Calibration of an agricultural-hydrological model (RZWQM2) using surrogate global optimization

¹Maolong Xi, ^{2,*}Dan Lu, ^{3,*}Dongwei Gui, ⁴Zhiming Qi, ⁵Guannan Zhang

Abstract

Robust calibration of an agricultural-hydrological model is critical for simulating crop yield and water quality and making reasonable agricultural management. However, calibration of the agricultural-hydrological system models is challenging because of model complexity, the existence of strong parameter correlation, and significant computational requirements. Therefore, only a limited number of simulations can be allowed in any attempt to find a near-optimal solution within an affordable time, which greatly restricts the successful application of the model. The goal of this study is to locate the optimal solution of the Root Zone Water Quality Model (RZWQM2) given a limited simulation time, so as to improve the model simulation and help make rational and effective agricultural-hydrological decisions. To this end, we propose a computationally efficient global optimization procedure using sparse-grid based surrogates. We first used advanced sparse grid (SG) interpolation to construct a surrogate system of the actual RZWQM2, and then we calibrate the surrogate model using the global optimization algorithm, Quantum-behaved Particle Swarm Optimization (QPSO). As the surrogate model is a polynomial with fast evaluation, it can be efficiently evaluated with a sufficiently large number of times during the optimization, which facilitates the global search. We calibrate seven model parameters against five years of yield, drain flow, and NO_3^- -N loss data from a subsurface-drained corn-soybean field in Iowa. Results indicate that an accurate surrogate model can be created for the RZWQM2 with a relatively small number of SG points (i.e., RZWQM2 runs). Compared to the conventional QPSO algorithm, our surrogate-based optimization method can achieve a smaller objective function value and better calibration performance using a fewer number of expensive RZWQM2 executions, which greatly improves computational efficiency.

Keywords: RZWQM2; Sparse grid; Surrogate model; QPSO algorithm; Global optimization

1 Introduction

Agricultural-hydrological models are important tools in quantifying and improving our understanding of hydrologic processes and evaluating the influence of agronomic management practices on the water cycle, water quality, and agricultural production. Several agricultural-hydrological models have been developed and each model has its own features. For example, the SWAT model evaluates effects of alternative management decisions on water resources and nonpoint-source pollution in large river basins (Arnold et al., 2012; Wang et al., 2015a); the HYDRUS model simulates water, heat, and solute movement in variably saturated media (Šimůnek et al., 2008); and a newly developed model in Alam and Dutta (2012) focuses on nutrient dynamics in river basin. In this study, we considered the Root Zone Water Quality Model (RZWQM2), which simulates plant growth and water, nutrient, and pesticide movement based on soil physical characteristics and hydraulic properties. The RZWQM2 was developed by the U.S. Department of Agriculture, and it has been widely used to investigate effects of different agricultural management practices on crop yield and water quality. The model performance has been evaluated in several U.S. states (e.g., Colorado, Georgia, Iowa, Minnesota, Missouri, Montana, Nebraska and Ohio —Ghidey et al., 1999; Wu et al., 1999; Landa et al., 1999; Abrahamson et al., 2006; Saseendran et al., 2008; Thorp et al., 2008; Qi et al., 2011; Ma et al., 2012; Qi et al., 2013), and in other countries (e.g., Canada, China and Portugal — Ahmed et al., 2007; Cameira et al., 2005; Fang et al., 2014; Sun et al., 2016). Recently, RZWQM2 has been used to quantify climate change impacts on the hydrologic cycle and agro-environments such as cultivated fields (Ko et al., 2011; Islam et al., 2012; Wang et al., 2015b). In most cases, the model performed satisfactorily, but its performance is sensitive to particular and sometimes

poorly identified parameter values. Thus, calibration of RZWQM2 is crucial to its successful application.

Traditionally, RZWQM2 has been calibrated by trial-and-error methods. While this straightforward and simple method continues to be widely used (Qi et al., 2011; Ma et al., 2012; Malone et al., 2014; Shresthaa and Dattab, 2015), it is time-consuming and the termination process, heavily dependent on modelers' experience and expertise, suffers from subjectivity. Faced with the weakness inherent to manual methods, gradient-based automatic calibration tools, such as PEST (Doherty, 2004), have recently been employed to calibrate RZWQM2 (Malone et al., 2010; Fang et al., 2012). PEST adjusts model parameters to reduce the objective function value until the fit between model simulation results and measurement data is optimized. However, as a local optimizer, the use of PEST may result in different optimal parameter estimates when starting with different initial values, i.e., calibration results rely on the procedure initialization. In fact, for most gradient-based optimization methods, becoming trapped in a local objective function minimum is a common problem. To address this issue, Xi et al. (2015) applied a global search method, termed quantum-behaved particle swarm optimization (QPSO), to calibrate the RZWQM2 and obtained promising results.

Proposed by Sun et al. (2004), QPSO is a population-based swarm intelligence algorithm theoretically guaranteed to find optimal solutions in search space. Given its strong global convergence, the QPSO algorithm has been applied to many studies in recent years (Davoodi et al., 2014; Xi et al., 2015; Hassani and Lee, 2016). A review on its application can be found in Fang et al. (2010). Many numerical results indicated that with sufficiently large iterations (typically thousands or even hundred thousand), the QPSO can successfully identify globally optimal parameters (Sun et al., 2004; Omkar et al., 2009). However, in practice, a large number

of iterations are usually unaffordable, especially for complex system models such as the RZWQM2 where each model simulation typically takes several minutes or even hours. Consequently, application of the global QPSO algorithm may end up with providing a local optimum given the limited search resulting from the intensive expense of model runs.

In this study, the problem of the high computational cost of global optimization is resolved by combining surrogate modeling with the optimization operation to develop a surrogate-based optimization algorithm. The surrogate modeling involves constructing a cheap-to-evaluate surrogate model, which provides an accurate and efficient approximation to the input-output relation of the actual simulation model. Several surrogate methods have been developed including sparse-grid stochastic collocation that uses the sparse-grid interpolation (Nobile et al., 2008a, 2008b) and probabilistic collocation that uses the finite dimensional polynomial chaos expansion (Marzouk et al., 2007; Li and Zhang, 2007; Shi et al., 2009). Chang and Zhang (2009) provided a comprehensive comparison of the accuracy and efficiency of these two methods.

The idea of sparse-grid (SG) methods is to place a grid in the parameter space with sparse parameter samples (as opposed to a full tensor-product grid). Then the simulation model is solved only at these sparse parameter samples to construct an interpolant and this interpolant is the SG-based surrogate of the actual simulation model. The SG methods have been demonstrated to be efficient and effective in dealing with uncertainty quantification problems. For example, Shi and Yang (2009) and Lin and Tartakovsky (2009, 2010) used SG methods to estimate mean and covariance of groundwater state variables such as hydraulic head and solute concentrations. Ma and Zabaras (2009) and Zeng et al. (2012) used SG methods to build surrogate of geophysical models that were then employed to evaluate parameter distributions. Zhang et al. (2013) developed an adaptive SG method to accelerate Bayesian inference in groundwater

reactive transport modeling. Similarly, Zeng et al. (2016) recently evaluated two SG surrogates for groundwater Bayesian uncertainty quantification. However, the SG based surrogate approach has rarely been employed in the context of parameter estimation and never in agricultural-hydrological models.

Considering the importance of the parameter optimization in the RZWQM2 and the challenging in the calibration of the model, this work explores a computationally efficient global optimization scheme by combining SG-based surrogate methods with the QPSO algorithm and applies it to the RZWQM2. The developed method takes advantage of the global convergence of the QPSO while overcoming its drawbacks in poor computational efficiency by using surrogate modeling. The key idea is to use SG interpolation to construct a surrogate of the RZWQM2 in a polynomial form, and then evaluate the cheap-to-run surrogate model in the global optimization process so as to improve overall computational efficiency. The main contribution of our work lies in exploring the combination of a state-of-the-art SG surrogate method with a global optimization technique, and successfully applying this efficient method to find better solutions of the RZWQM2 than previous study (Qi et al. 2011, Xi et al., 2015), which greatly improves model calibration performance and helps make rational and effective agricultural-hydrological decisions.

The paper is organized as follows. The RZWQM2 and the surrogate optimization method are described in Section 2. In Section 3, we apply the approach to calibrating the RZWQM2, and we examine the effectiveness and efficiency of the method in comparison with the conventional QPSO algorithm. In Section 4, we further discuss the optimization results and show some insight on future studies. Lastly, we conclude this paper in Section 5.

2 Materials and Methods

2.1 Description of the RZWQM2 and calibration parameters

The Root Zone Water Quality Model (RZWQM2) is a one-dimensional system model that simulates major physical, chemical, and biological processes in an agricultural crop production system. It consists of components for hydrology, nutrition and pesticide transport and transformation, plant growth and crop production, and management activities (Ahuja et al., 2000; Ma et al., 2005; Ma et al., 2006). Each component is simulated by sub-models. For example, infiltration from rainfall, irrigation, or snowmelt is calculated using a modified Green-Ampt model. Water redistribution in the soil profile is simulated via the Richards equation by treating surface evaporation and plant root water uptake as sinks. Water stored in the soil profile, if exceeding the field capacity, is drained to build up a water table above the impermeable layer and the subsequent tile drainage flux is computed using the steady state Hooghoudt equation. In addition, lateral flow and seepage are quantified by user-defined parameters for constant bottom layer water flux rate and hydraulic gradient, respectively. For the upper boundary, soil evaporation and plant transpiration are estimated by the double layer model of Shuttleworth and Wallace (1985), which is an extension of the Penman-Monteith concept. Nutrient chemistry processes are simulated by OMNI (Shaffer et al., 2000), a state-of-the-art model for carbon and nitrogen cycling in soils. The DSSAT cropping system models (Jones et al., 2003) are incorporated to predict crop establishment and water and nutrient uptake.

