Supplementary materials

1. Proof that the exponential covariance model is permissible for river distances on directed trees

We provide here a proof that the exponential covariance model is permissible for river distances on directed trees, using the powerful procedure outlined in the works of Ver Hoef et al. (2006) and Ver Hoef and Peterson (2008). We have defined $X(l,i)$ at longitudinal coordinate $l$ along reach $i$ as the moving-average of a white noise random process $W(u,j)$ downstream of point $(l,i)$ using the following equation

$$X(l,i) = \int_{-\infty}^{l} du \ g(u-l) \ W(u,V_i(u))$$

where $g(u-l)$ is a moving average function defined on $\mathbb{R}$, $V_i(u)\{j\}$ designate the reach at longitudinal coordinate $u$ downstream of reach $i$, and $W(u,j)$ is a white noise process with mean zero, i.e. $E[W(u,j)]=0$ where $E[.]$ is the expectation operator, and with covariance $\text{cov}[W(u,j), W(u',j')] = \delta_{j,j'} \delta(u-u')$, where $\delta_{j,j'}$ is the kronecker function ($\delta_{j,j'}=1$ if $j=j'$, and $\delta_{j,j'}=0$ otherwise), and $\delta(u-u')$ is the Dirac function (with property $\int_{-\infty}^{\infty} du' f(u') \delta(u-u') = f(u)$ for sufficiently smooth functions $f(u)$ defined on $\mathbb{R}$).

We now restrict ourselves to the case of the exponential moving average function $g(h)= \sqrt{2} \exp(-|h|)$. Without loss of generality we assume that $l' \geq l$. The covariance between two points $r=(s,l,i)$ and $r'=(s',l',i')$ is then given by

$$\text{cov}(r,r') = \text{cov}(X(l,i), X(l',i'))$$
\begin{align*}
&= E \left[ \int_{-\infty}^{l'} du \ g(u-l) \ W(u, V_i(u)) \int_{-\infty}^{l'} du' \ g(u'-l') \ W(u', V_i(u')) \right] \\
&= 2 \int_{-\infty}^{l} du \ \exp(u-l) \int_{-\infty}^{l'} du' \exp(u'-l') \ E[W(u, V_i(u)) \ W(u', V_i(u'))] \\
&= 2 \int_{-\infty}^{l} du \ \exp(u-l) \int_{-\infty}^{l'} du' \exp(u'-l') \delta_{V_i(u), V_i(u')} \delta(u-u') \\
&= 2 \int_{-\infty}^{l} du \ \exp(u-l) \exp(u-l') \delta_{V_i(u), V_i(u)}
\end{align*}

where \( l' \geq l \) was used in the last line to obtain the upper bound of the integral.

First consider the case where \( i \) and \( i' \) are flow-connected, i.e. \( i' \) is upstream of \( i \), or equivalently \( V_i(l) = \{i\} \). Then \( \delta_{V_i(u), V_i(u')} = 1 \) for all \( u \leq l \) and therefore in that case

\[
\text{cov}(r, r') = 2 \int_{-\infty}^{l} du \ \exp(u-l) \exp(u-l') = 2 \int_{-\infty}^{0} dv \ \exp(v) \exp(v - (l'-l))
\]

\[
= \exp(-(l'-l)) \int_{-\infty}^{0} dv \ \exp(2v) = \exp(-(l'-l))
\]

\[
= \exp(-d_R(r, r'))
\]

where \( d_R(r, r') = l' - l \) was used to obtain the last line since \( i \) and \( i' \) are flow-connected.

Next consider the case where the points \( r \) and \( r' \) are not flow-connected, i.e. \( i \) and \( i' \) are on different branches of the river network. In that case the confluence node of these two branches is at a longitudinal coordinate \( l'' \) such that \( l'' \leq l \) and \( l'' \leq l' \), and the river distance between \( r \) and \( r' \) is \( d_R(r, r') = (l - l'') + (l' - l'') \). It follows that \( \delta_{V_i(u), V_i(u')} = 1 \) for \( u \leq l'' \) and \( \delta_{V_i(u), V_i(u')} = 0 \) for \( l'' < u \leq l \). Therefore in that case we have

\[
\text{cov}(r, r') = 2 \int_{-\infty}^{l''} du \ \exp(u-l) \exp(u-l')
\]
Hence we have shown that whether or not two points are flow-connected, their covariance is \( \exp(-d_R(r,r')) \). Since the covariance of the moving-average of a white noise random process is a permissible covariance model (Ver Hoef et al., 2006), then the exponential covariance is permissible with the river metric.

