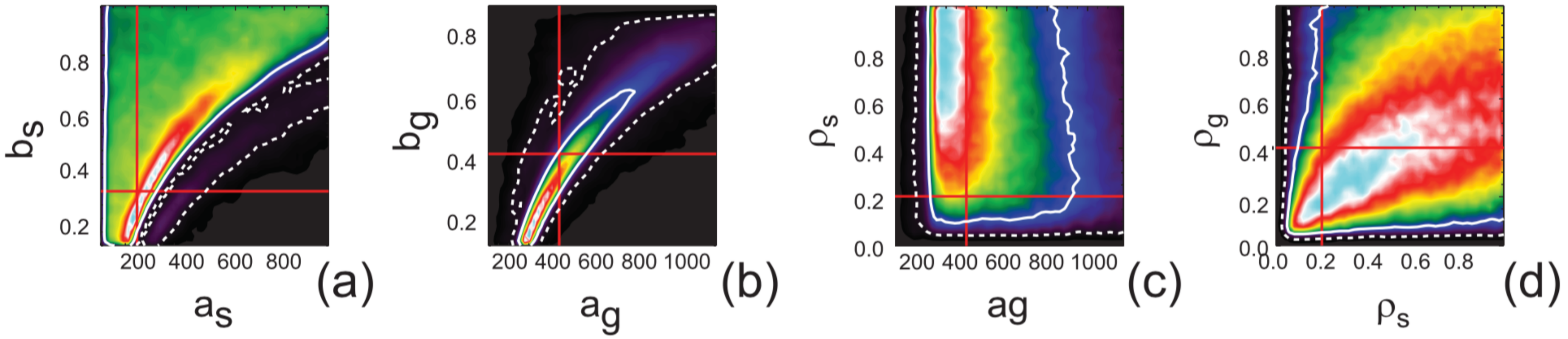
$$p(\mathbf{x} \,|\, \mathbf{y}) \propto p(\mathbf{y} \,|\, \mathbf{x})\, p(\mathbf{x})$$

Posselt and Vukicevic (2010, Mon. Wea. Rev.), Posselt and Bishop (2012, Mon. Wea. Rev.), van Lier-Walqui et al. (2012, 2014 Mon. Wea. Rev.), Posselt et al. (2014, Mon. Wea. Rev.), Posselt (2016, J. Atmos. Sci.), Posselt and Bishop (2018, QJRMS)

Convection Parameters and Observations

Parameter Sensitivity and Identifiability

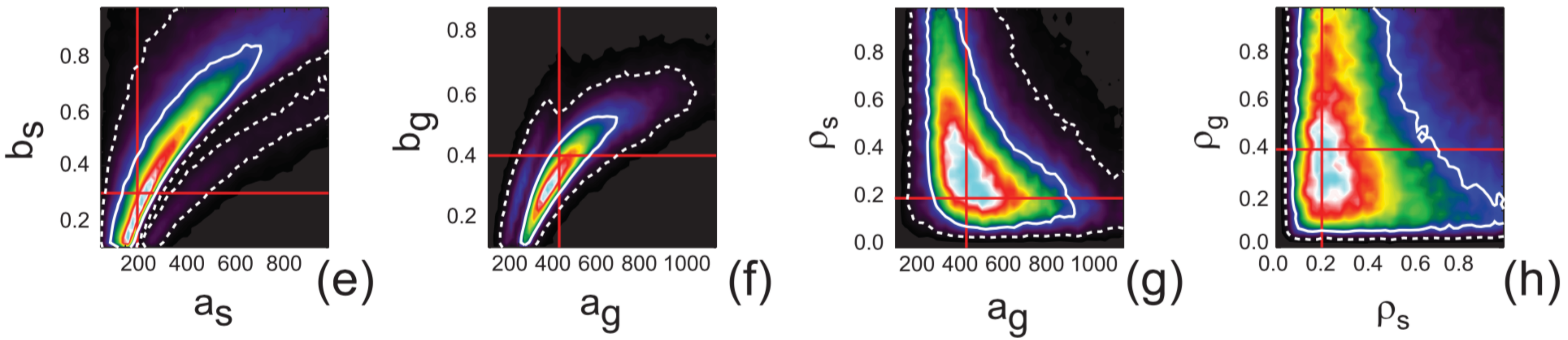
- Observe hydrologic cycle (precipitation rate, liquid and ice)
- Few of the parameters are well constrained by observations



Posselt and Vukicevic (2010, Mon. Wea. Rev.)

Parameter Sensitivity and Identifiability

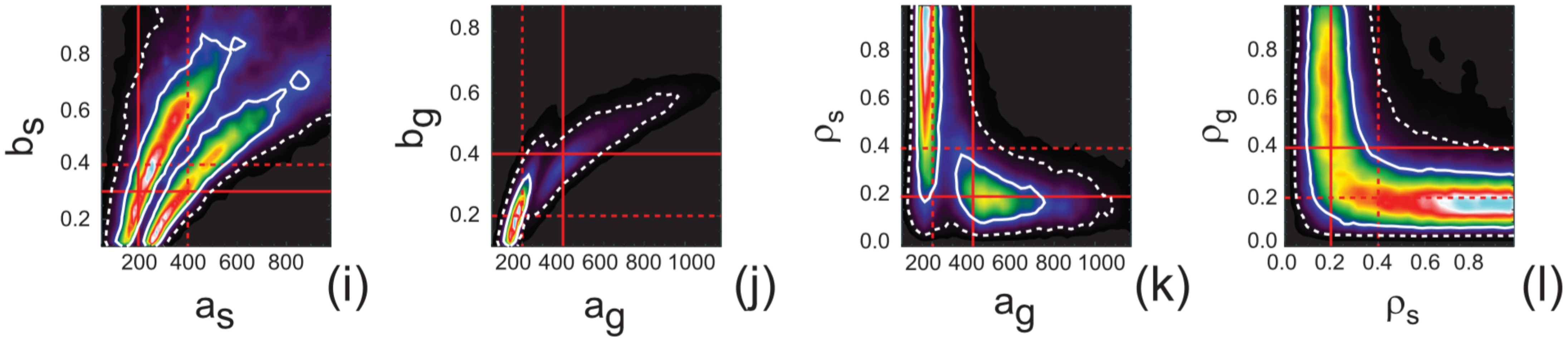
- Add observations of radiative flux (infrared and visible)
- Parameter constraint improves



Posselt and Vukicevic (2010, Mon. Wea. Rev.)

Parameter Sensitivity and Identifiability

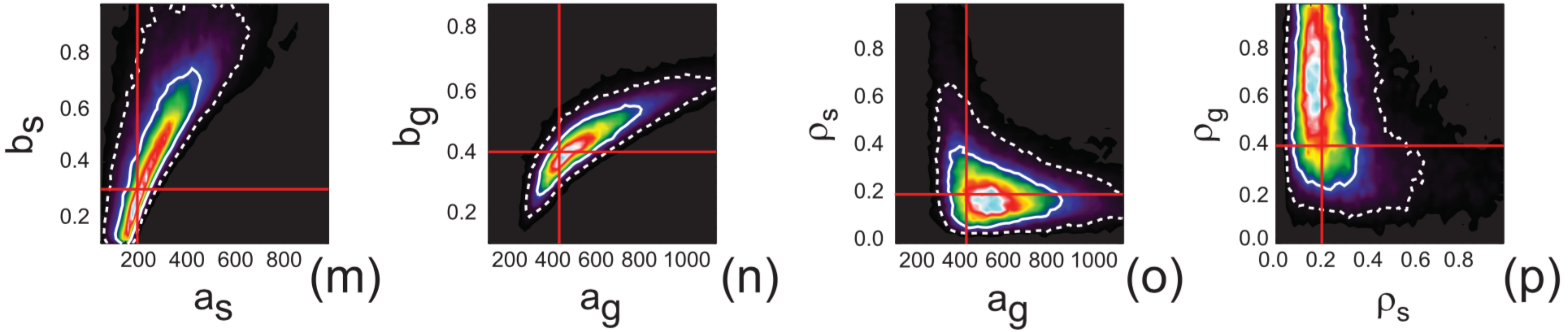
- Assume more accurate observations are available
- Lose parameter identifiability - there is non-uniqueness built into the system



Posselt and Vukicevic (2010, Mon. Wea. Rev.)

Parameter Sensitivity and Identifiability

- Apply physical constraints (graupel falls faster than snow)
- Nearly all parameters are now uniquely identifiable from observations

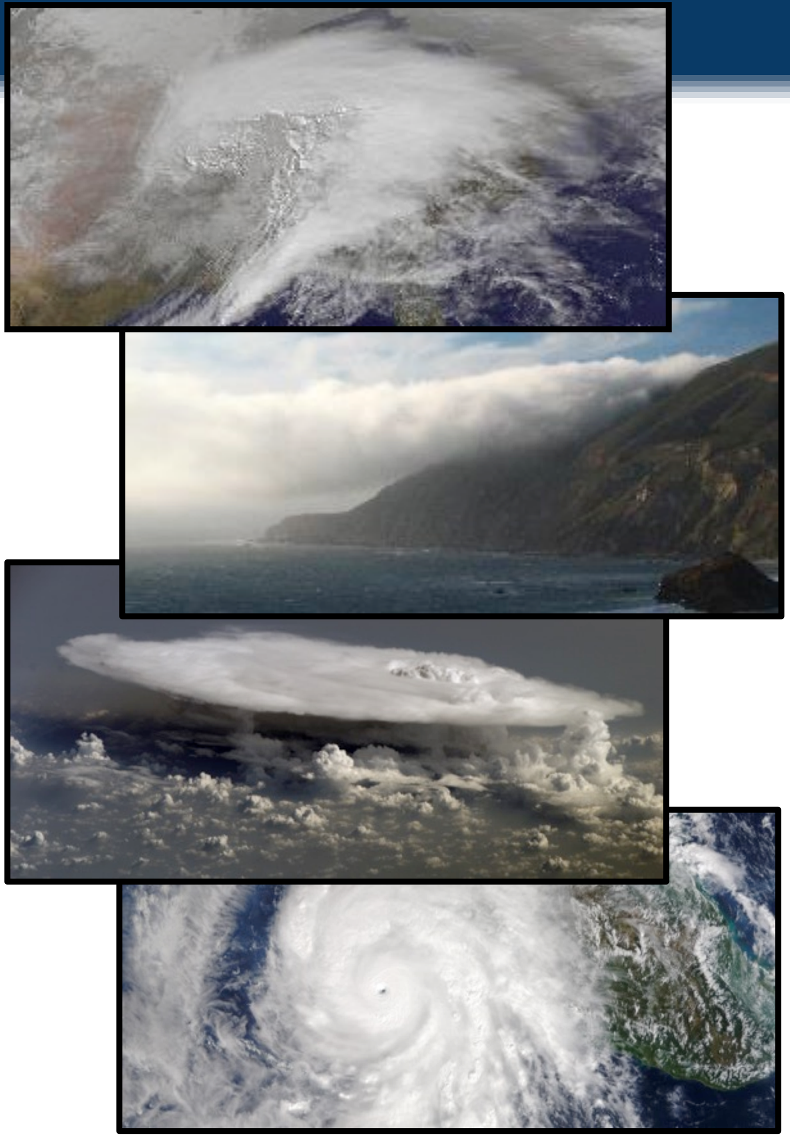


Posselt and Vukicevic (2010, Mon. Wea. Rev.)

Ensemble Filters for Parameter Estimation

- MCMC provides a sample of the unapproximated posterior PDF, but is too computationally expensive for most applications
- Evaluate the capability of ensemble filters for estimation of model physics parameters
  - Produce a posterior analysis distribution and compare with MCMC
  - Examine performance in the presence of nonlinearity
- Two algorithms
  - Perturbed-obs EnKF (Posselt and Bishop, 2012; Posselt et al. 2014)
  - Gamma – Inverse Gamma (GIG) filter (Bishop, 2016)
- Single analysis update (not cycling)

Perturbed-Obs Ensemble Kalman Filter



- Conduct a set of experiments using different assumed true sets of microphysical parameters

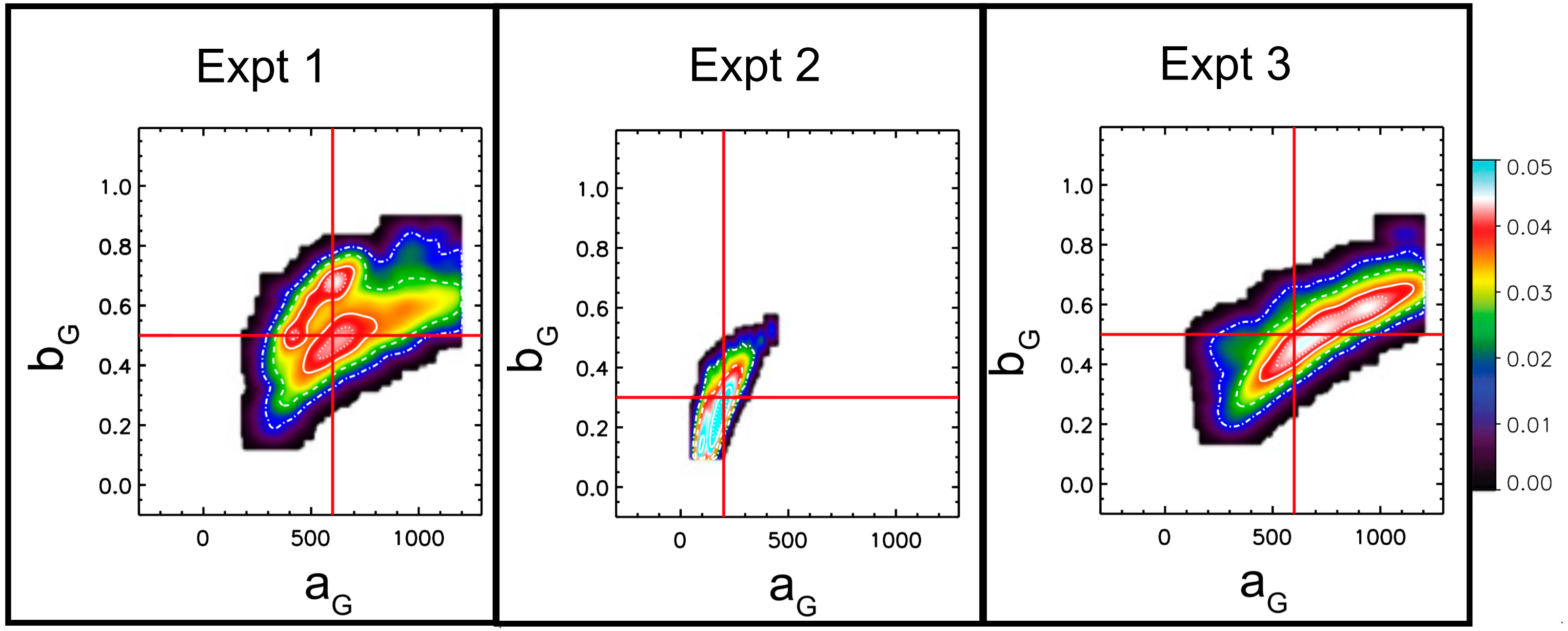
$$\bar{\mathbf{x}}_a = \bar{\mathbf{x}}^f + \mathbf{P}^f\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\mathbf{y} - \mathbf{H}\bar{\mathbf{x}}^f],$$

$$\boldsymbol{\varepsilon}_i^a = \boldsymbol{\varepsilon}_i^f + \mathbf{P}^f\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\boldsymbol{\varepsilon}_i^o - \mathbf{H}\boldsymbol{\varepsilon}_i^f].$$

- Determine how the solution space changes as the true parameters change
  - Experimenting with regional differences in processes
  - Do the posterior parameter distributions change?
  - Does EnKF track these changes?