In this study, the RZWQM2 was used to simulate crop growth, hydrology, and nitrate loss in a subsurface-drained corn-soybean field in Iowa. For this problem, the model involves about 230 parameters, most of which are measured or estimated, some for which default values are used; however, still a significant number of parameters require calibration against observed data.

Here, we focus on adjusting seven parameters that are related to crop growth, soil-root growth, and hydraulic gradient. They are denoted as G2, G3, PHINT, SRGF_Corn, LFMAX, SRGF_Soybean, and LHG, and described in Table 1. According to sensitivity analysis, the seven parameters are sensitive to the crop yields, drain flow, and NO_3 -N loss whose observation data were used for model calibration as described in Section 2.2. For example, the crop growth parameters directly control crop yields, biomass, and crop N uptake; and indirectly affect evapotranspiration, subsurface drainage, and NO_3 -N loss. Crop evapotranspiration is a function of leaf area, subsurface drainage is determined through water balance, and NO_3 -N loss is computed as a product of subsurface drainage volume and NO_3 -N concentration. The soil-root growth factor determines crop water uptake, which, in turn, indirectly affects drainage flow, N uptake, and N loss. The product of the hydraulic gradient and water table depth controls lateral water loss, which combined with deep seepage are two major factors influencing subsurface drainage flow. In the simulation, the deep seepage rate was set to zero. In addition, the seven parameters were the target in the previous studies of parameter estimation for the RZWQM2 and their accuracy significantly determines the model performance (Qi et al. 2011; Xi et al., 2015). Parameters defined in the RZWQM2 but not considered in the calibration were specified using measured or default values or drawn from similar studies (Bakhsh et al., 2001; Ma et al., 2007; Thorp et al, 2007). Reasonable ranges of the seven calibration parameters, listed in Table 1, were determined based on a previous study (Xi et al., 2015). These ranges were set large enough to cover all the possible values for all the known crops being physically reasonable (Ma et al., 2000).

2.2 Surrogate optimization method

Five years (2005-2009) of yield, drain flow, and NO_3 -N loss measurements from a subsurface-drained corn-soybean field near Gilmore City in Iowa, i.e., total 15 data, were employed for parameter calibration. The goal is to minimize the difference between model simulations of the three outputs and their corresponding measurements by adjusting the model parameters, so as to improve the model performance. In this section, we first formulate the objective function and then introduce our surrogate-based global optimization algorithm to minimize the objective function.

2.2.1 Objective function formulation

The objective function for a single output component is defined as the root mean squared weighted difference between model simulations and the corresponding field measurements. And the objective function for the three outputs is formulated as the weighted sum of the one for an individual component, i.e.,

$$\sum_{j=1}^m \gamma_j \cdot \sqrt{\frac{1}{n} \sum_{i=1}^n [\omega_{j,i} \cdot (Y_{j,i}^{obs} - Y_{j,i}^{sim}(\theta))]^2} \quad (1)$$

where $Y_{j,i}^{sim}(\theta)$ represents the model simulations based on parameters θ ; $Y_{j,i}^{obs}$ represents the field measurements; i is the year index for the measured data, and total $n=5$ years data are used for calibration; j is the index of model output component, and a total $m=3$ components are considered. The weight of the measurements for a certain year i is calculated as product of its inverse value and the maximum measurement over the five years:

$$\omega_{j,i} = \frac{\max(Y_{j,i}^{obs})}{Y_{j,i}^{obs}}. \quad (2)$$

We use a weight γ_j to balance the effect of different magnitudes of different components on the objective function. The weight is calculated as,

$$\gamma_j = \frac{\sum_{i=1}^5 Y_{1,i}^{obs}}{\sum_{i=1}^5 Y_{j,i}^{obs}}, j = 1, 2, 3. \quad (3)$$

According to the measurement data, the γ_1 , γ_2 , and γ_3 in Eq. (3) have values of 1.0, 204.0, and 153.4, respectively.

2.2.2 QPSO algorithm for global optimization

The QPSO algorithm is derived from particle swarm optimization (PSO), which is a population-based swarm intelligence algorithm for optimization over a continuous search space (Kennedy and Eberhart, 1995). In both PSO and QPSO, every particle in the parameter space explores a possible solution. The particles move around in the space with state constantly updated by the particle's own experience and the experience of the entire swarm. The personal best position is the best solution that is found so far by the particle in the course of the movement, denoted as *pbest*. The best position discovered by the whole swarm is the global best solution, denoted as *gbest*. The algorithms evaluate the objective function at all particles in each iteration and updates the *pbest* and *gbest* based on the minimum values found to that point. As the objective function decreases, the particles move closer to the best solution; the search ends when the maximum number of iterations is reached or the change of the objective function values in a certain number of iterations satisfies some threshold. Then the position of the particle corresponding to *gbest* is taken to be the optimal parameter solution. In this process, as the number of iterations is increasing, the objective function value is decreasing, i.e., the objective function value in the next iteration will be no larger than that in the current iteration. Therefore, the longer the search is, the higher the possibility that the global solution will be located. This

general procedure applies to both the PSO and QPSO algorithms; the difference between them is the way they update the state of the particles, as discussed below.

The PSO algorithm uses velocity and position to describe the state of a particle. For S particles, $\theta_1, \theta_2, \dots, \theta_S$, given initial positions $\{\theta_i^t\}_{i=1}^S$ and velocities $\{V_i^t\}_{i=1}^S$, the velocity and position of particle i at $(t+1)^{th}$ iteration are updated by the following equations:

$$V_i^{t+1} = w \cdot V_i^t + c_1 \cdot r_1^t(pbest_i^t - \theta_i^t) + c_2 \cdot r_2^t(gbest^t - \theta_i^t) \quad (4)$$

$$\theta_i^{t+1} = \theta_i^t + V_i^{t+1} \quad (5)$$

where w is the inertia factor; c_1 and c_2 are two positive constants controlling the relative proportion of cognition and social interaction, respectively; r_1 and r_2 are two independent random numbers uniformly distributed in the range $[0, 1]$. So the update in Eq. (4) is comprised of three portions: current state of the swarm, individual particle's experience, and information of the whole swarm.

The PSO algorithm is computationally inexpensive, but its main disadvantage is that global convergence cannot be guaranteed because each particle in the PSO converges to the best global position independently (Bergh, 2001). The quantum-behaved PSO algorithm was developed to address this issue (Sun et al., 2004). In the QPSO algorithm, the state of a particle is depicted by its wave function $\psi(\theta, t)$ instead of its position and velocity, resulting in the dynamic behavior of the particle in QPSO being distinctly different from that in the PSO system, since the particle's exact position and velocity cannot be determined simultaneously. We can only learn the probability of the particle's appearing at a certain position from its probability density function $|\psi(\theta, t)|^2$. By employing sampling methods such as Monte Carlo techniques, the particle's position is updated according to the following equations:

$$\theta_i^{t+1} = P_i^t \pm \beta \cdot |mbest^t - \theta_i^t| \cdot \ln(1/\mu_i^t) \quad (6)$$

248 where,

$$P_i^t = \alpha_i^t \cdot pbest_i^t + (1 - \alpha_i^t) \cdot gbest^t, \quad (7)$$

$$mbest^t = \frac{1}{S} \sum_{i=1}^S pbest_i^t. \quad (8)$$

249 ***mbest*** is mean best position defined as the mean of all the best positions of the particle swarm.

250 The α and μ are random numbers distributed uniformly in the range [0, 1]. The contraction-

251 expansion coefficient β is the only parameter in the QPSO algorithm that needs to be tuned to

252 control the algorithm performance.

253 Compared to the traditional PSO scheme, the QPSO algorithm guarantees global

254 convergence but at the cost of a slower rate (Omkar et al., 2009). Due to the introduction of the

255 ***mbest*** concept, each particle in QPSO cannot converge to the global best position without

256 considering other particles in the swarm; this avoids the independent convergence of the

257 individual particles and greatly improves the global search ability. As the distance between the

258 particle's current position and the ***mbest*** (Eq. (6)) determines the position distribution of the

259 particle for next iteration, it also slows down the convergence. For example, when the personal

260 best positions ***pbest*** of several particles (called lagged particles) are far away from the global best

261 position and some other particles (called good particles) are closer to the ***gbest***, the position

262 ***mbest*** will be pulled away from the ***gbest*** by the lagged particles. In this situation, the time spent

263 by the lagged particles in chasing their colleagues in the swarm deteriorates the convergence of

264 the ***mbest*** to the ***gbest***, which in turn decelerates the decrease of the distance between the ***mbest***

265 and the ***pbest*** of the good particles. So the good particles spend quite a bit time on local

266 exploration waiting for the lagged particles to approach the ***gbest***. The wait mechanism among

particles significantly enhances the global search ability of the QPSO algorithm but on the other hand, decelerates its convergence.

