Rigorous modelling of nonlocal interactions determines a macroscale advection-diffusion PDE

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Abstract A slowly-varying or thin-layer multiscale assumption empowers macroscale understanding of many physical scenarios from dispersion in pipes and rivers, including beams, shells, and the modulation of nonlinear waves, to homogenisation of micro-structures. Here we begin a new exploration of the scenario where the given physics has non-local microscale interactions. We rigorously analyse the dynamics of a basic example of shear dispersion. Near each cross-section, the dynamics is expressed in the local moments of the microscale non-local effects. Centre manifold theory then supports the local modelling of the system's dynamics with coupling to neighbouring cross-sections as a non-autonomous forcing. The union over all cross-sections then provides powerful new support for the existence and emergence of a macroscale model advection-diffusion PDE global in the large, finite-sized, domain. The approach quantifies the accuracy of macroscale advection-diffusion approximations, and has the potential to open previously intractable multiscale issues to new insights.

1 Introduction

This paper introduces a new rigorous approach to the multiscale challenge of systematically modelling by macroscale PDEs the dynamics of microscale, *spatially nonlocal*, systems. This approach provides a novel quantified error formula. Previous research using this type of approach rigorously modelled systems that were expressed as PDEs on the microscale. This previous research encompassed both cylindrical multiscale domains (Roberts 2015a) and more general multiscale domains (Roberts and Bunder 2017; Bunder and Roberts 2018). But recall that PDEs are themselves mathematical idealisations of physical processes that typically take place on mi-

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croscale length scales. Hence, here we begin to address the challenges arising when the given mathematical model of a system encodes microscale physical interactions over finite microscale lengths.

Physical systems with nonlocal, microscale, spatial interactions arise in many applications. In neuroscience, a spatial convolution expresses the excitatory/inhibitory effects of a neurone on a nearby neurone, giving rise to nonlocal neural field equations, and "have been quite successful in explaining various experimental findings" (Ermentrout 2015, e.g.). Models of free crack propagation in brittle materials invoke microscale *nonlocal* stress-strain laws, called peridynamics (Silling 2000, e.g.): one challenge is to derive the effective mesoscale PDEs from the nonlocal laws (Silling and Lehoucq 2008; Lipton 2014, e.g.). Nonlocal dispersal and competition models arise in biology (Omelyan and Kozitsky 2018; Duncan et al. 2017, e.g.). Other examples are non-local cell adhesion models (Buttenschön and Hillen 2020, e.g.). In this introduction we begin by exploring the specific example of a so-called 'Zappa' dispersion in a channel (Section 2) in which material is transported by finite jumps along the channel, and also is intermittently thoroughly mixed across the channel.

General scenario

Zappa dispersion is a particular case of the following general scenario—a scenario that is the subject of ongoing research. In generality we consider a field $u(x,y,t)$, on a 'cylindrical' spatial domain $\mathbb{X}\times\mathbb{Y}$ (where $\mathbb{X}\subseteq\mathbb{R}$ and where $\mathbb{Y}$ denotes the cross-section). We suppose the field u is governed by a given autonomous system in the form

$$\frac{\partial u}{\partial t} = \int_{\mathbb{Y}}\int_{\mathbb{X}} k(x,\xi,y,\eta)u(\xi,\eta,t)\,d\xi\,d\eta\,, \tag{1}$$

where the given kernel $k(x,\xi,y,\eta)$ expresses both nonlocal and local physical effects at position (x,y) from the field at position (ξ,η), both within the cylindrical domain $\mathbb{X}\times\mathbb{Y}$. We allow the kernel to be a generalised function so that local derivatives may be represented by derivatives of the Dirac delta function δ: for example, a component $\delta'(x-\xi)\delta(y-\eta)$ in the kernel k encodes the differential term $-\partial u/\partial x$ in the right-hand side of (1). In general the physical effects encoded in the kernel k may be heterogeneous in space. But, as is common and apart from boundaries, Zappa dispersion is homogeneous in space (translationally invariant) in which case some significant simplifications ensue.

The nonlocal system (1) is linear for simplicity, but we invoke the framework of centre manifold theory so the approach should, with future development, apply to nonlinear generalisations as in previous work on such modelling where the system is expressed as PDEs on the microscale (Roberts 2015a).

Our aim is to rigorously establish that the emergent dynamics of the nonlocal system (1) are captured over the 1D spatial domain $\mathbb{X}$ by a mean/averaged/coarse/macroscale variable $U(x,t)$ that satisfies a macroscale, second-order, advection-diffusion PDE of the form

$$\frac{\partial U}{\partial t} \approx A_1 \frac{\partial U}{\partial x} + A_2 \frac{\partial^2 U}{\partial x^2}, \quad x \in \mathbb{X}, \tag{2}$$

for some derived coefficients A_1 and A_2.[1] This macroscale PDE (2) is to model the dynamics of the microscale nonlocal (1) after transients have decayed exponentially quickly in time, and to the novel quantified error (6d).

