Holistic discretisation of dynamical PDEs: some theory

Tony Roberts

April 2005

Computational simulation is a key enabling technology in engineering, science and other quantitative fields. Coherent spatio-temporal dynamics, the main focus of application of this project, is the preeminent example of complex system behaviour as it emerges from the interactions of many similar components at each locale in space.

For the purposes of discussion consider that the microscopic model is one in the wide class of PDE's in the form

$$\mathbf{u}_t = \mathcal{L}\mathbf{u} + \mathbf{f}(\mathbf{u}) + \mathbf{q}(\mathbf{u}, t) \tag{1}$$

where: $\mathbf{x}$ is position in one or more spatial dimensions; $\mathbf{u}(\mathbf{x}, t)$ is some scalar or vector field, such as fluid velocity and pressure; $\mathcal{L}$ is a *dissipative* linear operator, such as ∇^2; $\mathbf{f}(\mathbf{u})$ includes other autonomous terms representing nonlinear advection, reaction, etc.; and $\mathbf{q}(\mathbf{u}, t)$ is some time dependent control or possibly stochastic forcing [22]. Among many physically relevant examples are Burgers' equation [1, e.g.], the Brusselator [9, §3], Liouville's equation [13] and the Swift–Hohenberg equation [4, e.g.].

Consider forming a numerical solution of (1) by implementing the method of lines through discretising in the spatial variable x and integrating in time

as a set of ordinary differential equations, sometimes called a semi-discrete scheme [5, 6, e.g.]. A finite difference approximation to the spatial structure of (1) on a 1D regular grid is straightforward; for example, a linear diffusion term on a regular grid, say $x_j = jh$ for some grid spacing h, is

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + \mathcal{O}\left(h^2\right) ,$$

where u_j is the value of u at the grid points x_j. However, there are many differing valid alternatives for a nonlinear term such as the self-advection uu_x: two possibilities are

$$u\frac{\partial u}{\partial x} = \frac{u_j(u_{j+1} - u_{j-1})}{2h} + \mathcal{O}\left(h^2\right) = \frac{u_{j+1}^2 - u_{j-1}^2}{4h} + \mathcal{O}\left(h^2\right) ;$$

and a third is the $1:2$ mix of the above two suggested by Fornberg [7] and used to improve stability [5, e.g.]. *The best choice depends upon how the discretisation of the nonlinearity interacts with the dynamics of other terms.* The traditional approach of considering the discretisation of each term in the equation separately does not answer. To find the best discretisation we consider the complex interaction of all terms in the PDE (1) in a "holistic" approach that involves resolving microscale subgrid structures and their evolution. Centre manifold techniques construct approximations based upon the principle of *capturing an exponentially attractive manifold of actual solutions*. The approximation is consequently invariant under any valid algebraic rewriting of the governing equations *and preserves symmetries*. Jones [11] argue that quite generally there exist good approximations to such attractive inertial manifolds. One core challenge of this project is to actually construct effective approximations and to give general theoretical support so that modern ideas become practical tools for engineers and scientists.

Centre manifold theory is a powerful tool for the modelling of complex dynamical systems [17, 18, 8, e.g.] such as dispersion [24, 16, e.g.], thin fluid films [2, 19, 25, e.g.], stochastic systems [27, 28], control [12, e.g.] and turbulent floods [15]. Based upon modifying linear dynamics the theory guarantees

that an accurate and relevant low-dimensional description of the nonlinear dynamics may be deduced. We currently place the discretisation of a nonlinear PDE such as (1) within the purview of centre manifold theory by the following artifice; such adaptation also proves effective in thin fluid flows [19] and dispersion [23]. Tessellate the spatial domain into finite size elements, say there are m elements of size h, and then introduce a homotopy parameter γ, $0 \le \gamma \le 1$, parametrising "internal boundary conditions" (IBC) [13, 20] between each element:

$$\frac{\partial u^o}{\partial n} = \frac{\partial u^i}{\partial n}\,, \quad (1-\gamma)\frac{h}{2}\left(\frac{\partial u^o}{\partial n} + \frac{\partial u^i}{\partial n}\right) = \gamma\left(u^o - u^i\right)\,, \tag{2}$$