Hence, QPSO algorithm requires a computational improvement, especially when applied to complex problems with long model executions, e.g., the RZWQM2 considered in this study that takes 3 to 4 minutes per simulation on a PC. In addition, the QPSO algorithm evaluates the objective function for every particle at each iteration, so the total number of model executions is the product of the number of particles and the maximum iterations. As the algorithm takes a relatively long period of global exploration, the total number of model runs can be very large. Two strategies can reduce the computational cost, one is to reduce the number of particles and iterations, and the other is to reduce the computational time of a single model execution. The first strategy may result in a near-optimal parameter estimate when the particles are not sufficient for parameter space exploration and when the iterations are not large enough to guarantee global convergence. In this study, we adopt the second strategy, building a cheap-to-evaluate surrogate of the computationally expensive RZWQM2 based on sparse grid interpolation.

2.2.3 Sparse-grid based surrogate method

In this section, we introduce the sparse grid (SG) interpolation to construct a surrogate model of the RZWQM2. In construction, the RZWQM2 is treated as a black box, with input θ and output $Y^{sim}(\theta)$ defined in Eq. (1). Based on a set of θ and $Y^{sim}(\theta)$ values, the surrogate system is constructed to approximate the relation between the input and output of the RZWQM2. The main idea of the SG-based surrogate method is to build a surrogate model using a sparse tensor product, as opposed to a full tensor product, of a hierarchy of one-dimensional interpolation rules (Zhang et al., 2015, 2016). In this way, the sparse grid interpolation has

comparable accuracy to the full tensor interpolation but with fewer samples of $\boldsymbol{\theta}$, thus improving the computational efficiency.

For notation simplicity, we denote the black-box model of RZWQM2 as $\eta(\boldsymbol{\theta})$. We first introduce a hierarchy of interpolation rules in one dimension case ($d = 1$); then move to a high-dimensional interpolation, where we introduce the full tensor interpolation first and then step into the sparse grid interpolation naturally. For a function $\eta(\boldsymbol{\theta}): [0,1] \rightarrow \mathbb{R}$, where the standard domain $[0,1]$ can be rescaled to any bounded domain by translation and dilation, a 1-D hierarchical Lagrange interpolation operator, denoted by $\mathcal{U}^{N_\ell}[\cdot]$, can be represented as

$$\mathcal{U}^{N_\ell}[\eta](\theta) := \sum_{j=1}^{N_\ell} \eta(\theta_j^\ell) \phi_j^\ell(\theta), \quad (9)$$

where $\ell \in \mathbb{N}_+$ is called the *resolution level* of the operator $\mathcal{U}^{N_\ell}$, N_ℓ is the number of degrees of freedom on level ℓ , $\{\phi_j^\ell\}_{j=0}^{N_\ell}$ is the set of Lagrange basis functions, and $\{\theta_j^\ell\}_{j=0}^{N_\ell}$ is the set of corresponding interpolation points. Note that N_ℓ grows monotonically with ℓ , i.e., $N_{\ell'} < N_\ell$ if $\ell' < \ell$. In addition, we define the difference operator

$$\Delta^\ell := \mathcal{U}^{N_\ell} - \mathcal{U}^{N_{\ell-1}},$$

with $\mathcal{U}^{N_0} := 0$, such that $\mathcal{U}^{N_\ell} = \sum_{\ell'=0}^{\ell} \Delta^{\ell'}$.

In the multidimensional case ($d > 1$), the tensorized operator can be defined by

$$\mathcal{U}^{N_{\ell_1}} \otimes \cdots \otimes \mathcal{U}^{N_{\ell_d}}[\eta](\boldsymbol{\theta}) := \sum_{j_1=1}^{N_{\ell_1}} \cdots \sum_{j_d=1}^{N_{\ell_d}} \eta(\theta_{j_1}^{\ell_1}, \dots, \theta_{j_d}^{\ell_d}) \left(\prod_{i=1}^d \phi_{j_i}^{\ell_i}(\theta_i) \right), \quad (10)$$

where, for each dimension $i = 1, \dots, d$, the notations N_{ℓ_i} , $\{\theta_{j_i}^{\ell_i}\}_{j_i=1}^{N_{\ell_i}}$ and $\phi_{j_i}^{\ell_i}$ have the same meaning as in the one-dimensional case. Prior to the development of sparse tensorization, an isotropic tensor-product operator was the most common way to handle multidimensional

307 interpolation. The isotropy refers to that we set $N_L = N_{\ell_1} = \dots = N_{\ell_d}$, i.e., $L = \ell_1 = \dots = \ell_d$. In
 308 this case, the interpolation operator in Eq. (10) can be represented by a full tensor product of the
 309 difference operators, i.e.,

$$\mathcal{U}^{N_L} \otimes \dots \otimes \mathcal{U}^{N_L} = \sum_{|\boldsymbol{\ell}|_\infty \leq L} \Delta^{\ell_1} \otimes \dots \otimes \Delta^{\ell_d}, \quad (11)$$

310 where $\boldsymbol{\ell} := (\ell_1, \dots, \ell_d)$ and $|\boldsymbol{\ell}|_\infty := \max_{1 \leq i \leq d} \ell_i$. For the full tensor interpolant in Eq. (11), the
 311 total number of interpolation points is N_L^d , which grows *exponentially* with the dimension d .
 312 Thus, the full tensor interpolation usually applies to low dimensional problems (typically for
 313 $d \leq 3$) and is computationally infeasible for high-dimensional cases. Then, the sparse-grid
 314 interpolation was developed with the aim of using fewer interpolation points to achieve a
 315 comparable accuracy with the full tensor interpolation (Barthelmann et al., 2000, Gunzburger et
 316 al. 2016):

$$\begin{aligned} \mathfrak{I}^{L,d}[\eta] &:= \sum_{|\boldsymbol{\ell}|_1 \leq L} \Delta^{\ell_1} \otimes \dots \otimes \Delta^{\ell_d}[\eta] \\ &= \sum_{L-d+1 \leq |\boldsymbol{\ell}|_1 \leq L} (-1)^{L-|\boldsymbol{\ell}|_1} \binom{d-1}{L-|\boldsymbol{\ell}|_1} \mathcal{U}^{N_{\ell_1}} \otimes \dots \otimes \mathcal{U}^{N_{\ell_d}}[\eta], \end{aligned} \quad (12)$$

317 where $|\boldsymbol{\ell}|_1 := \ell_1 + \ell_2 + \dots + \ell_d$. The main difference between Eq. (11) and Eq. (12) is the way
 318 to select $\Delta^{\ell_1} \otimes \dots \otimes \Delta^{\ell_d}$. Compared to using the infinity norm $|\boldsymbol{\ell}|_\infty$ in the full tensor interpolant,
 319 the SG interpolant uses the one norm $|\boldsymbol{\ell}|_1$, which causes the set of indices satisfying $|\boldsymbol{\ell}|_1 \leq L$
 320 much smaller than the set satisfying $|\boldsymbol{\ell}|_\infty \leq L$. Therefore, for any given L , the SG interpolation
 321 requires much fewer interpolation points than the full tensor interpolation. Generally speaking,
 322 the SG interpolation needs approximately $\mathcal{O}(N_L \cdot (\log N_L)^{d-1})$ grid points with $N_L =$
 323 $\max_{i=1,\dots,d} (N_{\ell_i})$ while the full tensor interpolation needs $\mathcal{O}(N_L^d)$ (Bungartz and Griebel, 2004).

The sparse grid interpolant in Eq. (12) is uniquely determined by the choice of the one-dimensional rule in Eq. (9), i.e., the type of interpolation points, and the growth rule of N_ℓ . Several rules have been proposed to construct the sparse grid, among which the most common choice is the Chebyshev rule. The Chebyshev rule has optimal stability and the Chebyshev points can result in nested sparse grid when setting $N_1 = 1, N_2 = 3$, and $N_\ell = 2N_{\ell-1} - 1$, for $\ell > 2$. The nestedness has been proven to be critical in controlling the total number of the SG points and in the SG construction. Here, we use a two-dimensional example to illustrate the SG construction based on the Chebyshev rule; the procedure is depicted in Fig. 1. For a function $\eta(\boldsymbol{\theta})$ with two parameters ($d = 2$), given $L = 5$, to satisfy $|\boldsymbol{\ell}|_1 := \ell_1 + \ell_2 \leq 5$, the resolution level in one dimension can be $\ell_1 = 1, 2, 3, 4$, as shown in top horizontal lines of Fig. 1(a); and the other dimension, correspondingly, can also be $\ell_2 = 1, 2, 3, 4$, as listed on left vertical lines of Fig. 1(a). Different combinations of ℓ_1 and ℓ_2 with $\ell_1 + \ell_2 \leq 5$ construct ten coarse grids. For the i -th dimension with level ℓ_i in any coarse grid, the number of interpolation points N_{ℓ_i} is calculated as $N_1 = 1, N_2 = 3$, and $N_{\ell_i} = 2N_{\ell_i-1} - 1$, for $\ell_i > 2$ according to the nested Chebyshev rule. For example, the top-right coarse grid in Fig. 1(a) with $\ell_1 = 4$ and $\ell_2 = 1$ has a total of $N_4 \times N_1 = 9$ points. Each coarse grid in Fig. 1(a) corresponds to an interpolant $\mathcal{U}^{N_{\ell_1}} \otimes \mathcal{U}^{N_{\ell_2}}[\eta]$ in Eq. (12). Taking the union of the ten coarse grids, we get the final sparse grid shown in Fig. 1(b). Likewise, taking the weighted sum of the ten interpolants, we get the final SG interpolant in Eq. (12) for the function $\eta(\boldsymbol{\theta})$. The use of Chebyshev points and the definition of N_{ℓ_i} result in many redundant points in the ten coarse grids, making the final sparse grid have only 29 points. Compared to the full tensor grid with 81 points (Fig. 1(c)), the reduction is significant even though the maximum number of interpolation points in each dimension is the same for both grids. With a much smaller number of points, however, the accuracy of the spares-

grid interpolant is not greatly deteriorated compared to the full tensor grid, as proven in Barthelmann et al. (2000).