2 Zappa shear dispersion

This section introduces a basic example system (non-dimensional) of nonlocal microscale jumps by a particle (inspired by W. R. Young, private communication). Section 3 systematically derives an advection-diffusion PDE (2) for the particle that is valid over macroscale space-time. Consider a particle in a channel $-1 < y < 1$, $\mathbb{Y} = (-1, 1)$, and of notionally infinite extent in x, $\mathbb{X} = \mathbb{R}$. Let $u(x, y, t)$ be the probability density function (PDF) for the particle's location: equivalently, view $u(x, y, t)$ as the concentration of some continuum material.

The 'Zappa' dynamics of the particle's PDF is encoded by

$$\frac{\partial u}{\partial t} = \Big[\tfrac{1}{v(y)} \underbrace{\int_{-\infty}^{x} e^{-(x-\xi)/v(y)} u(\xi, y, t)\, d\xi}_{= e^{-x/v(y)} \star u, \text{ the convolution (5)}} - u\Big] + \Big[\tfrac{1}{2}\int_{-1}^{1} u\, dy - u\Big] \tag{3}$$

for some jump profile $v(y) > 0$—$v(y)$ is an effective velocity along the channel. That is, the kernel of the Zappa system is the generalised function

$$\begin{aligned} k(x, \xi, y, \eta) = &\Big[\tfrac{1}{v(y)} e^{-(x-\xi)/v(y)} H(x-\xi) - \delta(x-\xi)\Big]\, \delta(y-\eta) \\ &+ \big[\tfrac{1}{2} - \delta(y-\eta)\big]\, \delta(x-\xi), \end{aligned} \tag{4}$$

where $H(x)$ is the unit step function. The nonlocal equation (3) governs the PDF of the particle in Zappa dispersion through the following two physical mechanisms.

- We suppose that, at exponentially distributed time intervals with mean one, the particle gets 'zapped' across the channel (by a burst of intermittent turbulence for example) and lands at any cross channel position y with uniform distribution. Consequently the Fokker–Planck PDE (3) for the PDF contains the terms $u_t = \big[\frac{1}{2}\int_{-1}^{1} u\, dy - u\big] + \cdots$.
- Further, suppose that, at exponentially distributed time intervals with mean one, the particle jumps in x a distance to the right, a distance which is exponentially distributed with some given mean $v(y)$. Consequently the Fokker–Planck PDE (3) for the PDF contains the terms $u_t = \big[\frac{1}{v(y)} e^{-x/v(y)} \star u - u\big] + \cdots$, in terms of the upstream convolution

[1] Ongoing research aims to generalise the approach here to certify the accuracy of PDEs truncated to Nth-order for every N.

$$e^{-x/v(y)} \star u = \int_{-\infty}^{x} e^{-(x-\xi)/v(y)} u(\xi,y,t)\,d\xi\,. \tag{5}$$

We derive the macroscale model that the cross-sectional mean field $U(x,t)$ evolves according to an advection-diffusion PDE: $U_t \approx A_1 U_x + A_2 U_{xx}$. The field $U(x,t)$ may be viewed as the marginal probability density of the particle being at x, averaged over the cross-section y. Innovatively, we put the macroscale modelling on a rigorous basis that additionally quantifies the error.

In particular, say we choose $v(y) := 1-y^2$ then computer algebra (Section 6) readily derives that over large space-time scales, and after transients decay roughly like e^{-t}, from every initial condition the Zappa system (3) has the quasistationary distribution (Pollett and Roberts 1990, e.g.)

$$u(x,y,t) \approx U + (y^2 - \tfrac{1}{3})\frac{\partial U}{\partial x} + (2y^4 - \tfrac{8}{3}y^2 + \tfrac{22}{45})\frac{\partial^2 U}{\partial x^2}\,, \tag{6a}$$

$$\text{such that} \qquad \frac{\partial U}{\partial t} = -\frac{2}{3}\frac{\partial U}{\partial x} + \frac{28}{45}\frac{\partial^2 U}{\partial x^2} + \rho\,, \tag{6b}$$

in terms of a macroscale variable here chosen to be the cross-sectional mean,

$$U(x,t) := \frac{1}{2}\int_{-1}^{1} u(x,y,t)\,dy\,. \tag{6c}$$

The macroscale PDE (6b) is a precise equality because we include the error terms in our analysis to find a precise, albeit complicated, expression for the final error ρ. The remainder error ρ in (6b) has the form

$$\begin{aligned}\rho :=\ & r_0 + \langle Z_0, \mathscr{W}_{0:}\mathscr{B}e^{\mathscr{B}t}\star\mathbf{r}'\rangle + \langle Z_0, \mathscr{W}_{0:}\mathbf{r}'\rangle \\ & - A_1\langle Z_0, \mathscr{W}_{1:}e^{\mathscr{B}t}\star\mathbf{r}'\rangle - A_2\langle Z_0, \mathscr{W}_{2:}e^{\mathscr{B}t}\star\mathbf{r}'\rangle\end{aligned} \tag{6d}$$

where here the convolutions are over time, $f(t)\star g(t) = \int_0^t f(t-s)g(s)\,ds$, and other symbols are introduced in the next Section 3. We anticipate this error ρ is

- 'small' in regions of slow variations in space, small gradients, and
- 'large' in regions of relatively large gradients such as spatial boundary layers.

