

Improving the Efficiency of Monte Carlo Bayesian Calibration of Hydrologic Models via Model Pre-emption

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Abstract

Bayesian inference via Markov Chain Monte Carlo (MCMC) sampling and Sequential Monte Carlo (SMC) sampling are popular methods for uncertainty analysis in hydrological modelling. However, application of these methodologies can incur significant computational costs. This study investigated using model pre-emption for improving the computational efficiency of MCMC and SMC samplers in the context of hydrological modelling. The proposed pre-emption strategy facilitates early termination of low-likelihood simulations and results in reduction of unnecessary simulation time steps. The proposed approach is incorporated into two samplers and applied to the calibration of three rainfall-runoff models. Results show that overall pre-emption savings range from 5% to 21%. Furthermore, results indicate that pre-emption savings are greatest during the pre-convergence “burn-in” period (*i.e.*, between 8% and 39%) and decrease as the algorithms converge towards high likelihood regions of parameter space. The observed savings are achieved with absolutely no change in the posterior set of parameters.

Keywords: calibration, uncertainty analysis, pre-emption, DREAM, SMC, AR

1. Introduction

This paper focuses on improving the computational efficiency of calibration and uncertainty analysis – two essential components of *model assessment*, defined as the use of robust procedures to determine the suitability of a given model for a given purpose (Matott et al., 2009). Investigations of uncertainty in hydrological modelling have emphasized the use of automatic calibration methods, which develop expressions for parameter uncertainty, ranging from simple Monte Carlo simulations such as GLUE (Beven and Binley, 1992) to statistical approaches based on Bayesian inference (Box and Tiao, 1973; Kuczera, 1983). Due to the complexity of large-scale hydrological models, Bayesian inference is facilitated through Markov Chain Monte Carlo (MCMC) sampling from parameters’ posterior distributions (e.g. Haario et al., 2001; Kavetski et al., 2006; Kuczera and Parent, 1998; Vrugt et al., 2003; Vrugt et al., 2009).

Sequential Monte Carlo (SMC) simulations have also become very attractive in hydrological modelling in recent years (Hsu et al., 2009; Jeremiah et al., 2011; Moradkhani et al., 2005; Salamon and Feyen, 2010). SMC samplers combine data assimilation principles with a particle filtering strategy (e.g., Moradkhani et al., 2005; Smith et al., 2008), and generally resemble previous developed Sampling Importance Resampling (SIR) approaches (e.g., Del Moral et al., 2006). More Recently, Jeremiah et al. (2011) compared an example SMC sampler with an adaptive MCMC sampler and found that both methods displayed robustness and convergence.

Despite the common use of MCMC and SMC approaches, their application can incur high computational costs. Therefore, strategies for improving the efficiency of such samplers are an ongoing area of research. In MCMC sampling, efforts to improve efficiency include utilizing prior information (Mertens et al., 2004; Sikorska et al., 2012), developing adaptive algorithms

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4 53 (e.g., *Craiu et al.*, 2009; *Haario et al.*, 2001; *Vrugt et al.*, 2003; *Vrugt et al.*, 2009), and using
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7 54 “limited - memory” sampling (*Kuczera et al.*, 2010). Efforts for overcoming practical SMC
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10 55 issues include using importance sampling (*Cheng and Druzdzal*, 2000) and seeding initial
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12 56 solutions using empirical Bayes (*Chen et al.*, 2004).