The Chebyshev rule is straightforward and commonly used, but it is not the most efficient one. Recently, Leja points have been introduced for SG construction and shown that the sparse grid constructed on the Leja points is superior to more standard SG constructions including the Chebyshev points (Calvi and Manh, 2012; Narayan and Jakeman, 2014). The Leja points maintain the nestedness but achieve it using the fast linear growth rule, i.e., $N_\ell = N_{\ell-1} + 1$, which greatly reduces the required points for interpolation. For example, the problem defined in Fig. 1 requires 29 Chebyshev points, but only 15 Leja points can achieve the comparable accuracy. Here we use the standard Chebyshev rule for explanation and demonstration due to its simplicity and nice visualization. In the numerical example, we apply the Leja rule for its efficiency. The SG constructed based on Leja rule is a global SG. Some adaptive local SG methods (Zhang et al., 2013) can also be applied, which start from an initial coarse grid and then add more points in the area with more variability. The adaptive SG methods work efficiently in low-dimensional functions ($d < 4$) with irregular behavior, but it is rather computationally expensive when applied to high dimensional cases by conducting mesh refinement. In this study, the adaptive SG method was also applied for the RZWQM2, but it turned out that its performance was worse than the SG using Leja points. The SG construction is implemented using TASMANIAN, a toolkit for adaptive stochastic modeling and non-intrusive approximation developed by the authors and their colleagues in the Oak Ridge National Laboratory (Stoyanov and Webster, 2016). The TASMANIAN implements several interpolation rules and can be used to reproduce the SG constructed in this study.

After the surrogate system is constructed, we use the surrogate model, $\mathfrak{T}^{L,d}[\eta]$ defined in Eq. (12), instead of the actual RZWQM2, to evaluate the objective function in the QPSO algorithm. As the evaluation of the surrogate model is very computationally fast (<1 sec), our surrogate-based optimization method can be affordably conducted for a sufficiently large number of iterations to ensure global convergence, but still with reduced computational cost compared to the conventional QPSO algorithm.

3 Results

3.1 Numerical experiments

To illustrate the effectiveness and efficiency of the proposed sparse-grid based surrogate global optimization method, it was applied to calibrate seven RZWQM2 parameters (Table 1). Two numerical experiments were conducted, one evaluating the surrogate global optimization method (S-QPSO), the other evaluating the conventional QPSO algorithm without surrogate modeling (R-QPSO). In a first step, simulations between the surrogate and the RZWQM2 model were compared to assess how well the constructed surrogate system captures the actual model. The computational efficiency of the surrogate was then assessed from two perspectives: (i) comparing the number of model executions required by the S-QPSO and R-QPSO methods to obtain a similar optimization performance, and (ii) comparing the calibration performance between the two approaches for a given number of model runs. These two criteria are complementary in that the first represents the situation where a large number of model runs are affordable, while the second addresses a situation where a limited number of model executions are affordable. Finally, we applied the calibrated RZWQM2 based on the S-QPSO and R-QPSO methods, respectively, to predict a different set of treatment data, so as to assess model performances in a contrasted crop growth conditions.

The optimization performance of S-QPSO and R-QPSO methods was evaluated by comparing their objective function values and their model fits to the observed data, based on the calibrated parameters. The goal of the optimization problem was to find the best set of parameters that minimizes the objective function, therefore, the method providing the smaller objective function values was considered to have better performance. Four statistical metrics served to assess model fit: percent bias (PBIAS), coefficient of determination of the linear relationship between simulated and observed values (R^2), Nash-Sutcliffe efficiency (NSE), and the ratio of root mean squared error to standard error (RSR) (Qi et al., 2011):

$$PBIAS = \frac{\sum_{i=1}^n (Y_i^{obs} - Y_i^{sim}) * (100)}{\sum_{i=1}^n Y_i^{obs}}, \quad (13)$$

$$R^2 = \frac{[\sum_{i=1}^n (Y_i^{obs} - \bar{Y})(Y_i^{sim} - \bar{Y}^{sim})]^2}{\sum_{i=1}^n (Y_i^{obs} - \bar{Y})^2 \cdot \sum_{i=1}^n (Y_i^{sim} - \bar{Y}^{sim})^2}, \quad (14)$$

$$NSE = 1 - \frac{\sum_{i=1}^n (Y_i^{obs} - Y_i^{sim})^2}{\sum_{i=1}^n (Y_i^{obs} - \bar{Y})^2}, \quad (15)$$

$$RSR = \frac{\sqrt{\sum_{i=1}^n (Y_i^{obs} - Y_i^{sim})^2}}{\sqrt{\sum_{i=1}^n (Y_i^{obs} - \bar{Y})^2}}. \quad (16)$$

Y_i^{obs} is the i^{th} observation, Y_i^{sim} is the corresponding simulated value, $\bar{Y}$ is the mean of all observations, n is the number of observations, and $\bar{Y}^{sim}$ is the mean of the simulated values.

The four metrics were also used to evaluate the model performance in the prediction phase. According to Moriasi et al. (2007), when $NSE > 0.50$, $RSR < 0.70$, and PBIAS is within $\pm 25\%$, the model fit is considered to be “satisfactory”. Recently, Ritter and Muñoz-Carpena (2013) recommended that the “satisfactory” model fit should have NSE value greater than 0.65. We will consider both criteria when we discuss the results. In addition, in evaluating the model we will

not only assess the goodness-of-fit but also analyze the physical reasonableness and realism of the optimized parameters.

3.2 Accuracy of surrogate model

The surrogate system was constructed using a five level sparse grid with 792 Leja points, i.e., 792 model executions of the RZWQM2. Based on 100 parameter samples randomly selected throughout the parameter space, a comparison between the surrogate model and the RZWQM2 in simulating different years' drainage, NO_3 -N loss and yield indicates that the surrogate model is sufficiently accurate to approximate the computationally intensive RZWQM2. As shown in Fig. 2, simulations of the two models correspond to each other almost perfectly with correlation coefficients up to 1.0; all points in the scatter plot lie close to or sit on the straight line that represents agreement of the two simulations. The averaged relative errors over the 100 samples are 0.3%, 0.8%, and 0.9%, respectively, for the three model outputs, which again indicates a minor difference between the simulations of the surrogate model and the RZWQM2 model.

3.3 Parameter optimization results

In both R-QPSO and S-QPSO, 20 particles were used; they were initialized randomly from uniform distributions with the ranges shown in Table 1. The maximum iteration for the R-QPSO was set to 50, while for the S-QPSO it was set to 500 given the computationally cheap surrogate model runs. Therefore, the total computational cost for the R-QPSO was $20 \times 50 = 1000$ RZWQM2 runs, but for the S-QPSO the cost was only 792 RZWQM2 runs, which were used for the surrogate construction. After that, no further RZWQM2 runs were required by S-QPSO but some negligible computational time spent for the polynomial evaluations. The question of how many iterations need to be conducted in order to obtain prescribed optimization accuracy is problem dependent. The simple answer is that the more iteration one does, in general, the better

results he can obtain. However, the point here is, for the R-QPSO, the more iterations mean more model evaluations and correspondingly greater computational costs; whereas for S-QPSO, the number of iterations can be easily extended at the cost of negligible computational time. In fact, results for many difficult and computationally expensive optimization problems indicated that surrogate global optimization methods can usually obtain more accurate results compared to non-surrogate methods within the same limited computational time (Mugunthan et al., 2005; Muller et al., 2015).

Fig. 3 plots the optimization progress of the R-QPSO and S-QPSO methods, where 50 iterations of R-QPSO in Fig. 3(a) takes 1000 RZWQM2 runs and 500 iterations of S-QPSO in Fig. 3(b) takes 792 RZWQM2 runs. The figure illustrates decrease of the smallest objective function value among particles recorded at each iteration. Fig. 3(b) shows that the objective function value of the S-QPSO is reduced significantly from 6000 to less than 4000 within 100 iterations, and continues decreasing as the search process proceeds; finally, it hits the value of 2071 at the end of the optimization. The rapid decrease of the objective function indicates that the surrogate optimization algorithm is very efficient at finding improved solutions. In contrast, Fig. 3(a) shows that the objective function value of the R-QPSO has a relatively slow improvement at the beginning of the process, and gently decreases to the value of 3134 when the optimization is done. The comparison of the objective functions between the two optimization schemes suggests that our S-QPSO method is more efficient and effective, in the sense of using the less computational time to achieve better calibration results.