Then, simply, the macroscale PDE model (6b) is valid whenever and wherever the error ρ is small enough for the application purposes at hand. The next section includes deriving this error term and clarifies the notation.

3 Many kernels generate local models

Inspired by earlier research (Roberts 2015a, Proposition 1), this section's aim is to rigorously derive and justify the model (6) that governs the emergent macroscale evolution of Zappa dispersion. The algebra starts to 'explode'—Section 4 discusses

how to compactly do the algebra in physically meaningful forms, and connect to other mathematical methodologies.

To derive the advection-diffusion model (6b) we truncate the analysis to second order quadratic terms. Higher-orders appear to be similar in nature, but much more involved algebraically, and are left for later development.

3.1 Rewrite the equations for local dynamics

Let's analyse the dynamics in the spatial locale about a generic longitudinal cross-section $X \in \mathbb{X}$. Then invoke Lagrange's Remainder Theorem—which empowers us to track errors—to expand the PDF as

$$u(x,y,t) = u_0(X,y,t) + u_1(X,y,t)(x-X) + u_2(X,x,y,t)\frac{(x-X)^2}{2!}, \tag{7}$$

where $u_0 := u$ and $u_1 := \partial u/\partial x$ both evaluated at the cross-section $x = X$, and where $u_2 := \partial^2 u/\partial x^2$ evaluated at some point $x = \hat{x}(X,x,y,t)$ which is some definite (but usually unknown) function of cross-section X, longitudinal position x, cross-section position y, and time t. By the Lagrange Remainder Theorem, the location $\hat{x}$ satisfies $X \lesseqgtr \hat{x} \lesseqgtr x$. The function $\hat{x}$ is implicit in our analysis because it is hidden in the dependency upon x of the second derivative $u_2(X,x,y,t)$.

Substitute (7) into the Zappa nonlocal equation (3) to obtain

$$\begin{aligned}
&\frac{\partial u_0}{\partial t} + \frac{\partial u_1}{\partial t}(x-X) + \frac{\partial u_2}{\partial t}\frac{(x-X)^2}{2!} \\
&= \int_{\mathbb{Y}} \left[\int_{\mathbb{X}} k(x,\xi,y,\eta)\, d\xi \right] u_0(X,\eta,t)\, d\eta \\
&\quad + \int_{\mathbb{Y}} \left[\int_{\mathbb{X}} k(x,\xi,y,\eta)(\xi - X)\, d\xi \right] u_1(X,\eta,t)\, d\eta \\
&\quad + \int_{\mathbb{Y}} \int_{\mathbb{X}} k(x,\xi,y,\eta)\frac{(\xi-X)^2}{2!} u_2(X,\hat{\xi},\eta,t)\, d\xi\, d\eta\,.
\end{aligned} \tag{8}$$

The effect at cross-section x of the nth moment of the kernel at cross-section X is summarised in the integrals $\int_{\mathbb{X}} k(x,\xi,y,\eta)\frac{(\xi-X)^n}{n!}\, d\xi$. So define the local nth moment of the kernel to be, for every $n \geq 0$,

$$\begin{aligned}
k_n(X,y,\eta) &:= \int_{\mathbb{X}} k(X,\xi,y,\eta)\frac{(\xi-X)^n}{n!}\, d\xi \\
&= \left[(-v)^n - \delta_{n0}\right]\delta(y-\eta) + \left[\tfrac{1}{2} - \delta(y-\eta)\right]\delta_{0n}
\end{aligned} \tag{9}$$

upon substituting the Zappa kernel (4). This Zappa problem is homogeneous in x, as are many problems, and so the kernel moments k_n are independent of the cross-section X (except near the boundary inlet and outlet).