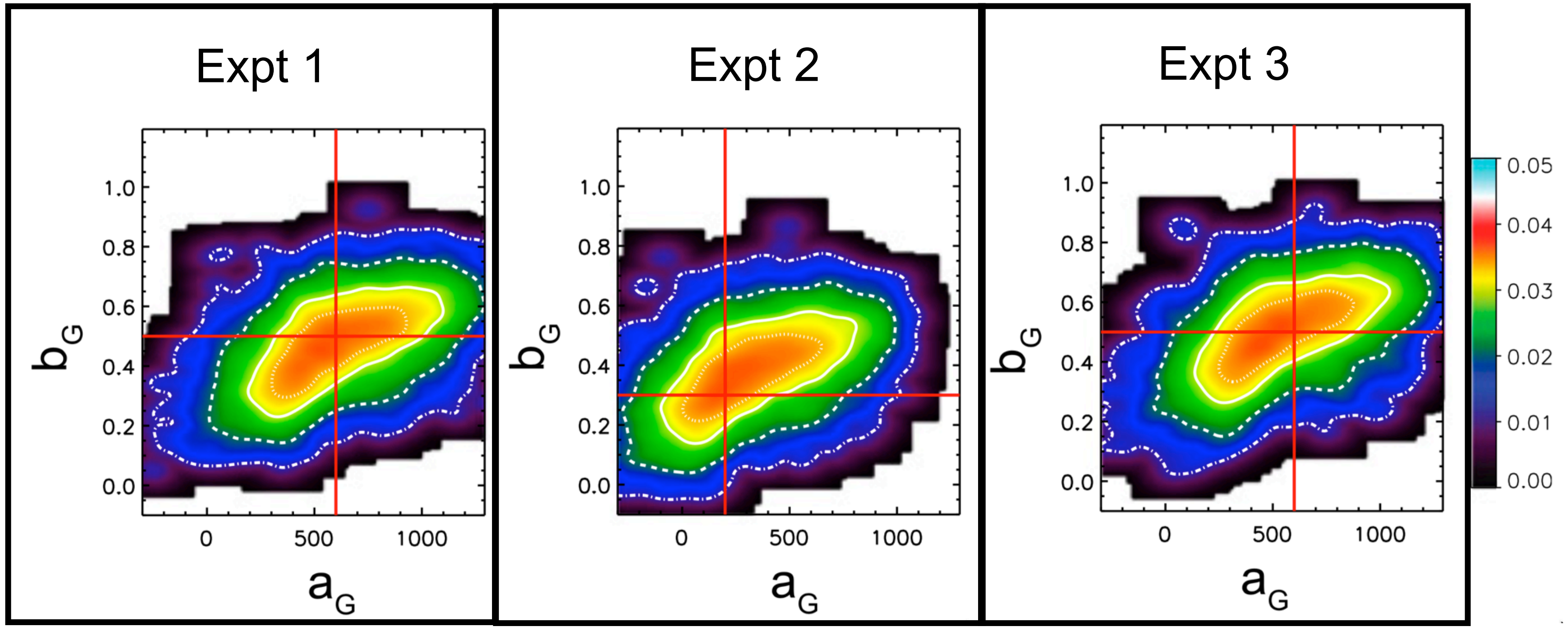
MCMC $p(\mathbf{x}|\mathbf{y})$

- Determine how the analysis changes for different (true) parameter values
- MCMC analysis ensemble is shown (at right) for three experiments
- Posterior distribution depends strongly on the parameter values
- Variance increases with parameter value



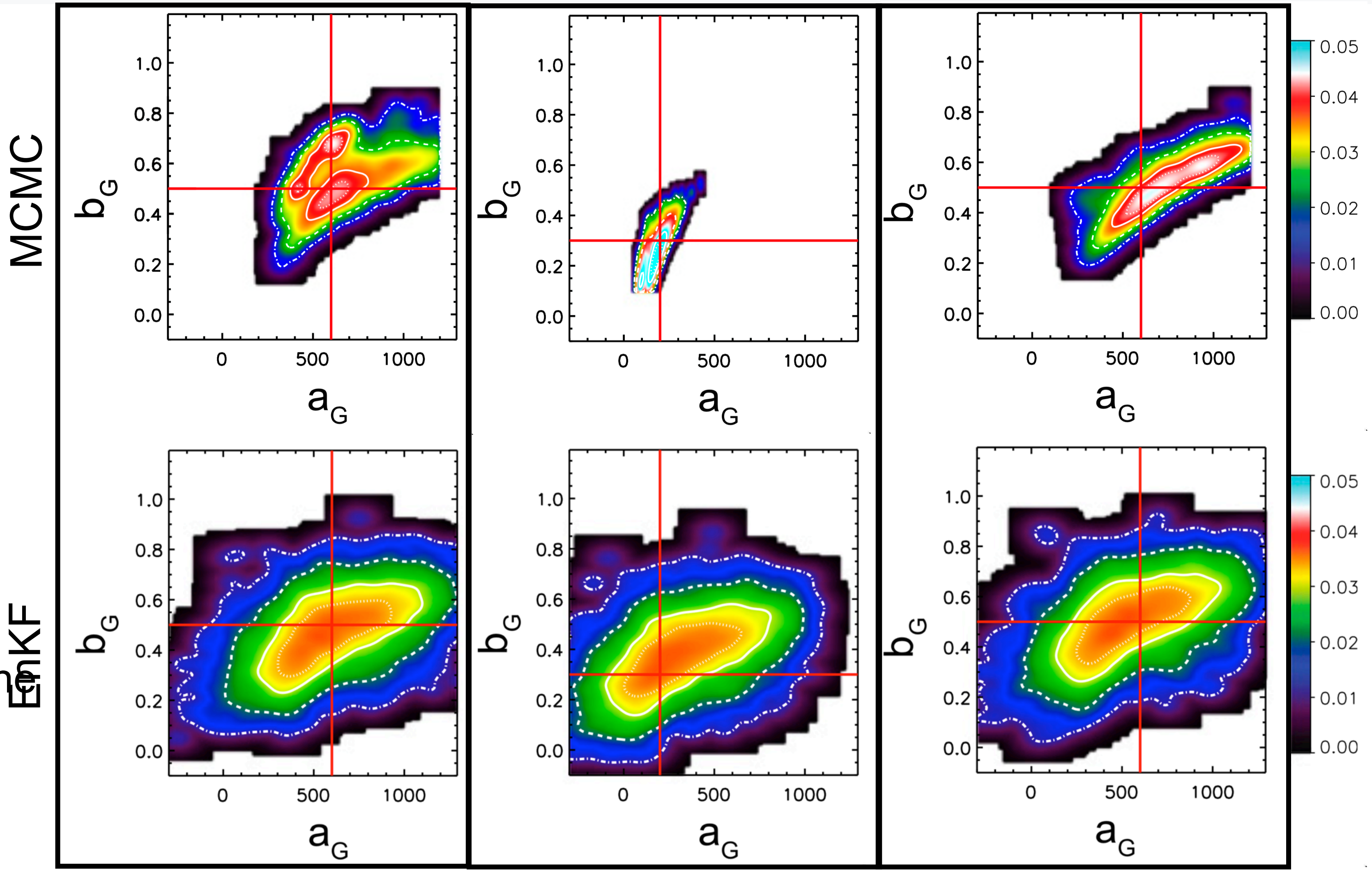
EnKF $p(\mathbf{x}|\mathbf{y})$

- EnKF analysis ensemble *shape* does not change
- Analysis mean shifts according to the true parameter value, but there is no change in higher moments
- When true parameter values are near zero, much of the analysis ensemble is non-physical



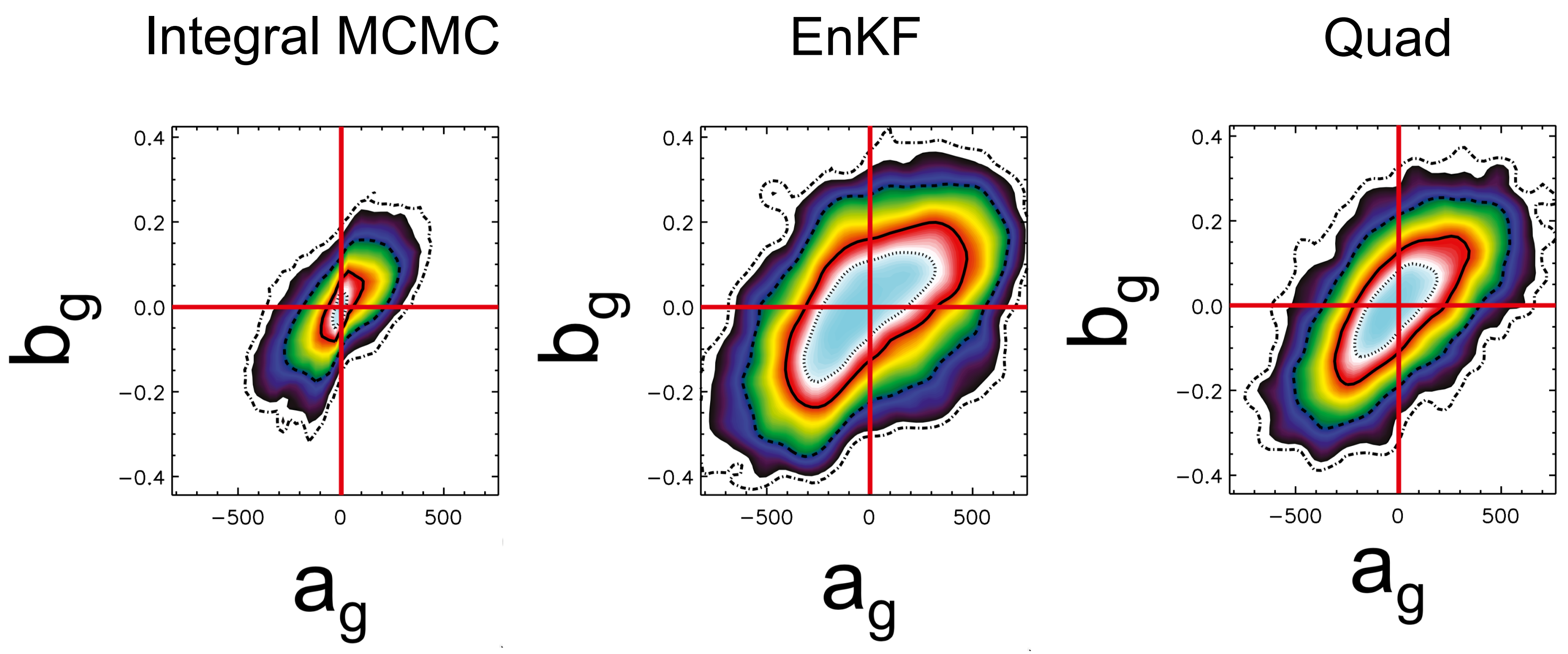
EnKF as an Integral Solution

- Compare MCMC with EnKF
- EnKF analysis looks like an integral over the set of possible posterior distributions
- Integral experiment:
  - Randomly draw 100 sets of parameter values
  - Simulate observations
  - Run MCMC to obtain 100 analysis distributions
  - Remove the mean and combine to produce integral over 100 realizations



EnKF as an Integral Solution

- EnKF better reflects the integral over all possible parameter sets
- The variance is still too large, due to the fact that the EnKF only knows about the 1st and 2nd moment of the distribution
- Hodyss (2012)'s quadratic ensemble filter accounts for the 3rd moment – produces a solution closer to MCMC



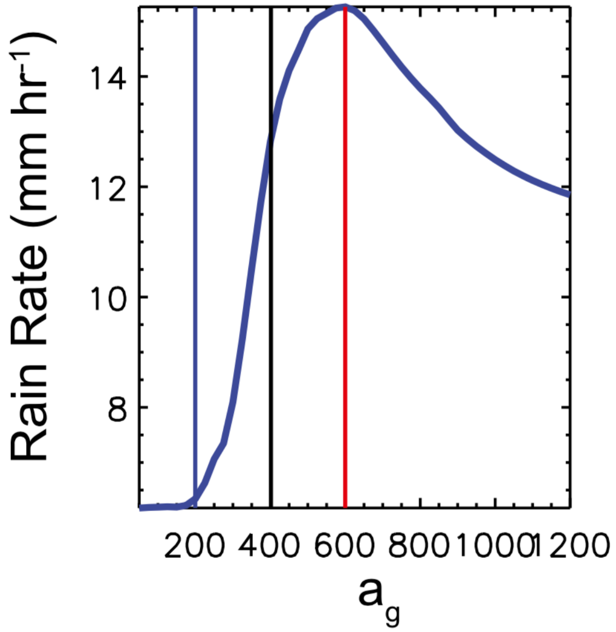
Posselt, Hodyss, and Bishop (2014, Mon. Wea. Rev.)

Nonlinear Parameter Estimation

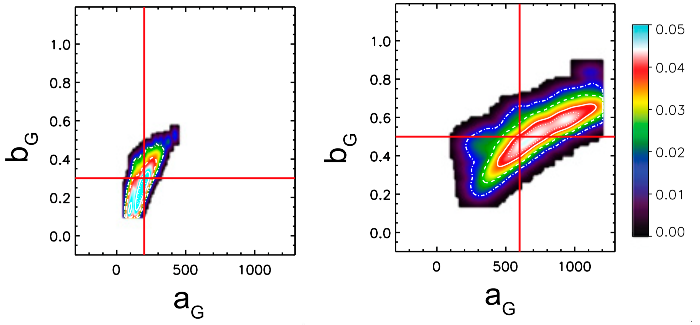
- EnKF successfully tracks the analysis mean
- The linear update does not handle changes in parameter sensitivity (distribution *p*(**x**|**y**) shape)

$$\bar{\mathbf{x}}_a = \bar{\mathbf{x}}^f + \mathbf{P}^f\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\mathbf{y} - \mathbf{H}\bar{\mathbf{x}}^f],$$

$$\boldsymbol{\varepsilon}_i^a = \boldsymbol{\varepsilon}_i^f + \mathbf{P}^f\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{P}^f\mathbf{H}^{\mathrm{T}} + \mathbf{R})^{-1}[\boldsymbol{\varepsilon}_i^o - \mathbf{H}\boldsymbol{\varepsilon}_i^f].$$



- Does not easily accommodate positive definite observations or parameters
- Note that, given a more informative prior, it is possible that the EnKF could have produced a more robust solution

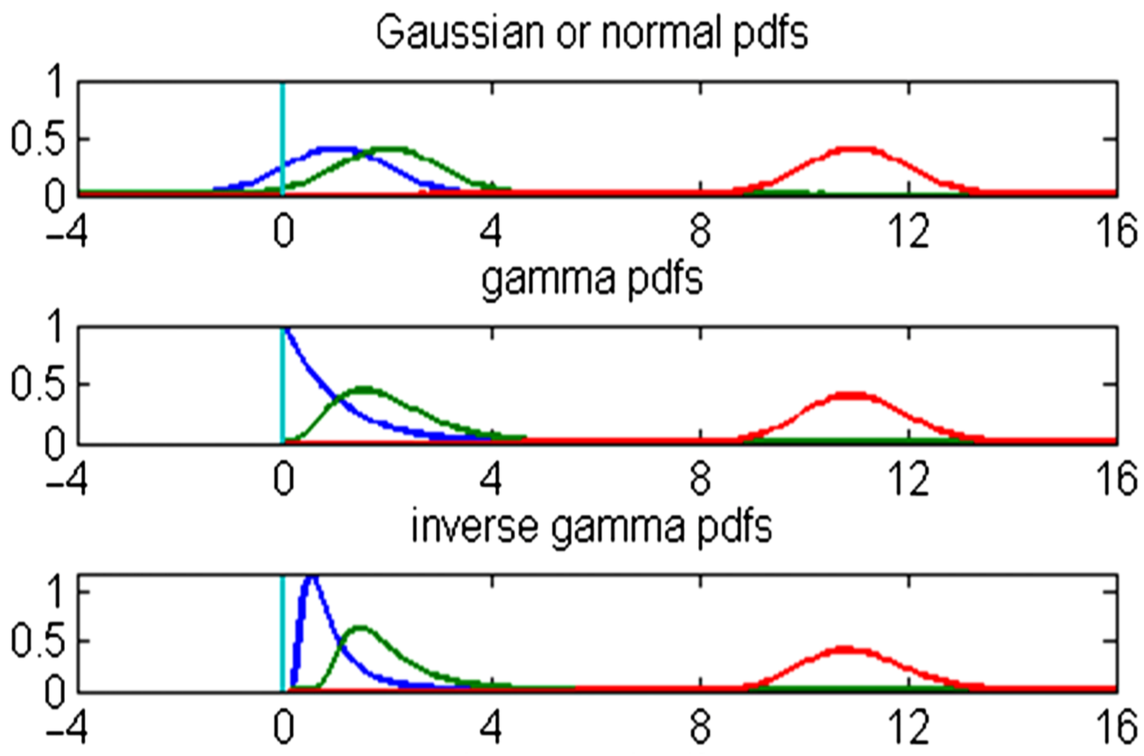


Gamma– Inverse Gamma Filter

Bishop (2016, QJRMS)

