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An accurate discretization for an inhomogeneous transport equation with arbitrary coefficients and source

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ABSTRACT

A new way of obtaining the algebraic relation between the nodal values in a general one-dimensional transport equation is presented. The equation can contain an arbitrary source and both the convective flux and the diffusion coefficient may vary arbitrarily. Contrary to the usual approach of approximating the derivatives involved, the algebraic relation is based on the exact solution written in integral terms. The required integrals can be speedily evaluated by approximating the integrand with Hermite splines or applying Gauss quadrature rules. The startling point about the whole procedure is that a very high accuracy can be obtained with few nodes, and more surprisingly, it can be increased almost up to machine accuracy by augmenting the number of quadrature points or the Hermite spline degree with little extra cost.

1. Introduction

Transport equations are partial differential equations (PDE) that are ubiquitous in many branches of science, in particular Fluid Mechanics. They govern the evolution of flow variables whose values, for one reason or another, are required to be known in a certain domain. Unfortunately, an analytical solution to these equations is seldom possible, so in order to know the field at a discrete number of points one has to resort to numerical techniques that provide an approximate solution. The computational techniques employed for the fluid mechanics equations gave birth to a branch called computational fluid dynamics (CFD) that nowadays has almost constituted a separate subject.

There has been a huge effort along the years to improve the algorithms devised to obtain the flow field solutions with general numerical methods: finite differences, elements, volumes or spectral. Finite differences and volumes employ a numerical approximation to the derivatives present in the equation, whereas, generally speaking, finite elements or spectral techniques use a kind of solution expansion either in a local or global basis. Usually these approaches are one-dimensional: the discretization along one coordinate is independent of the others. For a standard discretization it is worth pointing out that none of these methods uses the solution of the ordinary differential equation (ODE) that can be obtained if the multidimensional partial differential equation (PDE) is integrated over an interval along a given coordinate. As a result of this integration the PDE converts into a nonhomogeneous first-order ODE whose solution can be written in terms of its homogeneous and particular solutions via the general theory of first-order ODEs. The method proposed in this work uses the exact integral solution of the first-order ODE to obtain the algebraic nodal equations of the second-order PDE, and it is different in that sense from previous methods. The examples presented in this paper are however limited to one-dimensional convection–diffusion problems, that is, second-order ODEs.

There have been several attempts to use the exact solution of a transport equation in the derivation of the algebraic coefficients. The pioneering paper is that of Raithby at al. [1] in which they assessed the sources of errors in their 2D discretization by comparing it with the local unidirectional exact solution in which all cross-stream fluxes were lumped together into a pseudo-source. This source was constant in the interval between two consecutive nodes and the coefficients at the interface prevailed over the whole interval length. Based on this they proposed LOADS (Locally Analytic Differencing Scheme) where they made the exact equation to match the values at two consecutive nodes, thereby obtaining the numerical fluxes for each face of the control volume and, by summing up the fluxes, an algebraic equation for every node. This scheme basically was a conservative extension of the Allen and Southwell scheme [2] which was nonconservative. Thiart [3,4] used a collocated grid to implement the same idea for the Navier–Stokes equations. In the first paper only the external source was considered to form part of the exact solution but in the second he also included the cross-stream terms in the modified source. In these two papers the source was constant in every subinterval that belonged to a control volume and discontinuous at

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the interfaces. Harms et al. [5] and later Wang et al. [6] extended this scheme to interfaces not located midway between two consecutive nodes as Thiart's scheme required.

In the early 1990s two schemes that used the exact solution were LECUSSO (locally exact consistent upwind scheme of second order) and LENS (locally exact numerical scheme) [7,8]. The second one can deal with a wider range of problems because the exact solution for a constant-coefficient, linear absorption, polynomial-source ODE was employed in its derivation. When the absorption is zero and the source is constant LENS transforms into LECUSSO. All algebraic coefficients are obtained by adjusting the exact solution over five nodes. Later Sakai put forward an optimized version of both [9,10]. A final improvement of LENS was to incorporate four different zones of piecewise-constant diffusion and absorption coefficients within a three-node region [11]. A linearly varying diffusion and absorption coefficients were also considered by Kriventsev et al. [12].

In order to mimic the exact solution a set of methods used a test function inside the control volume that contained a sum of three terms: a constant, an exponential of the Péclet number based on a local coordinate x and a linear term of the same. The associated constants were determined by requiring the function to pass through the nodal values. All of them were logical inhomogeneous extensions of the exponential scheme which is known to be exact in 1D with constant coefficients and no source. The third term appeared because the exact solution with a constant source in the control volume contains a linear term related to the source. Amongst these approaches is the UNIFAES scheme [13,14] and the scheme adopted by Sheu et al. [15]. In the latter a linear absorption term was also included. The UNIFAES was again based in Allen and Southwell scheme with the constant in the source-related term being linearly interpolated at the interface from its values at the nodes, these latter obtained following Allen and Southwell's idea. This interpolation makes the whole scheme conservative yet it is based on a nonconservative one.