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14 57 As a complementary approach to the aforementioned efforts, this study explores the use
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16 58 of model ‘pre-emption’ to improve the computational efficiency of MCMC and SMC samplers
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19 59 in the context of hydrological modelling. Model pre-emption is a relatively simple strategy for
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22 60 identifying low-quality simulations and terminating them early before the entire simulation run
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24 61 time completes. Previous research by Razavi et al. (2010) establishes that model pre-emption can
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26 62 yield substantial computational savings when applied to various optimization-based calibration
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29 63 strategies (DDS and PSO) and various *informal* uncertainty-based calibration strategies (e.g.,
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31 64 GLUE (*Beven and Binley*, 1992) and DDS-AU (*Tolson and Shoemaker*, 2007)). In contrast, this
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34 65 study investigated model pre-emption for use within *formal* likelihood functions embedded
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36 66 within the MCMC and SMC sampling algorithms. These pre-emption enabled formal samplers
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39 67 were then applied to the calibration and uncertainty analysis of three rainfall-runoff models. To
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41 68 the best of our knowledge, such an implementation has not been considered in previous studies
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44 69 on the use of MCMC and SMC sampling in hydrological modelling.

45 46 47 70 **2. Methods**

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50 71 Model pre-emption was applied to two algorithms, *i.e.* an MCMC implementation known
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52 72 as DiffeRential Evolution Adaptive Metropolis or DREAM (*Vrugt et al.*, 2009) and an SMC
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55 73 implementation described by Jeremiah et al. (2011) and referred to herein as JSMC. DREAM
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57 74 runs multiple Markov chains simultaneously to facilitate efficient global exploration of the
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60 75 parameter space and its convergence is monitored using the Gelman-Rubin metric (\hat{R}) (*Gelman*

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4 76 *and Rubin, 1992*), *i.e.*, values less than 1.2 indicate convergence. The JSMC sampling process
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6 77 propagates a population of parameter vectors (or particles) of size N from an initial sampling
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8 78 distribution to the desired posterior distribution. For more information on the JSMC sampler
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11 79 refer to Jeremiah et al. (2011).
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14 80 Both DREAM and JSMC are designed to take samples from the Bayesian posterior
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16 81 distributions of model parameters. Two Bayesian formulations were investigated in this study, as
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19 82 described below. Consider a time series of N streamflow observations, Y_t $t=1, \dots, N$ (or \mathbf{Y} in
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21 83 vector notation) used to calibrate hydrologic model $h(\boldsymbol{\theta})$ given its parameter vector ($\boldsymbol{\theta}$).
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24 84 Assuming the model errors are uncorrelated and Gaussian distributed with zero mean and
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27 85 variance σ_ε^2 , the posterior probability density function $p(\boldsymbol{\theta} | \mathbf{Y})$ has the following form (after
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30 86 integrating out σ_ε^2):
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$$33 \quad p(\boldsymbol{\theta} | \mathbf{Y}) \propto \left(\sum_{t=1}^N \varepsilon_t^2 \right)^{-\frac{N}{2}} \quad (1)$$

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37 88 where $\boldsymbol{\varepsilon}_t = Y_t - h(\boldsymbol{\theta})$ is a vector of residuals. Equation (1) assumes that errors are uncorrelated,
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40 89 but this is not a very realistic assumption in the context of hydrologic modelling. One approach
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43 90 to account for auto-correlation is to use a first-order Auto-Regressive (AR) scheme for the error
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45 91 series (*Sorooshian and Dracup, 1980*):
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$$47 \quad \varepsilon_t = \rho \varepsilon_{t-1} + v_t \quad t = 1, \dots, N \quad (2)$$

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50 93 where $\varepsilon_0 = 0$, ρ is the first-order correlation coefficient, and v_t is the remaining error
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53 94 prescribed to have a zero mean and constant variance σ_v^2 . The resulting joint posterior
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56 95 distribution of $\boldsymbol{\theta}$ and ρ in this case would be:
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$$96 \quad p(\boldsymbol{\theta}, \rho | \mathbf{Y}) \propto \left(\varepsilon_1^2 (1 - \rho^2) + \sum_{t=2}^N \delta_t^2 \right)^{-\frac{N}{2}} \quad (3)$$

97 where $\delta_t(\boldsymbol{\theta}, \rho | \mathbf{Y}) = \varepsilon_t(\boldsymbol{\theta} | \mathbf{Y}) - \rho \varepsilon_{t-1}(\boldsymbol{\theta} | \mathbf{Y}) \quad t = 1, \dots, N$. It is observed in both Equations (1) and
98 (3) that the posterior density will monotonically decrease when residuals are incorporated time
99 step by time step into the equations. Since the posterior densities calculated with Equation (1)
100 and (3) monotonically degrade as the simulation proceeds through time, both formulations are
101 suitable for adopting a model pre-emption approach (*Razavi et al.*, 2010).