Bishop (2016) – GIGG-EnKF

- Unified formulation
  - Gaussian
  - Gamma – Inverse Gamma
  - Inverse Gamma – Gamma
- GIG and IGG
  - As in Anderson (2003), extended observation + state space solution
  - Allow for observations with fractional errors (constant *relative* error variance)
  - Naturally bound observation values at zero

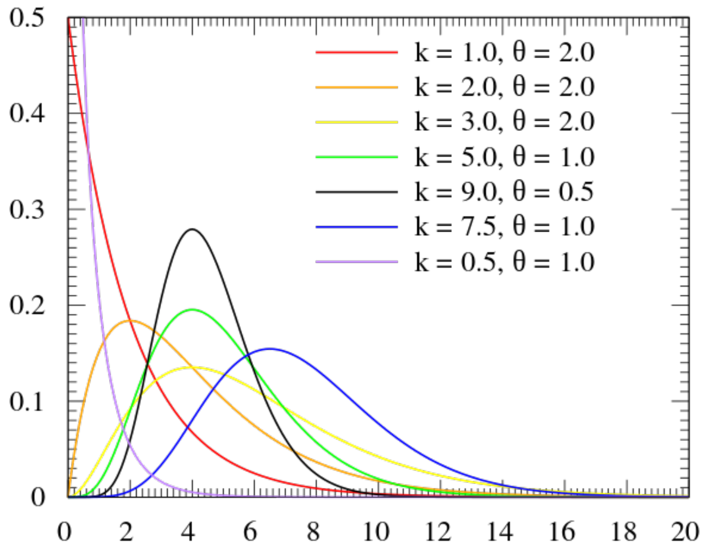


Bishop (2016, QJRMS), Fig. 1

Gamma– Inverse Gamma Filter

Bishop (2016, QJRMS)

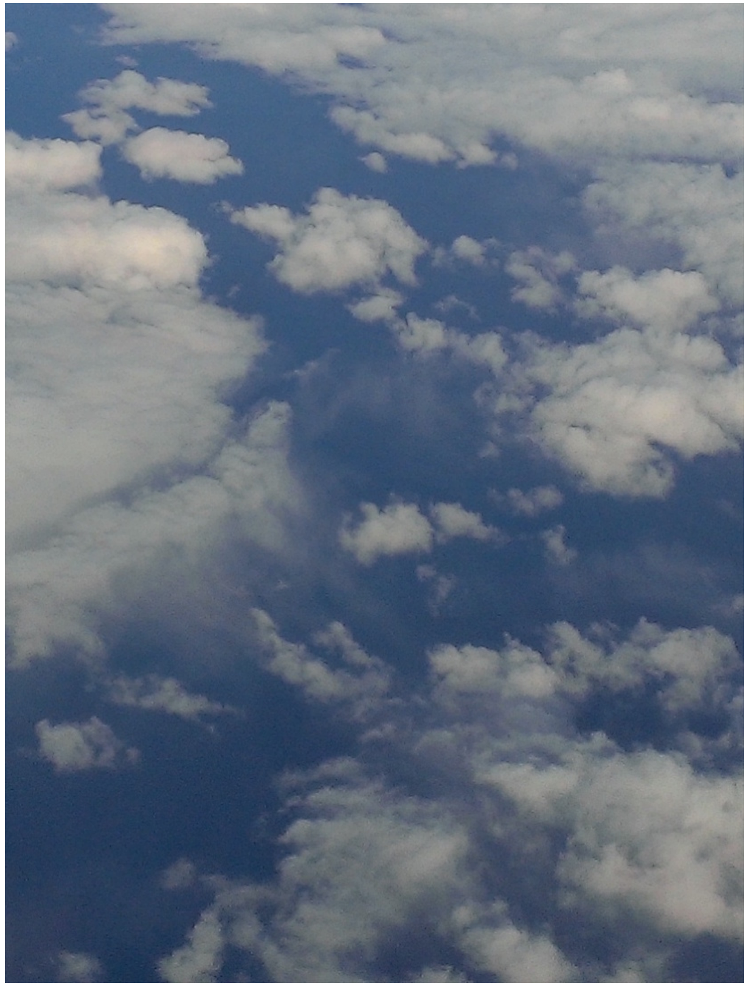
- Gamma (and Inverse Gamma) PDFs defined by 2 parameters: shape and scale, which define the distribution mean $\mu_x = k\theta$ and variance $\mathrm{var}(x) = k\theta^2$
- Parameters also set the shape – varying from exponential (large skewness) to nearly symmetric
- If $p(\mathbf{x})$ ~ Gamma, and $p(\mathbf{y}|\mathbf{x})$ ~ Inverse Gamma, then $p(\mathbf{x}|\mathbf{y})$ ~ Gamma
- Specified scale and shape leads to constant *fractional* error: constant *relative obs error variance*



$$R_j^r = \frac{\mathrm{var}(\varepsilon^o)}{(y_j)^2}$$

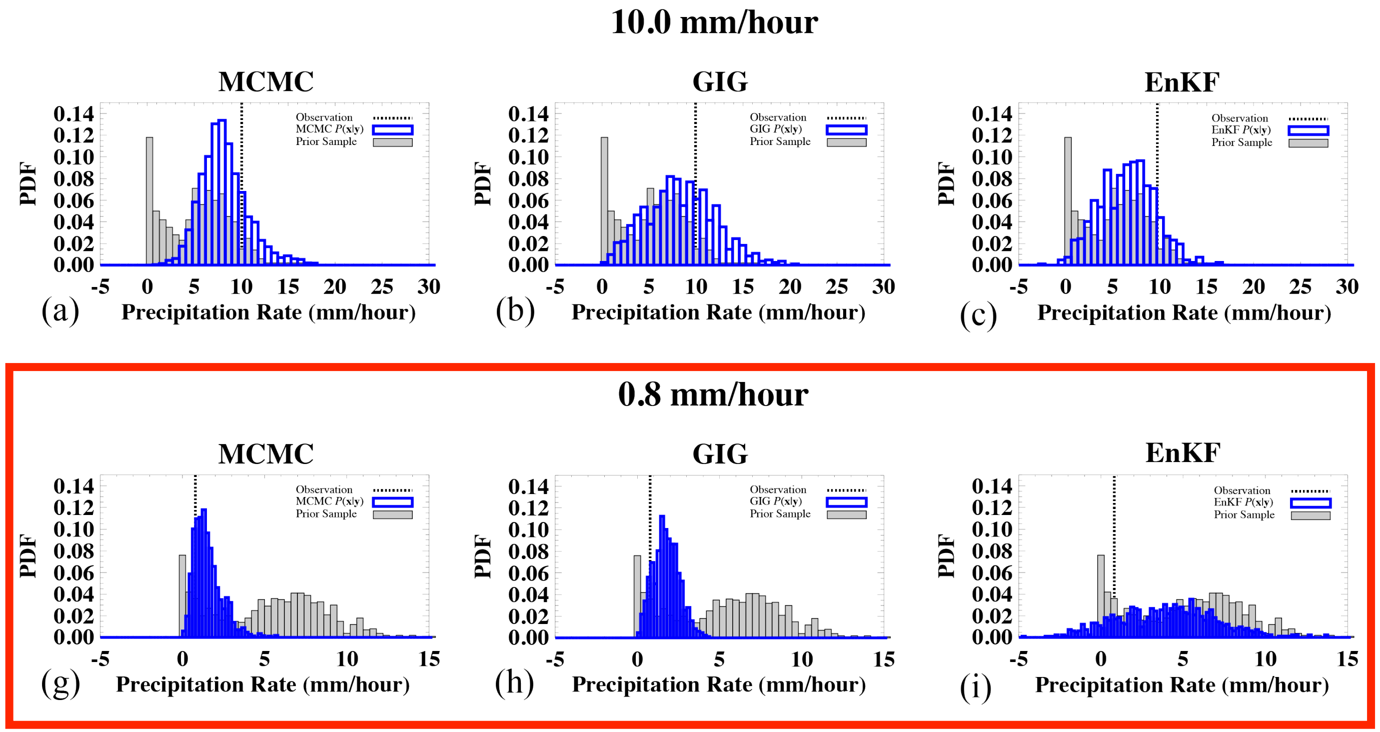
Evaluating the GIG vs. MCMC and EnKF

- Conduct a very simple experiment:
  - Estimate two warm rain parameters (N_{0R}, q_{c0})
  - Use one observation of precipitation rate
- Consider three different precipitation rates: low, medium, and high (0.8, 5.0, and 10.0 mm/hr)
- 100% relative error $\boldsymbol{\sigma}$ for MCMC and GIG
- Constant error $\boldsymbol{\sigma}$ = 5.7 mm/hour for EnKF *Posselt and Bishop (2018, QJRMS, in review)*
- Prior: Gamma, Obs: Inverse Gamma



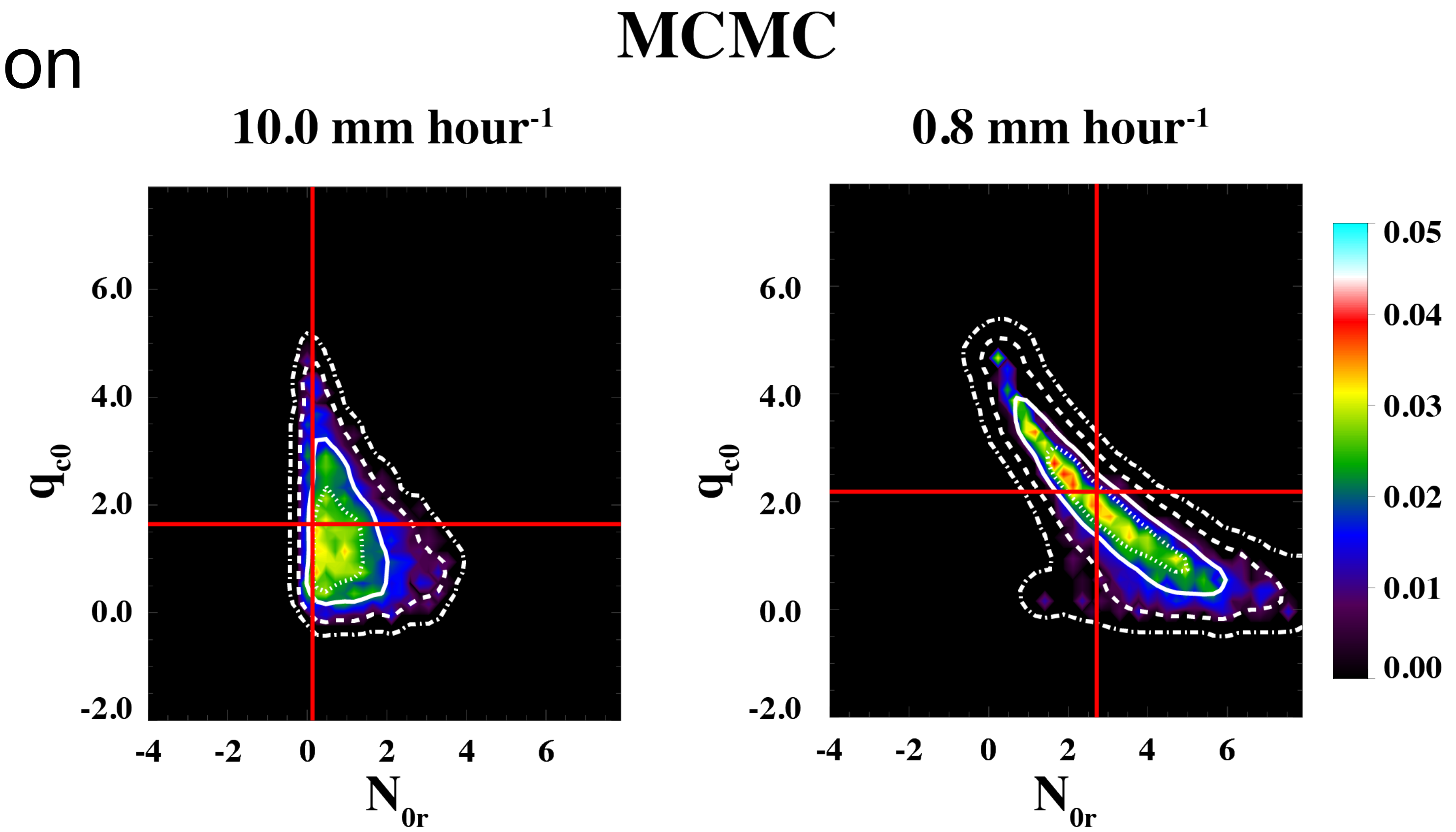
Observation Space Solution

- Prior PDF is **gray**, posterior obs-space solution in **black**
- Fractional obs error: posterior analysis variance scales with the obs value
- GIG reproduces this scaling, especially pronounced at low obs



State Space Solution: MCMC

- Observation-space formulation requires mapping back to state space for analysis (and forecast). In MCMC, this is automatic
- EnKF and GIG: linear regression from obs to state space
- EnKF analysis distribution shape does not change
- GIG analysis distribution changes with observation value, but does not reproduce the MCMC posterior distribution



State Space Solution: EnKF

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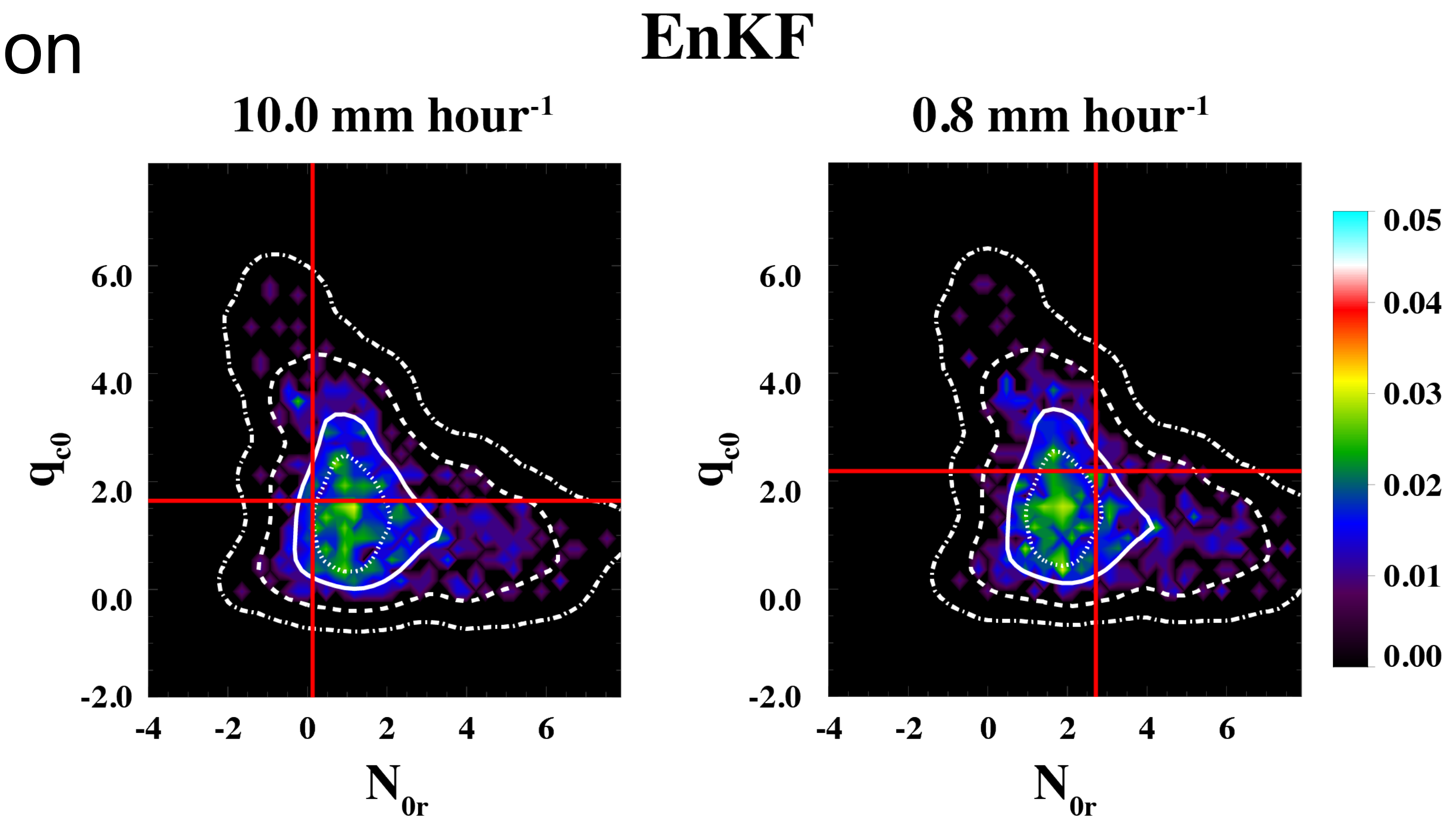

