

# Supplementary Material: Advection, diffusion and delivery over a network.

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In the Supplementary Material we detail the mathematical machinery involved in solving the advection, diffusion and delivery equation over a network. In Section A we describe how to solve the particular case of stepwise constant initial conditions. In Section B we show how to calculate the concentration of resource that leaves its initial edge over the time step in question. In Section C we show how to calculate the concentration of resource that remains in the edge in which it started, and in Section D we describe how to calculate the total quantity of resource in each section of the network. Finally, in Section E we describe the Gaver-Stehfest algorithm for inverting our solutions from Laplace space into the time domain.

## SOLVING ADVECTION, DIFFUSION AND DELIVERY IN LAPLACE SPACE

We are interested in calculating how the quantity of resource in a network changes over time, given that the resource decays or is delivered out of the network at a given rate, and is subject to advection and diffusion. In other words, we wish to solve a system of equations defined over a network, where the resource in edge  $ij$  of the network is governed by an equation of the form

$$\frac{\partial q_{ij}}{\partial t} + R_{ij}q_{ij} + u_{ij}\frac{\partial q_{ij}}{\partial x} - D_{ij}\frac{\partial^2 q_{ij}}{\partial x^2} = 0, \quad (1)$$

where  $q_{ij}$  is the quantity of resource per unit length,  $u_{ij}$  is the mean velocity,  $D_{ij}$  is the dispersion coefficient and  $R_{ij}$  is the rate at which a unit of resource is lost, or delivered out of the network. As we are interested in the case where the advective velocities  $u_{ij}$  may vary over several orders of magnitude, it is convenient to operate in Laplace space, and invert our solutions back into the time domain by using the Gaver-Stehfest algorithm. Note that after taking Laplace transforms  $\mathcal{L}(q_{ij}(x, t)) = \int_0^\infty q_{ij}(x, t)e^{-st} dt = Q_{ij}(x, s)$ , the fundamental Equation (1) becomes

$$(s + R_{ij})Q_{ij} + u_{ij}\frac{\partial Q_{ij}}{\partial x} - D_{ij}\frac{\partial^2 Q_{ij}}{\partial x^2} = q_{ij}(x, 0). \quad (2)$$

Also note that as in the Main Text, for each edge  $ij$  and every  $s > 0$  we let

$$\alpha_{ij}(s) = \sqrt{u_{ij}^2 + 4D_{ij}(s + R_{ij})},$$

$$g_{ij} = \frac{u_{ij}l_{ij}}{2D_{ij}} \quad \text{and} \quad h_{ij}(s) = \frac{\alpha_{ij}(s)l_{ij}}{2D_{ij}}.$$

### A. Stepwise constant initial conditions

We are interested in calculating how the quantity of resource in a network changes over time, given that the resource is subject to the fundamental Equation (1). In particular, it is convenient to consider a stepwise constant initial condition, as we can then calculate how the total quantity of resource in each segment of the network has changed by time  $t$ . The first step in this calculation is to find the Laplace transform of the concentrations at each node  $\bar{C}(s)$ . As we have seen, to calculate  $\bar{C}(s)$  we must first find  $\mathbf{M}_{ij}(s)$  and  $\tilde{\mathbf{Y}}(s)$ , which do not depend on the initial condition. For each sample point  $s$  and each edge  $ij$  we must also calculate  $\beta_{ij}(s)$  and  $\beta_{ji}(s)$ , which capture the effect of the initial condition  $q_{ij}(x, 0)$ . In particular, we start this subsection by considering the case where the initial condition is

$$q_{ij}(x, 0) = \begin{cases} k & \text{if } \frac{n-1}{N}l_{ij} \leq x < \frac{n}{N}l_{ij} \\ 0 & \text{otherwise,} \end{cases}$$

where  $n \leq N$ , before moving on to consider the more general case of stepwise constant initial conditions. For the sake of clarity we drop the subscripts  $ij$  from  $l_{ij}$ ,  $N_{ij}$ ,  $R_{ij}$ ,  $\alpha_{ij}$ ,  $g_{ij}$  and  $h_{ij}$ , and ignore the dependence on  $s$  of the terms  $\alpha_{ij}$  and  $h_{ij}$ . Now, to find a particular solution to the fundamental Equation (2) we use the method of