The parameter values corresponding to the lowest objective functions are recorded as the optima and listed in Table 2. As expected, the optimized parameter values of the R-QPSO and S-QPSO are different, where the values of G3 and PHINT are higher in the S-QPSO. Both sets of

optima are within the reasonable parameter ranges. This investigation is very important because it is possible that the calibration process may push the parameters to some physically unreasonable values to get a good fit. On the other hand, for a nonlinear optimization problem, the difference between two sets of optima from two schemes does not necessary suggest that one optimization is better than the other; since, for insensitive parameters, different values could produce similar model fits.

Thus, we further evaluate the calibration performance by comparing the goodness-of-fit of the actual RZWQM2 based on the optimal parameters found by the two optimization schemes. The results of the four statistics measuring fitness are summarized in Table 3. Both schemes produced “satisfactory” results as $NSE > 0.65$, $RSR < 0.70$, and $PBIAS$ within $\pm 25\%$. However, the S-QPSO showed a better calibration performance than the R-QPSO, especially for the model output of crop yield. The progress plot of Fig. 3 implies that a large number of additional iterations will be required by the R-QPSO before it converges to the best objective function value obtained by the S-QPSO. The increase of one iteration in the R-QPSO means the RZWQM2 simulations will increase in the magnitude of the number of swarm particles. Thus, to achieve the similar calibration performance as the S-QPSO, the algorithm without surrogate modeling needs significantly more computational cost, especially for the problems having long model execution and a lot of required particles.

On the other hand, note that the better optimization performance of the S-QPSO is obtained based on 792 RZWQM2 executions. With the similar computational cost, the calibration result of the S-QPSO is rather poor. As depicted in Fig. 3(a), after 40 iterations (i.e., 800 RZWQM2 runs), the smallest objective function value obtained by the R-QPSO is about 3274, much greater

than the value of 2071 achieved by the S-QPSO. This comparison once again demonstrates that our S-QPSO algorithm is computationally more efficient than the R-QPSO.

The improvement of computational efficiency by using the surrogate method can be more outstanding when more iterations are conducted since its optimization does not require any actual model executions. In addition, the construction of the surrogate model can be fully parallel, which can further reduce the computational cost of the S-QPSO. For example, if we have 792 processors available, the construction of the current surrogate model will only take the simulation time of a single RZWQM2 run. Moreover, the surrogate model can be reused when solving a modified optimization problem with different objective functions.

3.4 Model prediction results

The calibrated RZWQM2 based on S-QPSO and R-QPSO methods, respectively, were used to predict a different set of 15 data. They were collected in the same years for the same three outputs as the calibration data but under different crop growth conditions. In the dataset for prediction, the corn was planted in even years and soybean in odd years (denoted as CTRL2), while the dataset with corn in odd years and soybean in even years (denoted as CTRL1) was used for calibration. The predictive performance was evaluated using the four statistical criteria as listed in Table 4. Results indicate that both optimizations had an over prediction in the model outputs. The S-QPSO over predicted the yield less than the R-QPSO, but it gave a relatively poor predictive performance in drainage and NO_3 -N loss.

The results are not surprising. Actually, several studies have shown that calibrating models on a certain dataset does not necessarily imply that predictive skills are improved on another dataset, especially when the two datasets associate with different physical and chemical treatments or weather conditions (Hill et al., 1998; Hui et al., 2003; Richardson et al., 2007; Ma

et al., 2012). The reasons are multiple, possibly caused by definition of the objective function, model uncertainty, and difference in the datasets for calibration and prediction. We explore the reasons in detail below.

4 Discussion

The goal of parameter optimization is to efficiently and robustly locate the global minimum of an objective function with respect to model parameters. With complex models, such as RZWQM2, the achievement is not straightforward, because the objective function can contain multiple local minima and the evaluation of the objective function can be computationally expensive which can result in a near-optimal solution within an acceptable time. Thus, a better optimization algorithm should produce a smaller objective function value and better model fit to the same set of calibration data using less computational time. In this sense, the proposed surrogate optimization is a superior approach to effectively solving parameter optimization problems.

However, the optimized parameters from a formal optimization are not guaranteed to be optimal in reality. That is, the optimized parameters may not truly represent the underlying physical system and any simulations based on these parameters may not produce the as good performance as in the calibration. The reason is that the optimization is tuning model parameters with respect to an objective function that is defined based on the model and calibration data. First, choice of the objective function is crucial for identification of optimal parameters. Järvinen et al. (2010) showed that different definition of objective functions resulted in different optimized parameters and correspondingly different model performance in their climate model calibration. Formulation of a reasonable objective function is an open question (Hill and Tiedeman, 2007). Generally, a reasonable objective function should be physically justified in two perspectives: (1)

being capable of distinguishing accurate model simulations from inaccurate ones, and (2) being able to produce physically optimal parameters. In this study, the objective function was defined using the calibration data solely, based on which the good surrogate optimization method produces good model fits to the calibration data. However, the optimized parameters based on this definition of the objective function may not be physically optimal. For example, the parameter G2, which represents the maximum possible number of kernels per plant, has optimized values of 284.0 and 278.55 based on R-QPSO and S-QPSO, respectively (Table 1). But the observed kernel number per year was approximately 400 to 600 (Iowa State University Extension) and the kernel number per plant could be even larger as some plants may produce two ears (Qi et al., 2011). In this case, although the optimized G2 is within the given range, it is much smaller than its observed value. To improve the parameter optimization, one way is to account for observations of the parameters in the formulation of the objective function (Lu et al., 2012). Formulation of such an advanced objective function is one of our future works, and it is expected that the new calibration can be efficiently implemented with the proposed surrogate optimization method as we build the surrogate of the model itself, not the objective function.

In addition, the difference of the calibration and prediction data, and model uncertainty could be other reasons for the relatively poor predictive performance (Lu et al., 2015). When we calibrate parameters against a dataset, the parameters are tuned to fit the calibration data; when the prediction data are dramatically different from the calibration data, the simulation results based on the calibrated parameters may also deviate from the prediction data quite a bit. This may not be the situation for an “ideal” model that perfectly represents the system and can capture all its changes under different conditions, but it could be an issue for an inadequate model as the optimization may reflect over-fitting to compensate for model uncertainties.

In this study, we optimized the seven parameters of RZWQM2 against the dataset CTRL1, which has different land cover treatments from the dataset CTRL2 used for prediction. Results indicated that the calibrated model based on S-QPSO fits the dataset CTRL1 pretty well but produces a relatively poor performance in fitting the CTRL2 data. This finding may suggest model uncertainty in RZWQM2. Although RZWQM2 has included the DSSAT 4.0 cropping system models to improve the simulation of the crop production process, the agricultural-hydrological system is still too complex to be perfectly represented. Therefore, the optimization may compensate for the model uncertainties in simulating the crop growth by adjusting related parameters, and these calibrated parameters could deteriorate model performances in contrasted crop growth conditions (Santaren et al., 2014). In this work, six of seven calibrated parameters are directly related to the crop types (corn or soybean) as shown in Table 1. When CTRL1 data used for parameter optimization, the parameters were tuned to fit the crop growth conditions and crop yields when corn was planted in odd years and soybean in even years. But these conditions may not be consistent with those when the CTRL2 data were collected, thus resulting in inconsistent model fits to CTRL1 and CTRL2 datasets. Hence, it is suggested calibrating a model with multiple treatments and multiple years of data so that the calibrated parameters can be adapted to other management conditions. And it is expected that this calibration process can be efficiently implemented with the proposed surrogate optimization method.

5 Conclusions

This paper presented a surrogate-based global optimization approach for calibrating parameters of a multi-physics and multi-scale agricultural-hydrological system model, RZWQM2. As the model execution is computationally intensive and global optimization methods can only find a near-optimal result within an affordable time, our goal was to explore

the use of a surrogate-based optimization method for model calibration in a computationally efficient way by minimizing the root mean squared errors between the observations and model results. We first used advanced sparse-grid interpolation to construct a surrogate system of the actual RZWQM2, and then we calibrated the surrogate model in the optimization process. As the surrogate model is a polynomial whose evaluation is fast, it can be efficiently evaluated with a sufficiently large number of times in the optimization, which facilitates the global search. Results indicated that the surrogate-based optimization method gave a smaller objective function value and better calibration performance by using less computational time than the conventional optimization without surrogating. The surrogate approach is critical to the practical application of global optimization to time-consuming hydrological and agricultural models. Due to the nonintrusive nature of the method, it can be used together with many models and optimization schemes used in hydrology and agriculture community. In the future, we plan to define an advanced objective function and calibrate the RZWQM2 with multiple treatments and multiple years of data to further improve the model performance. Beneficial from the surrogate-based optimization method proposed in this study, the future work can be efficiently implemented.

Acknowledgements

The research work was supported by the National Natural Science Foundation of China (Project Number: 41471031, 61170119), partly by Natural Science Foundation for College and Universities in Jiangsu Province (Project Number: 16KJB520051), as well as the Qing Lan Project of Jiangsu and Wuxi Institute of Technology. The second author thanks the Climate Change Science Institute in Oak Ridge National Laboratory for the support.