State Space Solution: GIG

- Observation-space formulation requires mapping back to state space for analysis (and forecast). In MCMC, this is automatic
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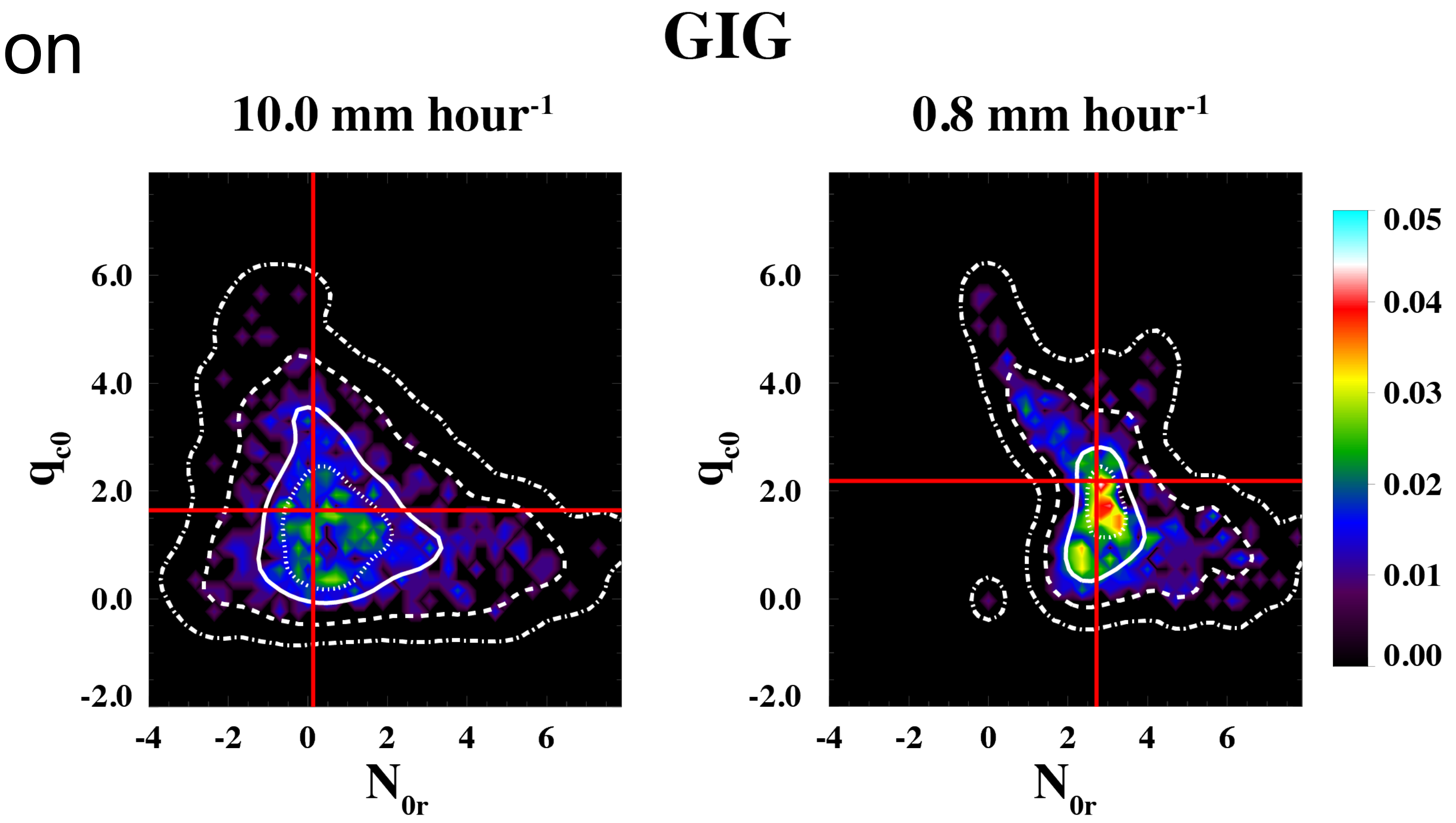
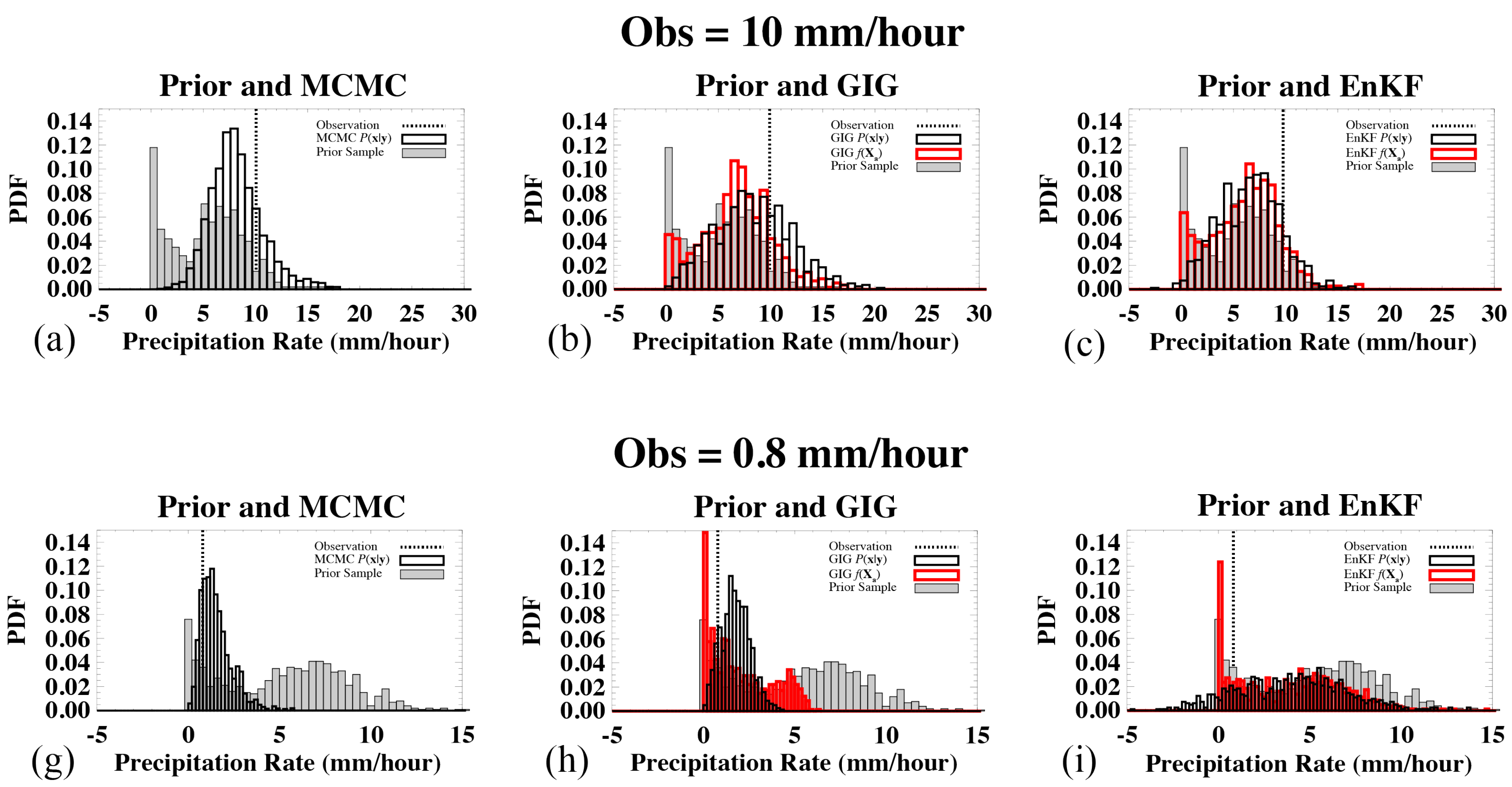


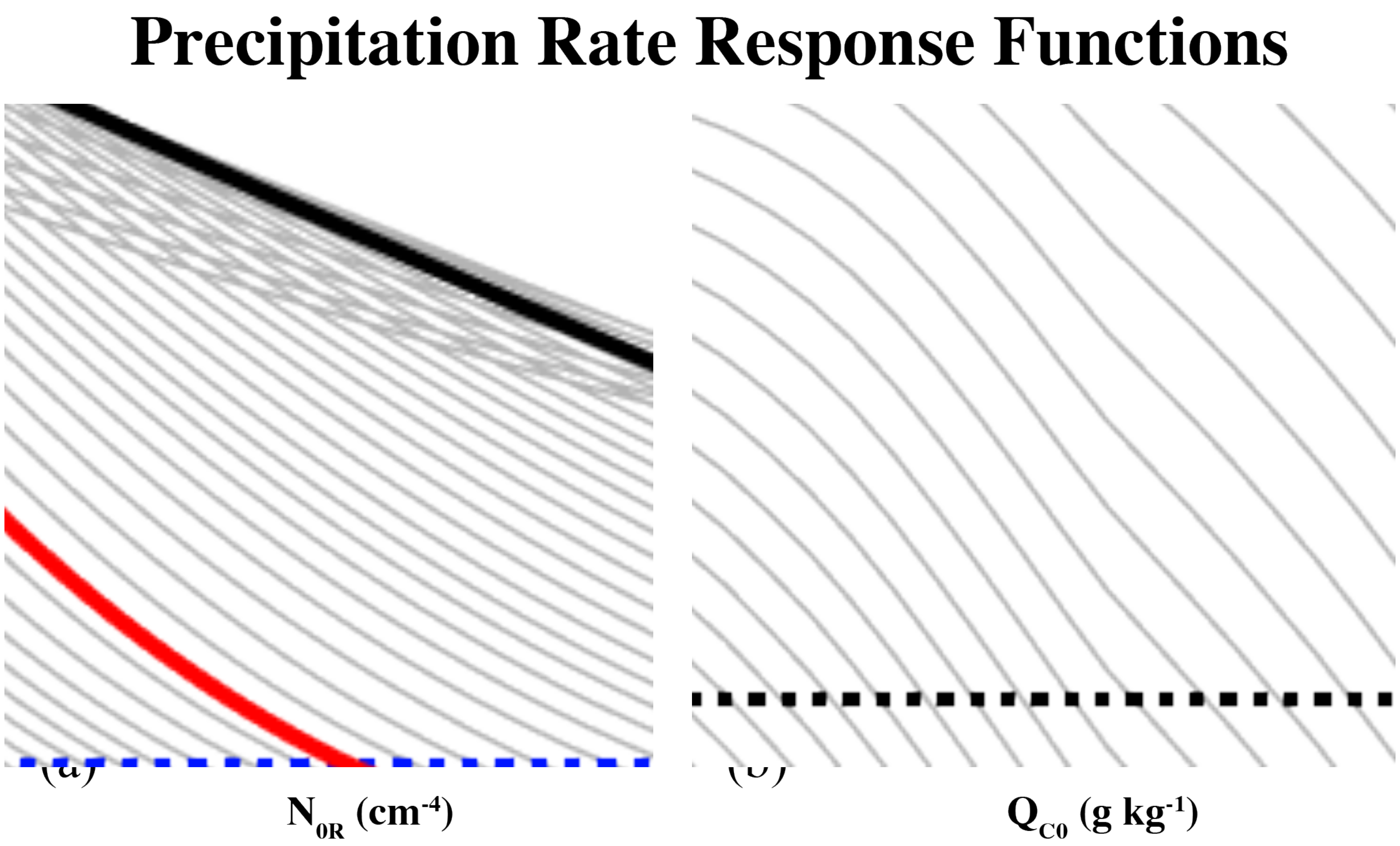
State Space Solution

- Forward model the state space analysis into observation space
- Note an inconsistency between state and observation space analyses for both EnKF and GIG
- Due to non-monotonic response function that changes slope and sign with parameter value



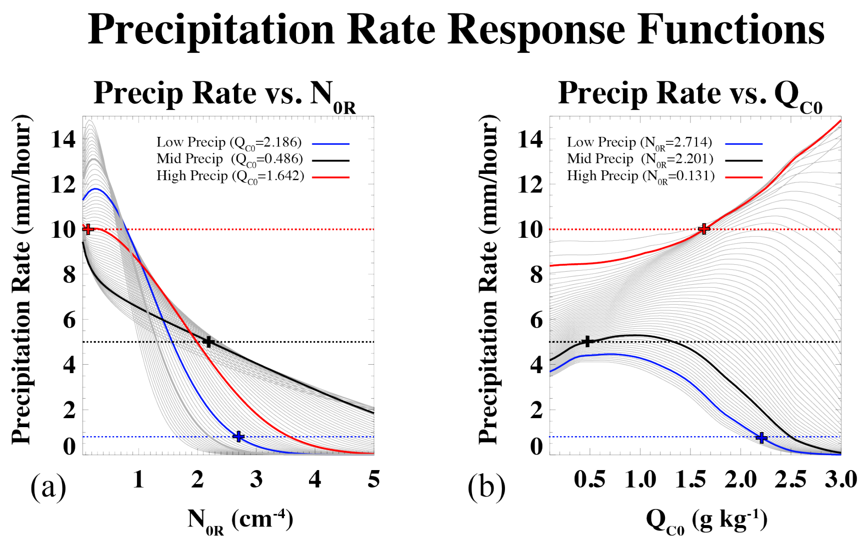
State Space Solution

- Consider response function
- Change in precipitation with a change in parameter value
- Slope of N_{0r} vs precip relationship changes, but the sign does not
- Slope and sign of q_{c0} vs precip relationship changes
- Regression from observation to state space fails when done globally



Enforcing Consistency Between State – Observation Space

- Change in observation – state covariance causes problems for the regression
- Conduct a *local regression* that accounts for the local covariance
- Initial regression to state space is the first guess
  - Regress each member independently
  - Compute weights on all other members based on distance from current member
  - Distance weighting is Gamma, to maintain consistency with the assumed prior distribution.
  - Iterate until we achieve observation – state space analysis consistency
- Analogous to a 4DVAR outer loop – a tangent linear regression or ensemble outer loop



$$w_{ij} = \exp\left[-\frac{1}{2}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)^T \mathbf{D}_w^{-1}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)\right]\left\{\sum_{k=1}^{M}\exp\left[-\frac{1}{2}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)^T \mathbf{D}_w^{-1}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)\right]\right\}^{-1}$$

where $\mathbf{D}_w = \begin{pmatrix} d_{N_{0r}}^2 & 0 \\ 0 & d_{q_{c0}}^2 \end{pmatrix}$

