Technical note: Quadratic solution of the approximate reservoir equation (QuaSoARe) - Supplement

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S1. Application of QuaSoARe to flux functions that are not Lipschitz continuous

QuaSoARe is a method designed to solve the reservoir equation given an initial condition and a set of flux functions. The method is developed based on the assumption that the flux functions are all Lipschitz continuous (see Section 1 of the paper) which restricts the choice of potential flux functions. This section explores the impact of applying QuaSoARe to flux functions that are not meeting this condition. More precisely, a variant of the routing models CR and BCR presented in Table 1 of the paper is considered where the reservoir equation is:

$$\frac{dS}{dt} = Q_{inflow} - Q_{ref}\left(\frac{S}{\theta}\right)^{\kappa} \quad \textbf{Eq. 1}$$

Where Q_{inflow} and Q_{ref} are the river reach inflow and reference flow ($m^3\ s^{-1}$), respectively, θ is the scaling factor set to 43 200 Q_{ref} and κ is an exponent set to 0.5. The catchment selected here is Coopers Creek at Ewin Bridge (203024). In this case, the second flux function in the right-hand side of Eq 1 is not Lipschitz continuous in $S = 0$ because it becomes infinitely steep at this point due to the fact that κ is strictly lower than 1.

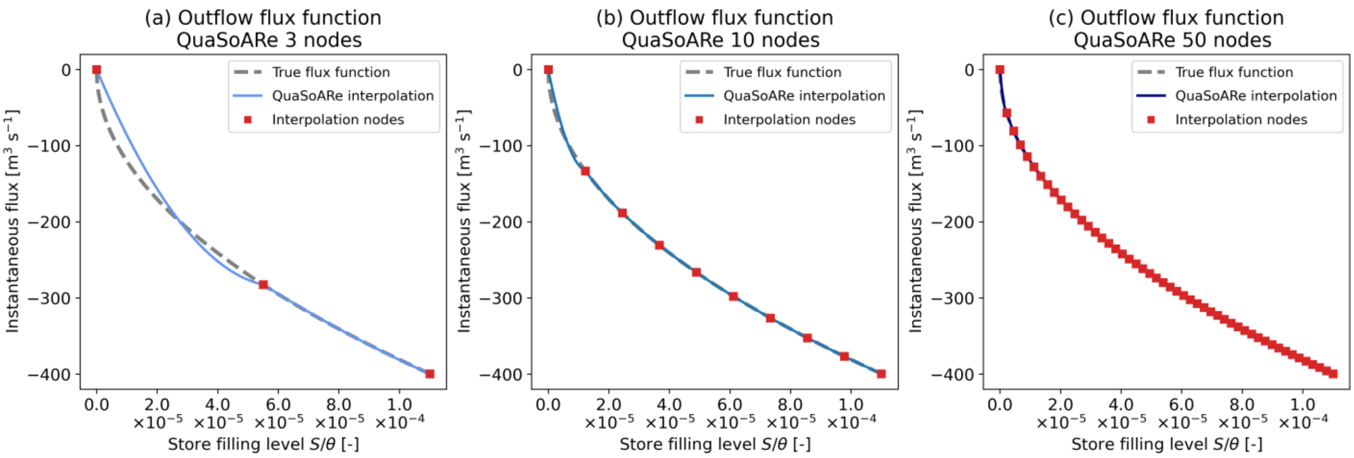

Figure S1: True and approximated flux functions of the routing reservoir equation with QuaSoARe interpolation using 3, 10 and 50 nodes.

Applying QuaSoARe requires to first interpolate the flux functions using a given set of interpolation nodes. Figure S1 shows the result of this process when using 3 (Figure S1.a), 10 (Figure S1.b) and 50 (Figure S1.c) nodes. Figure S1.a highlights the difficulty of interpolating a non-Lipschitz continuous function using a few quadratic polynomials: large discrepancies between the true (grey) and approximated (blue) functions appear close to the point $S = 0$. Increasing the number of nodes reduces these discrepancies significantly but cannot eliminate them completely as can be seen in Figure S1.c.