The last integral term in the local expansion (8) requires special consideration: apply Lagrange's Remainder Theorem to write $u_2(X,\xi,\eta,t) = u_2(X,X,\eta,t) + (\xi - X)u_{2x}(X,\hat{\xi},\eta,t)$ for some uncertain function $\hat{\xi}(X,\xi,\eta,t)$ that satisfies $X \leqslant \hat{\xi} \leqslant \xi$ for every η,t, and where $u_{2x} := \partial/\partial x[u_2(X,x,\eta,t)]$. Then the last term distributes into two:

$$\begin{aligned}
&\int_{\mathbb{Y}}\int_{\mathbb{X}} k(x,\xi,y,\eta)\frac{(\xi-X)^2}{2!}u_2(X,\hat{\xi},\eta,t)\,d\xi\,d\eta \\
&= \int_{\mathbb{Y}} \underbrace{\int_{\mathbb{X}} k(x,\xi,y,\eta)\frac{(\xi-X)^2}{2!}\,d\xi}_{k_2(X,y,\eta)} u_2(X,X,\eta,t)\,d\eta \\
&\quad + \underbrace{\int_{\mathbb{Y}}\int_{\mathbb{X}} k(x,\xi,y,\eta)3\frac{(\xi-X)^3}{3!}u_{2x}(X,\hat{\xi},\eta,t)\,d\xi\,d\eta}_{\text{a remainder, with a third } x \text{ derivative in } u_{2x}} .
\end{aligned}$$

Define $u_2(X,y,\eta) := u_2(X,X,y,\eta)$ for notational consistency with lower moments—see the definition (9).

The local equation (8) is exact everywhere, but is most useful in the vicinity of the cross-section X, that is, for small $(x-X)$. Notionally we want to 'equate coefficients' of powers of $(x-X)$ in (8), but to be precise we must carefully evaluate $\lim_{x\to X}$ of various x-derivatives of (8). For example, let $x \to X$ in (8), then

$$\begin{aligned}
\frac{\partial u_0}{\partial t} = &\int_{\mathbb{Y}} k_0(X,y,\eta)u_0(X,\eta,t)\,d\eta + \int_{\mathbb{Y}} k_1(X,y,\eta)u_1(X,\eta,t)\,d\eta \\
&+ \int_{\mathbb{Y}} k_2(X,y,\eta)u_2(X,\eta,t)\,d\eta \\
&+ 3\int_{\mathbb{Y}}\int_{\mathbb{X}} k(X,\xi,y,\eta)\frac{(\xi-X)^3}{3!}u_{2x}(X,\hat{\xi},\eta,t)\,d\xi\,d\eta .
\end{aligned}$$

Rewrite this conveniently and compactly as the integro-differential equation (IDE)

$$\frac{\partial u_0}{\partial t} = \mathfrak{L}_0 u_0 + \mathfrak{L}_1 u_1 + \mathfrak{L}_2 u_2 + r_0 , \tag{10}$$

for y-operators defined to be, from the moments (9),

$$\mathfrak{L}_n u := \int_{\mathbb{Y}} k_n(X,y,\eta)u|_{y=\eta}\,d\eta = \begin{cases} \frac{1}{2}\int_{-1}^{1} u\,dy - u , & n=0 , \\ [-v(y)]^n u , & n=1,2,\ldots . \end{cases} \tag{11}$$

The IDE (10) also has the remainder r_0 which couples the local dynamics to neighbouring locales via u_{2x} and is the $n=0$ case of

$$r_n(X,y,t) := 3\int_{\mathbb{Y}}\int_{\mathbb{X}} \frac{\partial^n k}{\partial x^n}\Big|_{x=X}\frac{(\xi-X)^3}{3!}u_{2x}(X,\hat{\xi},\eta,t)\,d\xi\,d\eta . \tag{12}$$

Now we can see how this approach to modelling the spatial dynamics works: given that the y-operators (11) are evaluated at X, the spatially local power series with remainder, in IDEs like (10), 'pushes' the coupling with neighbouring locales to a higher-order derivative term in r_0, here third-order via the u_{2x} factor. Hence the local dynamics in u_0, u_1, u_2 are essentially isolated from all other cross-sections whenever and wherever the coupling r_0 is small enough for the purposes at hand—here when third derivatives are small—that is, when the solutions are, in space, slowly varying enough.

The previous paragraph obtains the IDE for u_0 by simply taking the limit of (8) as $x \to X$. We straightforwardly and similarly obtain IDEs for u_1 and u_2 by finding the limits of spatial derivatives of (8):

$$\lim_{x\to X} \frac{\partial(8)}{\partial x} \implies \frac{\partial u_1}{\partial t} = \mathfrak{L}_0 u_1 + \mathfrak{L}_1 u_2 + r_1\,; \tag{13a}$$

$$\lim_{x\to X} \frac{\partial^2(8)}{\partial x^2} \implies \frac{\partial u_2}{\partial t} = \mathfrak{L}_0 u_2 + r_2\,; \tag{13b}$$

for local coupling remainders r_1 and r_2 defined by (12).

3.2 Local-to-global system modelling theory

This section considers the collection of 'local' systems as one 'global' (in space X) system. Then theory establishes that the advection-diffusion PDE (6b) arises as a globally valid, macroscale, model PDE.