### 2. Flow-weighted covariance models

The framework proposed in Ver Hoef et al (2006), and further used by Cressie et al. (2006) and Ver Hoef and Peterson (2008) was a break-through to obtain a large class of flow-weighted covariance models based on moving average constructions. We refer the reader to their papers for an in-depth presentation of the framework, but we provide here some mathematical steps using a slightly modified notation that can then be compared with the alternate framework proposed by Bernard-Michel and Fouquet (2006). Let’s define \( X(l,i) \) at longitudinal coordinate \( l \) along reach \( i \) as the moving-average of a white noise random process \( W(u,j) \) on the reaches upstream of point \( (l,i) \) using the following equation

\[
X(l,i) = \int_{\Omega(i,u)} du \sum_{j \in V_i(u)} \sqrt{\Omega(i,j)} g(u-l) W(u,j)
\]

where \( V_i(u) \) is the set of river reaches at longitudinal coordinate \( u \) upstream of reach \( i \), \( g(u-l) \) is a moving average function defined on \( R^1 \), \( W(u,j) \) is a white noise process with
mean zero, and \( \Omega(i,j) \) is real number between 0 and 1 expressing the amount of flow connection between reach \( i \) and \( j \) such that \( \sum_{j \in V_i(u)} \Omega(i,j) = 1 \) for \( u > l \). The flow connection between reach \( i \) and an upstream reach \( i' \) can be defined as the ratio \( \Omega(i,i') = \Omega(i')/\Omega(i) \) where \( \Omega(i) \) is function that increases in the direction of flow. In that case the property
\[
\sum_{i' \in V_i(u)} \Omega(i,i') = 1 \quad \forall \ u > l
\]
is verified if and only if \( \Omega(i) \) is a flow additive function, i.e. such that if two reaches \( i' \) and \( i'' \) combine into reach \( i \), then \( \Omega(i') + \Omega(i'') = \Omega(i) \). Flow discharges or watershed areas are physically meaningful variables that can be used to obtain \( \Omega(i) \) (see next section). The covariance between two points \( r=(s,l,i) \) and \( r'=(s',l',i') \) is then given by
\[
\text{cov}(r,r') = \text{cov}(X(l,i), X(l',i'))
\]
\[
= E \left[ \int du \sum_{j \in V_i(u)} \sqrt{\Omega(i,j)} g(u-l) W(u,j) \int_{l'} du' \sum_{j' \in V_i'(u')} \sqrt{\Omega(i',j')} g(u'-l') W(u',j') \right]
\]
\[
= \int_{l}^{\infty} du g(u-l) \int_{l'}^{\infty} du' g(u'-l') \sum_{j \in V_i(u)} \sqrt{\Omega(i,j)} \sum_{j' \in V_i'(u')} \sqrt{\Omega(i',j')} \delta_{j,j'} \delta(u-u') E[W(u,j)W(u',j')]
\]
\[
= \int_{l}^{\infty} du g(u-l) \int_{l'}^{\infty} du' g(u'-l') \sum_{j \in V_i(u)} \sqrt{\Omega(i,j)} \sum_{j' \in V_i'(u')} \sqrt{\Omega(i',j')} \delta_{j,j'} \delta(u-u')
\]
If \( r \) and \( r' \) are not flow-connected, then \( V_i(u) \cap V_i'(u') = \emptyset \ \forall \ u \geq l \) and \( u' \geq l' \), as a result
\( \delta_{j,j'} = 0 \ \forall \ j \in V_i(u) \) and \( j' \in V_i'(u') \), so that the double summation is zero and consequently \( \text{cov}(r,r') = 0 \). If \( r \) and \( r' \) are flow-connected let us assume without loss of generality that \( r \) is upstream of \( r' \), i.e. \( l \geq l' \). Then using the property of the Dirac function
\[
( \int_{-\infty}^{\infty} du' f(u') \delta(u-u') = f(u) \) for sufficiently smooth functions \( f(u) \) defined on \( \mathbb{R}^1 \) we obtain
\[
\text{cov}(r,r') = \int_{l}^{\infty} du g(u-l) g(u-l') \sum_{j \in V_i(u)} \sum_{j' \in V_{i'}(u)} \sqrt{\Omega(i,j)\Omega(i',j')} \delta_{j,j'}
\]

where \( l \geq l' \) was used in obtaining the lower bound of the integral. Since \( r \) and \( r' \) are flow-connected with \( r \) upstream of \( r' \), it follows that \( V_i(u) \subset V_{i'}(u) \neq \emptyset \ \forall \ u \geq l \), so that the double summation reduces to a single summation as follow

\[
\text{cov}(r,r') = \int_{l}^{\infty} du g(u-l) g(u-l') \sum_{j \in V_i(u)} \sqrt{\Omega(i,j)\Omega(i',j)}
\]