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variation of parameters. This tells us that

$$f(x, s, q_{ij}(y, 0)) = \frac{e^{(g-h)\frac{x}{l}}}{\alpha} \int_0^x e^{(h-g)\frac{y}{l}} q_{ij}(y, 0) dy - \frac{e^{(g+h)\frac{x}{l}}}{\alpha} \int_0^x e^{-(g+h)\frac{y}{l}} q_{ij}(y, 0) dy. \quad (3)$$

Equation (3) tells us that for the given initial condition

$$\begin{aligned} f(l, s, q_{ij}) &= -\frac{ke^{g+h}}{\alpha} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{-(g+h)\frac{x}{l}} dx \\ &\quad + \frac{ke^{g-h}}{\alpha} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{(h-g)\frac{x}{l}} dx, \\ &= \frac{2Dke^{g+h}}{\alpha(u+\alpha)} \left( e^{-\frac{n}{N}(g+h)} - e^{-\frac{(n-1)}{N}(g+h)} \right) \\ &\quad - \frac{2Dke^{g-h}}{\alpha(u-\alpha)} \left( e^{\frac{n}{N}(h-g)} - e^{\frac{(n-1)}{N}(h-g)} \right). \end{aligned} \quad (4)$$

As in the Main Text we let

$$\beta_{ij}(s) \equiv \frac{-\alpha_{ij}(s)e^{-g_{ij}}}{2 \sinh(h_{ij}(s))} f(l, s, q_{ij}(y, 0)). \quad (5)$$

Substituting Equation (4) into Equation (5) gives us

$$\begin{aligned} \beta_{ij}(s) &= \frac{ke^{\frac{1-n}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[ e^{\frac{N-n}{N}h} (e^{\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha - u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} (e^{-\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha + u) \right]. \end{aligned} \quad (6)$$

Recall that  $f(x, s, q_1+q_2) = f(x, s, q_1) + f(x, s, q_2)$ . Since Equation (5) is linear, it follows that if the initial condition contains several blocks of resource, each block makes its own separate contribution to  $\beta_{ij}(s)$  and  $\beta_{ji}(s)$ . Let  $x_0 = 0, x_1 = \frac{l}{N}, x_2 = \frac{2l}{N}, \dots, x_N = l$ , and suppose that for all  $1 \leq n \leq N$  we have

$$q_{ij}(x, 0) = k_{ij}^{(n)} \quad \text{for all } x_{n-1} < x < x_n. \quad (7)$$

Given such a stepwise constant initial condition, we can calculate  $\beta_{ij}(s)$  by summing the contribution of each of the blocks of resource. That is to say, in the case of stepwise constant initial conditions, Equation (6) becomes

$$\begin{aligned} \beta_{ij}(s) &= \sum_{n=1}^N \frac{k_{ij}^{(n)} e^{\frac{1-n}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[ e^{\frac{N-n}{N}h} (e^{\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha - u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} (e^{-\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha + u) \right]. \end{aligned} \quad (8)$$

We can find  $\beta_{ji}(s)$  by using the above formula, substituting  $-g_{ij}$  for  $g_{ji}$ ,  $-u_{ij}$  for  $u_{ji}$  and  $k_{ij}^{(N-n+1)}$  for  $k_{ji}^{(n)}$ . It follows that where  $g = g_{ij}$  and  $u = u_{ij}$

$$\begin{aligned} \beta_{ji}(s) &= \sum_{n=1}^N \frac{k_{ij}^{(N-n+1)} e^{\frac{n-1}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[ e^{\frac{N-n}{N}h} (e^{\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha + u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} (e^{-\frac{h}{N}} - e^{-\frac{g}{N}}) (\alpha - u) \right]. \end{aligned} \quad (9)$$