102 Pre-emption-enabled DREAM and JSMC sampling was applied to the calibration and
103 uncertainty analysis of three different rainfall-runoff models. Table 1 provides summary
104 information on these case-studies and lists corresponding case study reference papers containing
105 complete descriptions.

[Table 1 goes here]

107 **2.1. Model pre-emption**

108 In deterministic model pre-emption (*Razavi et al.*, 2010), model performance (in terms of
109 some monotonically degrading calibration objective function) is monitored during simulation,
110 and a given simulation is terminated early if it is recognized to be so poor that it will not
111 contribute to guiding the search strategy. In the present study, the DREAM and JSMC sampling
112 algorithms were modified to support deterministic model pre-emption. The first step in
113 implementing pre-emption is to select an appropriate objective function. As noted previously,
114 both Equations (1) and (3) are suitable choices for model pre-emption (*Razavi et al.*, 2010).

115 Another important factor in pre-emption implementation is the pre-emption threshold,
116 *i.e.*, a likelihood value where the solutions resulting in likelihood values worse than this

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4 117 threshold would be rejected even if the simulation is carried out completely. Both DREAM and
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7 118 JSMC decide to jump from a current state (θ_n) to a candidate state (θ^*) based on the ratio of the
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10 119 posterior densities of the two states, *i.e.*, $p(\theta^* | \mathbf{Y})/p(\theta_n | \mathbf{Y})$. θ^* is accepted if
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13 120 $p(\theta^* | \mathbf{Y})/p(\theta_n | \mathbf{Y}) > Z$, where Z is a random number uniformly distributed between 0 and 1;
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16 121 otherwise the sampler remains at θ_n . A move to θ^* is accepted only if $p(\theta^* | \mathbf{Y}) > Z \times p(\theta_n | \mathbf{Y})$.
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19 122 Thus, the posterior density value of $p(\theta^* | \mathbf{Y})_{\min} = Z \times p(\theta_n | \mathbf{Y})$ can be considered as the pre-
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21 123 emption threshold so long as the random number Z is generated *prior* to evaluating a given
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24 124 candidate solution. Algorithms can then determine, a priori, the minimum acceptable value of
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26 125 the candidate posterior density ($p(\theta^* | \mathbf{Y})_{\min}$) as the pre-emption threshold.
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29 126 Defining a pre-emption enabled version of DREAM and JSMC requires slight adjustment
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31 127 of the acceptance/rejection step in the Metropolis-Hastings algorithm, as illustrated in Figure 1.
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34 128 When a given parameter set θ_n is evaluated (box 1 in Figure 1), Z is generated and the pre-
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37 129 emption threshold for candidate θ^* or $p(\theta^* | \mathbf{Y})_{\min}$ is identified (box 2). At any time step (t) of
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40 130 the model simulation, the likelihood can be calculated as $p_t(\theta^* | \mathbf{Y})$ and evaluated against
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43 131 $p(\theta^* | \mathbf{Y})_{\min}$ (boxes 3-6). If the evaluated density of any candidate solution becomes lower than
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46 132 $p(\theta^* | \mathbf{Y})_{\min}$ at any point through the simulation, it is pre-empted (box 7); otherwise, the
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49 133 evaluation of θ^* terminates without any time saving (box 8). Note that a pre-empted candidate
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51 134 would never be accepted by the Metropolis-Hastings algorithm, even if the simulation had not
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53 135 been pre-empted. As such, the pre-emption strategy employed here is deterministic in that it has
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56 136 absolutely no influence, other than computational savings, on the behaviour of the algorithm.
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58 137 **[Figure 1 goes here]**
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4 138 Assuming computational cost is the same for all model time steps (*i.e.*, the simulation
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6 139 model takes identical amount of time during different time steps), the associated computational
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9 140 savings for a given application of DREAM or JSMC can be estimated as follows (*Razavi et al.*,
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11 141 2010):