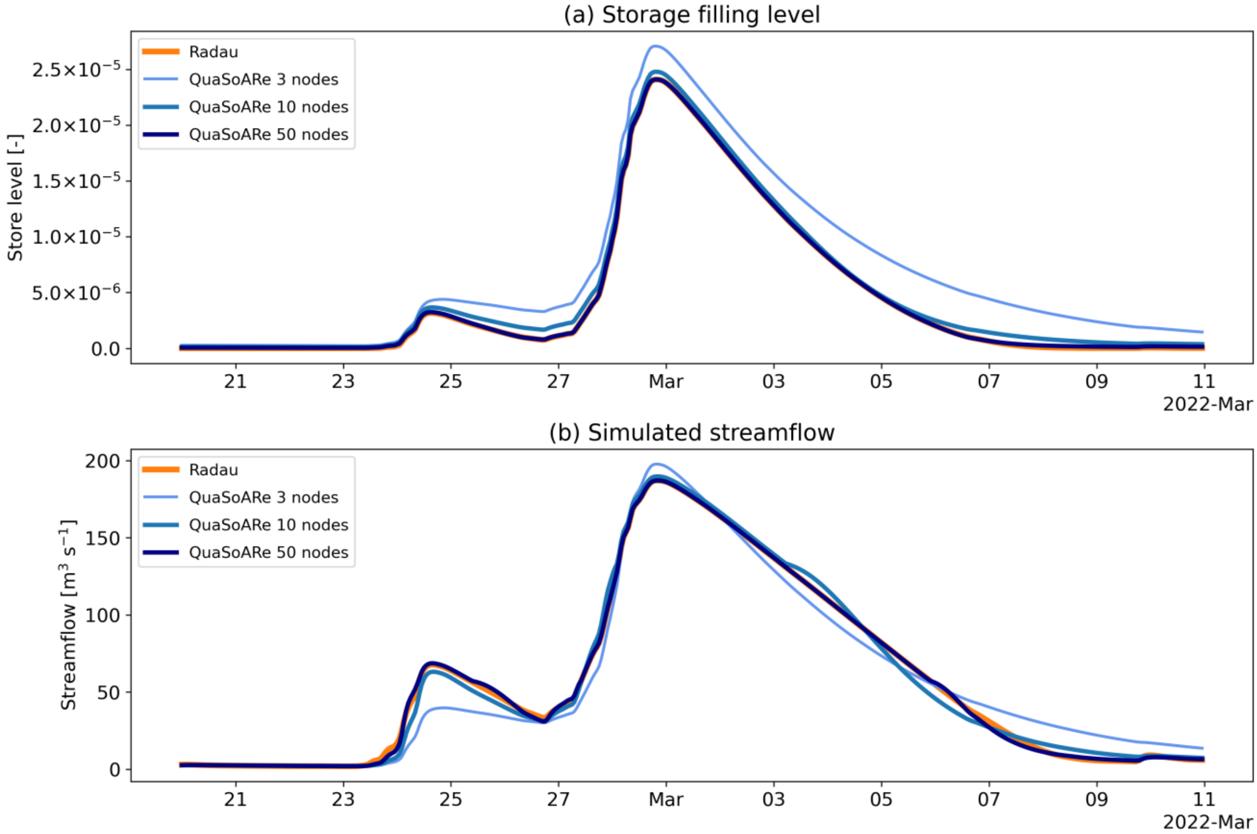

Figure S2: Radau and QuaSoARe storage level (plot a) and outflow flux (plots b) for the routing reservoir using data from the Coopers Creek at Ewing Bridge catchment. QuaSoARe is configured with 3, 10 and 50 interpolation nodes.

