

1 A comparison of methods for a priori bias correction in soil
2 moisture data assimilation

Sujay V. Kumar^{1,2}, Rolf H. Reichle³, Kenneth W. Harrison^{4,2},

Christa D. Peters-Lidard², Soni Yatheendradas^{4,2}, and Joseph A. Santanello²

Sujay V. Kumar, Hydrological Sciences Branch, NASA Goddard Space Flight Center, Greenbelt, MD
20771. Ph: 301-286-8663, Fax: 301-614-5808, email: Sujay.V.Kumar@nasa.gov

¹Science Applications International
Corporation, Beltsville, MD

²Hydrological Sciences Branch, NASA
Goddard Space Flight Center, Greenbelt, MD

³Global Modeling and Assimilation Office,
NASA Goddard Space Flight Center,
Greenbelt, MD

⁴Earth System Science Interdisciplinary
Center, College Park, MD

3 **Abstract.** Data assimilation is being increasingly used to merge remotely sensed
4 land surface variables such as soil moisture, snow and skin temperature with es-
5 timates from land models. Its success, however, depends on unbiased model pre-
6 dictions and unbiased observations. Here, a suite of continental-scale, synthetic
7 soil moisture assimilation experiments is used to compare two approaches that
8 address typical biases in soil moisture prior to data assimilation: (i) parameter
9 estimation to calibrate the land model to the climatology of the soil moisture
10 observations, and (ii) scaling of the observations to the model's soil moisture
11 climatology. To enable this research, an optimization infrastructure was added
12 to the NASA Land Information System (LIS) that includes gradient-based op-
13 timization methods and global, heuristic search algorithms. The land model cal-
14 ibration eliminates the bias but does not necessarily result in more realistic model
15 parameters. Nevertheless, the experiments confirm that model calibration yields
16 assimilation estimates of surface and root zone soil moisture that are as skill-
17 ful as those obtained through scaling of the observations to the model's clima-
18 tology. Analysis of innovation diagnostics underlines the importance of address-
19 ing bias in soil moisture assimilation and confirms that both approaches ade-
20 quately address the issue.

1. Introduction

21 Land data assimilation systems merge satellite or in situ observations of land surface fields
22 (such as soil moisture, snow and skin temperature) with estimates from land surface models.
23 Observations are often discontinuous in space and time, and their incorporation into the modeled
24 estimates helps generate spatially complete and temporally continuous estimates of land surface
25 fields. The process of combining observations and model forecasts is typically carried out by
26 weighting each based on their respective errors. The uncertainty in model states results from
27 model structural deficiencies, errors in model parameter specifications and input forcings. Simi-
28 larly, observational data also suffer from errors caused by instrument noise and errors associated
29 with the retrieval models. A key assumption in most data assimilation techniques is that the errors
30 in observations and model forecasts are strictly random and that on average, the observations
31 and model estimates agree with the true estimates. In reality, however, biases are unavoidable
32 and it is difficult to attribute the bias to the model or the observations. Nevertheless, the proper
33 treatment of such systematic errors is critical for the success of data assimilation systems (*Dee*
34 *and da Silva* [1998]).

35 A number of prior studies have described techniques to address the treatment of bias errors in
36 data assimilation systems. *Dee* [2005] characterizes the data assimilation systems as either “bias-
37 blind” or “bias-aware”, based on their treatment of systematic errors. The bias-blind systems
38 are designed to correct random, zero-mean errors and assume the use of unbiased observations
39 relative to the model-generated background. For soil moisture, the absolute levels of continental-
40 scale estimates from land surface models and satellite observations differ significantly (*Reichle*
41 *et al.* [2004, 2007]), which implies a need for “bias-aware” approaches to soil moisture assimi-

42 lation. An often used method to address such biases is to rescale the observations prior to data
43 assimilation in such a way that the observational climatology matches that of the land model
44 (*Reichle and Koster* [2004]; *Drusch et al.* [2005]; *Crow et al.* [2005]; *Slater and Clark* [2006];
45 *Reichle et al.* [2007]; *Draper et al.* [2009]; *Kumar et al.* [2009]; *Reichle et al.* [2010]; *Liu et al.*
46 [2011]; *Draper et al.* [2011]). Put differently, these so-called “a priori scaling” approaches as-
47 similate normalized deviates or percentiles instead of the raw observations. A priori scaling is
48 easy to implement as a preprocessing step to the data assimilation system and does not make
49 assumptions about whether the climatology of the model or that of the observations is more
50 correct. Although the resulting analyses are produced in the model’s climatology, they can be
51 scaled back to the observational climatology, if needed. However, since the computation of the
52 climatologies is conducted as a pre-processing step, the corrections cannot easily be adjusted to
53 dynamic changes in bias.

54 Dynamically bias-aware assimilation systems, on the other hand, incorporate specific assump-
55 tions about the nature of biases and are specifically built to estimate and correct them. These
56 strategies typically attribute the bias to either the model or the observations and use the analy-
57 sis increments in the data assimilation system to estimate the bias. Variants of such dynamic
58 bias correction strategies have been used in soil moisture assimilation studies (*De Lannoy et al.*
59 [2007a, b]) and for land surface temperature assimilation by *Bosilovich et al.* [2007] and *Reichle*
60 *et al.* [2010]. In these studies, the observations are assumed to be unbiased, and the bias is
61 attributed to model exclusively. In reality, however, the retrievals from different sensors may be
62 biased against each other (*Reichle et al.* [2007]; *Trigo and Viterbo* [2003]). The key advantage
63 of the dynamic bias estimation and correction approaches is their ability to adapt to transient
64 changes in bias.

65 In this article, we explore an alternative strategy for a priori bias correction that has not been
66 used for continental-scale soil moisture assimilation: the a priori calibration of land surface model
67 (LSM) parameters. We use optimization algorithms to estimate model parameters that minimize
68 the bias between model forecasts and observations. Similar to the a priori scaling methods
69 discussed above, the a priori calibration approach complements the state update steps of the
70 data assimilation system. In the latter, the model forecast is modified only when observations
71 are present. In the absence of observational information, the model will revert back to its
72 original climatology. Adjusting model parameters offers a way to bring the model's climatology
73 in line with that of the observations, including at times and locations where observations are
74 intermittently absent. Like a priori scaling, a priori model calibration does not adjust dynamically
75 to changes in model or observation bias.

76 Model parameters have long been recognized as a key source of errors in model predictions,
77 and many LSM studies have focused on the application of techniques to estimate them (*Duan*
78 *et al.* [1992]; *Burke et al.* [1997]; *Gupta et al.* [1999]; *Hogue et al.* [2005]; *Liu et al.* [2004, 2005];
79 *Santanello et al.* [2007]; *Peters-Lidard et al.* [2008]; *Lambot et al.* [2009]; *Gutman and Small*
80 [2010]; *Nearing et al.* [2010]). These studies estimate LSM parameters using independent
81 observations of variables such as soil moisture, streamflow and surface temperature. In addition,
82 data assimilation studies have also recognized the need to update and estimate model parameters
83 for improving the model's predictive skills. A number of studies have examined the potential
84 of parameter estimation in conjunction with state estimation in sequential data assimilation
85 systems (*Boulet et al.* [2002]; *Moradkhani et al.* [2005]). These approaches, known as joint
86 estimation or state augmentation methods, estimate the model parameters concurrently with
87 the model states. Such approaches, however, have difficulties in handling the relative time-

88 invariance of parameters (compared to model states) and very large parameter spaces (*Liu and*
89 *Gupta* [2007]). *De Lannoy et al.* [2007a] note that in some situations it may be better to estimate
90 the bias separately rather than correct it using state augmentation methods. An approach that
91 employs the simultaneous use of optimization and data assimilation was described by *Vrugt*
92 *et al.* [2005], where the model parameters are estimated through the recursive calibration over
93 a data assimilation instance. This method considers the estimation of model parameter sets for
94 generating the best possible forecasts, when model states are also adjusted through sequential
95 data assimilation. The advantages and limitations of these joint state and parameter estimation
96 approaches are discussed in detail in *Liu and Gupta* [2007].

97 Here we compare, in the context of data assimilation, the approach of bias mitigation through
98 the estimation of model parameters against a priori bias correction strategies that rescale the
99 observations to conform to the model's climatology. The parameter estimation is performed in
100 a "batch-calibration" mode, where a set of observational data is used to estimate time-invariant
101 model parameters with the objective of minimizing the climatological differences between the
102 model and the observations. The model with the calibrated parameters is subsequently employed
103 in the data assimilation system to assimilate the raw, unscaled observations. In contrast, the scal-
104 ing approaches essentially assimilate the anomaly information instead of the raw observations.
105 We investigate these methods with a soil moisture assimilation case study. A new generation of
106 satellite soil moisture retrievals are becoming available from the recently launched Soil Moisture
107 and Ocean Salinity (SMOS; *Kerr et al.* [2010]) and the planned Soil Moisture Active Passive
108 (SMAP; *Entekhabi et al.* [2010b]) missions. The results from our study are directly relevant to
109 the effective utilization of these new observations in land data assimilation systems.

110 The experiments presented in this paper are conducted using the NASA Land Information
111 System (LIS; *Kumar et al.* [2006]; *Peters-Lidard et al.* [2007]), which is a multiscale modeling
112 system for hydrologic applications developed with the goal of integrating satellite- and ground-
113 based observational data products and advanced land surface models and techniques to generate
114 improved estimates of land surface conditions. LIS includes a suite of subsystems to support
115 land surface modeling for a variety of applications, including a comprehensive sequential data
116 assimilation system, based on the NASA Global Modeling and Assimilation Office's infras-
117 tructure (*Reichle et al.* [2009]; *Kumar et al.* [2008b]). More recently, a generic optimization
118 subsystem has been developed within LIS, with the goal of combining the use of optimization
119 and data assimilation in an integrated framework. This new extension to LIS will be described
120 in detail below and was used to facilitate the experiments discussed here.

121 The paper is organized as follows. The design and capabilities of the optimization subsystem
122 within LIS are presented first (Section 2). This is followed by the description of the experiment
123 setup that evaluates the use of parameter estimation in data assimilation (Section 3). The results
124 from the data assimilation integrations are presented in Section 4. Finally, Section 5 discusses
125 the conclusions from the study.

2. Optimization subsystem in LIS

126 LIS is designed as an object-oriented framework, where all functional extensions (such as
127 land surface models, data assimilation algorithms, meteorological inputs, observational data,
128 etc.) are implemented as abstract, extensible components (*Kumar et al.* [2006, 2008a]). A large
129 suite of modeling extensions have been incorporated in LIS using this design paradigm. The
130 optimization subsystem in LIS is designed in a similar interoperable manner.

2.1. Optimization abstractions

131 Generically, an optimization instance can be stated as a problem of determining unknown
132 parameters by minimizing or maximizing an objective function subject to a number of constraints.
133 The optimization subsystem in LIS defines three functional abstractions based on this generic
134 form, shown in Figure 1: (1) objective function, (2) decision/parameter space and (3) algorithm
135 used to solve the optimization problem. In the instance of parameter estimation, the decision
136 space is defined by the list of LSM parameters (or a subset thereof). The objective function
137 object represents the function or criteria to be maximized or minimized. Examples include the
138 minimization of squared residuals and the maximization of likelihood measures. Finally, the
139 optimization algorithm abstraction represents the actual search strategy used to find the optimal
140 solution. The interconnections between these three generic pieces are handled within the LIS
141 core, which is the unit that enables the integrated use of various extensible components in LIS.
142 Custom implementations of each of these three abstractions constitute a specific instance of an
143 optimization problem.