$$142 \quad S = 100 \times \left[\frac{n - n_p}{n} \right] \quad (4)$$

143 where S is the computation savings (in percent), n is the total number of time steps in the
144 calibration period, and n_p is the number of time steps simulated before the simulation is
145 terminated by pre-emption. Note that the pre-emption approach outlined in this section is
146 applicable to any other MCMC or SMC samplers that utilize the Metropolis-Hastings
147 acceptance/rejection approach for evaluating candidate moves.

148 3. Results

149 3.1. Non-pre-emptive experiments

150 A “standard” (*i.e.*, non-pre-emptive) DREAM implementation was applied to three case
151 studies, thereby establishing baseline computational costs for the algorithm. Preliminary
152 investigation of model residuals indicated the standard Bayesian formulation of Equation (1) was
153 sufficient for calibrating the HYMOD case study. Conversely, the AR-based formulation of
154 Equation (3) was required for the WetSpa and SWAT case studies to accommodate correlation
155 among the residuals. The Gelman-Rubin convergence metric (\hat{R} -statistic) indicated that
156 DREAM converged after 7800, 4000, and 161000 simulations of the in HYMOD, WetSpa, and
157 SWAT case studies, respectively. After convergence, 10000 more samples were taken to form
158 the posterior distribution.

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159 A baseline set of non-pre-emptive JSMC sampling experiments were also applied to the
160 three case studies. Although JSMC convergence and model residuals are treated differently, the
161 same likelihood formulations as the DREAM experiments were used, and the same
162 computational budgets were considered. Note that the relative efficiencies of DREAM and
163 JSMC were compared previously by Jeremiah et al., (2011) and such inter-algorithm
164 comparisons were not pursued in the present study. Instead, the numerical experiments focused
165 on the application of pre-emption to reduce the computational burden of these methods.

166 3.2. Application of model pre-emption

167 Pre-emption-enabled versions of DREAM and JSMC were applied to the same
168 calibration problems as mentioned in Section 3.1. The pre-emptive DREAM and JSMC
169 experiments were performed using the same sequence of random numbers (generated by a
170 random number generator) applied in previous experiments. Moreover, the same computational
171 budgets were considered for corresponding pre-emptive and baseline experiments. These
172 identical settings ensured that a given samplers' search behaviour was the same with and without
173 pre-emption. As expected, the pre-emption-based DREAM and JSMC samplers yielded the same
174 sets of posterior parameter values as those obtained in the corresponding baseline (*i.e.*, non-pre-
175 emptive) experiments. In other words, use of model pre-emption did not change the calibration
176 results, and the only effect of using pre-emption was a reduction in the required amount of
177 computation.

178 Table 2 provides average computational savings (in percent) for the pre-emption-based
179 DREAM and JSMC experiments. The total average savings ranged from 5% to 21% in DREAM,
180 and from 16% to 18% in JSMC. Extrapolating based on average simulation model runtimes and
181 the percentage savings yields estimated wall-clock savings of up to 38 hours for our case studies.

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182 For more computationally demanding hydrologic models, such as fully distributed models
183 requiring hours of simulation time, the wall-time savings afforded by pre-emption would be even
184 more significant.