Ensemble Outer Loop

In each iteration *n*

- Update each ensemble member *i* using *weighted* linear regression
- Similar to update of ensemble mean in EnKF, but y_i^a (GIG analysis in obs space) does not change
- Weight for member *j* depends on distance from member *i*

for $n = 1:N$

  for $i = 1:M$

$$\mathbf{x}_i^{n+1} = \mathbf{x}_i^n + \left(\mathbf{PH}^T\right)_i^n\left[\left(\mathbf{HPH}^T\right)_i^n\right]^{-1}\left[y_i^a - H\left(\mathbf{x}_i^n\right)\right]$$

  end

end

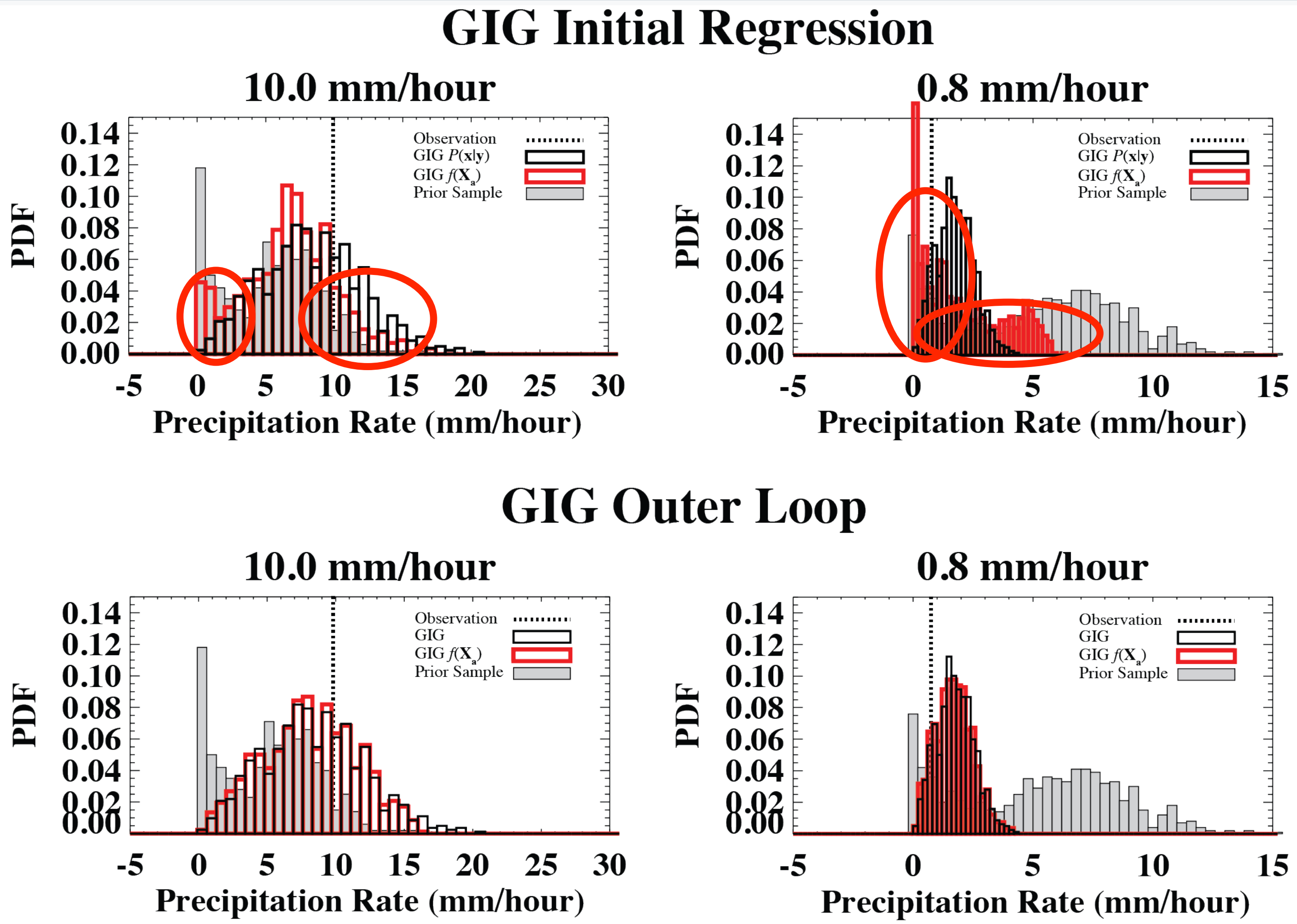
$$w_{ij} = \exp\left[-\frac{1}{2}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)^T \mathbf{D}_w^{-1}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)\right]\left\{\sum_{k=1}^{M}\exp\left[-\frac{1}{2}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)^T \mathbf{D}_w^{-1}\left(\mathbf{x}_j^n - \mathbf{x}_i^n\right)\right]\right\}^{-1}$$

where $\boxed{\mathbf{D}_w = \begin{pmatrix} d_{N_{0r}}^2 & 0 \\ 0 & d_{q_{c0}}^2 \end{pmatrix}}$

Controls radius of influence around current ensemble member *i*

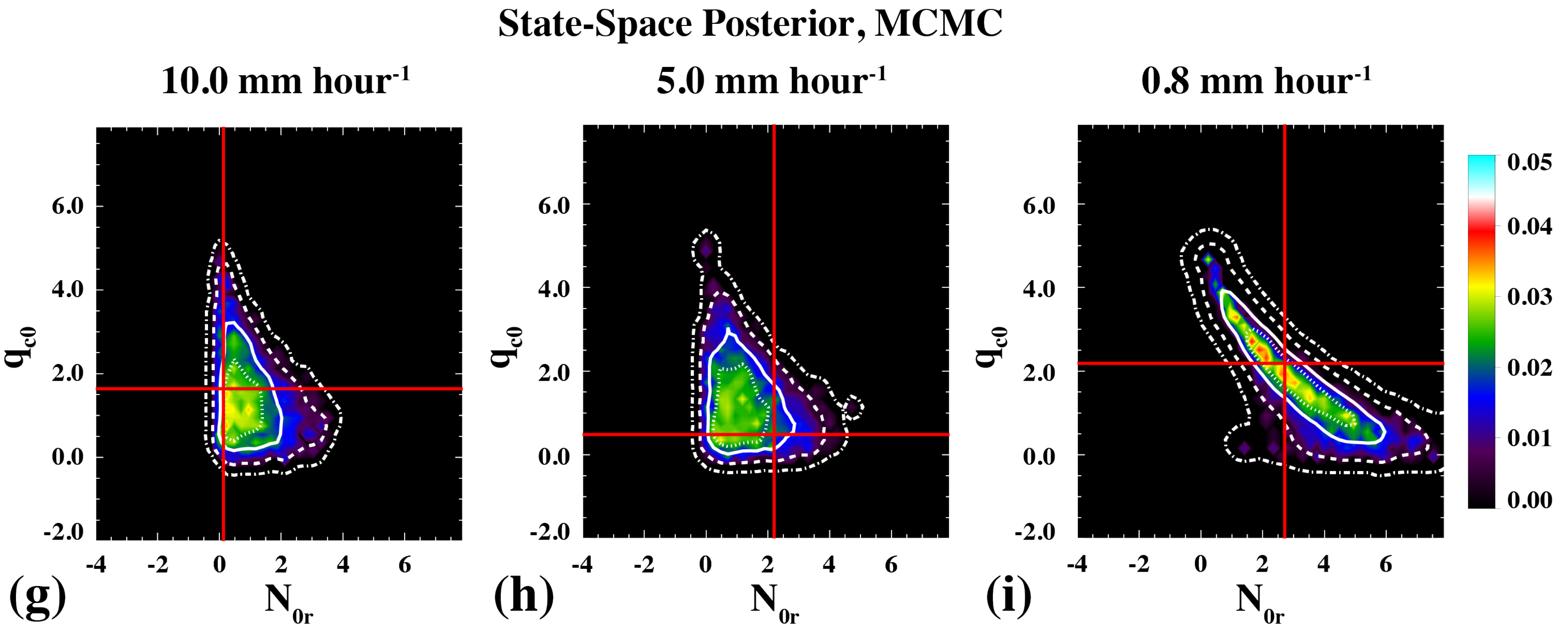
Ensemble Outer Loop: Observation Space

- Red = state space analysis mapped into observation space
- Iterative weighted regression leads to a state space analysis that is consistent with observation space
- Are there improvements in state space?



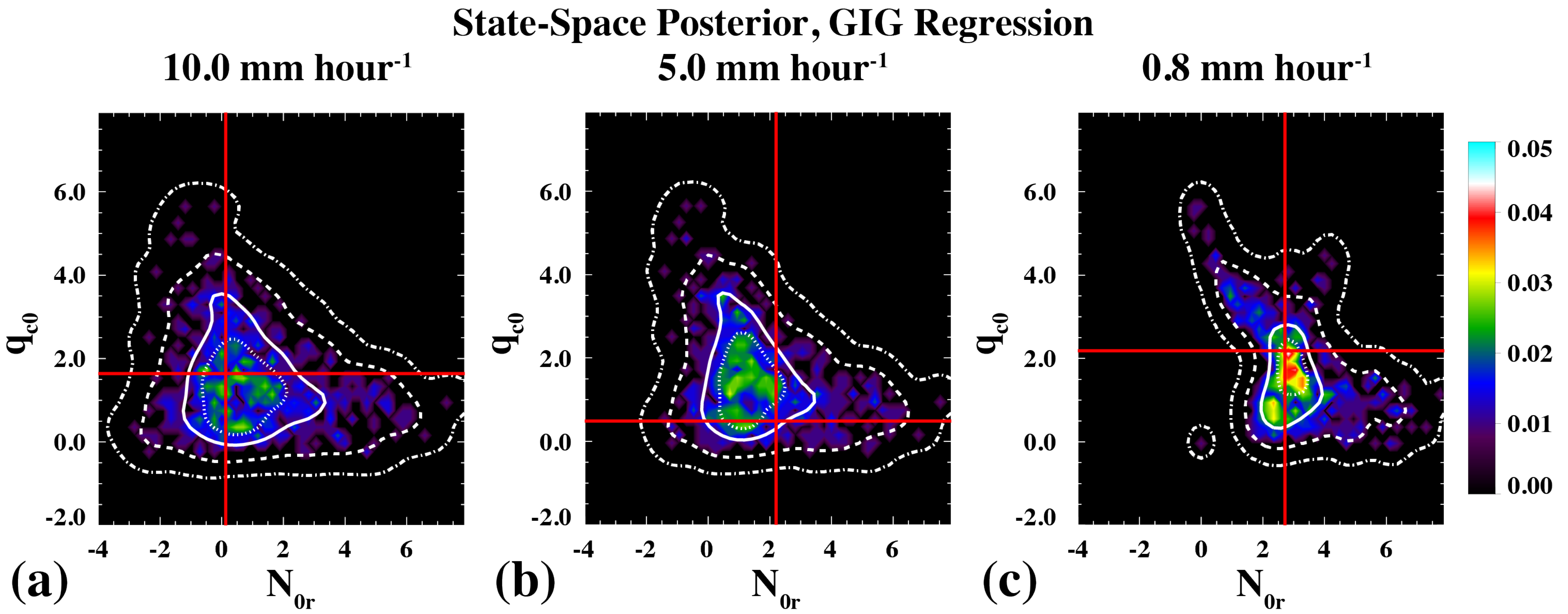
Bayesian State Space MCMC

- Bayesian posterior distribution from MCMC, for reference



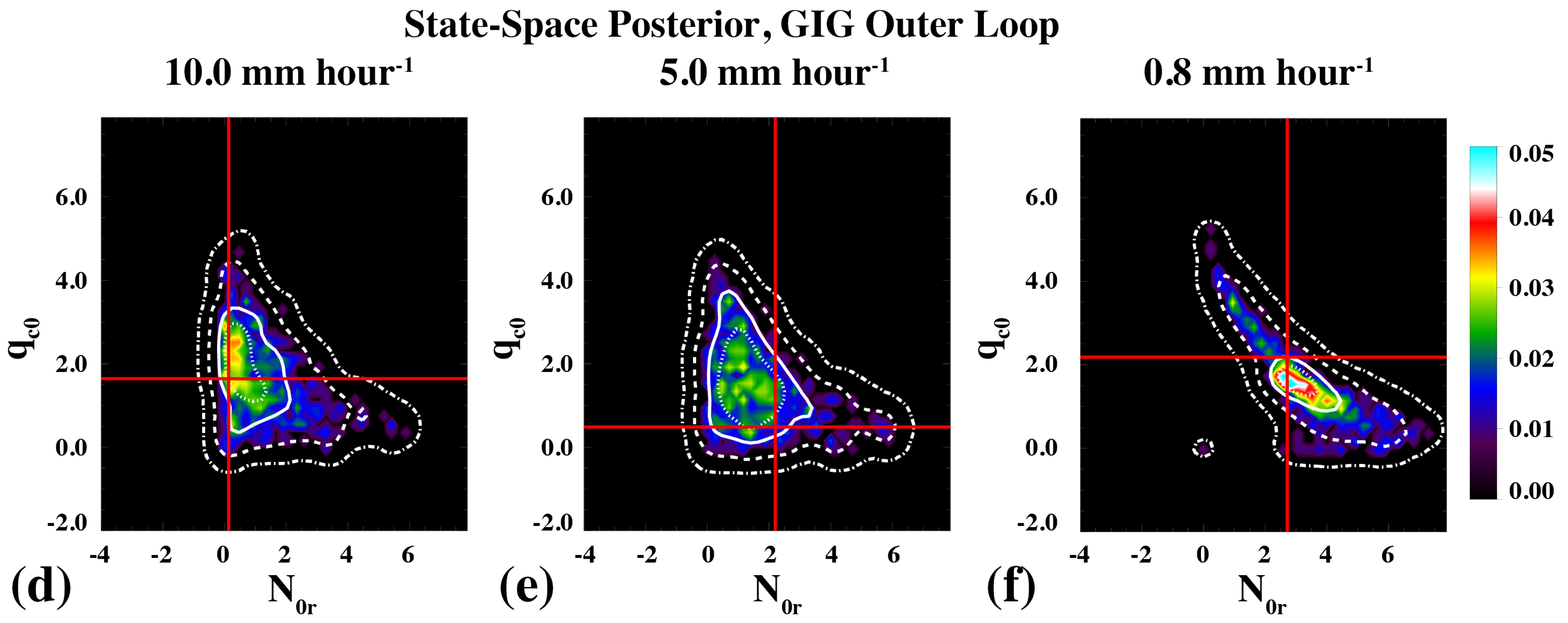
Initial Regression: State Space GIG

- The first guess regression has aspects of the true posterior distribution



Ensemble Outer Loop: State Space GIG

- Following 10 outer loop iterations, the state space looks quite similar to the Bayesian solution



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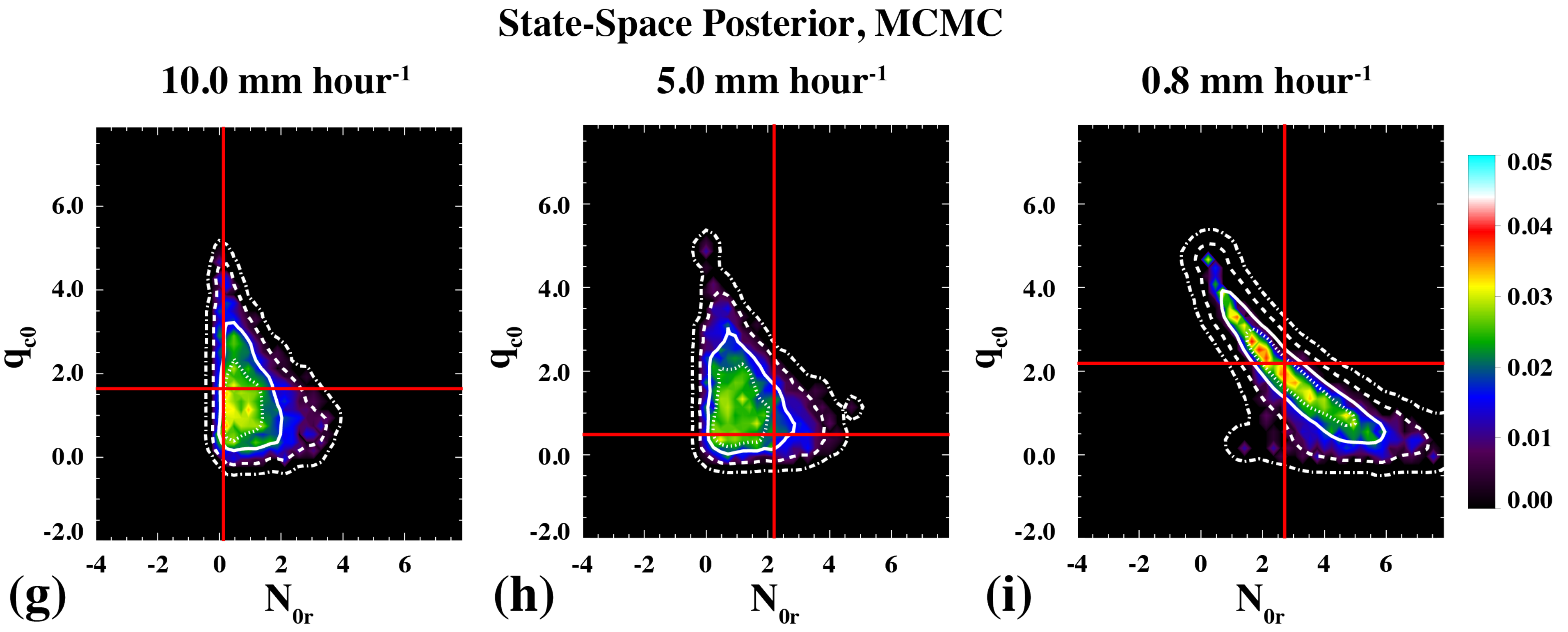
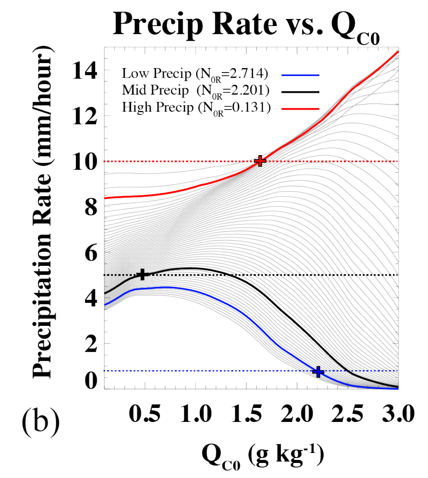
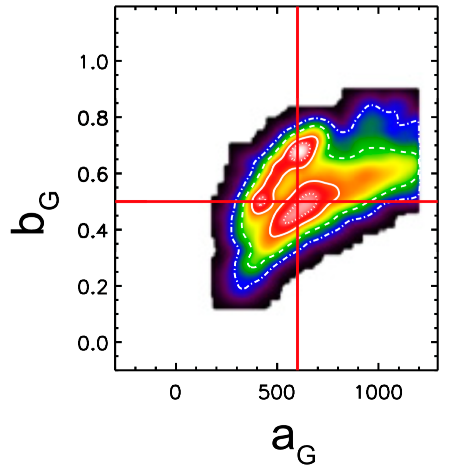