References

- Abrahamson, D. A., Radcliffe, D. E., Steiner, J. L., Cabrera, M. L., Endale, D. M., Hoogenboom, G., 2006. Evaluation of the RZWQM for simulating tile drainage and leached nitrate in the Georgia Piedmont. *Agron. J.* 98(3), 644-654. <http://dx.doi.org/10.2134/agronj2005.0074>.
- Ahmed, I., Rudra, R., McKague, K., Gharabaghi, B. Ogilvie, J., 2007. Evaluation of the Root Zone Water Quality Model (RZWQM) for Southern Ontario: Part I. Sensitivity Analysis, Calibration, and Validation. *Water Qual. Res. J. Canada.* 42(3), 202-218.
- Ahuja, L. R., Rojas, K.W., Hanson, J.D., Shaffer, M.J., Ma, L., 2000. Root Zone Water Quality Model: Modeling Management Effects on Water Quality and Crop Production. Water Resources Publications, Highlands Ranch, Colo.
- Alam, M. J., Dutta, D., 2012. A process-based and distributed model for nutrient dynamics in river basin: development, testing and applications. *Ecol. Model.* 247, 112-124.<http://dx.doi.org/10.1016/j.ecolmodel.2012.07.031>.
- Arnold, J. G., Moriasi, D. N., Gassman, P. W., Abbaspour, K. C., White, M. J., Srinivasan, R., Santhi, C., Harmel, R. D., Griensven, A., Liew, M. W., Kannan, N., Jha, M. K., 2012. SWAT: Model use, calibration, and validation. *Trans. ASABE.* 55 (4), 1491-1508.<http://dx.doi.org/10.13031/2013.42256>.
- Bakhsh, A., Kanwar, R. S., Jaynes, D. B., Colvin, T. S., Ahuja, L. R., 2001. Simulating effects of variable nitrogen application rates on corn yields and NO₃-N losses in subsurface drain water. *Trans. ASAE.* 44(2), 269- 276. <http://dx.doi.org/10.13031/2013.4688>.
- Barthelmann, V., Novak, E., Ritter, K., 2000. High dimensional polynomial interpolation on sparse grids. *Adv. Comput. Math.* 12(4), 273–288. <http://dx.doi.org/10.1023/A:1018977404843>

611 Bergh, F.V., 2001. An analysis of particle swarm optimizers. Ph.D. dissertation, University of
612 Pretoria, Pretoria, South Africa.

613 Bungartz, H. J., Griebel M., 2004. Sparse grids. *Acta Numerica*, 1-123. doi:
614 10.1017/S0962492904000182.

615 Calvi J. P., Manh, P., 2012. Lagrange interpolation at real projections of leja sequences for the
616 unit disk. *Proc. Amer. Math. Soc.* 140(2012), 4271–4284. [http://dx.doi.org/10.1090/S0002-](http://dx.doi.org/10.1090/S0002-9939-2012-11291-2)
617 9939-2012-11291-2.

618 Cameira, M.R., Fernando, R.M., Ahuja, L., Pereira, L., 2005. Simulating the Fate of Water in
619 Field Soil –Crop Environment. *J. Hydrol.* 315, 1-24.
620 <http://dx.doi.org/10.1016/j.jhydrol.2005.03.020>.

621 Chang, H., Zhang, D., 2009. A comparative study of stochastic collocation methods for flow in
622 spatially correlated random fields. *Commun. Computat. Phys.s.* 6(3), 509–535.

623 Davoodi, E., Hagh, M. T., Zadeh, S. G., 2014. A hybrid Improved Quantum-behaved Particle
624 Swarm Optimization–Simplex method (IQPSOS) to solve power system load flow
625 problems. *Appl. Soft Comput.* 21,171-179. <http://dx.doi.org/10.1016/j.asoc.2014.03.004>

626 Doherty, J. 2004. PEST: Model independent parameter estimation user manual. Watermark
627 Numerical Computing [R], Brisbane, Australia.

628 Fang, Q.X., Malonec, R.W., Mad, L., Jaynesc, D.B., Thorpe, K.R., Greend, T.R., Ahuja, L.R.,
629 2012. Modeling the effects of controlled drainage, N rate and weather on nitrate loss to
630 subsurface drainage. (PSET, RZWQM2). *Agr. Water Manage.* 103,150-
631 161.<http://dx.doi.org/10.1016/j.agwat.2011.11.006>.

632 Fang, W., Sun, J., Ding, Y, Wu, X., Xu, W., 2010. A Review of Quantum-behaved Particle
633 Swarm Optimization. IETC Tech. Rev. 27(4), 336-348.[http://dx.doi.org/10.4103/0256-](http://dx.doi.org/10.4103/0256-4602.64601)
634 [4602.64601](http://dx.doi.org/10.4103/0256-4602.64601).

635 Fang, Q. X., Ma, L., Flerchinger, G. N., Qi, Z., Ahuja, L. R., Xing, H. T., Li, J., Yu, Q., 2014.
636 Modelling Evapotranspiration and Energy Balance in a Wheat-Maize Cropping System
637 Using the Revised RZ-SHAW Model. Agric. Forest Meteorol. 194,218-229.
638 <http://dx.doi.org/10.1016/j.agrformet.2014.04.009>

639 Ghidry, F., Alberts, E. E., Kitchen, N. R., 1999. Evaluation of RZWQM using field measured
640 data from the Missouri MSEA. Agron. J. 91,183-192.
641 <http://dx.doi.org/10.2134/agronj1999.00021962009100020004x>.

642 Gunzburger M., Webster C., Zhang G., 2016. Sparse collocation methods for stochastic
643 interpolation and quadrature, Handbook of Uncertainty Quantification, 1-46, Springer
644 International Publishing, Switzerland. http://dx.doi.org/10.1007/978-3-319-11259-6_29-1.

645 Hassani, K., Lee, W., 2016. Multi-objective design of state feedback controllers using reinforced
646 quantum-behaved particle swarm optimization. Appl. Soft Comput., 41, 66-76.
647 <http://dx.doi.org/10.1016/j.asoc.2015.12.024>.

648 Hill, M. C., Cooley, R. L., Pollock, D. W., 1998. A controlled experiment in ground water flow
649 model calibration. Ground Water, 36(3), 520 - 535.[http://dx.doi.org/10.1111/j.1745-](http://dx.doi.org/10.1111/j.1745-6584.1998.tb02824.x)
650 [6584.1998.tb02824.x](http://dx.doi.org/10.1111/j.1745-6584.1998.tb02824.x).

651 Hill, M. C., Tiedeman, C. R., 2007. Effective calibration of ground water models, with analysis of
652 data, sensitivities, predictions, and uncertainty, 480 pp., John Wiley and Sons, New York.

653 Hui, D., Luo, Y., Katul, G., 2003. Partitioning interannual variability in net ecosystem exchange
 654 between climatic variability and functional change. *Tree Physiol.*, 23(7), 433–
 655 442. <http://dx.doi.org/10.1093/treephys/23.7.433>.
 656 Islam, A., Ahuja, L. R., Garcia, L. A. Ma, L., Saseendran, S. A., 2012. Modelling effect of
 657 climate change and elevated CO₂ on potential evapotranspiration demand using multi-
 658 model ensemble climate change scenarios. *Trans. ASABE*. 55, 2135-2146.
 659 Järvinen, H., Räisänen, R., Laine, M., Tamminen, J., Ilin, A., Oja, E., Solonen, A., Haario, H.,
 660 2010. Estimation of ECHAM5 climate model closure parameters with adaptive MCMC.
 661 *Atmos. Chem. Phys.*, 10, 9993-100002.
 662 Jones, J.W., Hoogenboom, G., Porter, C.H., Boote, K.J., Batchlor, W.D., Hunt, L.A., Wilkens,
 663 P.W., Singh, U., Gijisman, A.J., Ritchie, J.T., 2003. The DSSAT cropping system model.
 664 *Eur. J. Agron.* 18, 235-265. [http://dx.doi.org/10.1016/S1161-0301\(02\)00107-7](http://dx.doi.org/10.1016/S1161-0301(02)00107-7).
 665 Kennedy, J. Eberhart, R.C., 1995. Particle swarm optimization. In *Proceedings of the IEEE*
 666 *International Conference on Neural Networks*, Piscataway, NJ, Nov. 27-Dec. 1, 4, 1942-
 667 1948. <http://dx.doi.org/10.1109/ICNN.1995.488968>.
 668 Ko, J., Ahuja, L. R., Saseendran, S. A., Green, T. R., Ma, L., Nielsen, D. C., Walthall, C., 2011.
 669 Climate change impacts on dryland cropping systems in the Central Great Plains, USA.
 670 *Climatic. Change*. 111(2), 445-472. <http://dx.doi.org/10.1007/s10584-011-0175-9>.
 671 Landa, F. M., Fausey, N. R., Nokes, S. E., Hanson, J. D., 1999. Plant Production Model
 672 Evaluation for the Root Zone Water Quality Model (RZWQM 3.2) in Ohio. *Agron. J.*
 673 91,220-227. <http://dx.doi.org/10.2134/agronj1999.00021962009100020008x>.