Denote the vector of coefficients $\mathbf{u}(X,y,t) := (u_0, u_1, u_2)$, and similarly for the local coupling remainder $\mathbf{r}(X,y,t) := (r_0, r_1, r_2)$. Then write the IDEs (10) and (13), in the form of the 'forced' linear system

$$\frac{d\mathbf{u}}{dt} = \underbrace{\begin{bmatrix} \mathfrak{L}_0 & \mathfrak{L}_1 & \mathfrak{L}_2 \\ 0 & \mathfrak{L}_0 & \mathfrak{L}_1 \\ 0 & 0 & \mathfrak{L}_0 \end{bmatrix}}_{\mathscr{L}} \mathbf{u} + \mathbf{r}(X,t). \tag{14}$$

for upper triangular matrix/operator $\mathscr{L}$. The system (14) might appear closed, but it is coupled via the derivative u_{2x}, through the 'forcing' remainders $\mathbf{r}$, to the dynamics of cross-sections that neighbour X.

At each locale $X \in \mathbb{X}$, treat the remainder coupling $\mathbf{r}$ (third-order) as a perturbation (and if this was a nonlinear problem, then the nonlinearity would also be part of the perturbation). Thus to a useful approximation the global system satisfies the local linear ODEs $d\mathbf{u}/dt \approx \mathscr{L}\mathbf{u}$ for each $X \in \mathbb{X}$. Hence, the linear operator $\mathscr{L}$ is crucial to modelling the dynamics: all solutions are characterised by the eigenvalues of $\mathscr{L}$. Since $\mathscr{L}$ is block triangular, a structure exploited previously (Roberts 2015a,

§2), its spectrum is thrice that of $\mathfrak{L}_0 = \frac{1}{2}\int_{-1}^{1} u\,dy - u$ (definition (11)). Here it is straightforward to verify that the y-operator $\mathfrak{L}_0$ has:

- one 0 eigenvalue corresponding to eigenfunctions constant across the channel; and
- an 'infinity' of eigenvalue -1 corresponding to all functions with zero average across the channel.

Then globally in space, with $d\mathbf{u}/dt = \mathscr{L}\mathbf{u} + (\text{perturbation})$ at every $X \in \mathbb{X}$, and because of the 'infinity' of the continuum $\mathbb{X}$, the linearised system has a 'thrice-infinity' of the 0 eigenvalue, and a 'double-infinity' of eigenvalue -1. Consequently, the theory of Aulbach and Wanner (2000) asserts:

1. there exists a '(3∞)'-D slow manifold—the quasistationary (6a);
2. which is exponentially quickly attractive to all initial conditions, with transients roughly e^{-t}—it is emergent; and
3. which we approximate by approximately solving the governing differential equations (14)—done in encoded form by Section 6.

We obtain a useful approximation to the global slow manifold by neglecting the 'perturbing' remainder $\mathbf{r}$. Because the remainder $\mathbf{r}$ is the only coupling between different locales X this approximation may be constructed independently at each and every cross-section X. Further, because the Zappa system is homogeneous in space, the construction is identical at each and every $X \in \mathbb{X}$. These two properties vastly simplify the construction of the attractive slow manifold.

Neglecting the coupling remainder $\mathbf{r}$ gives the linear problem $d\mathbf{u}/dt = \mathscr{L}\mathbf{u}$. The approximate slow manifold is thus the zero eigenspace of $\mathscr{L}$. We find the zero eigenspace via (generalised) eigenvectors. With the (generalised) eigenvectors in the three columns of block-matrix $\mathscr{V}$, in essence we seek $\mathbf{u}(t) = \mathscr{V}\mathbf{U}(t)$ such that $d\mathbf{U}/dt = \mathscr{A}\mathbf{U}$ for 3×3 matrix $\mathscr{A}$ having all the zero eigenvalues. To be an eigenspace we need to solve $\mathscr{L}\mathscr{V} = \mathscr{V}\mathscr{A}$. Now let's invoke previously established results (Roberts 2015a, §2). The linear operator $\mathscr{L}$, defined in (14), has the same block Toeplitz structure as previously (Roberts 2015a, (7) on p.1496). Consequently (Roberts 2015a, Lemma 4), a basis for the zero eigenspace of $\mathscr{L}$ is the collective columns of

$$\mathscr{V} = \begin{bmatrix} V_0 & V_1 & V_2 \\ 0 & V_0 & V_1 \\ 0 & 0 & V_0 \end{bmatrix}, \qquad \text{and further, } \mathscr{A} = \begin{bmatrix} 0 & A_1 & A_2 \\ 0 & 0 & A_1 \\ 0 & 0 & 0 \end{bmatrix}.$$

The hierarchy of equations to solve for the components of these has been previously established (Roberts 2015a, Lemma 3): the hierarchy is essentially equivalent to the hierarchy one would solve if using the method of multiple scales, but the theoretical framework here is more powerful. The upshot is that for Zappa dispersion, in which overlines denote cross-channel averages,

$$\begin{aligned} V_0 &= 1, & V_1 &= \overline{v} - v, & V_2 &= 2(\overline{v}^2 - \overline{v^2} - \overline{v}v + v^2), \\ & & A_1 &= -\overline{v}, & A_2 &= \overline{(v-\overline{v})^2} + \overline{v^2}. \end{aligned} \tag{15}$$

In the specific case of $v(y) = 1 - y^2$, these expressions reduce to the coefficients and polynomials of the slowly varying, slow manifold, model (6).