Once the interpolation is done, QuaSoARe can be run. Figure S2 shows the simulation corresponding to four methods of integration: the Radau scheme (see Section 5.2 of the paper), and QuaSoARe using 3, 10 and 50 nodes. This figure reveals that QuaSoARe simulation using 3 nodes (light blue line) introduces large errors in the simulated outflow compared to the Radau outputs (orange line). This is not surprising considering the discrepancies between the true and approximated fluxes shown in Figure S1. However, the QuaSoARe simulation using 50 nodes (dark blue line) remains relatively close the Radau simulation in both plots of Figure S2, which suggests that it is possible to obtain a reasonable simulation using QuaSoARe even if the flux functions are not Lipschitz continuous. This is, however, highly dependent on the case considered and will probably require a much higher number of interpolation nodes compared to reservoirs where flux functions are smoother.

S2. Approximate computation of flux totals

In section 1.2 of the paper, it is mentioned that the flux totals O_i could be computed using simplified quadrature method as an alternative to expanding the reservoir equation into a system of differential equation or using QuaSoARe. If we assume that the reservoir equation is solved, i.e. that the two values S_0 (initial condition) and $S(\delta)$ are known, two of these quadrature methods suggested by one of the anonymous reviewers could be expressed as follows:

$$Mid\ point\ method\colon\ O_i = \int_0^{\delta} f_i\big(S,\tilde{V}\big)\,dt \approx \delta\, f_i\left(\frac{S_0 + S(\delta)}{2}, \tilde{V}\right) \qquad \textbf{Eq. 2}$$

$$Mid\ flux\ method\colon\ O_i \approx \delta\, \frac{f_i\big(S_0,\tilde{V}\big) + f_i\big(S(\delta),\tilde{V}\big)}{2} \qquad \textbf{Eq. 3}$$

Although computationally expeditive, both methods introduce an additional approximation to the solution of the reservoir equation which can lead to large errors if this approximation is poor. As an example, we applied the two approximate methods to GR4J production store (see Table 1 of the paper) when integrated with the Radau ODE solver (see Section 5.2 of the paper) and compared them with the system expansion method indicated in the paper (see Eq. 3). Note that we did not use QuaSoARe in this example.

The catchment selected is Coopers Creek at Ewin Bridge (203024). The store capacity θ is set to 50mm, which is outside of the parameter range reported in Table 1 of the paper (100 to 1000 mm). Based on our experience, such a small value of θ is rare in practice, but can happen during a calibration phase when a large number of parameters are tested. Intuitively, a GR4J store with a small capacity receiving a large rainfall input will react quickly and show large variations of the flux functions over the time step.