Parameter Estimation Summary I

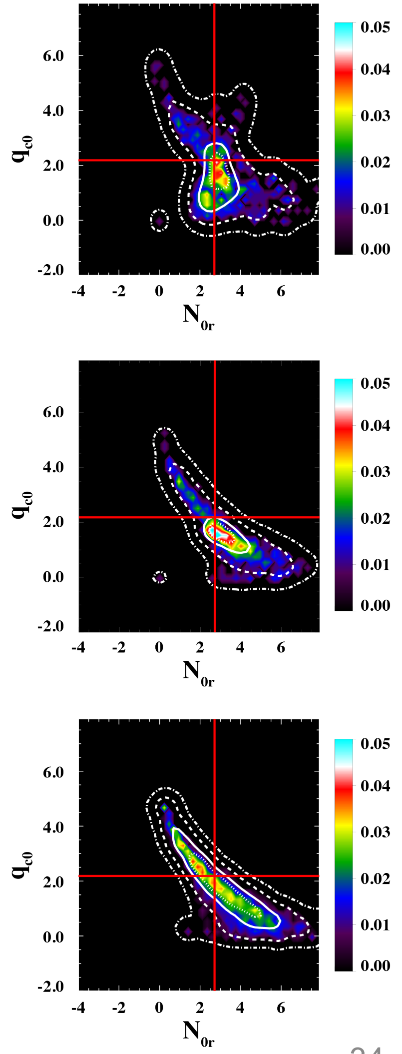
- Properties of model parameters
  - Many are positive definite
  - Values may be close to zero
  - Sensitivity may change according to context
- DA algorithms need to account for these properties
- MCMC provides the reference solution,
  a sample of $p(\mathbf{x}|\mathbf{y})$
  - Assessment of parameter sensitivity and identifiability
  - Evaluation of changes in both, with changes in physical context





Parameter Estimation Summary II

- EnKF distribution mean ~ correct, but linear update does not capture changes in distribution shape, and may produce negative (non-physical) parameter values.
- GIG filter can represent changes in parameter sensitivity, and naturally accommodates positive definite parameters and observations.
- A weighted ensemble outer loop ensures consistency between state and observation space.



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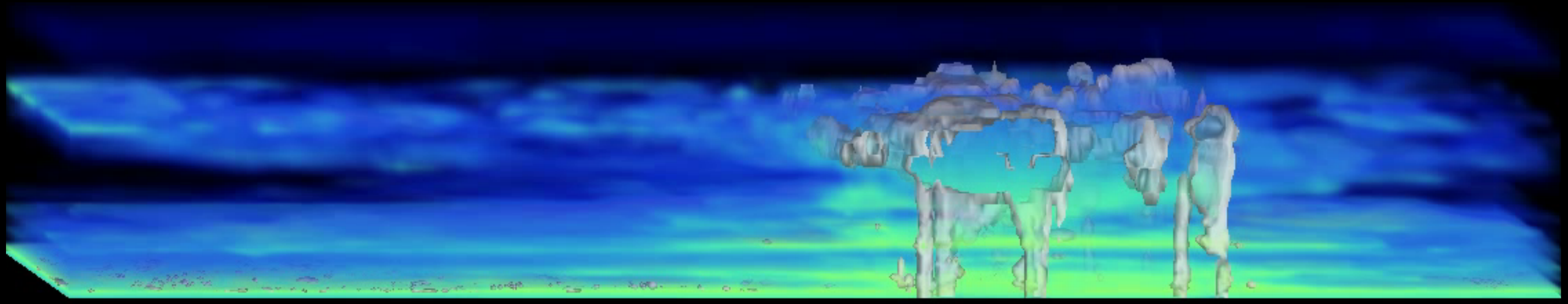
Influence of Model Parameters

Controls

- Liquid and ice particle size distribution
- Ice particle shape and density
- Aerosol content and chemistry
- Cloud process rates

Outcomes

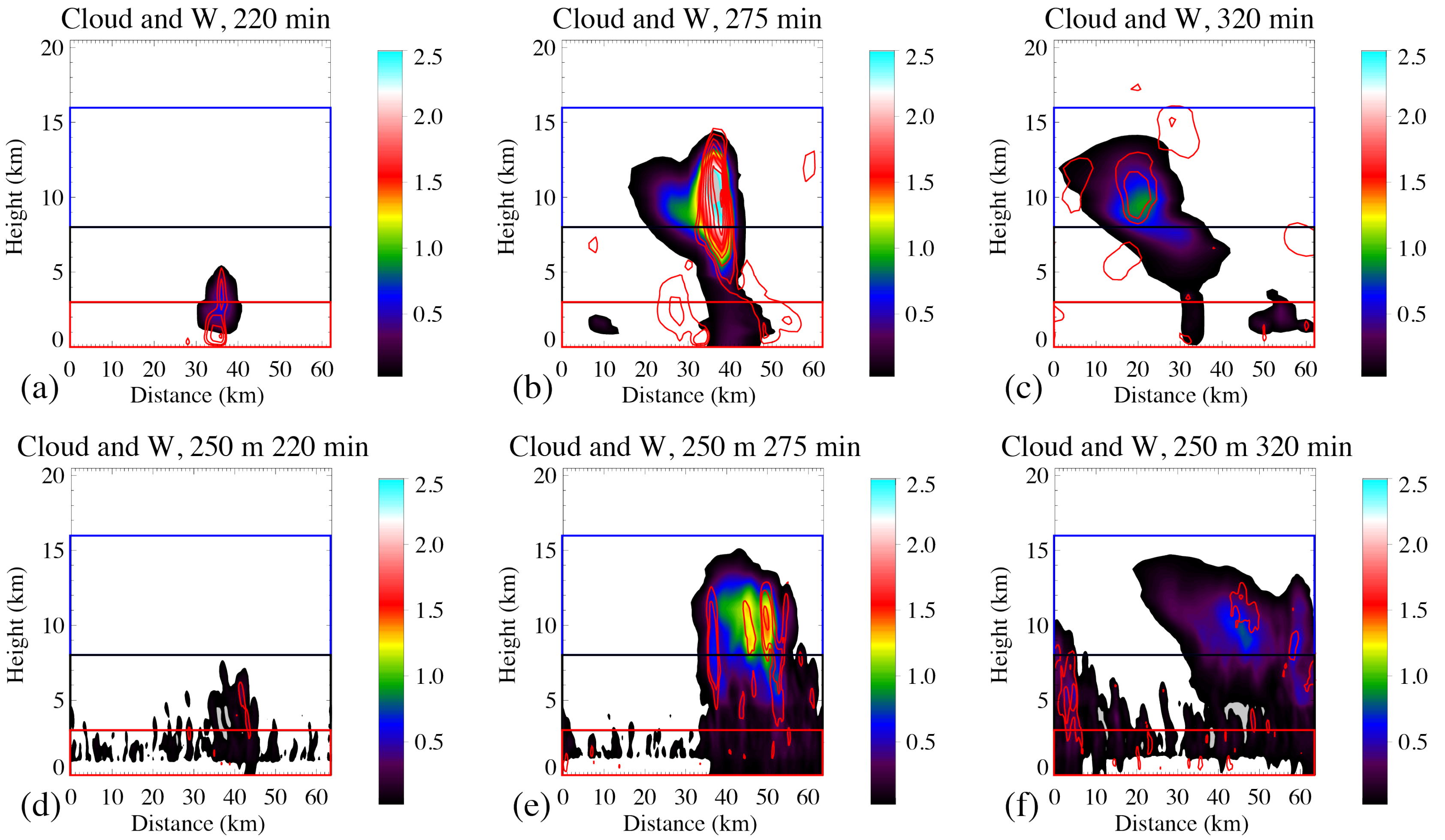
- Cold pools
- Updraft/downdraft strength
- Latent heat release
- Vertical condensate distribution
- Radiative fluxes and heating rates
- Precipitation rate and amount



Posselt et al., 2012 (J. Climate)

Case Study: Convective Squall Line

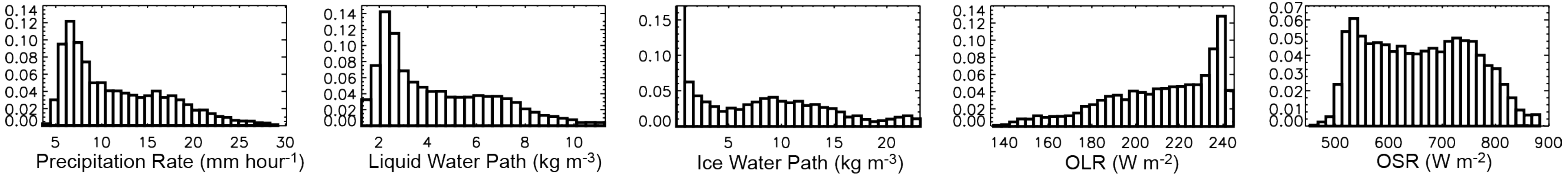
- Deep convective squall line
- Perturb cloud microphysics
- Three phases of development: initiation, maturity, dissipation
- Emulate convective development in 1D
- Simulate convection in 3D



Posselt (2016, Mon. Wea. Rev.)

Sensitivity to Changes in Parameters

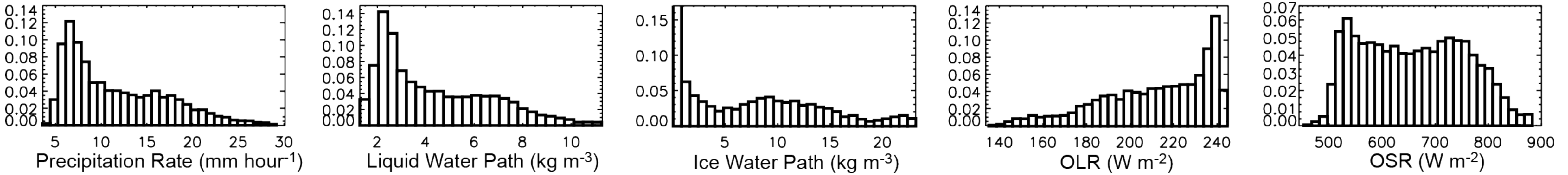
- Changes to microphysical parameters produce very large responses in hydrologic cycle and radiative fluxes
- Response in this system is limited to a single column – independent of 3D dynamics

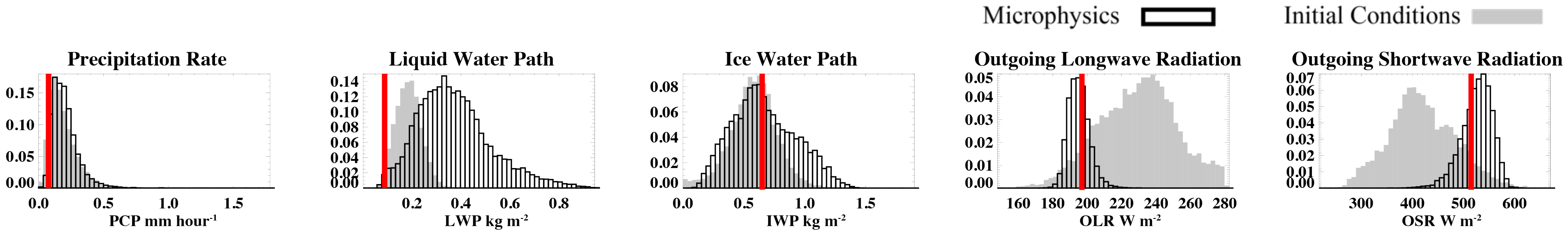


Posselt and Vukicevic (2010, Mon. Wea. Rev.)

Sensitivity to Changes in Parameters

- Response to changes in *parameters* in a 3D model is similar in magnitude to response to changes in *initial conditions*





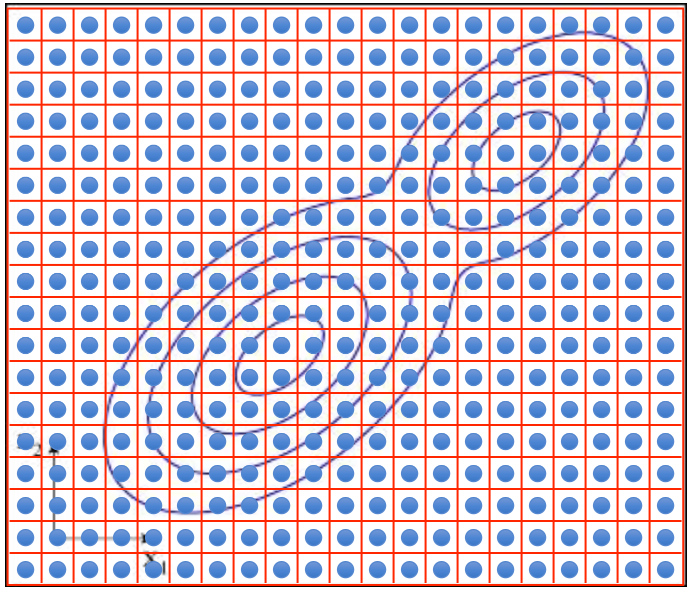
Posselt and Vukicevic (2010, Mon. Wea. Rev.); Posselt et al. (2017, in prep.)