So now we know that the evolution on the zero eigenspace, the approximate slow manifold, is $d\mathbf{U}/dt = \mathscr{A}\mathbf{U}$: let's see how this translates into the macroscale PDE (6b). Now, the first line of $d\mathbf{U}/dt = \mathscr{A}\mathbf{U}$ is the ODE $dU_0/dt = A_1U_1 + A_2U_2$. Defining $U_0 = U(X,t) := \overline{u(X,y,t)}$, Proposition 6 of Roberts (2015a) applies, and so generally $U(x,t)$ satisfies the macroscale effective advection-diffusion PDE (2)—a PDE that reduces to the specific (6b) in the case $v(y) = 1 - y^2$.

3.3 Account for the coupling remainder

Now we treat the exact 'local' system $d\mathbf{u}/dt = \mathscr{L}\mathbf{u} + \mathbf{r}$ as non-autonomously 'forced' by coupling to all cross-sections in $\mathbb{X}$ through the remainder (aka Mori–Zwanzig transformation, e.g., Venturi, Cho, and Karniadakis 2015). There are two justifications, both a simple and a rigorous, for being able to project such 'forcing' onto the local model. First, simply, the rational projection of initial conditions for low-dimensional dynamical models leads to a cognate projection of any forcing (Roberts 1989, §7). Second, alternatively and more rigorously, Aulbach and Wanner (2000) developed a general forward theory, that applies here, of centre manifolds for non-autonomous systems in suitable 'infinite-D' state spaces: the theory establishes the existence and emergence of an 'infinity-D' global centre manifold—a centre manifold whose construction (Potzsche and Rasmussen 2006, Prop. 3.6) happens to be symbolically identical at each $X \in \mathbb{X}$. Keep clear the contrasting points of view that contribute: on the one hand we consider the relatively low-dimensional system at each locale X in space, a system that is weakly coupled to its neighbours; on the other-hand we consider the relatively high-dimensional system of all locales $\mathbb{X}$ coupled together and then theory establishes global properties.

The upshot is that here we need to project the coupling remainder $\mathbf{r}(t)$ onto each local slow manifold. Fortunately, the structure of the linear local dynamics (14) is identical to that discussed by Roberts (2015a). Hence, many of the results reported there apply here. Linear algebra involving adjoint eigenvectors Z_0 and $\mathscr{W}_n$ ($\Omega_0^\dagger Z_0 = 0$ and $\mathscr{L}^\dagger\mathscr{W} = \mathscr{W}\mathscr{A}$, Roberts 2015a, §2.3), together with the history of the coupling remainder $e^{-t} \star \mathbf{r}$, leads to the error formula (6d) (equation (23) from Roberts 2015a). Then the general macroscale advection-diffusion model (2) becomes exact with the error term ρ included (here the error (6d) is third-order in spatial derivatives)

$$\frac{\partial U}{\partial t} = A_1\frac{\partial U}{\partial x} + A_2\frac{\partial^2 U}{\partial x^2} + \rho\,.$$

Then, simply, *the macroscale effective advection-diffusion model* PDE (2) *is valid simply whenever and wherever the error term* ρ *is acceptably small. There is: no* ε*; no limit; no required scaling; no 'balancing'; no ad hoc hierarchy of space-time variables.*

4 Compact analysis, and connect to well-known methodology

It is very tedious to perform all the algebraic machinations of Section 3 on the Taylor series coefficients. Instead, we may compactify the analysis by defining the quadratic *generating polynomial* (Roberts 2015a, §3.1)

$$\tilde{u}(X,\zeta,y,t) := u_0(X,y,t) + \zeta u_1(X,Y,t) + \tfrac{1}{2}\zeta^2 u_2(X,X,y,t) \tag{16}$$

(or a higher-order polynomial if the analysis is to higher-order). This generating polynomial then satisfies the exact differential equation (17). Consider $\partial\tilde{u}/\partial t$, at (X,ζ,y,t), and substitute the equations (14) for the Taylor coefficients at (X,y,t):