Recall that \( \Omega(i',j) = \Omega(j)/\Omega(i') \), \( \Omega(i,j) = \Omega(j)/\Omega(i) \) and \( \sum_{j \in V_i(u)} \Omega(i,j) = 1 \) for \( u > l \), from which we also get \( \sum_{j \in V_i(u)} \Omega(j) = \Omega(i) \) for \( u > l \). Using these relationships it follows that

\[
\sum_{j \in V_i(u)} \sqrt{\Omega(i,j)\Omega(i',j)} = \sum_{j \in V_i(u)} \sqrt{\Omega(i)} \Omega(i') = \sqrt{\Omega(i)} \\sqrt{\Omega(i')} = \sqrt{\Omega(i,i')} ,
\]

which when substituted in the equation above leads to

\[
\text{cov}(r,r') = \sqrt{\Omega(i,i')} \int_{0}^{\infty} du g(v) g(v+l-l')
\]

where the change of variable \( v = u-l \) was used in the integral. Noting that \( d_R(r,r')=l-l' \) when \( r \) and \( r' \) are flow-connected and \( l \geq l' \), and noting that \( \Omega(i,i')=0 \) when \( r \) and \( r' \) are not flow-connected, then a permissible model for the covariance between \( r \) and \( r' \) (whether they are flow-connected or not) is given by

\[
\text{cov}(r,r') = \sqrt{\Omega(i,i')} \ C_1( \ d_R(r,r') )
\]

where \( d_R(r,r')=|l-l'| \) is the river distance between \( r \) and \( r' \), and \( C_1( . \ ) \) is the class of permissible covariance functions in \( R^1 \) defined by \( C_1(h) = \int_{0}^{\infty} du g(v) g(v+h) \) for any
suitable moving average functions $g(v)$. This class of permissible covariance functions includes for example the strikingly beautiful Mariah (Ver Hoef, 2006) model.

De Fouquet and Bernard-Michel (2006) proposed a framework that can be used to expand the class of permissible flow-weighted covariance models. Along the lines of the framework they proposed, let us here define $X(l, i)$ at longitudinal coordinate $l$ along reach $i$ as

$$X(l, i) = \sum_{j \in V_i(\infty)} \sqrt{\Omega(i, j)} \ Y_j(l)$$

where $V_i(\infty)$ is the set of flow-connected leaf reaches (i.e. sources) upstream of reach $i$, $\Omega(i, j) \in [0, 1]$ quantifies the flow connection between reach $i$ and its source $j$ such that $\sum_{j \in V_i(\infty)} \Omega(i, j) = 1$, and $Y_j(l)$ are independent zero mean random processes on $R^1$ with covariance $\text{cov}(Y_j(l), Y_j(l')) = c_1(h)$, $h = |l-l'|$, where $c_1(h)$ may be any permissible covariance function in $R^1$ (i.e. such that it is the Fourier transform of a non-negative bounded function in $R^1$). The covariance between two points $r = (s, l, i)$ and $r' = (s', l', i')$ is then given by

$$\text{cov}(r, r') = \sum_{j \in V_i(\infty)} \sum_{j' \in V_i(\infty)} \sqrt{\Omega(i, j)} \sqrt{\Omega(i', j')} \ \text{cov}(Y_j(l), Y_j(l'))$$