185 For the selected algorithms (*i.e.*, DREAM and JSMC), most of the pre-emption savings
186 occurred during the initial sampling or “*burn-in*” period, defined as the period before the
187 Gelman-Rubin metric indicates convergence. As the samplers converge, candidate parameter sets
188 (θ^*) decreasingly differ from the current parameter sets (θ_n). This in turn increases the
189 likelihood ratio acceptance criteria, $p(\theta^* | Y)/p(\theta_n | Y)$, and reduces the probability of pre-
190 emption. To quantify this behaviour, the DREAM pre-emption savings were separated into burn-
191 in and post-burn-in periods, and the JSMC results were likewise divided into two halves. The
192 results are shown in brackets in Table 2.

[Table 2 goes here]

194 Figure 2 illustrates the empirical cumulative distribution function of the simulation time
195 at which model pre-emption terminated a given simulation. For DREAM in the post-burn-in
196 period, almost all pre-emption occurred after 85% of the simulation was completed. This
197 explains why the overall cumulative savings reported for DREAM in Table 2 are relatively low.
198 However, unacceptable simulations were terminated much earlier during the burn-in period and
199 there was considerable computational savings in this stage. Fairly similar pre-emption behaviour
200 was observed for the JSMC sampler (lower panel in Figure 2).

[Figure 2 goes here]

3.3. Sensitivity of pre-emption savings to calibration period

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203 The effectiveness of model pre-emption can be sensitive to the location of large storms
204 within the calibration period (*Razavi et al.*, 2010). For example, inferior parameter sets will
205 generally trigger early exceedance of the pre-emption threshold if major events happen early in
206 the calibration period. However, pre-emption will not help as much if a major storm occurs at the
207 end of a calibration period. This is because the simulation will need to cover most of the
208 calibration period before a pre-emption judgment can be made.

209 To explore the sensitivity of model pre-emption to the calibration period, the HYMOD
210 case-study was calibrated using pre-emption-enabled DREAM considering four different years
211 from the observation period. Results showed the pre-emption savings varied according to the
212 selected calibration period, and in some cases considerable savings were achieved. Overall pre-
213 emption savings in these experiments ranged from 8% to 35% during the entire simulation and
214 10% to 39% during the burn-in period.

215 **4. Discussion and Conclusions**

216 In view of the computational burden associated with samplers employed for Bayesian
217 inference (*e.g.* DREAM or JSMC), a model pre-emption approach was investigated for saving
218 computational time. The proposed approach (*i.e.*, avoiding unnecessary simulations) yielded on
219 average between 5 and 21% computational savings in the three selected case studies. In one of
220 the case studies, it was shown that savings could reach as high as 39% depending on the selected
221 calibration period. The time savings were larger during the initial stage of sampling, and ranged
222 from 8% to 39%. Such savings are considerable for simulation models that require several
223 minutes or hours to complete. Moreover, the pre-emption savings varied according to the
224 selected calibration period, and in some cases considerable savings were achieved. Implementing
225 pre-emption did not change the calibration results compared to when calibrating without pre-

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226 emption. Moreover, implementation was straightforward and our approach is generally
227 applicable to any samplers that utilize the Metropolis-Hastings acceptance/rejection approach for
228 evaluating candidate moves in the search space.

229 The case-study results presented here provide strong empirical evidence that a model pre-
230 emption approach is a good choice for application to other case studies involving formal
231 Bayesian calibration. Pre-emption will be most useful in calibration problems where it is very
232 hard to find good solutions and a lot of time is wasted fully evaluating bad solutions long after it
233 is known that they will contribute no new information to the sampling algorithm. Moreover, our
234 results suggest that pre-emption savings are most significant in cases where Bayesian samplers
235 do not converge. In practice, convergence failure is relatively common during the initial phases
236 of calibrating complex hydrological models where multiple applications of a Bayesian sampler
237 can be required. For example, refinement of the model, model input forcings and/or likelihood
238 function is often required before a satisfactory calibration result is obtained. The burn-in period
239 of the selected case-studies are representative of these no-converged situations and
240 corresponding results suggest that savings of up to 39% can be achieved. In this way, pre-
241 emption can accelerate model development by helping modellers more quickly determine when
242 there is an issue preventing MCMC or SMC algorithm convergence.