674 Li, H., Zhang, D., 2007. Probabilistic collocation method for flow in porous media: Comparisons
 675 with other stochastic methods. *Water Resour. Res.* 43(9), 6627-6632. [http://dx.doi.org/](http://dx.doi.org/10.1029/2006WR005673)
 676 10.1029/2006WR005673.

677 Lin, G., Tartakovsky, A., 2009. An efficient, high-order probabilistic collocation method on
 678 sparse grids for three-dimensional flow and solute transport in randomly heterogeneous
 679 porous media. *Adv. Water Resour.* 32(5), 712–722.
 680 <http://dx.doi.org/10.1016/j.advwatres.2008.09.003>.

681 Lin, G., Tartakovsky, A., 2010. Numerical studies of three dimensional stochastic Darcy's
 682 equation and stochastic advection diffusion-dispersion equation. *Journal of Scientific*
 683 *Computing.* 43, 92–117. <http://dx.doi.org/10.1007/s10915-010-9346-5>.

684 Lu, D., Ye, M., Hill, M. C., 2012. Analysis of regression confidence intervals and Bayesian
 685 credible intervals for uncertainty quantification. *Water Resour. Res.* 48, W09521,
 686 doi:10.1029/2011WR011289.

687 Lu, D., Ye, M., Curtis, G. P., 2015. Maximum likelihood Bayesian model averaging and its
 688 predictive analysis for groundwater reactive transport models. *J. of Hydro.* 529, 1859-1873.

689 Ma, L., Hoogenboom, G., Ahuja, L. R., Ascough II, J. C., Saseendran, S. A., 2006. Evaluation of
 690 the RZWQM-CERES-Maize hybrid model for maize production. *Agr. Syst.* 87, 274-295.
 691 <http://dx.doi.org/10.1016/j.agsy.2005.02.001>.

692 Ma, L., Hoogenboom, G., Ahuja, L. R., Nielsen, D. C., Ascough II, J. C., 2005. Development
 693 and evaluation of the RZWQM-CROPGRO hybrid model for soybean production. *Agron.*
 694 *J.* 97, 1172-1182. <http://dx.doi.org/10.2134/agronj2003.0314>.

695 Ma, L., Malone, R. W., Heilman, P., Ahuja, L. R., Meade, T., Saseendran, S. A., Ascough II, J.
 696 C., Kanwar, R. S., 2007. Sensitivity of tile drainage flow and crop yield on measured and

697 calibrated soil hydraulic properties. *Geoderma*. 140(3), 284-296.
 698 <http://dx.doi.org/10.1016/j.geoderma.2007.04.012>.

699 Ma, L., Trout, T.J., Ahuja, L.R., Bausch, W.C., Saseendran, S.A., Malone, R.W., Nielsen, D.C.,
 700 2012. Calibrating RZWQM2 model for maize response to deficit irrigation. *Agr. Water*
 701 *Manage.* 103,140-149. <http://dx.doi.org/10.1016/j.agwat.2011.11.005>.

702 Ma, X., Zabarar, N., 2009. An efficient Bayesian inference approach to inverse problems based
 703 on an adaptive sparse grid collocation method. *Inverse. Probl.* 25(3), 35013-35039.
 704 <http://dx.doi.org/10.1088/0266-5611/25/3/035013>.

705 Malone, R.W., Jaynes, D.B., Ma, L., Nolan, B.T., Meek, D.W., Karlen, D. L., 2010. Soil-Test N
 706 recommendations augmented with PEST-Optimized RZWQM simulations. *J. Environ.*
 707 *Qual.* 39(5), 1711-1723. <http://dx.doi.org/10.2134/jeq2009.0425>.

708 Malone, R.W., Nolan, B.T., Mac, L., Kanward, R.S., Pederson, C., Heilman, P., 2014. Effects
 709 of tillage and application rate on atrazine transport to subsurface drainage: Evaluation of
 710 RZWQM using a six-year field study. *Agr. Water Manage.* 132, 10-22.
 711 <http://dx.doi.org/10.1016/j.agwat.2013.09.009>

712 Marzouk, Y. M., Najm, H. N., Rahn, L. A., 2007. Stochastic spectral methods for efficient
 713 Bayesian solution of inverse problems. *J. Comput. Phys.* 224(2), 560–586.
 714 <http://dx.doi.org/10.1016/j.jcp.2006.10.010>.

715 Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Binger, R.L., Harmel, R.D., Veith, T.L., 2007.
 716 Model evaluation guidelines for systematic qualification of accuracy in watershed
 717 simulations. *Trans. ASABE*. 50 (3), 885-900. <http://dx.doi.org/10.13031/2013.23153>.

718 Muller, J., Paudel, R., Shoemaker, C.A., Woodbury, J., Wang, Y., Mahowald, N., 2015. CH4
 719 parameter estimation in CLM4.5bgc using surrogate global optimization. *Geosci. Model*
 720 *Dev.*, 8, 3285-3310.

721 Mugunthan, P., Shoemaker, C., Regis, R., 2005. Comparison of function approximation,
 722 heuristic, and derivative-based methods for automatic calibration of computationally
 723 expensive groundwater bioremediation models. *Water Resour. Res.*, 41, W11427.

724 Narayan A., Jakeman, J. D., 2014. Adaptive Leja sparse grid constructions for stochastic
 725 collocation and high-dimensional approximation. *Math. arXiv:1404.5663v2*.

726 Nobile, F., Tempone, R., Webster, C. G., 2008a. A sparse grid stochastic collocation method for
 727 partial differential equations with random input data. *Siam. J. Numer. Anal.* 46, 2309–
 728 2345. [http://dx.doi.org/ 10.1137/060663660](http://dx.doi.org/10.1137/060663660).

729 Nobile, F., Tempone, R., Webster, C. G., 2008b. An anisotropic sparse grid stochastic
 730 collocation method for elliptic partial differential equations with random input data. *Siam.*
 731 *J. Numer. Anal.* 46(5), 2411–2442. [http://dx.doi.org/ 10.1137/070680540](http://dx.doi.org/10.1137/070680540).

732 Omkar, S., Khandelwal, R., Ananth, T., Narayana, N., Gopalakrishnan, S., 2009. Quantum
 733 behaved particle swarm optimization (QPSO) for multi-objective design optimization of
 734 composite structures. *Expert. Syst. Appl.* 36 (8) , 11312-11322. [http://dx.doi.org/](http://dx.doi.org/10.1016/j.eswa.2009.03.006)
 735 [10.1016/j.eswa.2009.03.006](http://dx.doi.org/10.1016/j.eswa.2009.03.006).

736 Qi, Z., Helmers, M.J., Malone, R.W., Thorp, K.R., 2011. Simulating long-term impacts of winter
 737 rye cover crop on hydrological cycling and nitrogen dynamics for a corn-soybean crop
 738 system. *Trans. ASABE.* 54(5), 1575-1588. [http://dx.doi.org/ 10.13031/2013.39836](http://dx.doi.org/10.13031/2013.39836).

739 Qi, Z., Bartling, P.N.S., Jabro, J.D., Lenssen, A.W., Iversen, W.M., Ahuja, L.R., Ma, L., Allen,
 740 B.L., Evans, R.G., 2013. Simulating dryland water availability and spring wheat

production in the northern Great Plains. *Agron. J.* 105, 37-50. <http://dx.doi.org/10.2134/agronj2012.0203>.

Richardson, A. D., Hollinger, D. Y., Aber, J. D., Ollinger, S. V., Braswell, B. H., 2007. Environmental variation is directly responsible for short- but not long-term variation in forest-atmosphere carbon exchange. *Glob. Change Biol.* 13(4), 788–803.<http://dx.doi.org/10.1111/j.1365-2486.2007.01330.x>.

Ritter, A., Muñoz-Carpena, R., 2013. Performance evaluation of hydrological models: statistical significance for reducing subjectivity in goodness-of-fit assessments. *J. Hydrol.* 480, 33–45.<http://dx.doi.org/10.1016/j.jhydrol.2012.12.004>.

Santaren, D., Peylin, P., Bacour, C., Ciais, P., Longdoz, B., 2014. Ecosystem model optimization using in situ flux observations: benefit of Monte Carlo versus variational schemes and analyses of the year-to-year model performances. *Biogeosciences*. 11 (24), 7137-7158.<http://dx.doi.org/10.5194/bg-11-7137-2014>.

Saseendran, S. A., Ahuja, L. R., Nielsen, D. C., Trout, T., Ma, L., 2008. Use of crop simulation models to evaluate limited irrigation management options for corn in a semiarid environment. *Water Resour. Res.* 44(7), 137-149. <http://dx.doi.org/10.1029/2007WR006181>.

Shaffer, M.J., Rojas, K.W., Decoursey, D.G., Hebson, C.S., 2000. Chapter 5: Nutrient chemistry processes – OMNI. In: Ahuja, L.R., Rojas, K.W., Hanson, J.D., Shaffer, M.J., Ma, L., (Eds.), *Root Zone Water Quality Model: Modeling Management Effects on Water Quality and Crop Production*. Water Resources Publications, Highlands Ranch, CO, pp. 119-144.