If $r$ and $r'$ are not flow-connected, then $V_i(\infty) \cap V_i'(\infty) = \Phi$, as a result $\text{cov}(Y_j(l), Y_j(l')) = 0$ $\forall j \in V_i(\infty)$ and $j' \in V_i'(\infty)$, so that $\text{cov}(r, r') = 0$. If $r$ and $r'$ are flow-connected, assuming without loss of generality that $r$ is upstream of $r'$, i.e. $l \geq l'$, we have

$$\text{cov}(r, r') = \sum_{j \in V_i(\infty)} \sum_{j' \in V_i(\infty)} \sqrt{\Omega(i, j)} \sqrt{\Omega(i', j')} \ \delta_{j, j'} c_1(|l-l'|)$$

$$= \sum_{j \in V_i(\infty)} \sqrt{\Omega(i, j) \Omega(i', j)} c_1(|l-l'|)$$
Noting that \( \Omega(i,i')=0 \) when \( r \) and \( r' \) are not flow-connected, we obtain that a permissible model for the covariance between \( r \) and \( r' \) (whether they are flow-connected or not) is given by

\[
\text{cov}(r,r') = \sqrt{\Omega(i,i')} \ c_1(\ d_{R}(r,r') )
\]

where \( c_1(\ . \ ) \) can be any one dimensional permissible covariance function, which includes the functions \( C_1(\ . \ ) \) obtained with the moving average construction.

3 Flow additive functions used to calculate flow connectivity

As described above, the flow connection between reach \( i \) and an upstream reach \( i' \) can be defined as the ratio \( \Omega(i,i')=\Omega(i')/\Omega(i) \) where \( \Omega(i) \) is a flow additive function, i.e. such that if two reaches \( i' \) and \( i'' \) combine into reach \( i \), then \( \Omega(i')+\Omega(i'')=\Omega(i) \). We show here that the framework developed by Ver Hoef at al. (2006) to quantify flow-connection provides a flexible method to construct the flow additive function \( \Omega(i) \). Using their approach, let’s define the flow weight of a reach \( i' \) as \( \omega(i') \) such that if reaches \( i' \) and \( i'' \) combine at a river junction, then \( \omega(i')+\omega(i'')=1 \). Using this variable, Ver Hoef at al. (2006) originally defined the flow connection between reach \( i \) and an upstream reach \( i' \) as \( \Omega(i,i')=\prod_{j \in B_{i,i'}} \omega_j \), where \( B_{i,i'} \) is the set of reaches in the flow-path between reaches \( i \) and \( i' \), exclusive of the downstream reach \( i \) and inclusive of the upstream reach \( i' \). This construction is equivalent to defining the flow additive function as

\[
\Omega(i)=\prod_{j \in B_{i,i'}} \omega_j ,
\]
where $B_{1,i}$ is the set of reaches in the flow-path between the river outlet (on a river reach numbered 1 by convention) and reach $i$. Then it follows immediately that

$$\Omega(i,i') = \Omega(i')/\Omega(i) = \prod_{j \in B_{1,i}} \omega_j = \prod_{j \in B_{1,i}} \omega_j \prod_{j \in B_{1,i}} \omega_j = \prod_{j \in B_{1,i}} \omega_j,$$

which, after taking its square-root, leads to the multiplier $\sqrt{\Omega(i,i')} = \prod_{j \in B_{1,i}} \sqrt{\omega_j}$ defined in Ver Hoef et al. (2006) equation for flow-connected covariance models.

The weight of each combining reach can be calculated using a physically meaningful parameter that increases in the direction of flow. Examples include watershed area, discharge, cumulated river length, precipitation, pollution loading, etc. Let us denote the value of this parameter at the downstream end of any reach $i$ as $A_i$, and let $a_i$ be the contribution within reach $i$, such that if reaches $i'$ and $i''$ combine into reach $i$, then $A_i = A_{i'} + A_{i''} + a_i$. Using this parameter we can define the weights of combining reaches $i'$ and $i''$ as $\omega_{i'} = A_{i'}/(A_{i'} + A_{i''})$ and $\omega_{i''} = A_{i''}/(A_{i'} + A_{i''})$, respectively, which satisfies $\omega_{i'} + \omega_{i''} = 1$. The resulting flow additive function is then given by

$$\Omega(i) = \prod_{j \in B_{1,i}} \omega_j = \prod_{j \in B_{1,i}} \frac{A_j}{A_j + A_{C(j)}} = \prod_{j \in B_{1,i}} \frac{A_j}{A_{D(j)} - a_{D(j)}}$$

where $C(j)$ is the reach combining with reach $j$, and $D(j)$ is the reach immediately downstream of reaches $j$ and $C(j)$; so that $A_{D(j)} = A_j + A_{C(j)} + a_{D(j)}$. As can be seen in the example of Fig. S1, the construction shown allows us to account for the contribution of watershed area (or discharge, cumulated river length, etc.) within each reach.
Fig. S1: Example of a river with 5 reaches, indicating for each reach $i$ the contributing watershed area $a_i$, within reach $i$, the total watershed area $A_i$ at the downstream end of reach $i$, and the corresponding flow additive function $\Omega(i)$.