## B. Resource that leaves its initial edge

If a particle leaves edge  $ij$  and reaches node  $i$  or  $j$  over the relevant time scale, it contributes to  $\beta_{ij}(s)$  or  $\beta_{ji}(s)$ , and hence it contributes to our solution  $C_i(s)$ ,  $C_j(s)$  and  $\mathcal{L}(\hat{q}_{ij}(x, t)) = \hat{Q}_{ij}(x, s)$ . On the other hand, at time 0 none of the resource has reached the nodes, so the initial condition  $\hat{q}_{ij}(x, 0) = 0$ . It follows that the value of  $\hat{Q}_{ij}(x, s)$  is related to the boundary conditions  $X_{ij}(s)$  and  $X_{ji}(s)$  by the Main Text Equation (MT-18). In other words, we can find  $\hat{Q}_{ij}(x, s)$  by effectively considering an initially empty network, where resource is introduced at the nodes at a rate which exactly matches the rate at which resource reaches the nodes in the case where the network has the given non-zero initial condition. The propagation matrix described by Equation (MT-35) also accounts for the impact of any inlet nodes, in the case where resource is being added to the network.

We can therefore use Equations (MT-35), (8) and (9) to find  $\bar{C}(s) = \{C_1(s), \dots, C_m(s)\}$ , and in the case where the cross-sectional areas are constant, we can express  $\hat{Q}_{ij}(x, s)$  in terms of the boundary conditions  $X_{ij} = S_{ij}C_i(s)$  and  $X_{ji} = S_{ij}C_j(s)$ . In fact, we have

$$\begin{aligned} \hat{Q}_{ij}(x, s) &= S_{ij}C_i(s) \frac{\sinh(\frac{l-x}{l}h)}{\sinh(h)} e^{\frac{x}{l}g} \\ &\quad + S_{ij}C_j(s) \frac{\sinh(\frac{x}{l}h)}{\sinh(h)} e^{\frac{x-l}{l}g}, \end{aligned} \quad (10)$$

where the subscripts  $ij$  have been omitted for clarity. Since  $\mathcal{L}(\int \hat{q}_{ij}(x, t) dx) = \int \hat{Q}_{ij}(x, s) dx$ , we can find  $\int \hat{q}_{ij}(x, t) dx$  by letting  $s = \ln 2/t, \dots, N \ln 2/t$ , calculating  $\int \hat{Q}_{ij}(x, s) dx$  for each of these values of  $s$ , and applying the Gaver-Stehfest algorithm (see Section E).

As in Equation (7), we suppose that edge  $ij$  is divided into  $N_{ij}$  sections of equal length, and for the sake of clarity we drop the subscripts  $ij$  from  $D_{ij}$ ,  $l_{ij}$  and  $N_{ij}$ . We let  $y_{ij}^{(n)}(t)$  denote the mean value of  $\hat{q}_{ij}(x, t)$  in the  $n$ th section of edge  $ij$ , and note that by definition

$$y_{ij}^{(n)}(t) = \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \hat{q}_{ij}(x, t) dx. \quad (11)$$

Defining  $Y_{ij}^{(n)}(s) \equiv \mathcal{L}(y_{ij}^{(n)}(t))$  we have

$$\begin{aligned} Y_{ij}^{(n)}(s) &= \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \hat{Q}_{ij}(x, s) dx \\ &= \frac{ND}{l \sinh(h)} \left[ \frac{X_{ij}e^h - X_{ji}e^{-g}}{u - \alpha} e^{(g-h)\frac{x}{l}} \right. \\ &\quad \left. + \frac{X_{ji}e^{-g} - X_{ij}e^{-h}}{u + \alpha} e^{(g+h)\frac{x}{l}} \right] \frac{\frac{n}{N}l}{\frac{n-1}{N}l}, \end{aligned}$$

which implies that

$$\begin{aligned} Y_{ij}^{(n)}(s) &= \eta_{ij}(s)(\alpha + u) \times \\ &\quad \left[ X_{ij} \left( e^{\frac{n-1}{N}(g-h)} - e^{\frac{n}{N}(g-h)} \right) + X_{ji} \times \right. \\ &\quad \left. \left( e^{\frac{n-N}{N}g - \frac{n+N}{N}h} - e^{\frac{n-N-1}{N}g - \frac{n+N-1}{N}h} \right) \right] \\ &+ \eta_{ij}(s)(\alpha - u) \times \\ &\quad \left[ X_{ij} \left( e^{\frac{n-1}{N}g - \frac{2N-n+1}{N}h} - e^{\frac{n}{N}g - \frac{2N-n}{N}h} \right) \right. \\ &\quad \left. + X_{ji} \left( e^{\frac{n-N}{N}(g+h)} - e^{\frac{n-N-1}{N}(g+h)} \right) \right], \quad (12) \end{aligned}$$