Shi, L., Yang, J., 2009. Qualification of uncertainty for simulating solute transport in the
 heterogeneous media with sparse grid collocation method. *J. Hydrodyn.* 21(6), 779–789.
[http://dx.doi.org/10.1016/S1001-6058\(08\)60213-9](http://dx.doi.org/10.1016/S1001-6058(08)60213-9).

Shi, L., Yang, J., Zhang, D., Li, H., 2009. Probabilistic collocation method for unconfined flow
 in heterogeneous media. *J. Hydrol.* 365(1-2), 4–
[10.http://dx.doi.org/10.1016/j.jhydrol.2008.11.012](http://dx.doi.org/10.1016/j.jhydrol.2008.11.012).

Shresthaa, S., Dattab, A., 2015. Field measurements for evaluating the RZWQM and
 PESTFADE models for the tropical zone of Thailand. *J. Environ. Manage.* 147, 286-296.
<http://dx.doi.org/10.1016/j.jenvman.2014.09.017>

Shuttleworth W. J., Wallace J. S., 1985. Evaporation from sparse crops-an energy combination
 theory. *Q. J. Roy. Meteor. Soc.* 111, 839-855. <http://dx.doi.org/10.1002/qj.49711146910>.

Šimůnek J., van Genuchten, M., Sejna, M., 2008. Development and applications of the HYDRUS
 and STANMOD software packages and related codes. *Vadose Zone J.*, Vol. 7(2) , 587-
 600. <http://dx.doi.org/10.2136/vzj2007.0077>.

Stoyanov M.K., Webster C.G., 2016. A dynamically adaptive sparse grids method for quasi-
 optimal interpolation of multidimensional functions. *Comput. Math. Appl.*
<http://dx.doi.org/10.1016/j.camwa.2015.12.045>.

Sun, J., Feng, B., Xu, W., 2004. Particle swarm optimization with particles having quantum
 behavior. *CEC2004* , Portland OR, 20-23 June, 1, 326–331. <http://dx.doi.org/10.1109/CEC.2004.1330875>.

Sun, M., Zhang, X., Huo, Z., Feng, S., Huang, G., Mao, X., 2016. Uncertainty and sensitivity
 assessments of an agricultural–hydrological model (RZWQM2) using the GLUE method. *J.*
Hydrol. 534, 19-30. <http://dx.doi.org/10.1016/j.jhydrol.2015.12.045>.

785 Thorp, K. R., Jaynes, D. B., Malone, R.W., 2008. Simulating Long-Term Performance of
 786 Drainage water management in Midwestern United States. *Trans. ASABE*. 51(3), 961-976.
 787 <http://dx.doi.org/10.13031/2013.24534>.

788 Thorp, K.R., Malone, R.W., Jaynes, D.B., 2007. Simulating long-term effects of nitrogen
 789 fertilizer application rates on corn yield and nitrogen dynamics. *Trans. ASABE*. 50(4),
 790 1287-1303.

791 Wang, H., Wu, Z., Hu, C. 2015. A Comprehensive Study of the Effect of Input Data on
 792 Hydrology and non-point Source Pollution Modeling. *Water Resources Manag.* 29 (5):
 793 1505-1521. <http://dx.doi.org/10.1007/s11269-014-0890-x>.

794 Wang, Z., Qi, Z., Xue, L., Bukovsky, M., Helmers, M. J., 2015b. Modeling the impacts of
 795 climate change on nitrogen losses and crop yield in a subsurface drained field. *Climatic*.
 796 *Change*. 129(1), 323-335. <http://dx.doi.org/10.1007/s10584-015-1342-1>.

797 Wu, L., Chen, W., Baker, J. M., Lamb, J. A., 1999. Evaluation of the Root Zone Water Quality
 798 Model Using Field-Measured Data from a Sandy Soil. *Agron. J.* 91(2), 177-182.
 799 <http://dx.doi.org/10.2134/agronj1999.00021962009100020003x>.

800 Xi, M., Qi, Z., Zou Y., Vijaya, R. G.S., Sun, J., 2015. Calibrating RZWQM2 model using
 801 quantum-behaved particle swarm optimization algorithm. *Comput. Electron. Agr.* 113, 72–
 802 80. <http://dx.doi.org/10.1016/j.compag.2015.02.002>.

803 Zeng X., Ye M. Burkardt J., Wu J., Wang D., Zhu X., 2016. Evaluating two sparse grid
 804 surrogates and two adaptation criteria for groundwater Bayesian uncertainty quantification.
 805 *J. Hydrol.* 535,120-134. <http://dx.doi.org/10.1016/j.jhydrol.2016.01.058>.

806 Zeng, L., Shi, L., Zhang, D., Wu, L., 2012. A sparse grid based Bayesian method for
 807 contaminant source identification. *Adv. Water Resour.* 37, 1–9.
 808 <http://dx.doi.org/10.1016/j.advwatres.2011.09.011>.
 809 Zhang, G., Lu, D., Ye, M., Gunzburger ,M., Webster, C., 2013. An adaptive sparse-grid high-
 810 order stochastic collocation method for Bayesian inference in groundwater reactive
 811 transport modeling, *Water Resour. Res.* 49, 1-22. <http://dx.doi.org/10.1002/wrcr.20467>.
 812 Zhang, G., Webster, C., Gunzburger, M., Burkardt, J., 2015. A hyper-spherical adaptive sparse-
 813 grid method for high-dimensional discontinuity detection, *SIAM Journal of Numerical*
 814 *Analysis*, 53, 1508-1536. <http://dx.doi.org/10.1137/140971531>.
 815 Zhang, G., Webster, C., Gunzburger, M., Burkardt, J., 2016. Hyperspherical sparse
 816 approximation techniques for high-dimensional discontinuity detection, *SIAM Review*, 58,
 817 517-551. <http://dx.doi.org/10.1137/16M1071699>.
 818

819

List of Tables820 **Table 1.** Description of the seven parameters used for optimization in the RZWQM2 model.

	Parameter	Description	Range
Corn	G2	Maximum possible number of kernels per plant	[248, 990]
	G3	Kernel filling rate during the linear grain filling stage and under optimum conditions (mg d ⁻¹)	[5, 16.5]
	PHINT	Phylochron interval between successive leaf tip appearances	[30, 50]
	SRGF_Corn	Soil root growth factor parameter	[1.0, 3.5]
Soybean	LFMAX	Maximum leaf photosynthesis rate (mg CO ₂ m ⁻² s ⁻¹) at 30°C, 350 vpm CO ₂ , and high light intensity	[0.8, 1.5]
	SRGF_Soybean	Soil root growth factor parameter	[1.0, 3.5]
Lateral flow	LHG	Lateral hydraulic gradient	[0, 10 ⁻⁴]

821

822

823

Table 2. Optimized parameter values based on the R-QPSO and S-QPSO algorithms.

Parameter	R-QPSO	S-QPSO
G2	284.00	278.55
G3	14.11	15.56
PHINT	48.66	49.49
SRGF_Corn	1.41	1.39
LFMAX	1.09	0.93
SRGF_Soybean	3.27	3.05
LHG	4.24×10^{-7}	3.82×10^{-7}

824

825

Table 3. Statistical metrics used for evaluating optimization performance.

Statistics	Yield		Drainage		NO ₃ -N loss	
	R-QPSO	S-QPSO	R-QPSO	S-QPSO	R-QPSO	S-QPSO
PBIAS (%)	5.2	0.98	11.1	10.2	0.73	-0.58
R ²	0.93	0.99	0.98	0.98	0.99	0.99
NSE	0.86	0.98	0.88	0.96	0.99	0.99
RSR	0.38	0.13	0.34	0.32	0.11	0.06

826

827

Table 4.Statistical metrics used for evaluating prediction performance.

Statistics	Yield		Drainage		NO ₃ -N loss	
	R-QPSO	S-QPSO	R-QPSO	S-QPSO	R-QPSO	S-QPSO
PBIAS (%)	-18.19	-5.04	-24.01	-26.50	3.09	-20.91
R ²	0.98	0.99	0.85	0.84	0.84	0.70
NSE	0.89	0.97	0.51	0.44	0.78	0.06
RSR	0.34	0.16	0.70	0.75	0.47	0.97

828

Fig. 1. A comparison of a 5-level sparse grid (b) and the corresponding full tensor-product grid (c) based on Chebyshev points. The sparse grid (b) consists of 10 coarse grids in (a), each of which is a coarse tensor-product grid with $\ell_1 + \ell_2 \leq 5$. The use of Chebyshev points results in repeated points in the 10 coarse grids, so the sparse grid has only 29 points. The full tensor-product grid (c) is constructed by the grids with $\ell_1 = \ell_2 = 4$, which has 81 points. In building a surrogate system, one interpolation point means one original model execution.

Fig. 2. Pair wise comparison of the simulated drainage, NO₃ -N loss, and yield between the original RZWQM2 model and the surrogate model for 100 parameter samples randomly drawn from the parameter space.

Fig.3. Evolutionary progress of objective function values using (a) R-QPSO with 50 iterations of the expensive RZWQM2 model runs, and (b) S-QPSO with 500 iterations of the cheap-to-evaluate surrogate model runs. To get the smaller objective function value in (b), S-QPSO used 792 RZWQM2 runs, while R-QPSO used 1000 RZWQM2 runs to get the relatively large value in (a).