and its higher order analogues [14], where $\frac{\partial}{\partial n}$ is the derivative normal to the boundary, u^i is from the element under consideration (inside) and u^o is from the adjacent element (outside). When $\gamma = 1$ these reduce to conditions ensuring appropriate continuity between adjacent elements. When $\gamma = 0$ they reduce to effectively insulating conditions. We then treat terms multiplied by γ as "nonlinear" perturbations to the insulated dynamics. Thus in the "linear" dissipative dynamics governed by $u_t = \mathcal{L}u$ the field u in each element evolves exponentially quickly (typically in a time $\mathcal{O}(h^2)$ for a diffusive system) to some constant value in the jth element, say $u = u_j$. But in the presence of the nonlinear terms and the coupling between the elements when $\gamma \neq 0$, the values u_j associated with each element evolve in time. Centre manifold theory assures three things for the system of coupled elements: the existence of an m dimensional centre manifold parametrised by grid values u_j; the relevance of the m dimensional dynamics as an accurate and stable model of the original dynamics (1); and that we may systematically approximate the subgrid scale structures and the corresponding macroscale evolution. Importantly, symmetries of the PDE (1), compatible with the IBC (2), are fully maintained in the analysis. These dynamics on the centre manifold form a sound and systematic computational model on the macroscale h.

It might be argued that the dynamics of the PDE (1) recovered at $\gamma = 1$ is unrelated to that of the derived discrete model which is based upon asymptotics about $\gamma = 0$. But we routinely use asymptotic expansions at finite

values of a notionally small parameter. The practical issue here is whether the expansion converges at $\gamma = 1$. In application, our approach converges to a global spectral discretisation of Burgers' equation [20, Appendix]. We additionally ensure high order consistency in the limit $h \to 0$ [21] by the effectively near identity modification of the IBC's (2) to

$$u^o(x_{j\pm1}) - u^i(x_j) = \gamma[u^i(x_{j\pm1}) - u^i(x_j)]\,. \tag{3}$$

That the modelling process satisfies these two independent asymptotic limits provides wonderful support for the proposed approach. For example, in Burgers' equation it seems best to discretise the nonlinear advection uu_x [20] with a higher order correction which automatically improves the stability and accuracy of the numerical model. Indeed following Foias [5] [§2.1] we have found our holistic discretisation is nonlinearly stable when other discretisations are not. We need to be inventive in exploring and then analysing various options for the form of the coupling in order to ensure best performance of the resulting computational models.

This coupling between elements is a fundamental issue for multiscale modelling in general. Modification of the coupling of patches in the gap-tooth scheme [10, 26] achieves higher order consistency by being asymptotically consistent with (3). Further, the extension of the subgrid fields outside of the element, $u^i(x_{j\pm1})$ in (3) is analogous to the solution outside of their finite elements which Chen [3] required in their multiscale modelling.

References

[1] J. Baker, A. Armaou, and P. D. Christofides. Nonlinear control of incompressible fluid flow: application to Burgers' equation and 2d channel flow. *J. Math. Anal. and Appl.*, 252:230–255, 2000.

[2] H. C. Chang. Onset of nonlinear waves on falling films. *Phys. Fluids A*, 1:1314–1327, 1989.

[3] Zhiming Chen and Thomas Y. Hou. A mixed multiscale finite element method for elliptic problems with oscillating coefficients. *Math. Comp.*, 72:541–576, 2002.

[4] M. C. Cross, G. Tesauro, and H. S. Greenside. Wavenumber selection and persistent dynamics in models of convection. *Physica D*, 23:12–18, 1986.

[5] C. Foias, M. S. Jolly, I. G. Kevrekidis, and E. S. Titi. Dissipativity of numerical schemes. *Nonlinearity*, 4:591–613, 1991. http://dx.doi.org/10.1088/0951-7715/4/3/001.

[6] C. Foias and E. S. Titi. Determining nodes, finite difference schemes and inertial manifolds. *Nonlinearity*, 4:135–153, 1991. http://dx.doi.org/10.1088/0951-7715/4/1/009.

[7] B. Fornberg. On the instability of the leap-frog and Crank–Nicolson approximations of a nonlinear partial differential equation. *Maths of Comput.*, 27:45–57, 1973.

[8] J. Fujimura. Methods of centre manifold multiple scales in the theory of nonlinear stability for fluid motions. *Proc Roy Soc Lond A*, 434:719–733, 1991.

[9] B. García-Archilla and E. S. Titi. Postprocessing the Galerkin method: the finite element case. *SIAM J. Num. Anal.*, 37:470–499, 2000.