144 Similar to the design of the LIS data assimilation subsystem (*Kumar et al.* [2008b]), the data
145 exchanges between these abstractions are handled through the constructs of the Earth System
146 Modeling Framework (ESMF; *Hill et al.* [2004]). ESMF provides a standardized, self-describing
147 format for data exchange between these components. Three search algorithms of varying com-
148 plexity are implemented in this infrastructure: (1) Levenberg-Marquardt (LM; *Levenberg* [1944];
149 *Marquardt* [1963]) (2) Shuffled Complex Evolution from University of Arizona (SCE-UA; *Duan*
150 *et al.* [1992, 1993]) and (3) Genetic Algorithm (GA; *Holland* [1975]). LM is a gradient-based
151 search technique and is suited only for deterministic convex optimization problems, whereas

152 SCE-UA and GA are more suited for difficult combinatorial optimization problems such as
153 LSM parameter estimation.

2.2. Genetic Algorithm

154 In this article, we employ GA for estimating LSM parameters. GAs are stochastic search
155 techniques that use heuristics-based principles of natural evolution and genetics. The algorithm
156 works by employing a population of individuals (or candidate solutions), each of which is
157 represented by a set of values of the problem's variables that need to be estimated (also called
158 decision space). By applying operations that are based on natural evolution concepts, such
159 as selection, recombination and mutation, the population evolves towards better solutions over
160 several generations (or iterations).

161 Figure 2 depicts a flow chart showing the sequence of GA operations during optimization.
162 A fitness value that reflects the quality of the solution and its ability to satisfy constraints and
163 objectives of the problem is associated with each potential solution. The selection operator
164 simulates the "survival of the fittest" behavior by preferentially selecting the solutions with
165 higher fitnesses to be present in the subsequent populations. As a result, solutions with good
166 traits survive and solutions with bad traits are eliminated. Each pair of selected solutions then
167 undergoes the recombination step where two new solutions are generated by combining the
168 "genes" of the parent solutions. The mutation operator is used to infuse the population with gene
169 values that may not be present in the population. The recombination and mutation rates define
170 the probability of crossover between any two pairs and the probability of a gene undergoing
171 mutation, respectively. To ensure that the best solution in any generation is not lost through
172 these probabilistic recombination and mutation operations, a strategy named elitism is used.
173 Elitism ensures that the best solution from the previous generation is compared with the worst

174 solution in the current generation, replacing the current generation's solution, if better. These
175 steps are repeated through several iterations (or generations) until the specified convergence
176 criteria is met.

177 GAs do not rely upon local or gradient information and are able to deal with complexities in
178 the search space such as the presence of local optima and discontinuities. GAs are also well
179 suited to handle discrete decision variables and nonlinearity in the simulation models effectively.
180 The problem-independent structure of the algorithm has enabled its application in many areas
181 of science and engineering (*Goldberg* [1989]). GAs, however, require the evaluation of several
182 simulation runs to obtain the best solution, making them computationally intensive. The high
183 performance computing tools in LIS are employed for mitigating this limitation (section 4.3).

3. Experimental Setup

3.1. Experiment overview

184 In this section, we describe a suite of synthetic data assimilation experiments that examines
185 parameter estimation as an a priori bias mitigation scheme. In addition, two variants of the a priori
186 scaling method are used: standard-normal deviate scaling (*Crow et al.* [2005]) and cumulative
187 distribution function (CDF) matching (*Reichle and Koster* [2004]). The experiment setup is
188 similar to that of *Kumar et al.* [2009], but only two land surface models are used here. The Noah
189 land surface model (version 2.7.1; *Ek et al.* [2003]) employs the four-layer soil model of *Mahrt*
190 *and Pan* [1984] with thicknesses (listed from top to bottom) of 10, 30, 60 and 100cm. In the
191 Catchment LSM (*Koster et al.* [2000]), the vertical soil moisture profile is determined through
192 deviations from the equilibrium soil moisture profile between the surface and the water table.
193 Soil moisture in the 0-2 cm surface layer and in the 0-100 cm root zone layer is diagnosed from the
194 modeled soil moisture profile. The Catchment LSM typically employs hydrologically defined

195 catchments (or watersheds) as basic computational units. In this study, however, the Catchment
196 LSM is used on a regular latitude-longitude grid to facilitate the model intercomparison.

197 Using these land surface models, we conducted a suite of synthetic “fraternal twin” assimilation
198 experiments. The basic structure of the experiments is as follows: First, a soil moisture simulation
199 is conducted with the Catchment LSM to generate the assumed “true” state of the land surface,
200 referred to as the control (or “truth”) run. Second, the observations to be assimilated are generated
201 from this truth run by introducing realistic retrieval errors. Third, a suite of data assimilation
202 integrations are conducted by assimilating these synthetic observations into the Noah land surface
203 model, using different bias mitigation strategies. The Noah model integration without any data
204 assimilation is referred to as the “open loop” simulation. The assimilation integrations are
205 conducted using a one-dimensional Ensemble Kalman Filter (EnKF) algorithm (see *Reichle and*
206 *Koster [2003]* for details on 1d vs. 3d filtering). The performance of the assimilation approaches
207 is evaluated by comparing against the known true fields (from the Catchment LSM integration).

3.2. Experiment details

208 All model simulations are conducted on a gridded domain that roughly covers the Continental
209 United States (CONUS, from 30.5°N, 124.5°W to 50.5°N, 75.5°W) at 1° spatial resolution, using
210 a 30 minute model timestep. Surface meteorological boundary conditions from the Global Data
211 Assimilation System (GDAS; the global meteorological weather forecast model of the National
212 Centers for Environmental Prediction (*Derber et al. [1991]*)) are used to drive the LSMs. The
213 models are cycled three times through the period from 1 January 2000 to 1 January 2006 to ensure
214 that internal model states are in equilibrium with the forcing meteorology and parameters. The
215 initial conditions generated from this “spinup” process are used in the data assimilation and
216 open loop integrations except those that use the optimized parameters. The optimization based

217 integrations use the soil moisture initial conditions estimated through calibration (section 3.3).

218 All model and assimilation integrations are conducted over the above-mentioned six year period.

219 Each open loop or assimilation experiment with the Noah LSM consists of 12 ensemble
220 members (*Kumar et al.* [2008b]), and the mean of the ensemble is used in the evaluations. In
221 order to maintain an ensemble of model fields representing the uncertainty in soil moisture,
222 perturbations are applied to select meteorological and model prognostic fields. The parameters
223 used for these perturbations are based on previous work (*Reichle et al.* [2007]; *Kumar et al.*
224 [2009]) and are listed in Table 2. Zero-mean, normally distributed additive perturbations are
225 applied to the downward longwave radiation forcing, and log-normal multiplicative perturbations
226 with a mean value of 1 are applied to the precipitation and downward shortwave fields (Table 2).
227 Time series correlations are imposed via a first-order regressive model (AR(1)) with a time scale
228 of 24 hours. No spatial correlations are applied since this study uses the one-dimensional version
229 of the EnKF. Cross correlations are imposed on the perturbations of radiation and precipitation
230 fields using the values specified in Table 2.

231 In addition to the forcing perturbations, the Noah model prognostic variables for soil moisture
232 are perturbed with additive noise that is vertically correlated (Table 2). For the perturbations to
233 the model prognostics we impose AR(1) time series correlations with a 12 hour time scale. The
234 perturbation settings do not introduce systematic biases in the open loop integrations relative to
235 a standard, unperturbed, single-member model integration (not shown).

236 A set of preprocessing steps are applied to the synthetic retrievals generated from the Catchment
237 LSM integration. To account for difficulties in retrieving soil moisture products from microwave
238 sensors, the synthetic observations are masked out when the green vegetation fraction values
239 exceed 0.7 and when snow or precipitation are present. Random Gaussian noise with an error

240 standard deviation of $0.03 \text{ m}^3\text{m}^{-3}$ (volumetric soil moisture) is added to the Catchment model
241 surface soil moisture values to mimic measurement uncertainties. This error standard deviation
242 is chosen as an estimate of the expected error level in surface soil moisture retrievals from
243 upcoming space-borne L-band radiometers (*Kerr et al.* [2010]; *Entekhabi et al.* [2010b]).

244 Five different data assimilation integrations are conducted using these synthetic observations
245 (Table 1): (DA-NOSC) Using unscaled observations without any bias correction, (DA-STDN)
246 using a priori scaled observations based on standard normal deviate scaling, (DA-CDF) using
247 a priori scaled observations based on CDF matching, (DA-OPT1) using unscaled observations
248 with a calibrated model, where the model parameters were estimated using a single year of batch
249 calibration (year 2000), and (DA-OPT6) using unscaled observations with a calibrated model,
250 where model parameters were optimized using all 6 years (2000-2006) of observations.

The approaches that employ a priori scaling of observations (DA-STDN and DA-CDF) represent the commonly followed approaches of correcting biases prior to data assimilation by scaling the observations into the model climatology. The DA-CDF experiment follows the strategy of *Reichle and Koster* [2004] and matches the CDF of the observations to that of the model soil moisture. First, the observation and model CDFs are computed independently for each grid cell using the six year period. Next, the observations are rescaled, separately for each grid cell, such that their climatology matches that of the model soil moisture. In theory, this approach corrects all moments of the distribution regardless of its shape, although in practice the correction of higher order moments is naturally limited by the sample size. While the climatological differences between the model and the observations may change with season (*Drusch et al.* [2005]), our experiment DA-CDF is based on CDFs derived with data from all seasons lumped together as in *Reichle et al.* [2007]. The standard normal deviate-based scaling used in the DA-STDN ex-

periment is a simpler approach that matches only the first and second moments of the observation and model distributions but breaks the scaling down by calendar month to account for possible seasonal changes in the climatological differences. This approach is used, for example, by *Crow et al.* [2005]). For a given calendar month k and a given grid cell i , the scaling parameters are the multi-year mean ($\bar{\theta}_{i,k}^m$ and $\bar{\theta}_{i,k}^o$, for model and observations, respectively) and multi-year standard deviation ($\sigma_{i,k}^m$ and $\sigma_{i,k}^o$, for model and observations, respectively). For all observations θ_i from this particular calendar month (time subscript omitted), the scaled observations θ'_i are then given by:

$$\theta'_i = \bar{\theta}_{i,k}^m + (\theta_i - \bar{\theta}_{i,k}^o) \frac{\sigma_{i,k}^m}{\sigma_{i,k}^o} \quad (1)$$

251 In contrast, the calibration-based integrations (DA-OPT1 and DA-OPT6) assimilate raw (un-
 252 scaled) observations and rely on the calibrated model parameters to mitigate bias in the data
 253 assimilation system. Note that in the four experiments with bias correction, the information
 254 from the observation set is employed twice. In DA-STDN and DA-CDF, the observations are
 255 used once for deriving the climatology and then for assimilation, when the scaled observations
 256 are assimilated. Similarly in DA-OPT1 and DA-OPT6, the same set of observations is employed
 257 twice, once for the calibration of the model climatology and then again for the subsequent data
 258 assimilation. We do not separate the periods of model calibration and data assimilation in ex-
 259 periments DA-OPT1 and DA-OPT6 in order to provide an equivalent comparison to DA-STDN
 260 and DA-CDF.

261 Note that a priori scaling and model calibration are intended to address the *relative* bias
 262 between the model and the observations. The data assimilation system then works with a set
 263 of observations that are unbiased relative to the model background. In this sense, the synthetic
 264 experiment used here represents the issues in a “real” data assimilation system. The long-term

mean and variability of satellite, in-situ and model soil moisture estimates differ from each other due to representativeness differences (horizontal and vertical), limited sensor calibration, retrieval model assumptions and model deficiencies, implying that, in a climatological sense, none of the datasets is necessarily more correct than any other (*Reichle and Koster* [2004]; *Reichle et al.* [2007]). Consequently, our use of the “truth” label for the synthetic observations does *not* necessarily imply that satellite-based retrievals are unbiased.

3.3. Optimization formulation for parameter estimation

In experiments DA-NOSC, DA-STDN, and DA-CDF we use the Noah LSM with its native parameters that are mostly based on look up tables (as functions of vegetation and soil categories), the same parameters that are used in the operational environments at the National Centers for Environmental Prediction (NCEP) and the Air Force Weather Agency (AFWA). For experiments DA-OPT1 and DA-OPT6, by contrast, we estimate spatially distributed representations of Noah model parameters through GA optimization (section 4.1).