$$\text{where } \eta_{ij}(s) = \frac{N_{ij}e^{h_{ij}}(s)}{4(s + R_{ij})l_{ij} \sinh(h_{ij}(s))}. \quad (13)$$

### C. Resource that remains in its initial edge

Over the time scale  $t$ , not all of the resource will leave the edge in which it started. To find  $\tilde{q}_{ij}(x, t)$ , the quantity of resource that has not left edge  $ij$ , we must solve the advection, diffusion, delivery problem for each separate edge  $ij$ , where nodes  $i$  and  $j$  are absorbing boundaries and the initial condition  $\tilde{q}_{ij}(x, 0) = q_{ij}(x, 0)$ . The resulting solution accounts for those particles which do not reach a node in the relevant time-scale. In particular, we consider the case where the initial condition is stepwise constant, as in Equation (7).

The fundamental Equation (1) tells us that for each edge

$$\frac{\partial}{\partial t} \tilde{q}_{ij} = D_{ij} \frac{\partial^2}{\partial x^2} \tilde{q}_{ij} - u_{ij} \frac{\partial}{\partial x} \tilde{q}_{ij} - R_{ij} \tilde{q}_{ij}. \quad (14)$$

Furthermore, we are looking for a real valued function such that  $\tilde{q}_{ij}(0, t) = 0$  and  $\tilde{q}_{ij}(l_{ij}, t) = 0$  for all  $t$ . These conditions imply that we can express  $\tilde{q}_{ij}(x, t)$  in the following form:

$$\begin{aligned} \tilde{q}_{ij}(x, t) &= e^{\frac{u_{ij}}{2D_{ij}}x} \sum_{m=1}^{\infty} A^m e^{\lambda_{ij}^m t} \sin\left(\frac{m\pi x}{l_{ij}}\right), \\ \text{where } \lambda_{ij}^m &= -\left(m^2 \frac{D_{ij}\pi^2}{l_{ij}^2} + \frac{u_{ij}^2}{4D_{ij}} + R_{ij}\right). \quad (15) \end{aligned}$$

The parameters  $A^m$  can be found by taking Fourier transforms. More specifically, we know that  $\tilde{q}_{ij}(x, 0) = q_{ij}(x, 0)$ , so

$$\begin{aligned} \sum_{n=1}^{\infty} A^m \sin\left(\frac{m\pi x}{l_{ij}}\right) &= q_{ij}(x, 0) e^{-g_{ij} \frac{x}{l_{ij}}} \quad \text{and} \\ \int_0^l \sin\left(\frac{m\pi x}{l_{ij}}\right) \sin\left(\frac{n\pi x}{l_{ij}}\right) dx &= \begin{cases} 0 & \text{if } m \neq n, \\ \frac{l_{ij}}{2} & \text{if } m = n. \end{cases} \end{aligned}$$

It follows that for every positive integer  $m$ ,

$$A^m = \frac{2}{l_{ij}} \int_0^{l_{ij}} \sin\left(\frac{m\pi x}{l_{ij}}\right) q_{ij}(x, 0) e^{-g_{ij} \frac{x}{l_{ij}}} dx.$$