Bayesian Parameter Estimation

Goal: estimate $p(\mathbf{x}|\mathbf{y})$

Options:

- Discretize $p(\mathbf{y}|\mathbf{x})$ and $p(\mathbf{x})$ and compute $p(\mathbf{x}|\mathbf{y})$
  - Specify a range of parameter values
  - Run the model repeatedly in small increments of the control parameters



$$p(\mathbf{x} \mid \mathbf{y}) \propto p(\mathbf{y} \mid \mathbf{x})\, p(\mathbf{x})$$

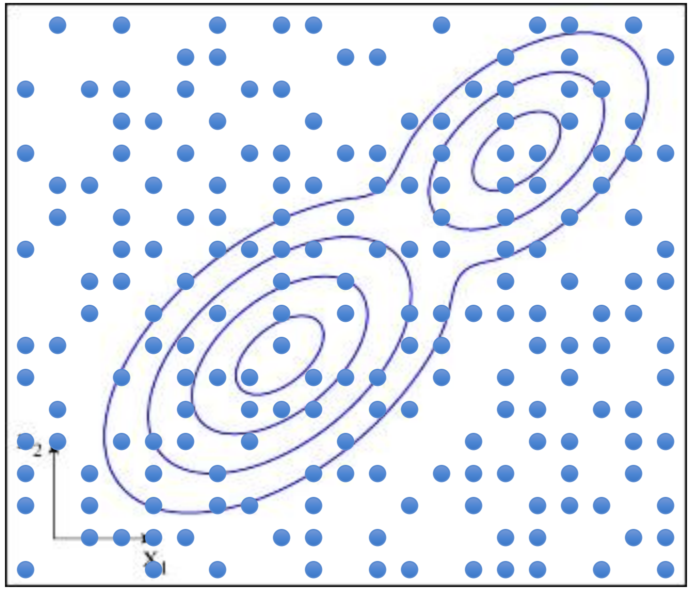
Thorough, but **very** computationally expensive

Bayesian Parameter Estimation

Goal: estimate $p(\mathbf{x}|\mathbf{y})$

Options:

- Randomly sample $p(\mathbf{x}|\mathbf{y})$
  (traditional Monte Carlo, latin hypercube)
  - Evaluate $p(\mathbf{y}|\mathbf{x})$ and $p(\mathbf{x})$ at points randomly distributed in parameter space
  - Compute sample of $p(\mathbf{x}|\mathbf{y})$
  - Fill the response surface using
    - Kernel density estimate
    - Interpolation
    - Function fitting



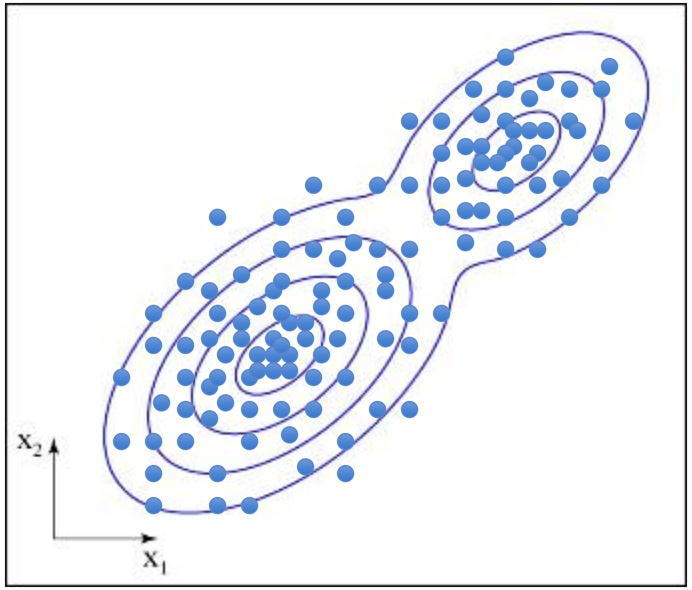
$$p(\mathbf{x}\,|\,\mathbf{y}) \propto p(\mathbf{y}\,|\,\mathbf{x})\,p(\mathbf{x})$$

Bayesian Parameter Estimation

Goal: estimate $p(\mathbf{x}|\mathbf{y})$

Markov chain Monte Carlo:

- Construct a Markov chain that samples $P(\mathbf{x}|\mathbf{y})$
- A random walk guided by information from observations and prior



Application:

- Characterize cloud microphysics (particle size, density, shape) effect
  - Bulk hydrologic cycle and radiative balance
  - Evaluate approximate ensemble algorithms

$$p(\mathbf{x}\,|\,\mathbf{y}) \propto p(\mathbf{y}\,|\,\mathbf{x})\,p(\mathbf{x})$$

Posselt and Vukicevic (2010, Mon. Wea. Rev.), van Lier-Walqui et al. (2012, 2014 Mon. Wea. Rev.), Posselt (2016, Mon. Wea. Rev.)

Cloud Retrievals via Bayesian Sampling (MCMC)

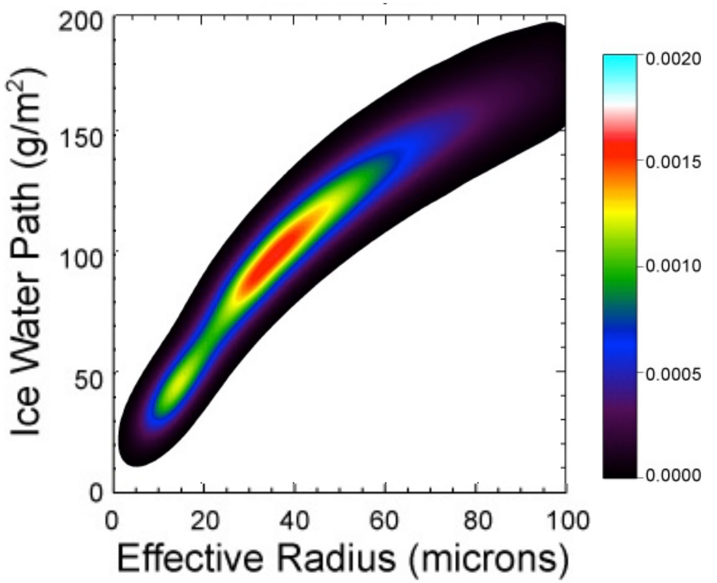
Goal: estimate $P(\mathbf{x}|\mathbf{y})$

Markov chain Monte Carlo:

- Construct a Markov chain that samples $P(\mathbf{x}|\mathbf{y})$
- A random walk guided by information from observations

Application:

- Characterize cloud microphysics retrieval uncertainty
  - Is there a unique solution?
  - How does solution change when we relax assumptions?



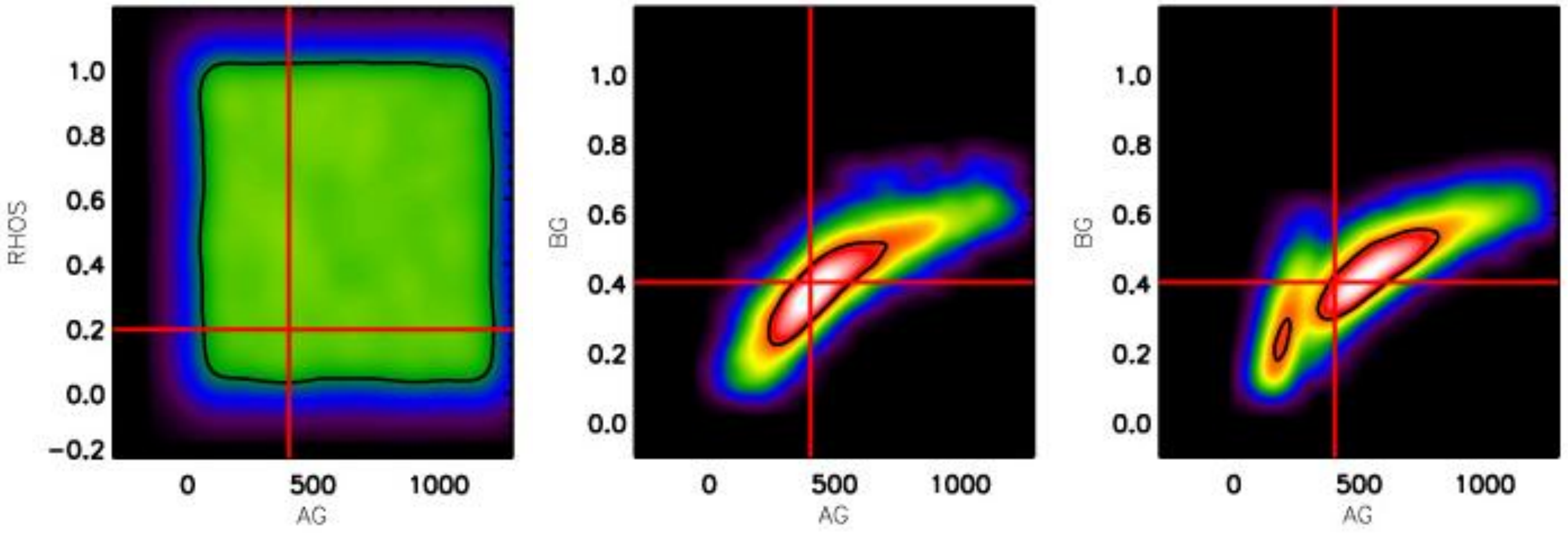
Posselt et al. 2008 (J. Geophys. Res.)

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

Haario et al. (1999, Comp. Stat.), Tamminen and Kyrola (2001, JGR); Tamminen (2004, JGR); Haario et al. (2006, Stat&Comp); Posselt et al. (2008, JGR), Posselt and Mace (2014, JAMC), Posselt et al. (2015, MWR), Posselt et al. (2017, JAMC)

Parameter Estimation: Posterior PDF

- Characteristics of analysis ensemble viewed from perspective of joint parameter PDF
- Difficult to visualize a 10-D space
- Use 2D marginals, examples at right



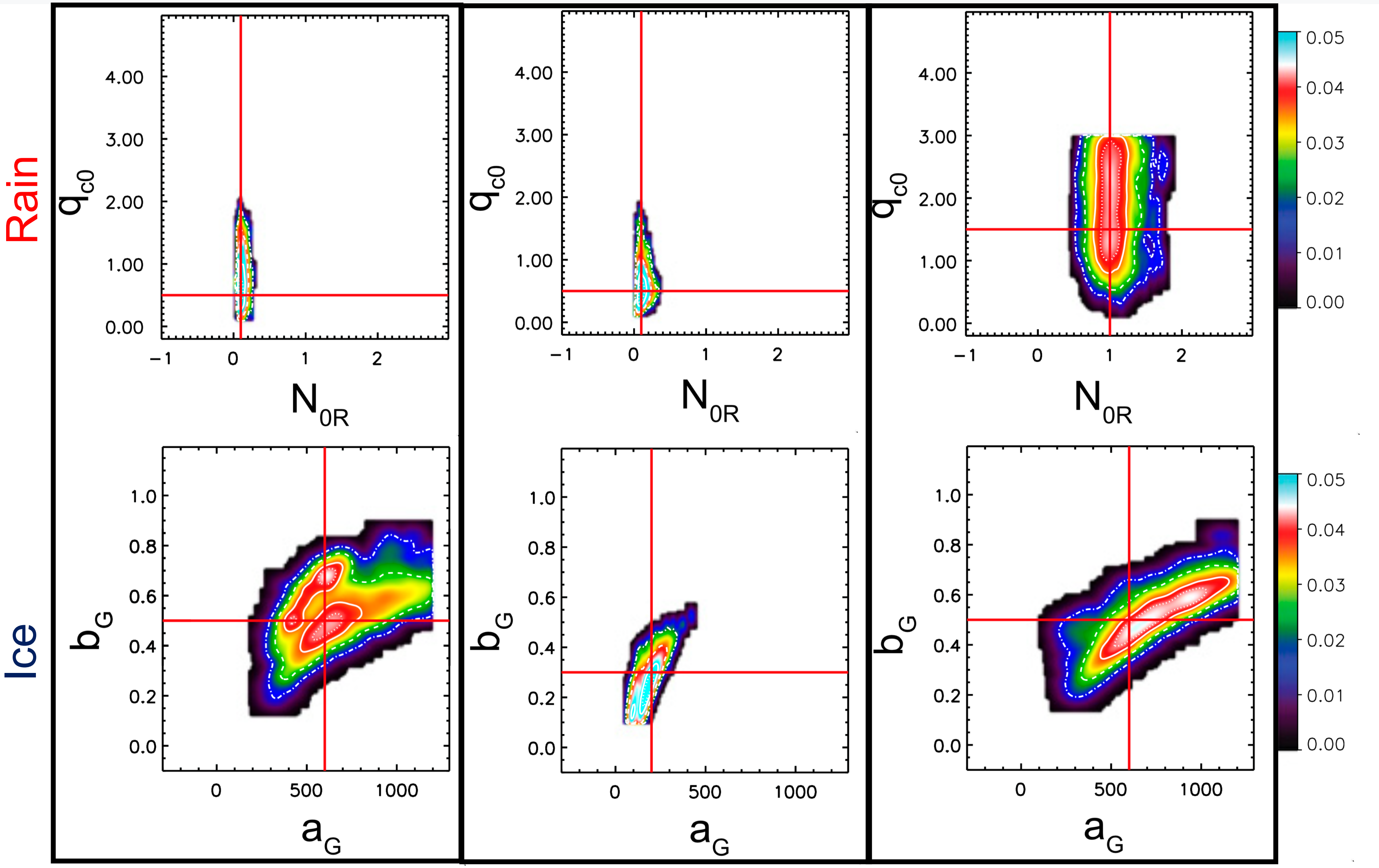
Model output not sensitive to changes in parameters

Model output sensitive to changes in parameters, parameters are correlated

Non-unique parameter-output relationship

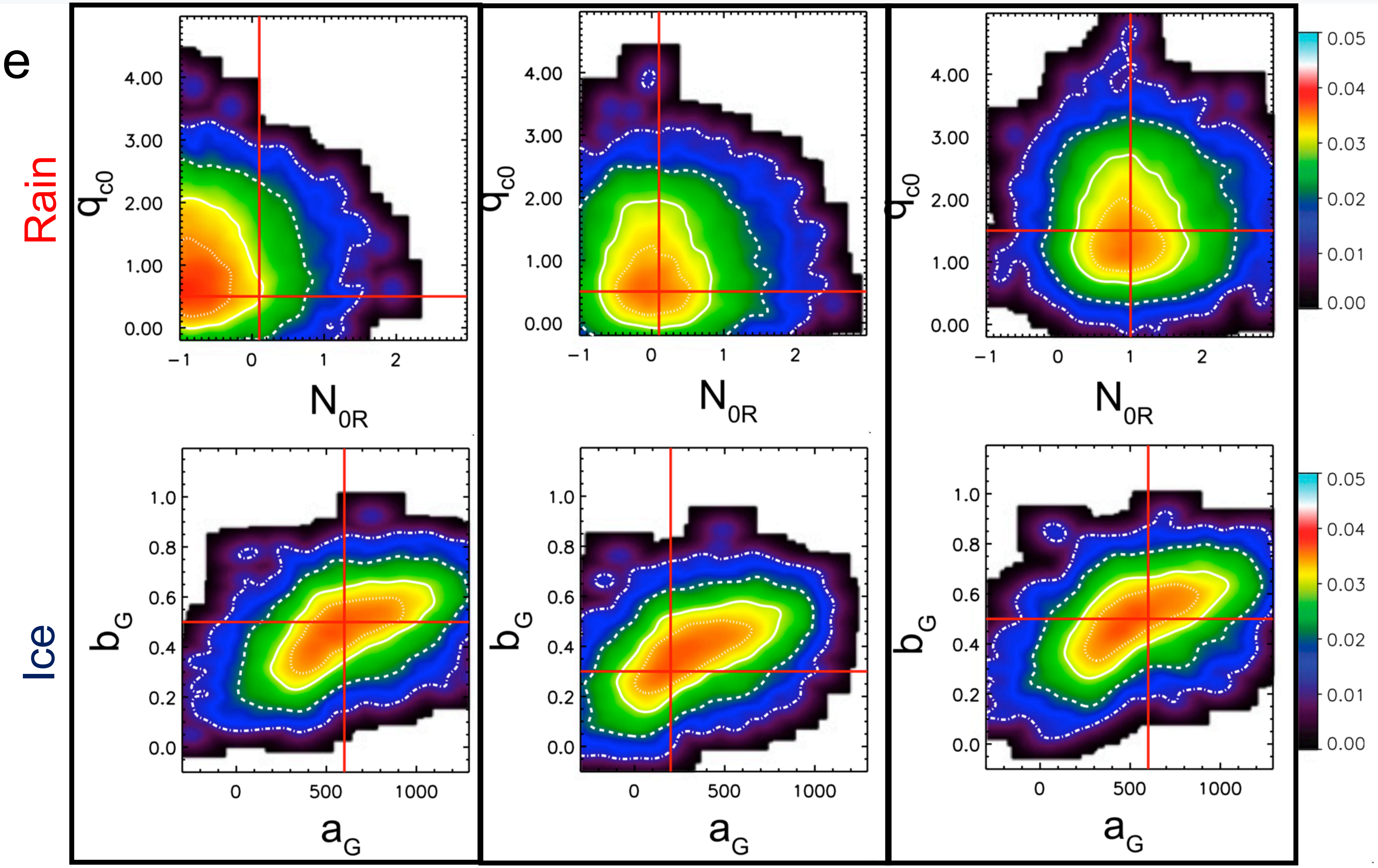
MCMC $p(\mathbf{x}|\mathbf{y})$

- Determine how the analysis changes for different (true) parameter values
- MCMC analysis ensemble is shown (at right) for three experiments
- Posterior distribution depends strongly on the parameter values
- Variance increases with parameter value