Table 3 lists the parameters included in the decision space in the optimization simulations based on *Hogue et al.* [2005]. The decision space includes a number vegetation and soil properties along with the initial soil moisture states. The initial set of potential solutions in GA is generated by randomly sampling from the range of each parameter as specified in Table 3. A population size of 50 is used in the GA simulations.

The objective function at each grid point is defined as the inverse of absolute difference in the mean soil moisture values of the observation and the model (Equation 2), where J_i is the fitness value for grid cell i , $\bar{\theta}_i^o$ and $\bar{\theta}_i^m$ are the the mean soil moisture values from the observations (from Catchment LSM), and simulated from Noah model, respectively, for grid cell i . The mean soil moisture values $\bar{\theta}_i^o$ and $\bar{\theta}_i^m$ are computed at each grid point i by averaging

287 the available soil moisture values over the course of the model simulation. The denominator of
288 the objective function thus represents the absolute soil moisture climatology difference between
289 the observations and the model.

$$J_i = \left(\frac{1}{|(\theta_i^o - \theta_i^m)|} \right) \quad (2)$$

290 This objective function is maximized independently for each grid cell i . The optimization
291 explores the decision space to maximize the fitness function values, subject to the the allowed
292 range of values for each parameter (Table 3).

293 The GA integrations use an elitism strategy to ensure that the current best solution is not
294 overwritten during GA evolution. A mutation rate of 0.005 and a recombination rate of 0.9 was
295 employed. The algorithm was found to converge after approximately 200 generations, when
296 the fitness of the best solution was found not to improve in the last 30 generations. These GA
297 parameters (including the mutation and recombination rates) are chosen largely from experience
298 and the success of the optimization simulations presented in Section 4.1 suggest that they are
299 reasonable.

4. Results

300 The results presented in this section focus first on the optimization simulations, that is, the
301 model calibration conducted prior to the DA-OPT1 and DA-OPT6 assimilation integrations.
302 Following this discussion, the different bias mitigation strategies are evaluated within the context
303 of soil moisture data assimilation.

4.1. Optimization simulations

304 Two separate optimization simulations are conducted: (1) using a single year of observational
305 data (OPT1; observations from year 2000) and (2) using observations from all six years (OPT6;
306 years 2000 - 2006). First, we compare the Noah model integrations using these two sets of
307 LSM parameters with the open loop simulation that employs the default values from the look
308 up table. Figure 3 presents maps of time series mean (climatological) differences in surface
309 soil moisture (which is essentially the inverse of the objective function used in the optimization
310 simulations). As discussed in section 3.3, the maps are computed by subtracting the mean Noah
311 LSM soil moisture values for each of the integrations shown in the figure from the corresponding
312 mean Catchment LSM surface soil moisture estimates. In computing these mean fields, we only
313 include the times and locations for which (synthetic) observations are available (section 3.2).
314 Further, only grid points with at least 600 observations for the evaluation period are considered
315 in the analysis of the results.

316 Figure 3 demonstrates that using the optimized parameters leads to reducing the systematic
317 differences in climatologies between the model and observations, throughout the domain. These
318 maps indicate that the Noah open loop integration generates on average (but not uniformly) drier
319 soil moisture values compared to the Catchment LSM. The use of optimized parameters helps
320 to correct the bias. Both OPT1 and OPT6 integrations improve this systematic underestimation
321 in the open loop by providing closer matches to the Catchment (“truth”) estimates, as seen in
322 the bottom two panels of Figure 3. The domain averaged soil moisture climatology difference
323 is reduced from $0.034 \text{ m}^3\text{m}^{-3}$ (for OL) to $0.006 \text{ m}^3\text{m}^{-3}$ for OPT1 and to $-0.003 \text{ m}^3\text{m}^{-3}$ for
324 OPT6. If absolute values of climatology differences are used, the improvements from OPT1 and
325 OPT6 are even more pronounced; the domain averaged absolute difference reduces from 0.047
326 m^3m^{-3} for OL to $0.010 \text{ m}^3\text{m}^{-3}$ for OPT1 and $0.009 \text{ m}^3\text{m}^{-3}$ for OPT6. The estimation of model

327 parameters thus enables the correction of systematic biases and leads to a closer match between
328 the soil moisture climatologies of the model (Noah) and the synthetic observations (Catchment).

329 Figure 4 shows maps of the parameters used in the open loop integration (prescribed using
330 look up tables) and the calibrated values from the OPT6 integration. Out of the parameters listed
331 in Table 3 we focus on three key parameters: porosity (θ_s), saturated matric potential (ψ_s) and
332 saturated hydraulic conductivity (K_s). The spatial patterns in the look up table-based parameters
333 are similar to each other, because they are determined based on the soil texture map. In contrast,
334 the optimized parameters show more spatial variability, because they are not constrained to soil
335 types or vegetation categories. Compared to the default parameters, the optimized parameters
336 in general show higher values of θ_s , ψ_s and K_s over the domain. This is consistent with the
337 optimization objective of correcting the dry bias in the open loop integration, as higher values
338 of θ_s , ψ_s and K_s would allow for more water to be held in the soil and more infiltration into the
339 soil, and correspondingly higher soil moisture values. Similar spatial trends are also observed
340 in other parameters (not shown).

341 Although these spatial trends are consistent with the patterns in soil moisture simulations, the
342 intent here is not to judge the veracity or physical realism of the estimated parameters. Instead,
343 our goal is to study how bias mitigation through parameter estimation helps in the subsequent
344 data assimilation performance. Though the typical approach in land surface models is to employ
345 look up table-based parameters that are derived from limited data samples (e.g. *Rawls et al.*
346 [1982]; *Cosby et al.* [1984]), these representations suffer from numerous issues, including lack
347 of spatial representativeness of the datasets on which they are based, errors in extrapolating the
348 point-scale to the modeling scales, and the large within-soil class variation of properties that is
349 on par with the variation across different texture classes (*Schaap* [2004]; *Braun and Schadler*

350 [2005]; *Doherty and Welter* [2010]; *Gutman and Small* [2010]). Further, the physical realism and
351 mismatch issues of the parameters are difficult to assess at large spatial scales because validating
352 in situ measurements of surface and root zone soil moisture that match the scale of the model
353 grid cells are not available.

354 In short, there is significant uncertainty associated with the default parameters, typically re-
355 garded as the “truth”. The optimization formulation in this article samples from the ranges of
356 parameters (Table 3) representing the full spectrum across all look up table categories. Additional
357 look up table category-based constraints can be introduced on these parameter ranges to ensure
358 that the estimated parameters conform to the traditional, category-based (e.g. soil texture-based)
359 notions of physical realism. Algorithms and approaches that incorporate notions of “equifinal”
360 solutions (e.g., *Gupta et al.* [1999]; *Hogue et al.* [2006]) may offer more effective ways to rep-
361 resent parameter uncertainty and to ensure physical consistency since they generate a range of
362 plausible model fits. The use of such methods is left for a future work. Here, the parameter
363 sets generated by the optimization simulations OPT1 and OPT6 may represent mismatches with
364 regard to the typical category-based definitions.

4.2. Data assimilation experiments

365 This section presents the results from data assimilation experiments that employ different
366 strategies for bias correction (section 3.2). Since the suite of experiments include simulations
367 that assimilate both unscaled (experiments DA-NOSC, DA-OPT1 and DA-OPT6) and scaled
368 observations (experiments DA-STDN and DA-CDF), we primarily use the anomaly time series
369 correlation coefficient (R), to quantify the skill of the model simulations.

370 The anomaly time series for each grid point is estimated as follows: The monthly-mean clima-
371 tology values are subtracted from the daily average raw data, so that the anomalies represent the

372 daily deviations from the mean seasonal cycle. The skill contribution from correctly identifying
373 the mean seasonal variation is therefore excluded. The anomaly R values are computed, sepa-
374 rately for each grid point, as the correlation coefficients between the daily anomalies from the
375 assimilation estimates and the corresponding truth data. Only anomalies at times and locations
376 for which observations are assimilated contribute to the computation of the R values. Similar
377 to the comparisons in Section 4.1, only grid points with at least 600 assimilated observations
378 during the evaluation period are included in the evaluations.

379 Figure 5 shows the comparison of the anomaly R values for surface soil moisture from different
380 model integrations. Overall, the assimilation experiments perform better than the open loop
381 simulation, and the assimilation skill systematically improves from experiment DA-NOSC to
382 experiment DA-OPT6. The domain averaged skill of the Noah model integration without any
383 data assimilation (OL) is 0.47. When observations are assimilated without bias correction (DA-
384 NOSC), the domain averaged skill improves to 0.63. The assimilation skill is further improved
385 in the integrations that employ a priori scaling of observations, with domain averaged skill values
386 of 0.71 and 0.73, for DA-STDN and DA-CDF, respectively. For the climatological differences
387 encountered in this synthetic experiment, the use of higher-order moments in the CDF matching
388 technique slightly outperforms the seasonally varying scaling parameters used in DA-STDN.
389 Finally, surface soil moisture skill values of 0.73 and 0.75 are obtained for experiments DA-
390 OPT1 and DA-OPT6, respectively, when assimilation integrations are conducted with optimized
391 parameters that conform to the Catchment LSM (truth) climatology.

392 The assimilation of surface soil moisture retrievals is often used as a way to generate superior
393 estimates of related states such as root zone soil moisture (*Reichle et al. [2007]; Kumar et al.*
394 [2009]). Figure 6 presents a comparison of the root zone soil moisture skill estimates from

395 different model integrations. Similar to the behavior observed for surface soil moisture, the
396 skill of root zone estimates from using the calibrated model is comparable to the skills from
397 a priori scaling approaches. The domain averaged open loop root zone skill estimate is 0.45
398 and it improves to 0.54 when assimilation is performed without bias correction (DA-NOSC).
399 The skill further improves to 0.62 and 0.63, through the use of a priori scaling of observations,
400 for integrations DA-STDN and DA-CDF, respectively. Finally, the use of a calibrated model
401 together with the assimilation of unscaled observations provides domain averaged skill values
402 of 0.62 and 0.63, for integrations DA-OPT1 and DA-OPT6, respectively. For root zone soil
403 moisture, the relative advantage of the a priori calibration strategy (DA-OPT1, DA-OPT6) over
404 the a priori scaling methods (DA-STDN, DA-CDF) is minimal. The 95% confidence intervals
405 of the domain averaged anomaly R values are in the range of 0.008 to 0.01, verifying that the
406 improvements obtained through data assimilation in both surface and root zone soil moisture are
407 statistically significant.

408 In a separate analysis (not shown), we also examined the skill improvements in surface fluxes
409 (latent, sensible and ground heat) from the data assimilation integrations. The assimilation runs
410 with bias correction (DA-STDN, DA-CDF, DA-OPT1, and DA-OPT6) were found to marginally
411 improve the surface flux skill values over the open loop and DA-NOSC integrations, with a priori
412 scaling and a priori calibration yielding comparable results.

413 Figures 5 and 6 also indicate that soil moisture skill values improve consistently across the
414 domain in the data assimilation integrations. To further illustrate this fact, Figure 7 shows
415 probability density functions (PDFs) for surface and root zone soil moisture skill values across the
416 modeling domain. Compared to the PDF for the OL integration, the PDFs from data assimilation
417 integrations show narrower distributions that are skewed towards higher skill values, due to

418 the improved soil moisture estimates from assimilation. For surface soil moisture, the PDF
419 for DA-NOSC is shifted towards higher R values, but shows only a marginal reduction in the
420 spread compared to the PDF for OL skill (The standard deviation of the PDF reduces from
421 0.156 to 0.142). The runs based on a priori scaling (DA-STDN and DA-CDF) yield a greater
422 reduction in the OL spread (standard deviation of 0.121 and 0.093, respectively) and a further
423 shift towards higher skill values. The DA-OPT1 and DA-OPT6 integrations provide similarly
424 reduced variability in skill estimates (that is, consistent improvements) across the domain with
425 standard deviations in PDFs of 0.113 and 0.091, respectively). Comparable but more muted
426 trends are observed for root zone soil moisture, where the variability in skill values also reduces,
427 gradually from the OL to DA-OPT6. In summary, Figure 7 indicates that a priori calibration and
428 a priori scaling yield comparable improvements in surface and root zone skill.