In particular, consider the case where the initial condition is stepwise constant, and of the form described by Equation (7). Dropping some of the subscripts  $ij$  for clarity, we have

$$\begin{aligned} A^m &= \mu_{ij}^m \sum_{n=1}^N k_{ij}^{(n)} \left[ e^{-g \frac{x}{l}} \times \right. \\ &\quad \left. \left( \frac{-g}{\pi m} \sin\left(\frac{m\pi x}{l}\right) - \cos\left(\frac{m\pi x}{l}\right) \right) \right] \frac{\frac{n}{N}l}{\frac{n-1}{N}l} \\ &= \mu_{ij}^m \left( k_{ij}^{(1)} - k_{ij}^{(N)} e^{-g} (-1)^m \right) \\ &\quad + \mu_{ij}^m \sum_{n=1}^{N-1} \left[ e^{-\frac{g}{N}x} \left( k_{ij}^{(n+1)} - k_{ij}^{(n)} \right) \times \right. \\ &\quad \left. \left( \frac{g}{\pi m} \sin\left(\frac{mn\pi}{N}\right) + \cos\left(\frac{mn\pi}{N}\right) \right) \right], \quad (16) \end{aligned}$$

where

$$\mu_{ij}^m = \frac{8D_{ij}^2 \pi m}{u_{ij}^2 l_{ij}^2 + 4D_{ij}^2 \pi^2 m^2}. \quad (17)$$

We are now in a position to find

$$z_{ij}^{(n)}(t) = \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \tilde{q}_{ij}(x, t) dx,$$

as Equation (15) implies that

$$\begin{aligned} z_{ij}^{(n)}(t) &= \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{\frac{g_{ij}}{2}x} \sum_{m=1}^{\infty} A^m e^{\lambda_{ij}^m t} \sin\left(\frac{m\pi x}{l}\right) dx \\ &= \frac{N}{2} e^{g \frac{x}{N}} \sum_{m=1}^{\infty} \mu_{ij}^m A^m e^{\lambda_{ij}^m t} \left[ \frac{g}{\pi m} \times \right. \\ &\quad \left. \left( \sin\left(\frac{mn\pi}{N}\right) - e^{-\frac{g}{N}} \sin\left(\frac{m(n-1)\pi}{N}\right) \right) \right. \\ &\quad \left. + \left( e^{-\frac{g}{N}} \cos\left(\frac{m(n-1)\pi}{N}\right) - \cos\left(\frac{mn\pi}{N}\right) \right) \right]. \quad (18) \end{aligned}$$

Note that  $\mu_{ij}^m \rightarrow \frac{2}{\pi m}$  as  $m \rightarrow \infty$ , and likewise  $A^m \in O(m^{-1})$ . In contrast  $e^{\lambda_{ij}^m t}$  tends to zero much

more rapidly. Indeed, we note that

$$\begin{aligned} \sum_{m=\Omega'}^{\infty} e^{\lambda_{ij}^m t} &= e^{-\left(\frac{u^2}{4D}+R\right)t} \sum_{m=\Omega'}^{\infty} e^{-\frac{D\pi^2 t}{l^2} m^2} \\ &< \frac{e^{-\left(\frac{u^2}{4D}+R\right)t}}{\Omega'} \int_{\Omega'}^{\infty} x e^{-\frac{D\pi^2 t}{l^2} x^2} dx \\ &< \frac{l^2}{2\Omega'\pi^2 D t} e^{\lambda_{ij}^{\Omega'} t}. \end{aligned} \quad (19)$$

It follows that the relative error

$$\left| \frac{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t} - \sum_{m=1}^{\Omega'} e^{\lambda_{ij}^m t}}{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t}} \right| < \frac{\sum_{m=\Omega'}^{\infty} e^{\lambda_{ij}^m t}}{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t}} < \epsilon$$

whenever we have

$$e^{\lambda_{ij}^{\Omega'} t} < \epsilon \frac{2\Omega'\pi^2 D_{ij} t}{l_{ij}^2} \sum_{m=1}^{\Omega'} e^{\lambda_{ij}^m t}. \quad (20)$$

We can therefore be confident that if we truncate the sum in Equation (18) at  $m = \Omega'$ , the relative errors in our estimates for  $z_{ij}^{(n)}(t)$  will be smaller than  $\epsilon$  provided that  $\Omega'$  satisfies Equation (20). Also note that Equation (15) tells us that if  $D_{ij} t > l_{ij}^2$  then  $e^{\lambda_{ij}^m t}$  decreases rapidly, so  $\Omega'$  does not need to be large unless  $D_{ij} t \ll l_{ij}^2$ . Furthermore, if  $u_{ij}^2 t^2 > l_{ij}^2$  then most of the resource will leave edge  $ij$  over the time scale  $t$ , and  $\tilde{q}_{ij}(x, t)$  will only make a small contribution to the total value of  $q_{ij}(x, t)$ .

