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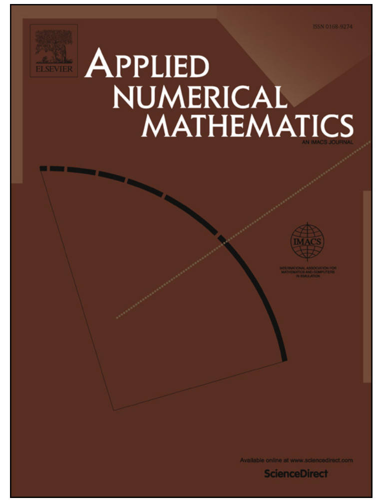

Smooth subgrid fields underpin rigorous closure in spatial discretisation of reaction–advection–diffusion PDEs

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Smooth subgrid fields underpin rigorous closure in spatial discretisation of reaction-advection-diffusion PDEs

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Abstract

Finite difference/element/volume methods of spatially discretising PDEs impose a subgrid scale interpolation on the dynamics. In contrast, the so-called holistic discretisation approach developed herein constructs a natural subgrid scale field adapted to the whole system out-of-equilibrium dynamics. Consequently, the macroscale discretisation is systematically informed by the underlying microscale dynamics. We establish a new proof that there exists an exact closure of the spatially-discrete dynamics of a general class of reaction-advection-diffusion PDEs. The approach also constructs new systematic approximations to the in-principle closure starting from a basis of simple, piecewise-linear, continuous approximation. Under inter-element coupling conditions that guarantee continuity of several field properties, the constructed holistic discretisation possesses desirable properties such as a natural cubic spline first-order approximation to the field, and the self-adjointness of the diffusion operator under periodic, Dirichlet and Neumann macroscale boundary conditions. As a concrete example, we demonstrate the holistic discretisation procedure on the well-known Burgers' PDE, and compare the theoretical and numerical stability of the resulting discretisation to other approximations. The approach developed here promises to empower systematic construction of good, macroscale discretisations to a wide range of dissipative and wave PDEs.

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