[10] C. W. Gear, Ju Li, and I. G. Kevrekidis. The gap-tooth method in particle simulations. *Phys. Lett. A*, 316:190–195, 2003. http://dx.doi.org/10.1016/j.physleta.2003.07.004.

[11] D. A. Jones and A. M. Stuart. Attractive invariant manifolds under approximation. Inertial manifolds. *J. Diff. Eqns*, 123:588–637, 1995.

[12] Der-Chang Liaw. Application of center manifold reduction to nonlinear system stabilization. *Appl. Maths. & Computation*, 91:243–258, 1998.

[13] T. MacKenzie and A. J. Roberts. The dynamics of reaction diffusion equations lead to a holistic discretisation. In R. L. May, G. F. FitzGerald, and I. H. Grundy, editors, *EMAC 2000 Proceedings. Proceedings of the fourth biennial Engineering Mathematics and Applications Conference*, pages 199–202, 2000.

[14] T. Mackenzie and A. J. Roberts. Holistic finite differences accurately model the dynamics of the Kuramoto–Sivashinsky equation. *ANZIAM J.*, 42(E):C918–C935, 2000. http://anziamj.austms.org.au/V42/CTAC99/Mack.

[15] Z. Mei, A. J. Roberts, and Zhenquan Li. Modelling the dynamics of turbulent floods. *SIAM J. Appl. Math.*, 63(2):423–458, 2003. http://epubs.siam.org/sam-bin/dbq/article/35886.

[16] G. N. Mercer and A. J. Roberts. A complete model of shear dispersion in pipes. *Jap. J. Indust. Appl. Math.*, 11:499–521, 1994.

[17] E. Meron and I. Procaccia. Theory of chaos in surface waves: The reduction from hydrodynamics to few-dimensional dynamics. *Phys. Rev. Lett.*, 56:1323–1326, 1986. http://dx.doi.org/10.1103/PhysRevLett.56.1323.

[18] I. Procaccia. Universal properties of dynamically complex systems: the organisation of chaos. *Nature*, 333:618–623, 1988. 16th June. http://dx.doi.org/10.1038/333618a0.

[19] A. J. Roberts. Low-dimensional models of thin film fluid dynamics. *Phys. Letts. A*, 212:63–72, 1996. http://dx.doi.org/10.1016/0375-9601(96)00040-0.

[20] A. J. Roberts. Holistic discretisation ensures fidelity to Burgers' equation. *Applied Numerical Modelling*, 37:371–396, 2001. http://dx.doi.org/10.1016/S0168-9274(00)00053-2.

[21] A. J. Roberts. A holistic finite difference approach models linear dynamics consistently. *Mathematics of Computation*, 72:247–262, 2002. http://www.ams.org/mcom/2003-72-241/S0025-5718-02-01448-5.

[22] A. J. Roberts. A step towards holistic discretisation of stochastic partial differential equations. In Jagoda Crawford and A. J. Roberts, editors, *Proc. of 11th Computational Techniques and Applications Conference CTAC-2003*, volume 45, pages C1–C15, December 2003. [Online] http://anziamj.austms.org.au/ojs/index.php/ANZIAMJ/article/view/869 [December 14, 2003].

[23] A. J. Roberts and D. V. Strunin. Rigorous zonal modelling of contaminant dispersion in shear flows. In N. Mastorakis, editor, *Recent Advances in Applied and Theoretical Mechanics*, pages 64–70. WSES Press, 2000.

[24] S. Rosencrans. Taylor dispersion in curved channels. *SIAM J. Appl. Math.*, 57:1216–1241, 1997.

[25] R. Valery Roy, A. J. Roberts, and M. E. Simpson. A lubrication model of coating flows over a curved substrate in space. *J. Fluid Mech.*, 454:235–261, 2002. http://dx.doi.org/10.1017/S0022112001007133.

[26] G. Samaey, I. G. Kevrekidis, and D. Roose. The gap-tooth scheme for homogenization problems. *SIAM Multiscale Modeling and Simulation*, 4:278–306, 2005. http://dx.doi.org/10.1137/030602046.

[27] G. Schöner and H. Haken. The slaving principle for Stratonovich stochastic differential equations. *Z. Phys. B—Condensed matter*, 63:493–504, 1986.

[28] N. Sri Namachchivaya and Y. K. Lin. Method of stochastic normal forms. *Int. J. Nonlinear Mechanics*, 26:931–943, 1991.