429 The anomaly R metric is indifferent to any bias in the mean or the amplitude of variations. By
430 contrast, the RMSE is highly sensitive to biases. As mentioned earlier, the long-term mean bias
431 with respect to the true conditions is difficult (if not impossible) to determine for continental-scale
432 soil moisture. To supplement the anomaly R skill values presented above, we now assess the
433 “unbiased” RMSE (ubRMSE) values, which are computed from the time series after removal of
434 the long-term mean bias (*Entekhabi et al. [2010a]*). Table 4 provides a comparison of the domain
435 averaged ubRMSE values from different model simulations, which shows similar trends to those
436 seen with the anomaly R metric. For surface soil moisture, the domain-averaged ubRMSE
437 for the OL integration is $0.052 \text{ m}^3\text{m}^{-3}$, which reduces to $0.041 \text{ m}^3\text{m}^{-3}$ for DA-NOSC. The
438 scaling-based DA runs DA-STDN and DA-CDF improve these estimates to $0.038 \text{ m}^3\text{m}^{-3}$ and
439 $0.037 \text{ m}^3\text{m}^{-3}$, respectively. The optimization-based runs DA-OPT1 and DA-OPT6 provide
440 comparable skills to those the scaling-based runs with domain averaged ubRMSE values of

441 0.037 and $0.036 \text{ m}^3\text{m}^{-3}$, respectively. The root zone soil moisture skill values follow similar
442 trends. The domain averaged ubRMSE for OL is $0.039 \text{ m}^3\text{m}^{-3}$, and it improves to 0.037
443 m^3m^{-3} in the DA-NOSC simulation. Both a priori scaling and optimization based approaches
444 provide systematic, statistically significant improvements (relative to OL) with domain-averaged
445 ubRMSE of 0.035, 0.034, 0.033 and $0.033 \text{ m}^3\text{m}^{-3}$, for integrations DA-STDN, DA-CDF, DA-
446 OPT1, and DA-OPT6, respectively.

447 An important aspect of a priori bias mitigation approaches is the fact that they require an a priori
448 estimate of the climatology of the observations. *Reichle and Koster* [2004] demonstrate that for
449 the a priori scaling approach, a single year of observations may be sufficient if some spatial
450 averaging over neighboring grid cells is employed to reduce sampling noise. In this context, it
451 is encouraging that the assimilation skill values from the DA-OPT1 and DA-OPT6 integrations
452 are comparable, with DA-OPT6 generating an additional domain averaged improvement of only
453 0.02 over DA-OPT1 for surface and root zone soil moisture. In other words, most of the benefit
454 of the a priori calibration method can be achieved with just one year's worth of observations,
455 provided the climatology can be reasonably approximated from the available data year, which is
456 the case here (not shown). This suggests that using a short time period for calibration can still
457 be an effective strategy, which is especially important for new types of satellite missions when
458 the period of available data is relatively short.

459 Further, note that the objective function formulation (equation 2) is designed to only correct the
460 first moment of the model and observation distributions, whereas the a priori scaling approaches
461 are designed to correct multiple moments of the distributions. Nevertheless, the assimilation
462 skills from the a priori scaling and a priori optimization approaches are already comparable,

463 indicating that further skill improvements may be achieved using objective function formulations
464 designed to correct multiple moments of the distributions.

4.3. Computational considerations

465 Data assimilation with bias mitigation through a priori calibration (DA-OPT1, DA-OPT6)
466 improves surface and root zone soil moisture estimates compared to bias mitigation through
467 a priori scaling (DA-STDN, DA-CDF). It should be noted, however, that the estimation of
468 the optimization parameters through batch calibration has an associated computational cost.
469 The scalable computing infrastructure in LIS helps in reducing this overhead through parallel
470 computation using multiple processors. The OPT6 integration requires 200 iterations of LIS
471 runs over the 2000-2006 period, which translates to wall clock times of approximately a week,
472 using 128 processors. In comparison, the OPT1 integration requires approximately a day (using
473 128 processors). The comparable skill of the short calibration-based run (DA-OPT1) relative to
474 the long calibration-based run (DA-OPT6) indicate that the high computational cost associated
475 with batch calibration can be considerably reduced by using a shorter time period of observations
476 that adequately represents the overall climatology. The dimensionality of the decision space can
477 be reduced by selecting a smaller number of parameters that are likely to be more sensitive to
478 the soil moisture simulations. The reduction in the dimensionality of the decision space vector
479 will also aid towards reducing the computational cost associated with optimization simulations.

4.4. Innovation metrics

480 In this section, we examine the filter innovations (observation minus model forecast residuals)
481 from the assimilation experiments. This analysis provides insights into the performance of the
482 data assimilation integrations (*Reichle et al.* [2002]; *Crow and Van Loon* [2006]; *Reichle et al.*

483 [2007]; *Kumar et al.* [2008b]). Strictly speaking, the EnKF provides optimal estimates only if
484 several assumptions hold, including linear system dynamics with model and observation errors
485 that are Gaussian and mutually and serially uncorrelated. If these assumptions hold, then the
486 distribution of normalized innovations (normalized with their expected covariance) follows a
487 standard normal distribution, $N(0, 1)$ (*Gelb* [1974]). The deviations from the expected mean
488 and variance of the normalized innovation distribution provides a measure of the degree of
489 suboptimality with which the assimilation system performs.

490 Unsurprisingly, the integration without a priori bias mitigation exhibits the largest innovation
491 biases, reflecting strong biases between the (synthetic) observations and the corresponding model
492 forecasts (not shown). The a priori scaling (DA-STDN, DA-CDF) and a priori calibration
493 approaches (DA-OPT1, DA-OPT6) clearly mitigate these biases (not shown). Figure 8 presents
494 maps of the variance of the normalized innovations. For the bias-blind assimilation integration
495 (DA-NOSC), the variance of the normalized innovations is on average 2.38 and far exceeds the
496 target value of 1, which reflects the strong underestimation of the actual errors by the assimilation
497 system because it ignores the bias. Adding a priori bias mitigation strategies brings the variance
498 of the normalized innovations much closer to the target value of 1. Based on this metric, the
499 assimilation using the CDF-based a priori scaling (DA-CDF) operates closer to optimality than
500 the simpler strategy that uses only the first and second order rescaling (DA-STDN). Likewise,
501 variance of the normalized innovations is closer to the target value of 1 when all years are used
502 in the a priori calibration (DA-OPT6) rather than just one year (DA-OPT1).

5. Summary

503 Data assimilation methods such as the EnKF require that the errors in the model and the ob-
504 servations are strictly random. As a result, the presence of systematic or bias errors needs to be

505 addressed separately within the data assimilation system. In this study, we evaluate a number of
506 bias mitigation strategies in the context of assimilating surface soil moisture retrievals. Specifi-
507 cally, we examine the use of land model parameter estimation as a bias correction strategy prior
508 to data assimilation. This strategy is compared to the approach of scaling the assimilated obser-
509 vations to the land model's climatology prior to data assimilation. The study is conducted using
510 a fraternal twin experiment setup, where synthetic observations generated using the Catchment
511 LSM are assimilated into the Noah LSM. Five different data assimilation experiments are con-
512 ducted, each using a different strategy to correct (or not) for bias prior to data assimilation. The
513 resulting soil moisture estimates are evaluated against the corresponding synthetic truth fields
514 from the Catchment LSM.

515 Our results indicate that a priori land model calibration is an effective strategy for bias mitiga-
516 tion in soil moisture assimilation. The domain averaged skill estimates (in terms of anomaly R
517 values) for the Noah open loop simulation without any data assimilation are 0.47 for surface soil
518 moisture and 0.45 for root zone soil moisture. These skill estimates improve to 0.63 for surface
519 soil moisture and 0.54 for root zone soil moisture. when assimilation is conducted without any
520 bias correction (DA-NOSC). When observations are assimilated after rescaling to the model
521 climatology, the assimilation skill improves further. Two approaches for a priori scaling are con-
522 sidered: (DA-STDN) using standard normal deviates and (DA-CDF) by matching the CDFs of
523 the observations to that of the model. Assimilation using these a priori scaling approaches yields
524 domain averaged skill values of 0.71 and 0.73 for surface soil moisture and 0.62 and 0.63 for root
525 zone soil moisture, respectively. Similar improvements in the surface and root zone soil moisture
526 estimates are observed with the assimilation runs that employ optimized model parameters but
527 ingest unscaled observations. Two sets of optimized parameters are used in the experiments:

528 (DA-OPT1) parameters estimated from a single year of calibration and (DA-OPT6) parameters
529 estimated from six years of calibration. When data assimilation is conducted using parameters
530 from a single year of calibration, skill estimates of 0.73 for surface soil moisture and 0.62 for
531 root zone soil moisture are obtained. The use of the six-year based parameters further improves
532 these skill measures to 0.75 for surface soil moisture and 0.63 for root zone soil moisture.

533 It was also observed that spatial variability in the skill scores across the domain is reduced
534 with the use of optimized parameters, resulting in more spatially consistent skill enhancements.
535 The skill improvements in surface fluxes were found to be comparable for data assimilation
536 following a priori scaling and a priori calibration. Similar trends in skill scores are also observed
537 if the unbiased RMSE metric is used instead of anomaly R for evaluating the results. Finally,
538 the analysis of innovation diagnostics also demonstrates that without the use of suitable bias
539 correction, the assimilation system performs in a less than optimal manner and that all four bias
540 mitigation strategies adequately address the bias issue.

541 In the suite of synthetic experiments presented in this article we are in effect calibrating the
542 Noah surface soil moisture climatology to that of the Catchment LSM. It must be stressed that
543 this approach is chosen not because one model (Catchment) is more correct than the other (Noah).
544 A similar argument holds when satellite soil moisture retrievals are assimilated. In that case, the
545 climatology of the retrievals is not necessarily more correct than that of the model. However,
546 when brightness temperatures are assimilated in radiance space instead of the retrievals, the model
547 should be calibrated to the observed brightness temperature climatology. The long-term biases
548 can be mitigated through calibration and the remaining shorter-term biases can be addressed
549 with a priori scaling. The combined use of these strategies will be examined in future radiance
550 based data assimilation experiments.

551 Though effective, the approach of using parameter estimation for bias correction also suffers
552 from the limitations of the a priori scaling approaches. Since the parameters are estimated in
553 advance of data assimilation, any subsequent changes in model behavior will not be captured,
554 unlike in the dynamic bias estimation algorithms. The optimization formulation does not con-
555 strain the estimated parameters to conform to the traditional, look up table-based definitions of
556 parameters. Here, no attempt was made to ensure the physical realism of the estimated param-
557 eters. The calibration might also require additional constraints to ensure that the behavior of
558 related variables is not adversely affected. Note, however, that we have found that the estimates
559 of the latent and sensible heat fluxes were comparable for the assimilation integrations with bias
560 correction (DA-STDN, DA-CDF, DA-OPT1, and DA-OPT6). Furthermore, our results suggest
561 that using model parameter estimation could be a viable strategy for bias mitigation in cases of
562 relatively short (i.e., one year) satellite records. This result is important for expediting the use
563 of soil moisture retrievals becoming available from SMOS and SMAP.

564 The study also demonstrates the advanced capabilities of the NASA LIS framework, including
565 the development of a new subsystem for optimization. This extension encapsulates a range of
566 advanced search algorithms suited for both convex and non-convex optimization problems. In
567 this particular study, the Genetic Algorithm, a heuristic search technique based on principles
568 of evolutionary computing, is employed for estimating model parameters. The optimization
569 infrastructure within LIS is currently being enhanced with a suite of uncertainty estimation algo-
570 rithms based on Bayesian methods. In contrast to the optimization techniques that have already
571 been implemented in LIS and generate a single solution for parameters, the newer uncertainty
572 estimation tools infer distributions of parameters based on the observational information. These
573 parameter distributions can then be used to condition the ensembles used in the data assimilation

574 system. The joint use of optimization and data assimilation tools presented here and future
575 LIS advancements will enable the increased exploitation of observational data for improving
576 hydrological modeling.