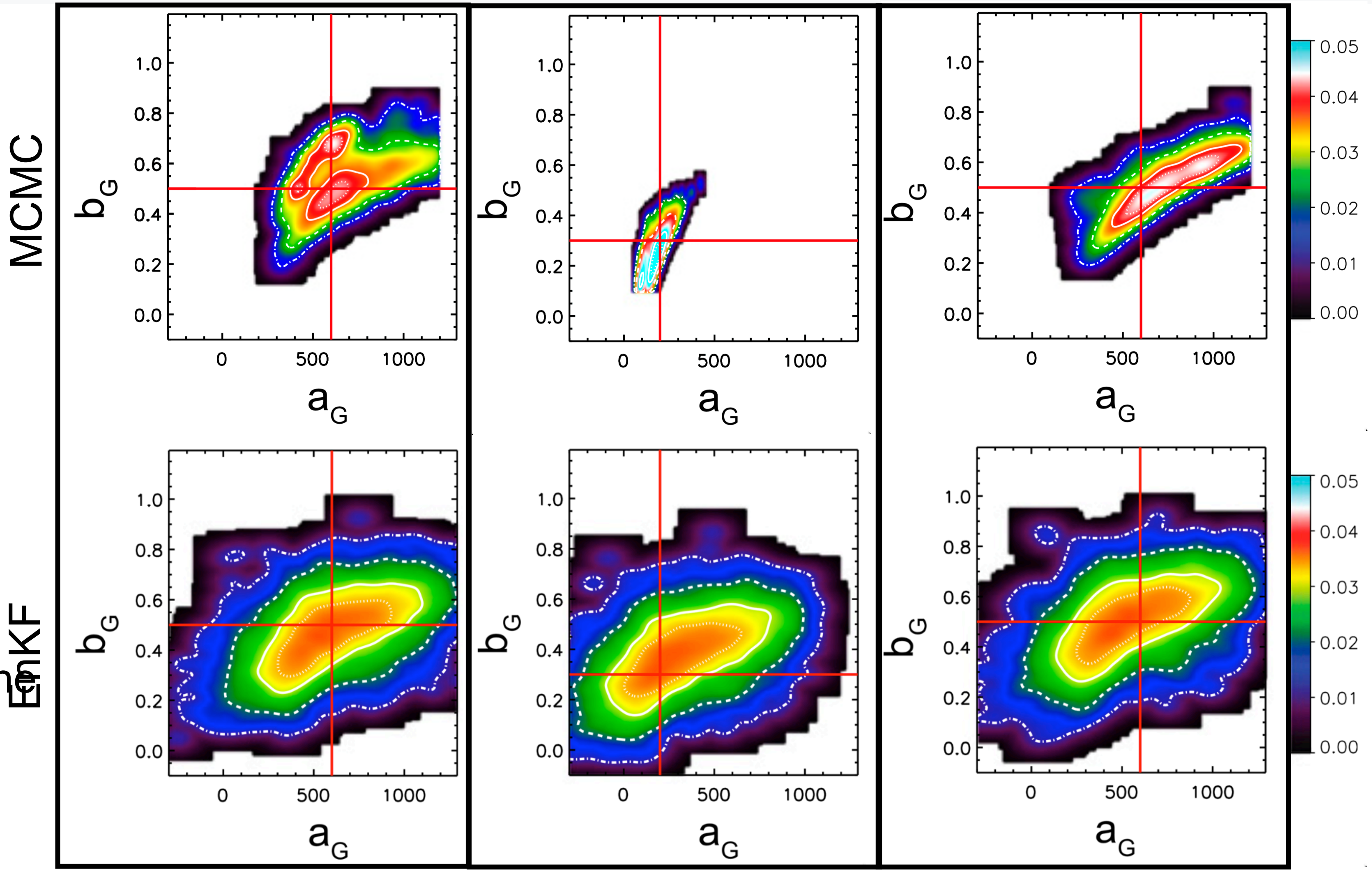
EnKF $p(\mathbf{x}|\mathbf{y})$

- EnKF analysis ensemble *shape* does not change
- Analysis mean shifts according to the true parameter value, but there is no change in higher moments
- When true parameter values are near zero, much of the analysis ensemble is non-physical



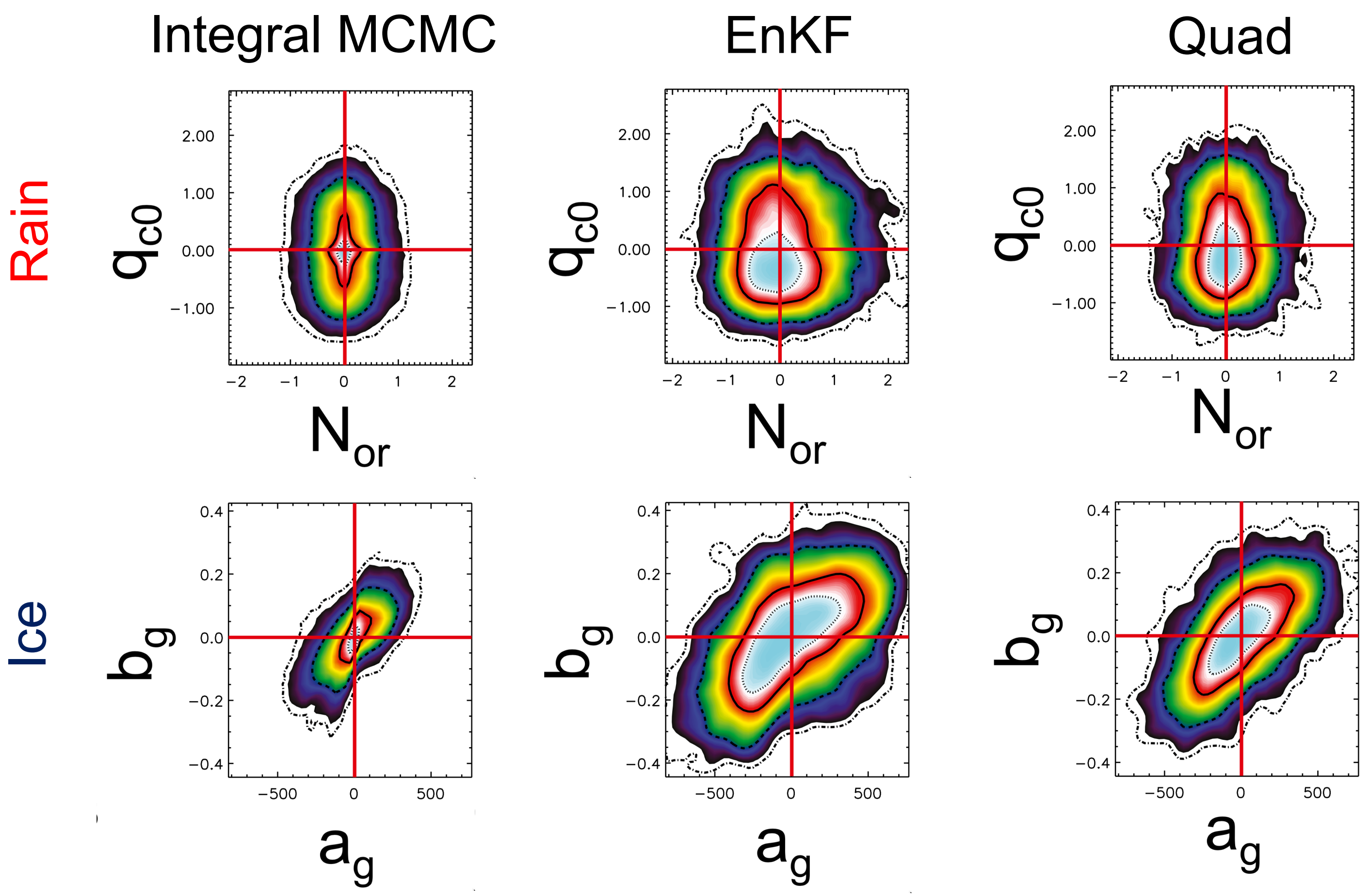
EnKF as an Integral Solution

- Compare MCMC with EnKF
- EnKF analysis looks like an integral over the set of possible posterior distributions
- Integral experiment:
  - Randomly draw 100 sets of parameter values
  - Simulate observations
  - Run MCMC to obtain 100 analysis distributions
  - Remove the mean and combine to produce integral over 100 realizations

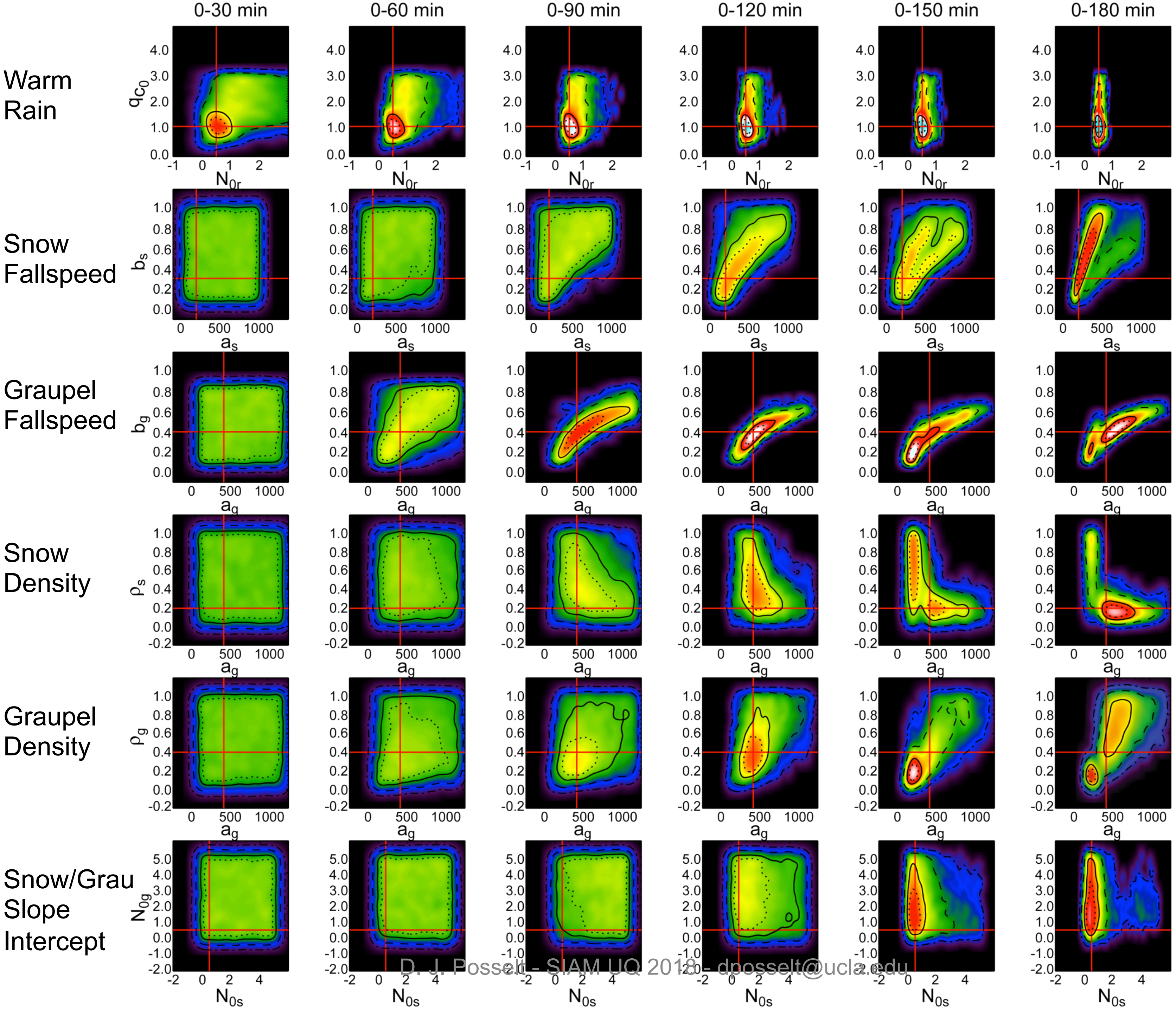


EnKF as an Integral Solution

- EnKF better reflects the integral over all possible parameter sets
- The variance is still too large, due to the fact that the EnKF only knows about the 1st and 2nd moment of the distribution
- Hodyss (2012)'s quadratic ensemble filter accounts for the 3rd moment – produces a solution closer to MCMC



Posselt, Hodyss, and Bishop (2014, Mon. Wea. Rev.)

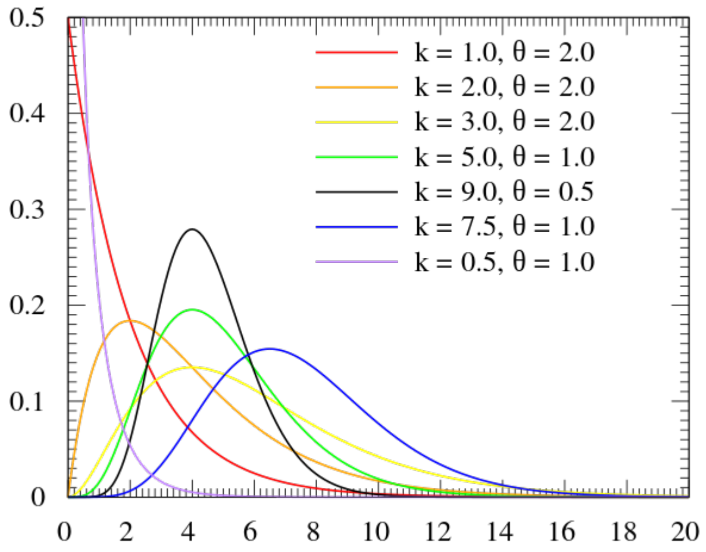


0-30 min
0-60 min
0-90 min
0-120 min
0-150 min
0-180 min
Warm Rain
Snow Fallspeed
Graupel Fallspeed
Snow Density
Graupel Density
Snow/Grau Slope Intercept
q_{c0}
N_{0r}
b_s
a_s
b_g
a_g
ρ_s
ρ_g
N_{0g}
N_{0s}

Gamma– Inverse Gamma Filter

Bishop (2016, QJRMS)

- GIG analysis equations are similar in form to the Kalman update equations



$$\Pi_j^{\mathrm{r}} = \{(\widetilde{R}_j^{\mathrm{r}})^{-1} + (\widetilde{P}_j^{\mathrm{r}})^{-1}\}^{-1} = \widetilde{P}_j^{\mathrm{r}} - \widetilde{P}_j^{\mathrm{r}}(\widetilde{P}_j^{\mathrm{r}} + \widetilde{R}_j^{\mathrm{r}})^{-1}\widetilde{P}_j^{\mathrm{r}},$$

$$\frac{1}{\langle y_j^{\mathrm{a}}\rangle} = \frac{1}{\langle y_j^{\mathrm{f}}\rangle} + \frac{\widetilde{P}_j^{\mathrm{r}}}{\widetilde{R}_j^{\mathrm{r}} + \widetilde{P}_j^{\mathrm{r}}}\left\{\frac{1}{y_j^{\mathrm{o}}} - \left(\widetilde{R}_j^{\mathrm{r}} + 1\right)\frac{1}{\langle y_j^{\mathrm{f}}\rangle}\right\}.$$

$$\tilde{R}_j^r = \frac{\mathrm{var}(\varepsilon^o)}{(y_j)^2 + \mathrm{var}(\varepsilon^o)} \qquad \tilde{P}_j^r = \frac{\mathrm{var}(y_j^f)}{\left\langle y_j^f \right\rangle^2 + \mathrm{var}(y_j^f)}$$