Because they have sparked lines of research of their own it is adequate to comment apart on two general approaches that employ in one way or another the exact solution: the finite analytic method (FA) [16,17] and the nodal integral method (NIM) [19,20]. The main idea of the FA method is applicable to any unsteady multidimensional transport equation. A local domain is considered around a generic node P. For any spatial boundary the method assumes that the solution contains the same three terms as before as well as a linear time dependence in the temporal boundaries. These boundary conditions are written in terms of the boundary nodes (those surrounding P). Applying separation of variables one is able to obtain the exact solution in the local domain. With this solution the coefficients that should multiply the boundary values to obtain the value at P can be obtained. For a detailed description and many applications of the FA method see [18]. NIM, on the other hand, uses the exact solution with constant coefficients to derive the solution of the variable obtained by line-averaging the original equation around P, either spatial or temporal. For instance, in a 1D spatial domain NIM integrates the variable over the spatial or the temporal coordinate producing two ODEs, one for the mean spatial value around P and other for the mean temporal value. All terms with derivatives with respect to the other coordinates are lumped into a pseudo-source term. The integration of this pseudo-source is performed by Legendre polynomials truncated at the desired degree. NIM then uses the exact solution to obtain that of these two first-order ODE, written in terms of the variable at the nodes. By algebraically manipulating these expressions and applying continuity constraints NIM is able to derive two coupled algebraic equations for both nodal means with a three-node stencil.

As a resumé, almost all attempts to use the exact solution of a nonhomogeneous convection–diffusion equation as a base for discretization schemes have been with constant coefficients and very simple polynomial sources. In this short review the only schemes that employ a varying diffusion coefficient are those of Sakai et al. [11] and Kriventsev et al. [12]. None of them considered varying convective flux even though in 2D or 3D the mass flux varies along a coordinate even if the divergence of the mass flux is zero.

In a former paper the first author developed a scheme named ENATE for a transport equation with constant coefficients that can handle arbitrary sources as long as they have continuous derivatives of any order in the working interval [22]. In this paper the exact integral solution of the transport equation is employed to extend this idea to arbitrary coefficients. The idea followed in this paper is very close to that proposed by ten Thije Boonkamp and Anthonissen [21] in its FV-CF scheme (finite volume-complete flux). They look for an integral representation of the homogeneous and inhomogeneous fluxes at control volume faces of a general steady conservation law in terms of the nodes that share the face. It can be checked that the integrals involved in both fluxes are the same as those that can be derived from the approach presented in this paper, apart from the very different nomenclature employed and the path taken for its derivation. It could not be otherwise as the solution of an inhomogeneous ODE with given boundary conditions is unique. The main differences with this paper are that they work with fluxes at the faces and we work with the exact solution between nodes that allows us to present the scheme in terms of an algebraic equation with three nodes. The coefficients of this algebraic equation are clearly defined in terms of integrals between nodes which facilitates their coding. On top of that, when it comes to computing the several cases presented, ten Thije Boonkamp and Anthonissen assume linear dependencies of the integrand, that is, the standard trapezoidal rule for integral evaluation, which overly reduces their accuracy.

This paper is structured as follows: firstly, the integral solution to a homogeneous transport equation will be derived. Then, how to deal with the source in a nonhomogeneous equation will be described. As the complete solution is the sum of the homogeneous and the particular solutions, the latter in integral terms will eventually be obtained in this section. The complete solution will then be employed to obtain the algebraic connections between nodes and the extra terms due to the source, with some discussion on the asymptotic regime of mesh Péclet going to infinity. The accuracy of the discretization is connected to a numerical integration problem and some integration alternatives employed in this paper will then be described. Finally the approach is applied to three test cases with spatially varying convective flux, diffusion coefficient and/or source, showing its excellent behaviour.

2. Integral solution of a 1D homogeneous transport equation

The nonhomogeneous convection–diffusion equation with variable coefficients can be written as

$$\frac{d}{dx}\left(\rho\upsilon\phi - \Gamma\frac{d\phi}{dx}\right) = S; \quad \rho\upsilon = \rho\upsilon(x); \quad \Gamma = \Gamma(x); \quad S = S(x) \tag{1}$$

In this section we will derive the integral solution of the homogeneous equation, $S = 0$, and its simplified variants, some of them well known. This integral solution is later employed as a constituent part of the solution of the general nonhomogeneous equation with arbitrary source. As will later be seen the homogeneous solution partly contributes to the coefficients that connect nodal values in the final algebraic equation.

The domain is split in N intervals, not necessarily of equal length, and $N+1$ nodes with locations x_i, $i = 0, \ldots, N$, with two nodes at the boundaries, x_0 and x_N. In order to obtain the homogeneous solution in every generic interval with left boundary (lb) and right boundary (rb), it is more convenient to work with normalized variables, defined as