6. Acknowledgments

577 We gratefully acknowledge the financial support from the NASA Earth Science Technology
578 Office (ESTO) (Advanced Information System Technology program award AIST-08-077). Rolf
579 Reichle was supported by the NASA program on Earth System Science Research using Data and
580 Products from Terra, Aqua, and ACRIMSAT Satellites and the SMAP Science Definition Team.
581 Thanks to James Geiger, Scott Rheingrover and Dr. Dalia Kirschbaum for helpful comments.
582 Computing was supported by the resources at the NASA Center for Climate Simulation.

References

- 583 Bosilovich, M., J. Radakovich, A. da Silva, R. Todling, and F. Verter, Skin temperature analysis
584 and bias correction in a coupled land-atmosphere data assimilation system, *J. Meteor. Soc.
585 Japan*, 85A, 205–228, 2007.
- 586 Boulet, G., Y. Kerr, and A. Chehbouni, Deriving catchment-scale water and energy balance
587 parameters using data assimilation based on extended kalman filtering, *Hydrol. Sci. J. Sci.
588 Hydrol.*, 47, 449–467, 2002.
- 589 Braun, F., and G. Schadler, Comparison of soil hydraulic parameterizations for mesoscale and
590 meteorological models, *Journal of Applied Meteorology*, 44(1116), 2005.
- 591 Burke, E., R. Gurney, L. Simmonds, and T. Jackson, Calibrating a soil water and energy budget
592 with remotely sensed data to obtain quantitative information about the soil, *Water Resources
593 Research*, 33(7), 1689–1697, 1997.
- 594 Cosby, B., G. Hornberger, R. Clapp, and T. Ginn, A statistical exploration of the relationships
595 of soil moisture characteristics to the physical properties of soils, *Water Resources Research*,
596 20(6), 682–690, 1984.
- 597 Crow, W., R. Koster, R. Reichle, and H. Sharif, Relevance of time-varying and time-invariant re-
598 trieval error sources on the utility of spaceborne soil moisture products, *Geophysical Research
599 Letters*, 32(L24405), doi:10.1029/2005GL024889, 2005.
- 600 Crow, W. T., and E. Van Loon, Impact of incorrect model error assumptions on the sequential
601 assimilation of remotely sensed surface soil moisture, *Journal of Hydrometeorology*, 7(3),
602 421–432, 2006.
- 603 De Lannoy, G., P. Houser, V. Pauwels, and N. Verhoest, State and bias estimation for soil
604 moisture profiles by an ensemble kalman filter: Effect of assimilation depth and frequency,

- 605 *Water Resources Research*, 43(W06401), doi:10.1029/2006WR005100, 2007a.
- 606 De Lannoy, G., R. Reichle, P. Houser, V. Pauwels, and N. Verhoest, Correcting for forecast
607 bias in soil moisture assimilation with the ensemble kalman filter, *Water Resources Research*,
608 43(W09410), doi:10.1029/2006WR005449, 2007b.
- 609 Dee, D., Bias and data assimilation, *Q.J.R. Meteorol.Soc.*, 131, 3323–3343, 2005.
- 610 Dee, D., and A. da Silva, Data assimilation in the presence of forecast bias, *Q.J.R. Meteorol.Soc.*,
611 124, 269–295, 1998.
- 612 Derber, J., D. Parrish, and S. Lord, The new global operational analysis system at the National
613 Meteorological Center, *Weather and Forecasting*, 6, 538–547, 1991.
- 614 Doherty, J., and D. Welter, A short explanation of structural noise, *Water Resources Research*,
615 46(W05525), doi:10.1029/2009WR008377, 2010.
- 616 Draper, C., J. Mahfouf, and J. Walker, An EKF assimilation of AMSR-E soil moisture into
617 the ISBA land surface scheme, *Journal of Geophysical Research-Atmospheres*, 114(D20104),
618 2009.
- 619 Draper, C., J. Mahfouf, and J. Walker, Root zone soil moisture from the assimilation of
620 screen-level variables and remotely sensed soil moisture, *Journal of Geophysical Research-*
621 *Atmospheres*, 116(D02127), 2011.
- 622 Drusch, M., E. Wood, and H. Gao, Observation operators for the direct assimilation of TRMM
623 microwave imager retrieved soil moisture, *Geophysical Research Letters*, 32(L15403), doi:
624 10.1029/2005GL023623, 2005.
- 625 Duan, Q., S. Sorooshian, and V. Gupta, Effective and efficient global optimization for conceptual
626 rainfall-runoff models, *Water Resources Research*, 28(4), 1015–1031, 1992.

- 627 Duan, Q., V. Gupta, and S. Sorooshian, A shuffled complex evolution approach for effective and
628 efficient global minimization, *J. Optim. Theory. Appl.*, 76(3), 501–521, 1993.
- 629 Ek, M., K. Mitchell, L. Yin, P. Rogers, P. Grunmann, V. Koren, G. Gayno, and J. Tarpley,
630 Implementation of Noah land-surface model advances in the NCEP operational mesoscale Eta
631 model, *Journal of Geophysical Research*, 108(D22), doi:10.1029/2002JD003296, 2003.
- 632 Entekhabi, D., R. Reichle, R. Koster, and W. Crow, Performance metrics for soil moisture
633 retrievals and application requirements, *Journal of Hydrometeorology*, 11, 832–840, doi:
634 doi:10.1175/2010JHM1223.1, 2010a.
- 635 Entekhabi, D., et al., The soil moisture active passive (SMAP) mission, *Proceedings of the IEEE*,
636 98(5), doi:10.1109/JPROC.2010.2043918, 2010b.
- 637 Gelb, A., *Applied Optimal Estimation*, MIT Press, Cambridge, MA, 1974.
- 638 Goldberg, D., *Genetic Algorithms in Search, Optimization and Machine Learning*, Addison-
639 Wesley, 1989.
- 640 Gupta, H., L. Bastidas, S. Sorooshian, W. Shuttleworth, and Z. Yang, Parameter estimation of a
641 land surface scheme using multicriteria methods, *Journal of Geophysical Research*, 104(D16),
642 19,491–19,503, 1999.
- 643 Gutman, E., and E. Small, A method for the determination of the hydraulic properties of soil
644 from MODIS surface temperature for use in land surface models, *Water Resources Research*,
645 46(W06520), doi:10.1029/2009WRF008203, 2010.
- 646 Hill, C., C. DeLuca, V. Balaji, M. Suarez, and A. da Silva, The architecture of the earth system
647 modeling framework, *Computing in Science and Engineering*, 6(1), 2004.
- 648 Hogue, T., L. Bastidas, H. Gupta, S. Sorooshian, K. Mitchell, and W. Emmerich, Evaluation and
649 transferability of the noah land surface model in semiarid environments, *Journal of Hydrom-*

- 650 *eteorology*, 6(1), 68–84, 2005.
- 651 Hogue, T., L. Bastidas, S. Sorooshian, and H. Gupta, Comparative evaluation of the perfor-
652 mance of land-surface schemes using multi-criteria methods, *Water Resources Research*,
653 42(W08430), doi:10.1029/2005WR004440, 2006.
- 654 Holland, J., *Adaptation in Natural and Artificial Systems*, University of Michigan Press, Ann
655 Arbor, Michigan, 1975.
- 656 Kerr, Y. H., et al., The SMOS mission: New tool for monitoring key elements of the global water
657 cycle, *Proceedings of the IEEE*, 98(5), 666–687, 2010.
- 658 Koster, R. D., M. J. Suarez, A. Ducharne, M. Stieglitz, and P. Kumar, A catchment-based
659 approach to modeling land surface processes in a general circulation model 1. model structure,
660 *Journal of Geophysical Research*, 105(D20), 24,809–24,822, 2000.
- 661 Kumar, S., C. Peters-Lidard, Y. Tian, R. H. Reichle, C. Alonge, J. Geiger, J. Eylander, and
662 P. Houser, An integrated hydrologic modeling and data assimilation framework enabled by
663 the Land Information System (LIS), *IEEE Computer*, 41, 52–59, doi:10.1109/MC.2008.511,
664 2008a.
- 665 Kumar, S., R. Reichle, C. Peters-Lidard, R. Koster, X. Zhan, W. Crow, J. Eylander,
666 and P. Houser, A land surface data assimilation framework using the Land Information
667 System: Description and applications, *Advances in Water Resources*, 31, 1419–1432,
668 doi:10.1016/j.advwatres.2008.01.013, 2008b.
- 669 Kumar, S., R. Reichle, R. Koster, W. Crow, and C. Peters-Lidard, Role of subsurface physics
670 in the assimilation of surface soil moisture observations, *Journal of Hydrometeorology*, doi:
671 10.1175/2009JHM1134.1, 2009.

- 672 Kumar, S., et al., Land information system: An interoperable framework for high resolution land
673 surface modeling, *Environmental Modeling and Software*, 21, 1402–1415, 2006.
- 674 Lambot, S., E. Slob, J. Rhebergen, O. Lopera, K. Jadoon, and H. Vereecken, Remote esti-
675 mation of the hydraulic properties of a sand using full-waveform integrated hydrogeophys-
676 ical inversion of time-lapse, off-ground gpr data, *Vadoze Zone Journal*, 8, 743–754, doi:
677 10.2136/vzj2008.0058, 2009.
- 678 Levenberg, K., A method for the solution of certain non-linear problems in least squares, *The*
679 *Quarterly of Applied Mathematics*, 2, 164–168, 1944.
- 680 Liu, Q., R. Reichle, R. Bindlish, M. Cosh, W. Crow, R. de Jeu, G. J. M. De Lannoy, G. Huffman,
681 and T. Jackson, The contributions of precipitation and soil moisture observations to the skill
682 of soil moisture estimates in a land data assimilation system, *Journal of Hydrometeorology*,
683 doi:10.1175/JHM-D-10-05000, in press, 2011.
- 684 Liu, Y., and H. Gupta, Uncertainty in hydrologic modeling: Toward an integrated data assimi-
685 lation framework, *Water Resources Research*, 43(W07401), 10.1029/2006WR005,756, 2007.
- 686 Liu, Y., H. Gupta, S. Sorooshian, L. Bastidas, and W. Shuttleworth, Exploring parameter sensitiv-
687 ities of the land surface using a locally coupled land-atmosphere model, *Journal of Geophysical*
688 *Research*, 109, 21,101–21,114, 2004.
- 689 Liu, Y., H. Gupta, S. Sorooshian, L. Bastidas, and W. Shuttleworth, Constraining land surface
690 and atmospheric parameters of a locally coupled model using observational data, *Journal of*
691 *Hydrometeorology*, 6, 156–172, 2005.
- 692 Mahrt, L., and H. Pan, A two-layer model of soil hydrology, *Boundary Layer Meteorology*, 29,
693 1–20, 1984.

- 694 Marquardt, D., An algorithm for least-squares estimation of nonlinear parameters, *SIAM Journal*
695 *on Applied Mathematics*, *11*, 431–441, 1963.
- 696 Moradkhani, H., S. Sorooshian, H. Gupta, and P. Houser, Dual state-parameter estimation of
697 hydrological models using ensemble kalman filter, *Advances in Water Resources*, *28*, 135–147,
698 2005.
- 699 Nearing, G., M. Moran, K. Thorp, C. Collins, and D. Slack, Likelihood parameter estimation
700 for calibrating a soil moisture model using radar bakscatter, *Remote Sensing of Environment*,
701 *114*, 2564–2574, 2010.
- 702 Peters-Lidard, C., D. Mocko, M. Garcia, J. Santanello, M. Tischler, and M. Moran, Role
703 of precipitation uncertainty in the estimation of hydrologic soil properties using remotely
704 sensed soil moisture in a semiarid environment, *Water Resources Research*, *44*(W05S18),
705 doi:10.1029/2007WR005884, 2008.
- 706 Peters-Lidard, C. D., et al., High-performance earth system modeling with NASA/GSFC's land
707 information system, *Innovations in Systems and Software Engineering*, *3*(3), 157–165, 2007.
- 708 Rawls, W., D. Brakensiek, and K. Saxton, Estimation of soil water properties, *Transactions of*
709 *the ASAE*, *25*, 1316–1320, 1982.
- 710 Reichle, R., Data assimilation methods in the earth sciences, *Advances in Water Resources*, *31*,
711 1411–1418, 2008.
- 712 Reichle, R., and R. Koster, Assessing the impact of horizontal error correlations in background
713 fields on soil moisture estimation, *Journal of Hydrometeorology*, *4*(6), 1229–1242, 2003.
- 714 Reichle, R., D. McLaughlin, and D. Entekhabi, Hydrologic data assimilation with the ensemble
715 kalman filter, *Monthly Weather Review*, *130*(1), 103–114, 2002.