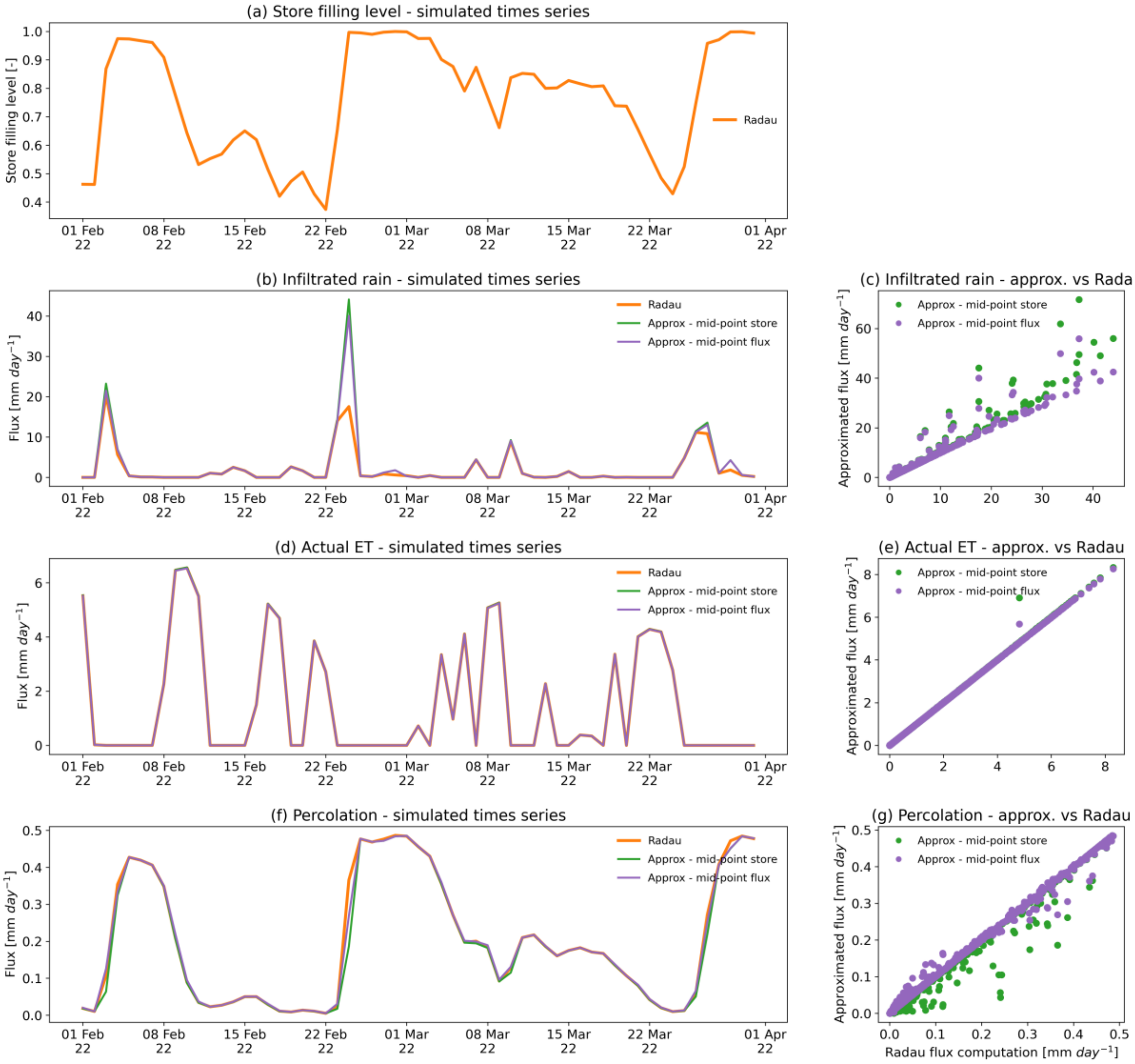

Figure S3: Comparison of flux computation using ODE system expansion method proposed in the paper and two approximate quadrature methods.

Figure S3 shows the simulations of the store level (figure a) and the three fluxes: infiltrated rain (b), actual evapotranspiration (d), and percolation (f). The Radau fluxes (orange lines) are compared with fluxes computed with the two approximate methods: mid-point method shown (green lines) and mid-flux method (purple lines). Scatter plots of Radau versus approximated values are shown in figures c, e and g using the same colour scheme.

Overall, the approximated fluxes appear close to the Radau fluxes, especially for the actual ET flux where the three lines are visually indistinguishable. For infiltrated rain, the three flux computation methods remain very close except for large rainfall events, especially on the 24th February where the Radau flux is less than 20mm whereas both approximated methods lead to values exceeding 40mm. The scatter plot in figure (c) confirms the large errors introduced by the two approximate methods with point deviating significantly from the 1:1 line. To understand the reason for these discrepancies, the Radau integrator was run at a finer time step of 30min during the 24th February starting from the initial condition extracted from the daily simulation. The resulting half-hourly simulations of store level and infiltrated rain are shown in Figure S4. Note that a constant rainfall rate is used throughout the day to match with the daily simulation.