243 **Acknowledgments**

244 This research was supported with funding from Bryan Tolson's NSERC Discovery Grant (50%).
245 The authors thank Dr. De Smedt (Vrije Universiteit Brussel - VUB) and Dr. Ali Safari (VUB) for
246 providing the WetSpa case study (and associated input and data files), and Dr. Vrugt (University
247 of California at Irvine) for their DREAM source code.

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Table 1. Three rainfall-runoff models and the catchments studied in this paper

Simulation Model (Type)	# of Para.	Catchment (Area km ²)	Forcing data	Calibration Period	Refs. for more info
HYMOD (lumped)	5	Leaf (1994)	Precipitation Temperature PET*	1953-1954	Boyle (2000); Vrugt et al. (2003)
WetSpa (semi-distributed)	6	Baron (965)		1995-2000	Safari et al. (2009)
SWAT (semi-distributed)	26	Cannonsville (37)	Precipitation Temperature PET* Sol. radiation Rel. humidity	1996-1998	Tolson (2005); Tolson and Shoemaker (2007)

* Potential Evapotranspiration

Table 2. Average computation saving (in percent) obtained from model pre-emption in different calibration problems

Method	Case Study		
	HYMOD	WetSpa	SWAT
MCMC	14* [17**]	21 [39]	5 [8]
JSMC	16 [21]	18 [28]	17 [25]

* During entire simulations

** During initial sampling stage (burn-in period in MCMC, and first half of JSMC simulations).

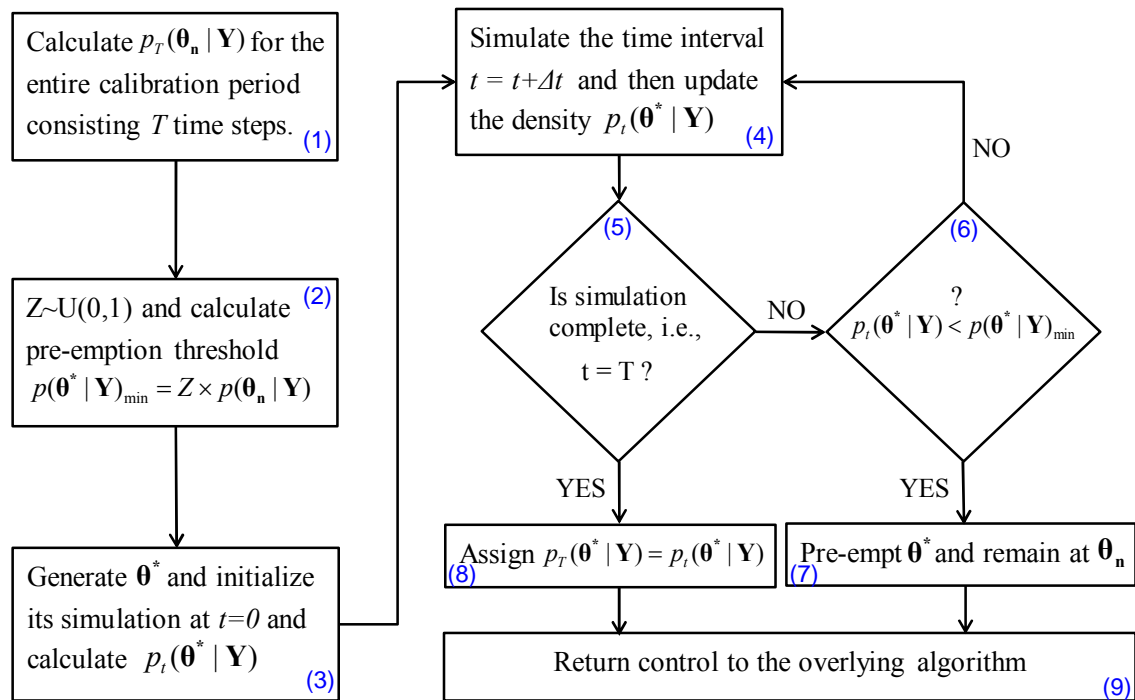


Figure 1. Modified acceptance/rejection step in Metropolis-Hastings component implemented in pre-emption