- 716 Reichle, R., R. Koster, J. Dong, and A. Berg, Global soil moisture from satellite observations,
717 land surface models, and ground data: implications for data assimilation, *Journal of Hydrometeorology*, 5, 430–442, 2004.
- 718
- 719 Reichle, R., R. Koster, S. Liu, P. and. Mahanama, E. Njoku, and M. Owe, Comparison
720 and assimilation of global soil moisture retrievals from the advanced microwave scanning
721 radiometer for the earth observing system (AMSR-E) and the scanning multichannel microwave radiometer (SMMR), *Journal of Geophysical Research-Atmospheres*, 112(D09108),
722 doi:10.1029/2006JD008033, 2007.
- 723
- 724 Reichle, R., M. Bosilovich, W. Crow, R. Koster, S. Kumar, S. Mahanama, and B. Zaitchick,
725 Recent advances in land data assimilation at the NASA Global Modeling and Assimilation
726 Office, in *Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications*, edited by
727 S. K. Park and L. Xu, pp. 407–428, Springer Verlag, doi:10.1007/978-3-540-71056-1, 2009.
- 728 Reichle, R., S. Kumar, S. Mahanama, R. Koster, and Q. Liu, Assimilation of satellite-derived
729 skin temperature observations into land surface models, *Journal of Hydrometeorology*, doi:
730 10.1175/2010JHM1262.1, 2010.
- 731 Reichle, R. H., and R. Koster, Bias reduction in short records of satellite soil moisture, *Geophys.*
732 *Res. Lett.*, L19501, doi:10.1029/2004GL020938, 2004.
- 733 Santanello, J., C. Peters-Lidard, M. Garcia, D. Mocko, M. Tischler, M. Moran, and D. Thoma,
734 Using remotely sensed estimates of soil moisture to infer spatially distributed soil hydraulic
735 properties, *Remote Sensing of Environment*, 110, 79–97, 2007.
- 736 Schaap, M., Accuracy and uncertainty in PTF predictions, *Developments in soil science*, 30, 33,
737 2004.

- 738 Slater, A., and M. Clark, Snow data assimilation via an ensemble kalman filter, *Journal of*
739 *Hydrometeorology*, 7, 478–493, 2006.
- 740 Trigo, I., and P. Viterbo, Clear-sky window channel radiances: A comparison between observa-
741 tions and the ECMWF model, *Journal of Applied Meteorology*, 42, 1463–1479, 2003.
- 742 Vrugt, J., C. Diks, H. Gupta, W. Bouten, and J. Verstaten, Improved treatment of uncertainty in
743 hydrologic modelling: Combining the strengths of global optimization and data assimilation,
744 *Water Resources Research*, 41(W01017), doi:10.1029/2004WR003059, 2005.

Table 1. Overview of model and assimilation integrations

OL	Noah model integration without assimilation (Open Loop)
OPT1	Noah model integration without assimilation and with model parameters optimized to reproduce one-year (2000) climatology of synthetic soil moisture observations
OPT6	Noah model integration without assimilation and with model parameters optimized to reproduce six-year (2000-2006) climatology of synthetic soil moisture observations
DA-NOSC	Noah assimilation integration without bias correction using unscaled observations
DA-STDN	Noah assimilation integration using a priori scaling of observations based on standard normal deviates
DA-CDF	Noah assimilation integration using a priori scaling of observations based on CDF matching
DA-OPT1	Noah assimilation integration using OPT1 model parameters and unscaled observations
DA-OPT6	Noah assimilation integration using OPT6 model parameters and unscaled observations

Table 2. Parameters for perturbations to meteorological forcings and model prognostic variables in the EnKF assimilation experiments

Variable	Perturbation Type	Standard Deviation	Cross Correlations with perturbations in			
			SW↓	LW↓	PCP	
Meteorological Forcings						
Downward Shortwave (SW↓)	Multiplicative	0.3 [-]	1.0	-0.5	-0.8	
Downward Longwave (LW↓)	Additive	50 W/m ²	-0.5	1.0	0.5	
Precipitation (PCP)	Multiplicative	0.50 [-]	-0.8	0.5	1.0	
Noah LSM soil moisture states			sm1	sm2	sm3	sm4
Total soil moisture - layer 1 (sm1)	Additive	6.0E-3 m ³ m ⁻³	1.0	0.6	0.4	0.2
Total soil moisture - layer 2 (sm2)	Additive	1.1E-4 m ³ m ⁻³	0.6	1.0	0.6	0.4
Total soil moisture - layer 3 (sm3)	Additive	0.60E-5 m ³ m ⁻³	0.4	0.6	1.0	0.6
Total soil moisture - layer 4 (sm4)	Additive	0.40E-5 m ³ m ⁻³	0.2	0.4	0.6	1.0

Table 3. List of Noah LSM parameters used in the optimization runs. The columns show the variable names, a brief description and the range of values (maximum and minimum values) of the parameters used in the optimization system.

No.	Variable	Description	Min value	Max value
1	smcmax	Porosity (-)	0.30	0.55
2	psisat	Saturated matric potential (-)	0.01	0.70
3	dksat	Saturated hydraulic conductivity (m/s)	0.05E-5	3.00E-5
4	dwsat	Saturated soil diffusivity (-)	5.71E-6	2.33E-5
5	bexp	The “b” parameter (-)	3.0	9.0
6	quartz	Soil quartz content (-)	0.10	0.90
7	rsmin	Minimum stomatal resistance (m)	40	1000
8	rgl	Parameter used in solar radiation term of canopy resistance (-)	30	150
9	hs	Parameter used in vapor pressure deficit term of canopy resistance (-)	36.35	55
10	z0	Roughness length (m)	0.01	0.99
11	lai	Leaf area index (-)	0.05	6.00
12	cfactr	Canopy water parameter	0.1	2.0
13	cmcmax	Canopy water parameter (m)	1E-4	2E-3
14	sbeta	Parameter used in the computation of vegetation effect on soil heat flux (-)	-4	-1
15	rsmax	Maximum stomatal resistance (m)	2000	10000
16	topt	Optimum transpiration air temperature (K)	293	303
17	refdk	Reference value for saturated hydraulic conductivity (m/s)	5E-7	3E-5
18	fxexp	Bare soil evaporation exponent (-)	0.2	4.0
19	refkdt	Reference value for surface infiltration parameter (-)	0.1	10.0
20	czil	Parameter used in the calculation of roughness length of heat (-)	0.05	0.8
21	csoil	Soil heat capacity for mineral soil component (-)	1.26E6	3.5E6
22	frzk	Ice threshold (-)	0.10	0.25
23	snup	Snow depth threshold that implies 100% snow cover (m)	0.02	0.08
24	sh2o1	Initial liquid soil moisture for soil layer 1 (m ³ m ⁻³)	0.05	0.50
25	sh2o2	Initial liquid soil moisture for soil layer 2 (m ³ m ⁻³)	0.05	0.50
26	sh2o3	Initial liquid soil moisture for soil layer 3 (m ³ m ⁻³)	0.05	0.50
27	sh2o4	Initial liquid soil moisture for soil layer 4 (m ³ m ⁻³)	0.05	0.50
28	smc1	Initial total soil moisture for soil layer 1 (m ³ m ⁻³)	0.05	0.50
29	smc2	Initial total soil moisture for soil layer 2 (m ³ m ⁻³)	0.05	0.50
30	smc3	Initial total soil moisture for soil layer 3 (m ³ m ⁻³)	0.05	0.50
31	smc4	Initial total soil moisture for soil layer 4 (m ³ m ⁻³)	0.05	0.50

Table 4. Comparison of domain averaged unbiased RMSE (ubRMSE) metric values from different model integrations (all with the 95% confidence intervals).

Experiment	Surface soil moisture (m^3m^{-3})	Root zone soil moisture (m^3m^{-3})
OL	0.052 ± 0.001	0.039 ± 0.001
DA-NOSC	0.041 ± 0.001	0.037 ± 0.001
DA-STDN	0.038 ± 0.001	0.035 ± 0.001
DA-CDF	0.037 ± 0.001	0.034 ± 0.001
DA-OPT1	0.037 ± 0.001	0.033 ± 0.001
DA-OPT6	0.036 ± 0.001	0.033 ± 0.001

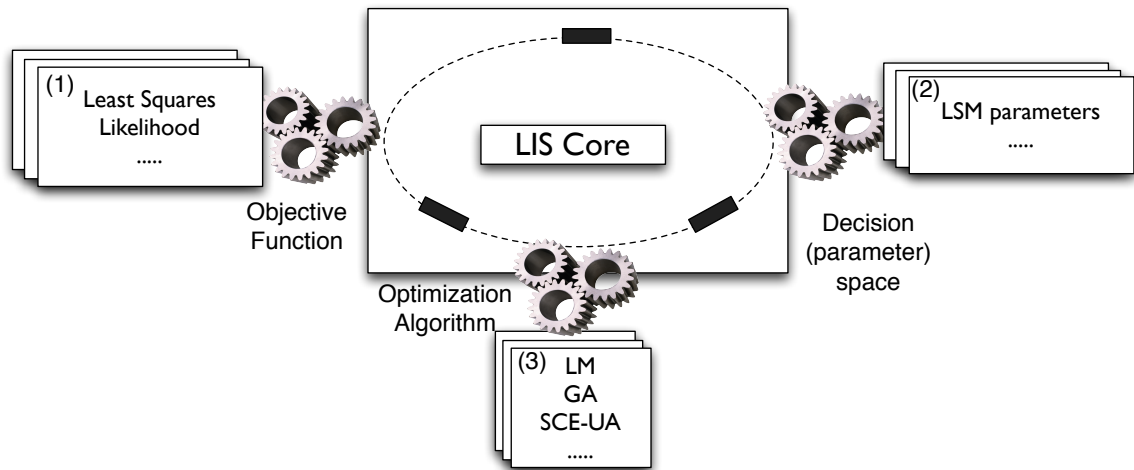


Figure 1. Optimization abstractions in LIS: (1) objective function, (2) decision/parameter space, and (3) optimization algorithm (LM - Levenberg-Marquardt, GA - Genetic Algorithm, SCE-UA - Shuffled Complex Evolution from University of Arizona). Dotted lines represent interconnections between the optimization abstractions enabled by the LIS core. Black boxes represent data exchanges between the three components through ESMF objects.