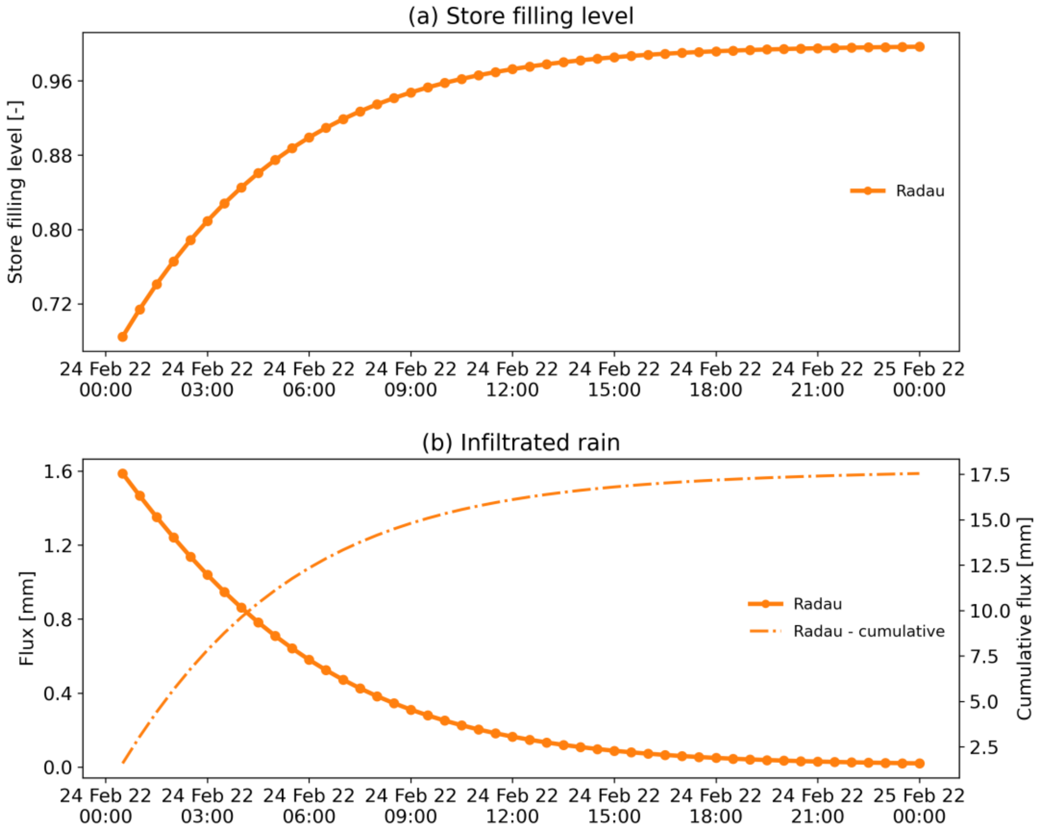

Figure S4: GR4J simulations obtained with the Radau integrator for the 24th of February. Figure a shows the production store level. Figure b shows the infiltrated rain flux times series and its cumulative sum on a secondary y axis.

Figure S4 reveals that the storage level $s(t)$ increases significantly during the simulation with most of the increase occurring during the first half of the day. As a result, the infiltrated rain, which is a decreasing quadratic function of s (see Table 1 of the paper), decreases quickly at first and progressively more slowly to reach a value close to 0 at the end of the day. Both store and flux are clearly not following a linear trend, which explains why the two approximate flux computation methods severely overestimate the Radau flux for this day.

Overall, the approximate computation methods appear valid if the store and fluxes do not vary significantly during the time step of integration. However, it is difficult to guarantee that such sudden changes will not occur and, hence, degrade the simulation quality for certain flow regimes (particularly high flow regimes). For this reason, we recommend computing fluxes analytically, like in QuaSoARe, or using the ODE integrator in conjunction with Eq 3, as indicated in Section 1.2 of the paper.