$$\begin{aligned}
\frac{\partial\tilde{u}}{\partial t} &= \frac{\partial u_0}{\partial t} + \zeta\frac{\partial u_1}{\partial t} + \tfrac{1}{2}\zeta^2\frac{\partial u_2}{\partial t}\\
&= \quad \mathfrak{L}_0 u_0 + \mathfrak{L}_1 u_1 + \mathfrak{L}_2 u_2 + r_0\\
&\quad + \mathfrak{L}_0\zeta u_1 + \mathfrak{L}_1\zeta u_2 \qquad + \zeta r_1\\
&\quad + \mathfrak{L}_0\tfrac{1}{2}\zeta^2 u_2 \qquad\qquad + \tfrac{1}{2}\zeta^2 r_2\\
&= \mathfrak{L}_0\tilde{u} + \mathfrak{L}_1\frac{\partial\tilde{u}}{\partial\zeta} + \mathfrak{L}_2\frac{\partial^2\tilde{u}}{\partial\zeta^2} + \tilde{r}\\
\implies \frac{\partial\tilde{u}}{\partial t} &= \left[\mathfrak{L}_0 + \mathfrak{L}_1\frac{\partial}{\partial\zeta} + \mathfrak{L}_2\frac{\partial^2}{\partial\zeta^2}\right]\tilde{u} + \tilde{r}
\end{aligned} \tag{17}$$

for the generating polynomial of the coupling remainder, $\tilde{r} := r_0 + \zeta r_1 + \frac{1}{2}\zeta^2 r_2$.

Appropriate analysis of the IDE (17) then reproduces the previous Section 3. But the algebra is done much more compactly as the separate components u_0, u_1, u_2 are all encompassed in the one generating polynomial $\tilde{u}$. One important property of the analysis is that although we normally regard the derivative $\partial/\partial\zeta$ as unbounded, in the analysis of IDE (17) the space of functions is just that of quadratic polynomials in ζ, and so here $\partial/\partial\zeta$ is bounded, as well as possessing other nice properties.

Indeed, since we are only interested in the space of quadratic polynomials in ζ, the analysis neglects any term $\mathcal{O}(\zeta^3)$. Equivalently, we would work to 'errors' $\mathcal{O}(\partial^3/\partial\zeta^3)$. This view empowers us to organise the necessary algebra in a framework where we imagine $\partial/\partial\zeta$ is 'small'. Note: in the methodology here $\partial/\partial\zeta$ is *not assumed* small, as we track errors exactly in the remainder $\tilde{r}$, it is just that we may organise the algebra as if $\partial/\partial\zeta$ was small. Such organisation then leads to the same hierarchy of problems as in Section 3.2, just more compactly.

Connect to extant methodology

Since the notionally small $\partial/\partial\zeta$ is effectively a small spatial derivative, we now connect to extant multiscale methods that a priori assume slow variations in space. That is, we now show that the non-remainder part of IDE (17) appears in a conventional multiscale approximation of the governing microscale system (1).

In conventional asymptotics we invoke restrictive scaling assumptions at the start. Here one would assume that the solution field $u(x,y,t)$ is slowly-varying in space x. Then the argument goes that the field may be usefully written near any $X \in \mathbb{X}$ as the local Taylor quadratic approximation[2]

$$u(\xi,y,t) \approx u|_{\xi=X} + (\xi - X)u_\xi|_{\xi=X} + \frac{(\xi-X)^2}{2!}u_{\xi\xi}|_{\xi=X}\,.$$

Substituting into the nonlocal microscale (1) gives, at (X,y,t) and letting dashes/primes denote derivatives with respect to the first argument,

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \int_{\mathbb{Y}}\int_{\mathbb{X}} k(X,\xi,y,\eta)u(\xi,\eta,t)\,d\xi\,d\eta \\
&\approx \int_{\mathbb{Y}}\int_{\mathbb{X}} k(X,\xi,y,\eta)\left[u|_{\xi=X} + (\xi-X)u'|_{\xi=X} + \frac{(\xi-X)^2}{2!}u''|_{\xi=X}\right]d\xi\,d\eta \\
&= \int_{\mathbb{Y}}\int_{\mathbb{X}} k(X,\xi,y,\eta)\,d\xi\,u(X,\eta,t) + \int_{\mathbb{X}} k(X,\xi,y,\eta)(\xi-X)\,d\xi\,u'(X,\eta,t) \\
&\qquad + \int_{\mathbb{X}} k(X,\xi,y,\eta)\frac{(\xi-X)^2}{2!}\,d\xi\,u''(X,\eta,t)\,d\eta \\
&= \int_{\mathbb{Y}} k_0(X,y,\eta)u(X,\eta,t) + k_1(X,y,\eta)u'(X,\eta,t) \\
&\qquad + k_2(X,y,\eta)u''(X,\eta,t)\,d\eta \\
&= \mathfrak{L}_0 u + \mathfrak{L}_1 u' + \mathfrak{L}_2 u''. \qquad (18)
\end{aligned}$$

Now the generating polynomial $\tilde{u}$, defined by (16), is such that $u(X+\zeta,y,t) = \tilde{u}(X,\zeta,y,t) + \mathscr{O}(\zeta^3)$. Hence, rewriting the *approximate* PDE (18) for $u(X+\zeta,y,t)$ at fixed X gives precisely the IDE (17) except that the remainder coupling $\tilde{r}$ is omitted. Consequently, extant multiscale methodologies continuing on from PDE (18) generate equivalent results to that of Section 3, but in a different framework—a framework without the error term (6d).