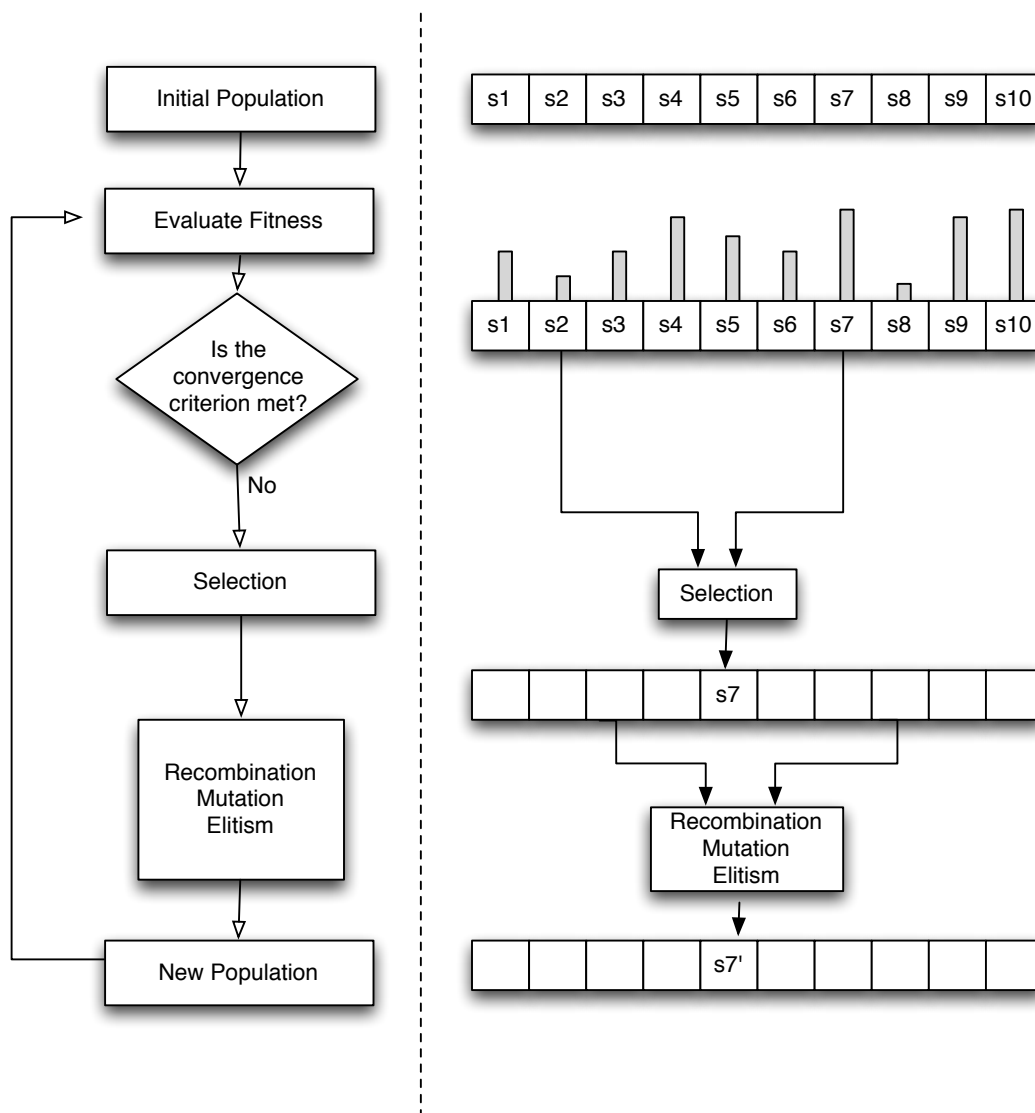


Figure 2. Sequence of GA operations. An example of the population evolution is shown on the right, with a population size of 10 potential solutions (s1, s2, ..., s10). The grey bars indicate the fitness values of the individual solutions. An example of the selection step shows the choice of s7 after comparing s2 and s7. After the selection step, the GA operations of recombination, mutation and elitism are conducted and a new population of solutions are generated. The algorithm continues until the convergence criteria are met.

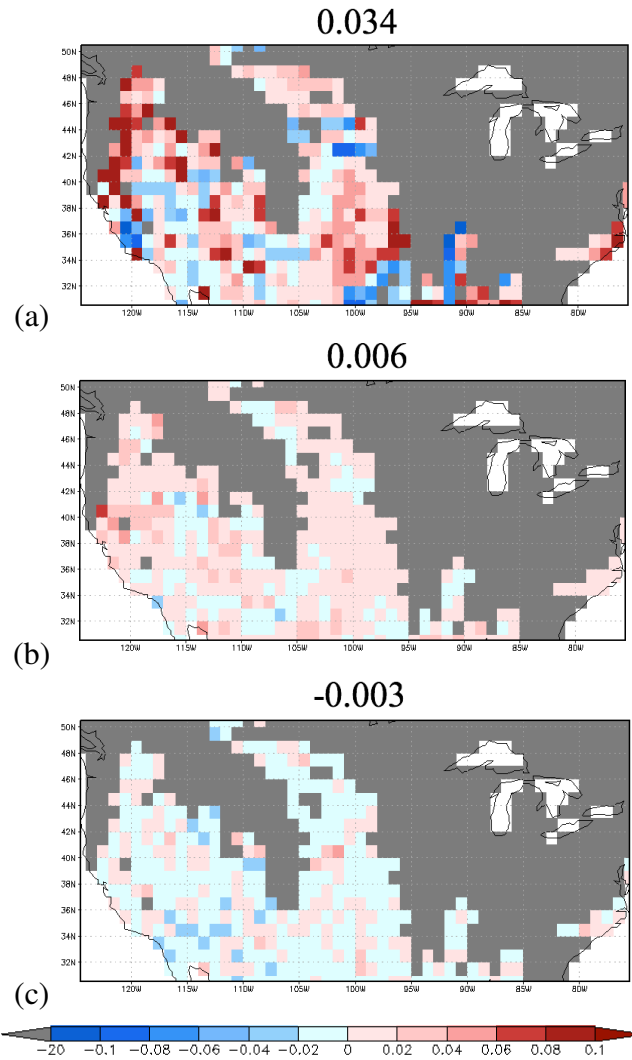


Figure 3. Comparison of the surface soil moisture climatology difference fields between the Catchment LSM truth and (a) OL (b) OPT1, and (c) OPT6 (see Table 1). The gray color represents grid cells excluded from the computations. Titles indicate domain averaged values. The units are m^3m^{-3}

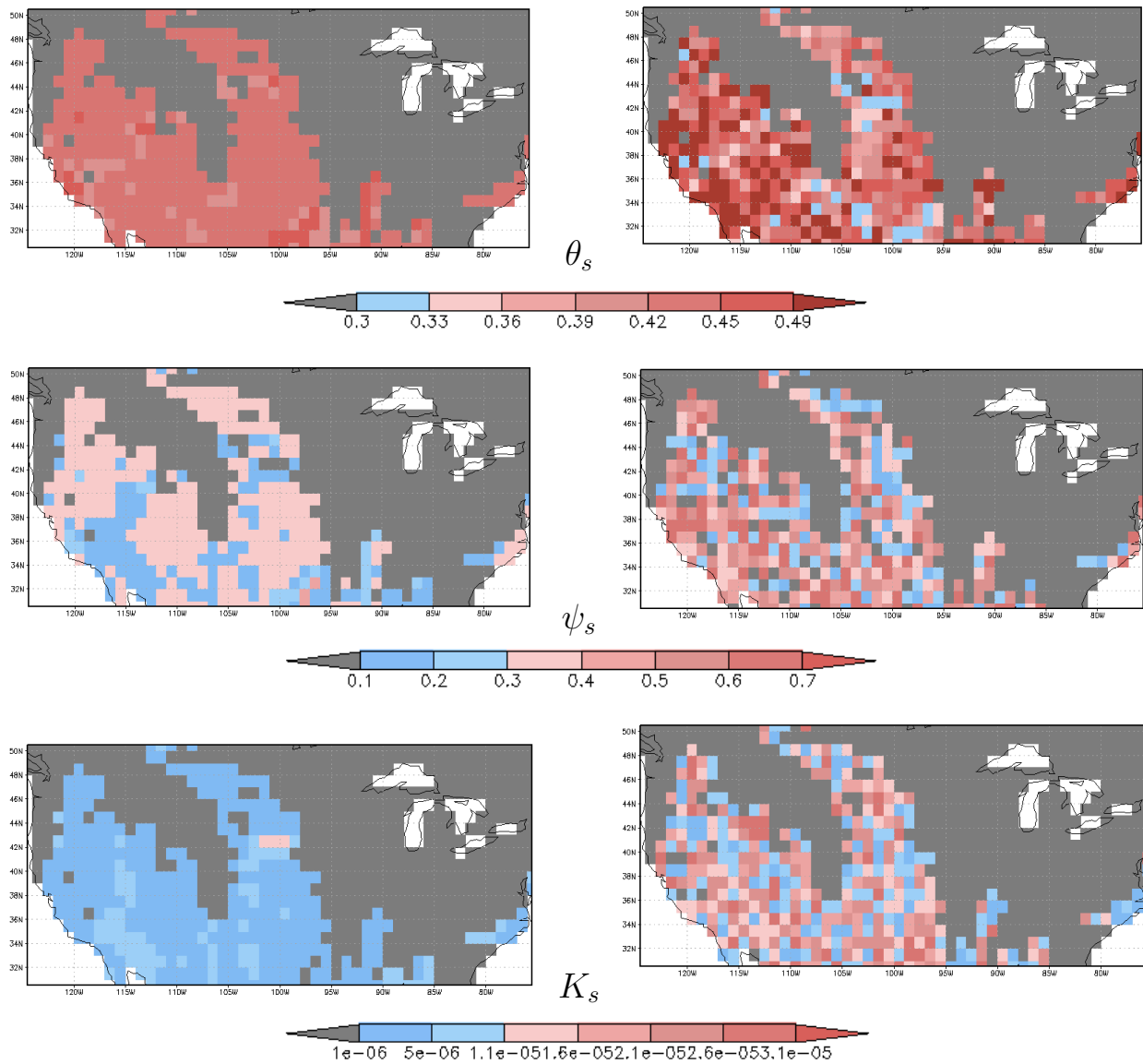


Figure 4. (Top) porosity (θ_s , unitless), (middle) saturated matric potential (ψ_s , unitless) and (bottom) saturated hydraulic conductivity (K_s , in units of m/s) from (left column) look up tables and (right column) estimated through optimization OPT6. The gray color represents grid cells for which parameters were not estimated.