#### D. Calculating the total quantity of resource in each segment of a network

Suppose that we wish to calculate the mean concentration per unit length in each segment of a network at time  $t$ , such that each part of our final answer has a relative error  $\epsilon < 10^{-0.45\Omega}$ , where  $\Omega$  is an even integer. The first step is to set  $s = \Omega \ln 2/t$ , and apply Equations (8) and (9) to find  $\beta_{ij}(s)$  and  $\beta_{ji}(s)$  for each edge  $ij$ . We then compute  $\mathbf{M}(s)$  and  $\bar{p}(s)$ , and employ the BiCGStab algorithm to find  $\bar{C}(s_{\Omega})$ , starting with the initial guess that for each  $i$ ,

$$C_i(s_{\Omega}) \approx \frac{\tau}{\Omega \ln 2} c_i(0) = \frac{\tau}{\Omega \ln 2} \frac{\sum_j k_{ij}^{(1)}}{\sum_j S_{ij}(0)}. \quad (21)$$

This initial guess for the value of  $\bar{C}(s_{\Omega})$  would be correct if the concentration at the nodes was constant, and making such a guess can help to speed up the process of finding the true value of  $\bar{C}(s_{\Omega})$ . At each step, when we have identified  $\bar{C}(s)$  such that  $\mathbf{M}(s)\bar{C}(s) = \bar{p}(s)$ , we store the vector  $\bar{C}(s)$  and repeat for  $s = s_{\Omega-1}, \dots, s_1$ , where  $s_n = n \ln 2/t$ . The only difference is that for subsequent applications of the BiCGStab algorithm, we can take advantage of the approximation

$$C_i(s_n) \approx \frac{n+1}{n} C_i(s_{n+1}). \quad (22)$$

This is generally a better initial guess than that provided by Equation (21), so the BiCGStab algorithm converges on the solution more rapidly. Given  $C_i(s_n)$  and  $C_j(s_n)$ , we can use Equation (12) to calculate  $Y_{ij}^{(m)}(s_n)$  for each section in the edge  $ij$ . Having found  $Y_{ij}^{(m)}(s_n)$  for each  $1 \leq n \leq \Omega$ , we can apply the Gaver-Stehfest algorithm to obtain  $y_{ij}^{(m)}(t)$  (see Section E), and we repeat this process for each edge in the network.

Finally, for each edge  $ij$  we can use Equations (15), (17) and (16) to calculate a sequence of values for  $e^{\lambda_{ij}^m t}$ ,  $\mu_{ij}^m$  and  $A^m$  until we reach an integer  $\Omega'$  such that  $e^{\lambda_{ij}^{\Omega'} t}$  satisfies Equation (20). We then employ Equation (18) to find  $z_{ij}^{(1)}(t), \dots, z_{ij}^{(N_{ij})}(t)$  (the mean quantity of resource in  $ij$  that has not reached a node), and note that for each section of the network the mean quantity of resource per unit length

$$k_{ij}^{(n)}(t) = y_{ij}^{(n)}(t) + z_{ij}^{(n)}(t). \quad (23)$$

#### E. Inverting from Laplace space

We have seen that we can calculate a sequence of real valued sample points in Laplace space, and we wish to calculate the corresponding value at a given point in time. Under these circumstances it is appropriate and efficient to apply the Gaver-Stehfest algorithm [1–6]. The key idea behind this algorithm (and other, related algorithms) is the notion of constructing a sequence of linear combinations of exponential functions, in order to form a weighted delta convergent sequence [1–6]. That is to say, we consider a sequence of functions  $\delta_n(x, t)$  such that for any function  $q$  that is continuous at  $t$ , we have

$$\int_0^{\infty} \delta_n(v, t) q(v) dv = t \tilde{q}_n(t), \quad (24)$$

where  $\tilde{q}_n(t) \rightarrow q(t)$  as  $n \rightarrow \infty$ . As we shall see, there are weighted delta convergent sequences of functions such that  $\delta_n(v, t)$  is of the form