Most extant multiscale analysis invokes, at the outset, balancing of scaling parameters, requires a small parameter, is only rigorous in the limit of infinite scale separation, and often invents heuristic multiple space-time variables. The approach developed herein connects with such analysis, but is considerably more flexible and, furthermore, justifies a more formal approach developed 30 years ago (Roberts 1988), and implemented in Section 6. Further this approach derives the rigorous error expression (6d) at finite scale separation.

[2] I continue to conjecture that truncations to orders other than quadratic give corresponding analysis and results. Ongoing research will elucidate.

5 Conclusion

This article initiates a new multiscale modelling approach applied to a specific basic problem. This article considers the scenario where the given physical problem (1) has non-local microscale interactions, such as inter-particle forces or dynamics on a lattice. Many extant mathematical methodologies derive, for such physical systems, an approximate macroscale PDE, such as the advection-diffusion (2). The novelty of our approach is that it derives a precise expression for the error of the macroscale approximate PDE, here (6d). Then, simply, and after microscale transients decay, the macroscale advection-diffusion PDE (2) is valid wherever and whenever the quantified error (6d) is acceptable.

Of course, in all such applications, we need the third moment of the microscale interaction kernel $k(x,\xi,y,\eta)$ to exist (see definition (12)) for the error analysis of Section 3.1 to proceed and provide the error term. All moments exist for the Zappa problem, see (9). If, in some application, the third moment does not exist, but the second moment does, then the advection-diffusion PDE (2) may be an appropriate macroscale model, but this work would not provide a quantifiable error.

Another important characteristic of our new approach is that the validity of the macroscale PDE is not confined by a limit '$\varepsilon \to 0$'—the approach holds for finite scale separation in the multiscale problem, in the large but finite domain $\mathbb{X}$. Further, and in contrast to most extant methodologies, the approach here should generalise in further research to arbitrary order models just as it does when the microscale is expressed as PDEs (Roberts 2015a).

The developed scenario here is that of linear nonlocal systems (1). However, key parts of the argument are justified with centre manifold theory (Aulbach and Wanner 2000; Potzsche and Rasmussen 2006; Haragus and Iooss 2011; Roberts 2015b, e.g.). Consequently, further research should be able to show that cognate results hold for nonlinear microscale systems.

With further research, correct boundary conditions for the macroscale PDEs should be derivable by adapting earlier arguments to derive rigorous boundary conditions for approximate PDEs (Roberts 1992; Chen, Roberts, and Bunder 2018).

Interesting applications of this novel approach would arise whenever there are microscale nonlocal interactions in the geometry of problems such as (e.g., Roberts 2015b) dispersion in channels and pipes, the lubrication flow of thin viscous fluids, shallow water approximations whether viscous or turbulent, quasi-elastic beam theory, long waves on heterogeneous lattices, and pattern evolution.

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6 Appendix: Computer algebra derives macroscale PDE

The following computer algebra derives the effective advection-diffusion PDE (6b), or any higher-order generalisation, for the microscale nonlocal Zappa system (3). This code uses the free computer algebra package Reduce.[3] Analogous code will work for other computer algebra packages, and/or for cognate problems (Roberts 2015b, e.g.).

```
% advection-diffusion PDE of Zappa transport in a channel
% AJR, 20 Jan 2017 -- 20 Jan 2020
on div; off allfac; on revpri; factor d,uu;

let d^5=>0; % truncate to this order of error
operator uu; depend uu,x,t; % uu(n):=df(uu,x,n)
let { df(uu(~n),x)=>uu(n+1), df(uu(~n),t)=>df(g,x,n)  };
operator mean; linear mean; % average across channel
let { mean(1,y)=>1, mean(y^~~p,y)=>(1+(-1)^p)/2/(p+1) };

% Preprocess nonlocal x-jumping: in essence finds the
% kernel integrals are (-v)^n
depend w,x; % dummy function for u(x)
% Taylor expand w(xi)=w(x+z) where z=xi-x
jmp:=for n:=0:deg((1+d)^99,d) sum d^n*df(w,x,n)*z^n/factorial(n)$
jmp:=int(exp(z/v)*jmp,z)$ % integrate exp((xi-x)/v)w(x)
% eval from z=-inf to 0 for the convolution
jmp:=sub(z=0,jmp/v)-w$

% iterate from quasi-equilibrium start
u:=uu(0)$ g:=0$
for it:=1:99 do begin
   res:=-df(u,t)+sub({w=u,v=1-y^2},jmp)+(-u+mean(u,y));
   write lengthres:=length(res);
   g:=g+(gd:=mean(res,y));
   u:=u+res-gd;
   if res=0 then write "Success: ",it:=it+10000;
end;
write "The resulting slow manifold and evolution is";
u:=u; duudt:=g;
end;
```

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[3] http://www.reduce-algebra.com/

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