Figure 2

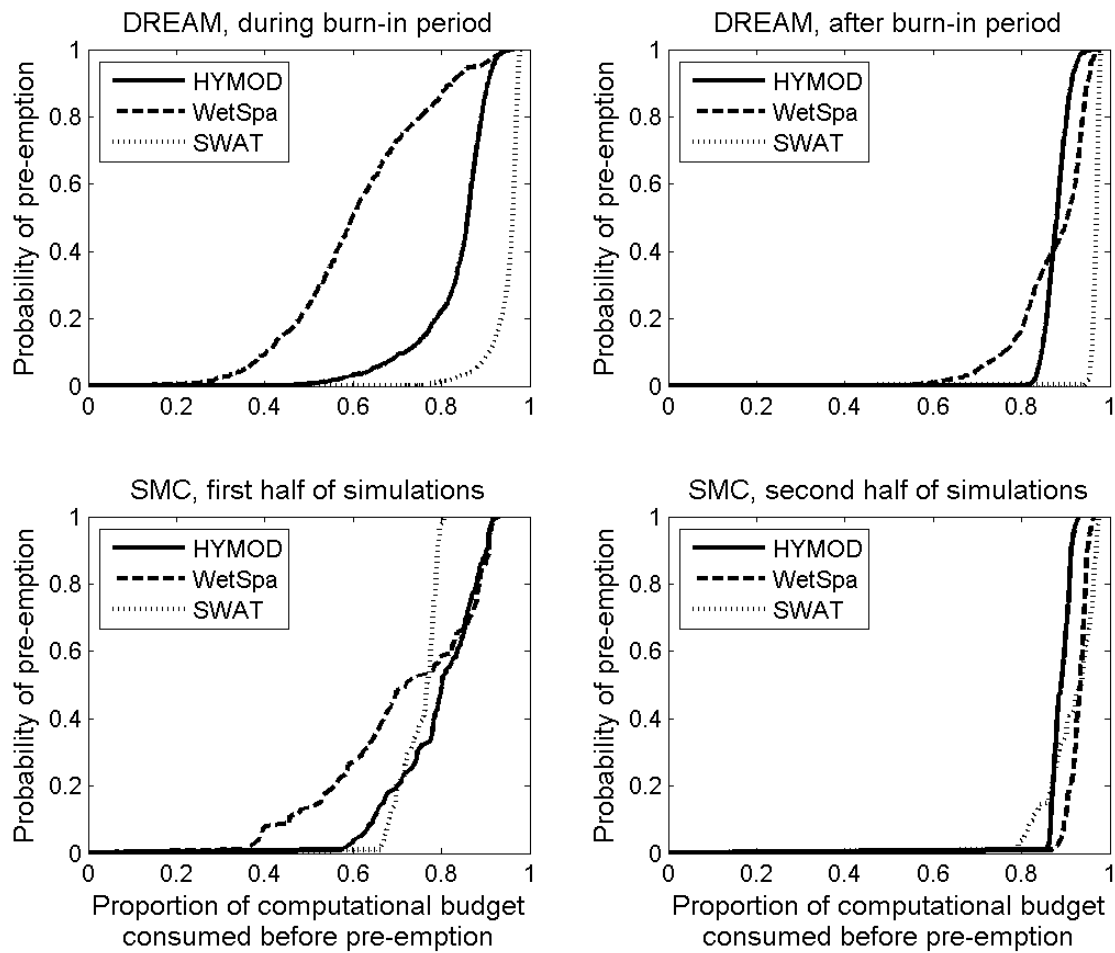


Figure 2. Empirical cumulative distribution function of the simulation time at which model pre-emption is applied in different calibration problems