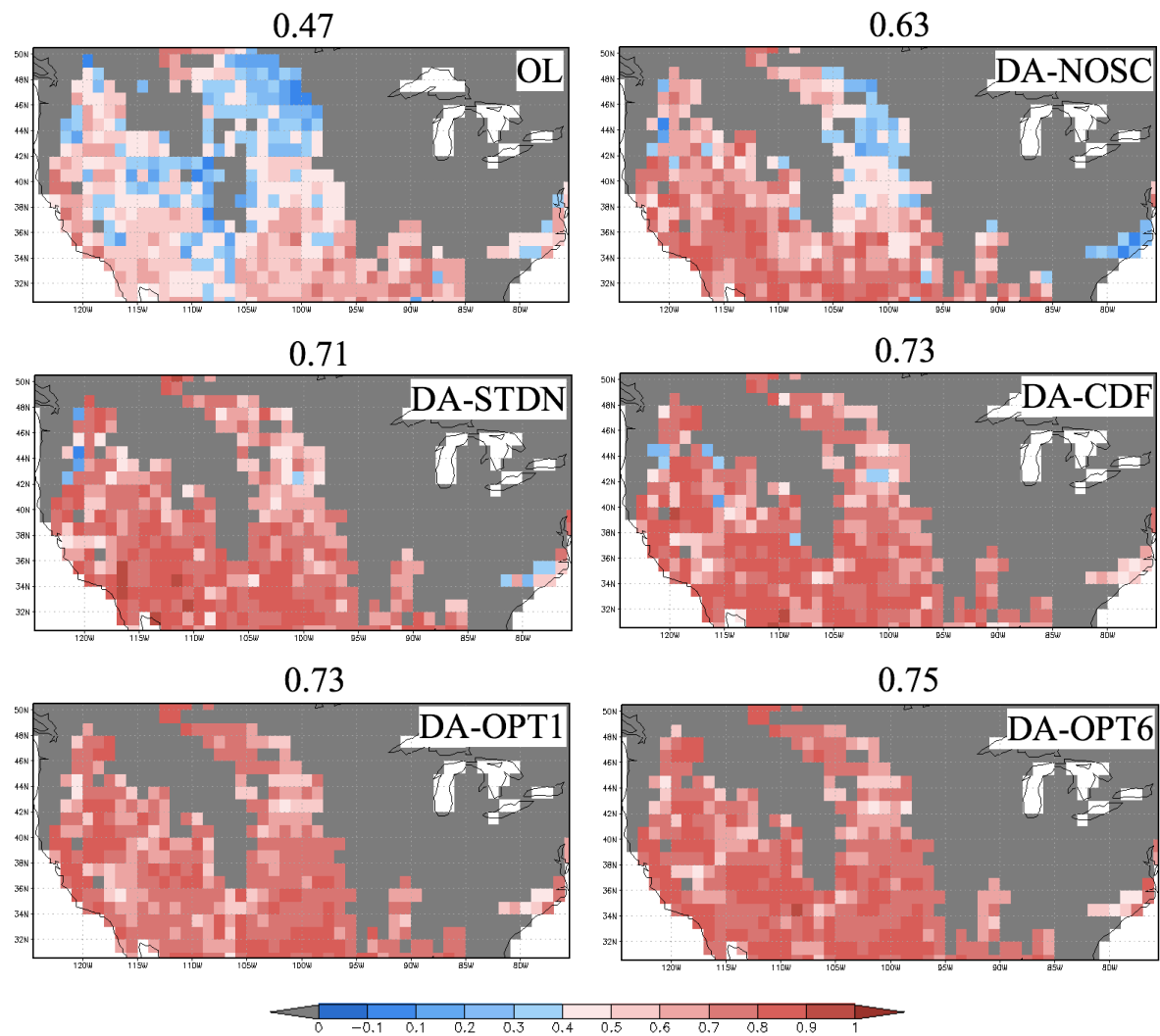


Figure 5. Surface soil moisture skill in terms of anomaly time series correlation coefficients. See table 1 for definition of experiments. The gray color represents grid cells excluded from the computations. Titles show domain averaged values.

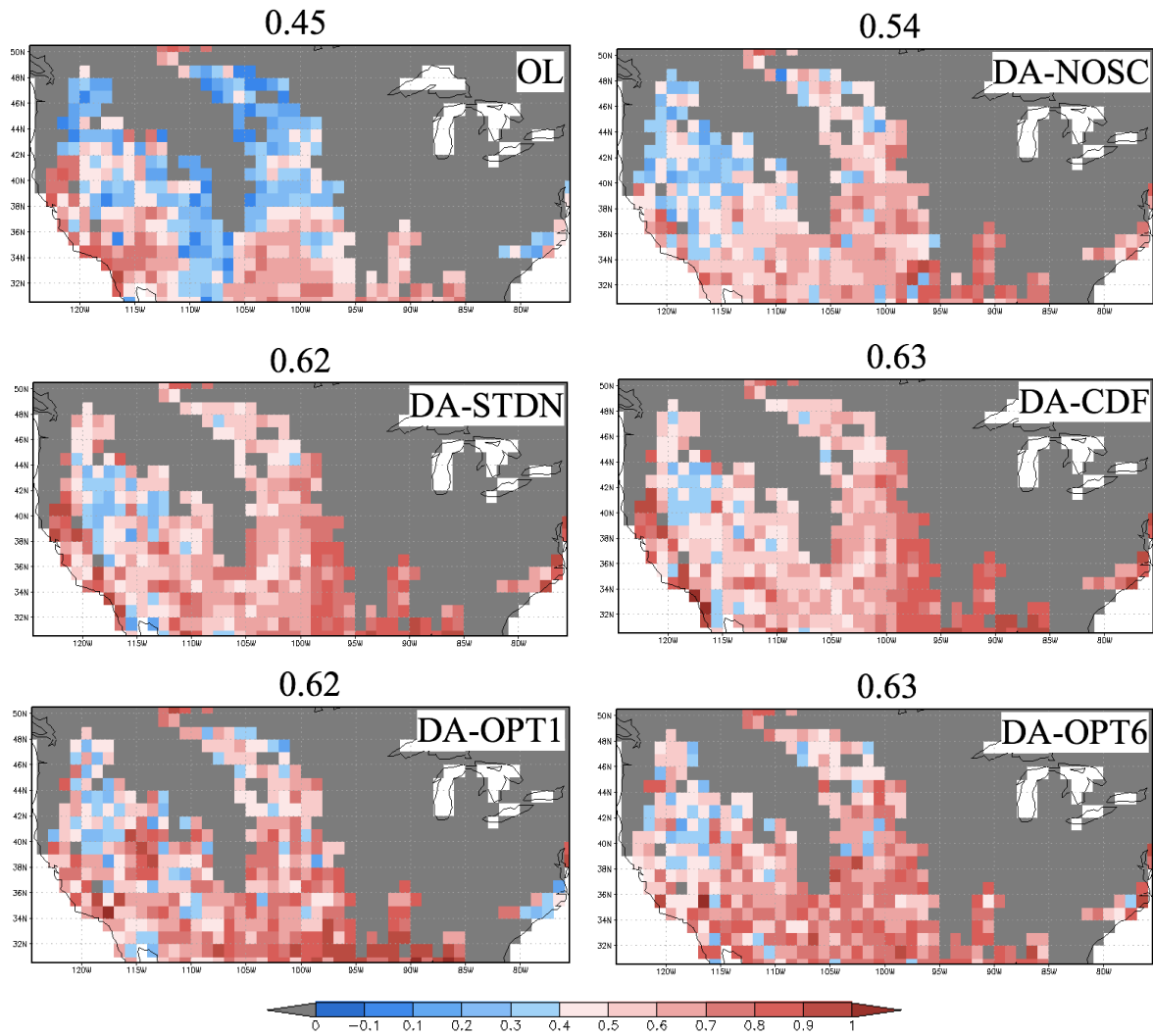


Figure 6. Same as Figure 5, but for root zone soil moisture.

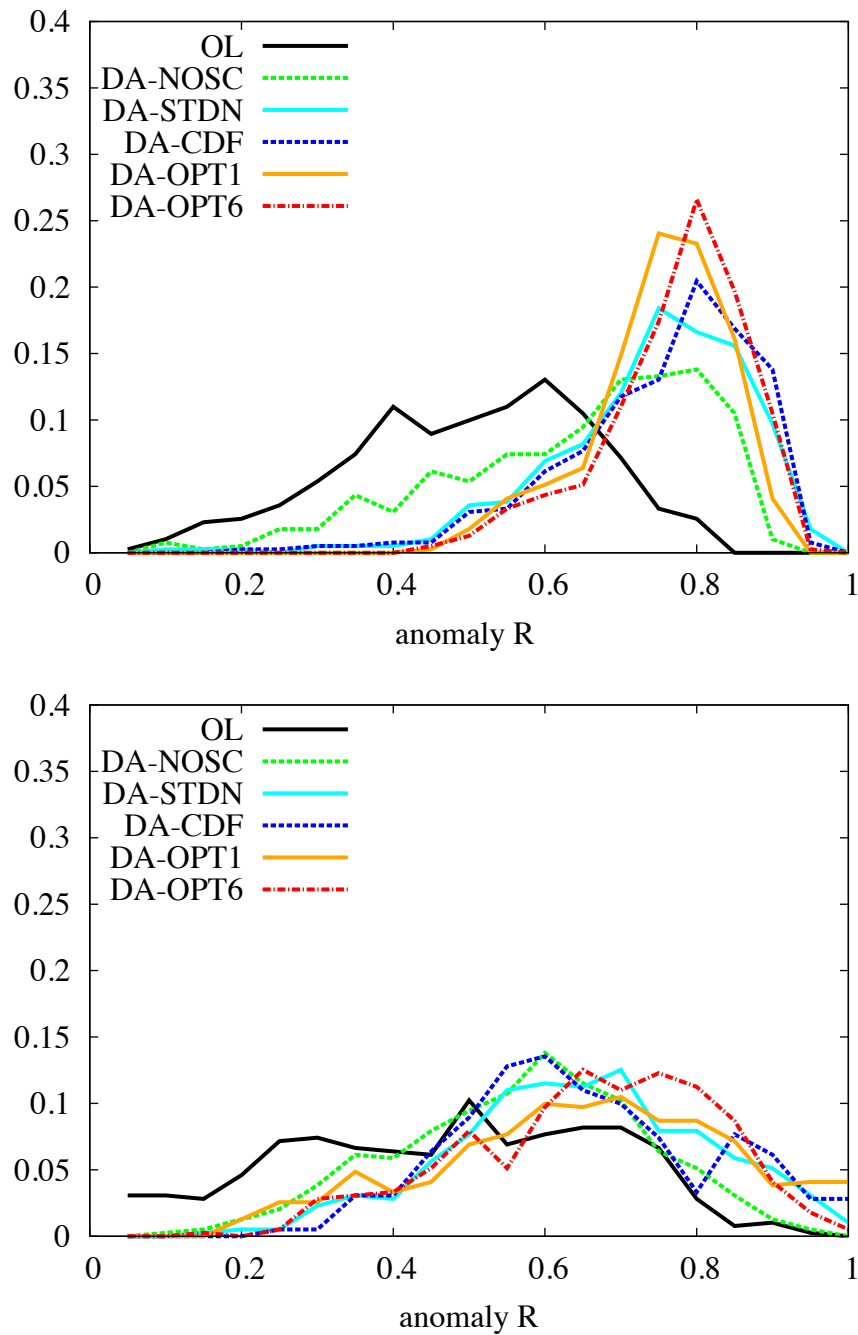


Figure 7. PDFs of skill (anomaly R) values across the domain from different model integrations for (top) surface soil moisture and (bottom) root zone soil moisture.

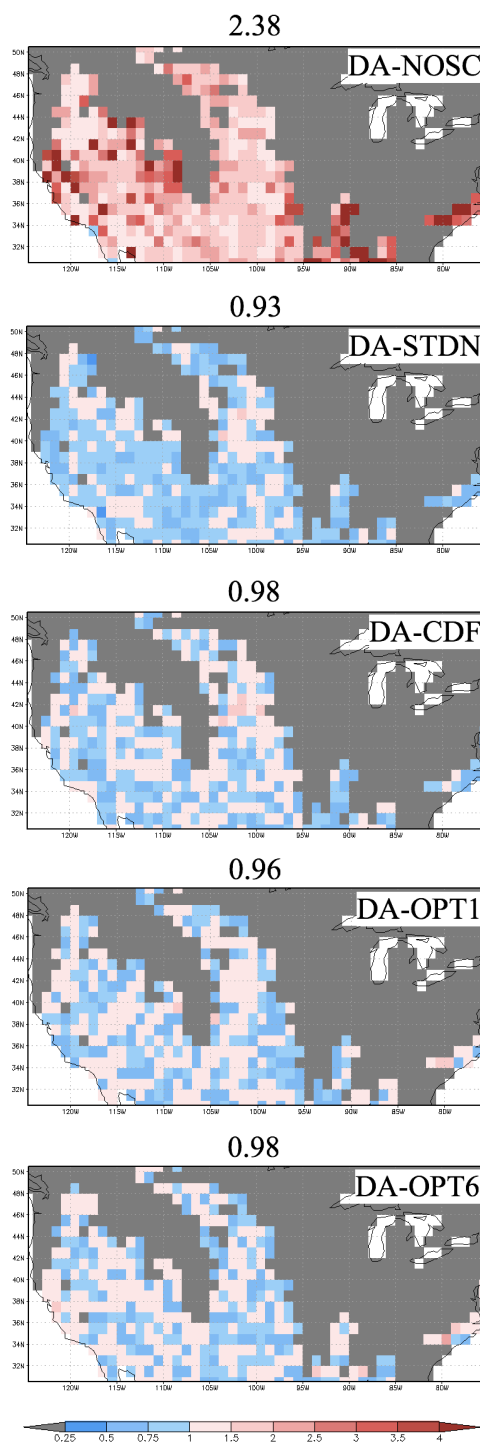


Figure 8. Variance of normalized innovations from different assimilation experiments. The gray color represents grid cells excluded from the computations. The titles indicate domain averaged values.