A simplified construction might consist in setting $a_i=1$ for each leaf reaches, and setting the contribution of non-leaf reaches to zero, i.e. $a_D(i)=0 \ \forall \ i>1$. In this case $A_i$ corresponds to the additive stream-order number used in Cressie et al. (2006), and the flow additive function simplifies to $\Omega(i)=A_i/A_1$. For illustration purposes, this corresponds to setting $a_5=a_4=a_3=1$ and $a_2=a_1=0$ in the example of Fig. S1, resulting in the stream-order numbers $A_5=A_4=A_3=1$, $A_2=2$ and $A_1=3$, and in the flow additive function values $\Omega(5)=1/3$, $\Omega(4)=1/3$, $\Omega(3)=1/3$, $\Omega(2)=2/3$, $\Omega(1)=1$. This construction provides a convenient way to obtain flow-connectivity if no information is available about the
contribution of watershed area (or discharge, cumulated river length, etc.) within each reach.

Another simplification consists in weighting each reach equally, i.e. \( \omega(i) = \frac{1}{2} \forall i > 1 \), which leads to \( \Omega(i) = \prod_{j \in B_{i,j}} \frac{1}{2} \). This would correspond to using \( \Omega(5) = \frac{1}{4}, \Omega(4) = \frac{1}{4}, \Omega(3) = \frac{1}{2}, \Omega(2) = \frac{1}{2}, \Omega(1) = 1 \) in the example of Fig. S1, which is a slightly different representation of flow-connectivity than that of based on stream-order number.

4 Implementation of river distance calculation in BMElib

In this work an algorithm is developed and implemented in BMElib (Christakos et al. 2002) that efficiently calculates the isotropic river distance between points on a downstream-only combining network. Other tools exist within GIS software to calculate distances and spatial weights. However, since this research aims at an efficient space/time implementation of the river metric, it is necessary to implement an algorithm within the BME space/time numerical library. Within MATLAB\textsuperscript{TM}, river reach segments are checked for downstream \( \rightarrow \) upstream connectivity relative to the basin outlet, and re-organized into river reaches, which are defined as single continuous polylines connecting river reach segments that approximately delineate the centerline of a stream between its upstream and downstream confluence nodes. Each river reach is identified by a unique ID. These re-organized sets of unique river reaches are then saved as the “organized” networks to continue with the analysis.

The organized networks are used to obtain the river topology for each basin using a branching measure of complexity. The branching level of a reach is defined by starting at 1 for the most downstream reach, and each time a reach splits at a node, the
resulting reaches will be assigned the next branching level (2 and so on). The end result is a topology file that consists of four columns: (1) the unique reach ID; (2) the reach branching level; (3) the downstream reach ID; and (4) the reach length (i.e. the linear length of the reach) (Fig. S2).

Using this information each monitoring data point is associated with the underlying river network by ‘snapping’ the data geographical location to the closest polyline point making up one of the river network reaches. The resulting ‘river’ space/time coordinate of each point is stored in a file consisting of 5 columns, which are (1) the x spatial coordinate (e.g. Easting or longitude) of the point; (2) its y spatial coordinate (e.g. Northing or latitude); (3) the unique ID of the reach onto which the point was snapped; (4) the linear distance from the data point on that reach to its downstream node, and; (5) the time of measurement.

Fig. S2. River network in (a) raw format, (b) re-organized so flow (arrows) point towards the basin outlet (blue circle) and each reach is assigned a unique reach ID, and (c) with river topology information including reach ID, branching level and ID of the connecting downstream reach, as well as reach length (not shown).
This river topology provides the information necessary to efficiently calculate the river distances between any two points along the river network. The steps of the algorithm used to calculate this distance are shown in Fig. S3.

Fig. S3. Flow Chart of the calculation of the distance between two points using isotropic river distance for downstream-only combing river networks within the BME space/time numerical package.

This river metric was then numerically implemented in BMElib by modifying all the core BME functions dealing with the distance between points, including experimental covariance calculation and estimation.