$$\delta_n(v, t) = \sum_{i=1}^n \omega_i e^{-\frac{\theta_i v}{t}}, \quad (25)$$

where  $\theta_i > 0$  for all  $i$ , and the terms  $\theta_i$  and  $\omega_i$  do not depend on  $t$ . Now, if we suppose that our function  $q$  does not increase exponentially, then the Laplace transform  $Q(s) = \int_0^{\infty} e^{-sv} q(v) dv$  is well defined for all positive numbers  $s$ . Hence the existence of  $Q(s)$  for all positive  $s$  is a reasonable assumption, given the context in which our functions  $q$  arise. Assuming that  $Q(s)$  is well defined for all positive numbers  $s$ , Equations (24) and (25) imply that

$$\begin{aligned} \tilde{q}_n(t) &= \frac{1}{t} \int_0^{\infty} \sum_{i=1}^n \omega_i e^{-\frac{\theta_i v}{t}} q(v) dv \\ &= \frac{1}{t} \sum_{i=1}^n \omega_i Q\left(\frac{\theta_i}{t}\right). \end{aligned}$$

Gaver [7] employed the sequence of functions

$$\delta_n(v, t) = \ln 2 \frac{(2n)!}{n!(n-1)!} (1 - e^{-\frac{v \ln 2}{t}})^n (e^{-\frac{v \ln 2}{t}})^n,$$

but the resulting terms  $\tilde{q}^n(t)$  converge to  $q(t)$  logarithmically slowly. Gaver also showed that the quantity  $\tilde{q}^n(t) - q(t)$  can be expanded in terms of inverse powers of  $n$ , which enabled him to accelerate the convergence of his original sequence of approximations [7]. The most useful formula for finding an accurate estimate of  $q(t)$  based on a linear combination of the Gaver estimates was derived by Stehfest [4], who stated that

$$q(t) \approx \tilde{q}_\Omega(t) = \frac{\ln 2}{t} \sum_{n=1}^{\Omega} \kappa_n Q\left(n \frac{\ln 2}{t}\right), \quad \text{where} \quad (26)$$

$$\kappa_n = (-1)^{n+\Omega/2} \sum_{k=\lceil(n+1)/2\rceil}^{\min(n, \Omega/2)} \frac{k^{\Omega/2} (2k)!}{(\Omega/2 - k)! k! (n - k)! (2k - n)!},$$

and  $\Omega$  is even. Note that the terms  $\kappa_n$  can be extremely large, and that the value of  $\kappa_n$  depends on the parameter  $\Omega$ . Furthermore, increasing the parameter  $\Omega$  increases the accuracy of our estimate  $q(t) \approx \tilde{q}_\Omega(t)$ , provided that

we have sufficient system precision to utilize the exact values for  $\kappa_n$ .

The Gaver-Stehfest algorithm is very efficient and accurate, but it requires high system precision for the weights  $\kappa_n$  if it is to yield accurate estimates for  $q(t)$ . Indeed, if we wish to produce an estimate of  $q(t)$  that is accurate to  $N$  significant digits, we must calculate the values of  $\kappa_n$  with an accuracy of about  $2.5N$  significant digits [1, 2]. Fortunately, to calculate  $q(t)$  accurately we do not require such a disproportionately high level of accuracy in the values of  $Q(s)$ .

If the transform  $Q(s)$  has all its singularities on the negative real axis, and if the function  $q(t)$  is infinitely differentiable for all  $t > 0$ , extensive experimentation [1, 2] indicates that the relative error

$$\left| \frac{q(t) - \tilde{q}_\Omega(t)}{q(t)} \right| \approx 10^{-0.45\Omega} \quad (27)$$

provided that the values  $\kappa_n$  have been calculated with sufficient precision [1, 2]. If the function  $q$  does not satisfy the above conditions  $\tilde{q}_\Omega(t)$  may converge to  $q(t)$  rather more slowly, but as a rule of thumb setting  $\Omega = 10$  and using standard double precision for the weights  $\kappa_n$  will ensure that the Gaver-Stehfest algorithm produces inversions that are accurate to at least three significant digits.

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