Journal of Computational Physics 274 (2014) 432–454

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Diagonal-norm summation by parts operators for finite difference approximations of third and fourth derivatives

Ken Mattsson

ARTICLE INFO

Article history:
Received 20 December 2013
Received in revised form 13 June 2014
Accepted 15 June 2014
Available online 20 June 2014

Keywords:
Finite difference methods
High-order derivative
High-order accuracy
Stability
Boundary treatment
Nonlinear waves

ABSTRACT

High-order accurate finite difference operators for third and fourth derivatives are derived. The closures are based on the summation-by-parts (SBP) framework, thereby guaranteeing linear stability. Stability for nonlinear equations that support a convex extension can be achieved if the SBP operators are based on a diagonal norm. The boundary conditions are imposed using a penalty technique. The accuracy and stability properties of the newly derived SBP operators are demonstrated for both linear and nonlinear dispersive wave propagation problems.

1. Introduction

Wave-propagation problems frequently require far-field boundaries to be positioned many wavelengths away from the disturbance source. Efficient simulation of these problems requires numerical techniques capable of accurately propagating disturbances over long distances. It is well know that high-order finite difference methods (HOFDMs) are ideally suited for problems of this type. (See the pioneering paper by Kreiss and Oliger [23].) Not all high-order spatial operators are applicable, however. For example, schemes that are G-K-S stable [13], while being convergent to the true solution as $\Delta x \to 0$, may experience nonphysical solution growth in time [4], thereby limiting their efficiency for longtime simulations. Thus, it is imperative to use HOFDMs that do not allow nonphysical solution growth in time—a property termed "strict stability" [12]. Deriving a strictly stable, accurate, and conservative HOFDM is a significant challenge that has received considerable past attention. (For examples, see [25,43,40,1,3,16,42,15].)

A robust and well-proven high-order finite difference methodology that ensures the strict stability of time-dependent partial differential equations (PDEs) is the summation-by-parts–simultaneous approximation term (SBP–SAT) method. The SBP–SAT method combines semi-discrete operators that satisfy a summation-by-parts (SBP) formula [21], with physical boundary conditions implemented using the simultaneous approximation term (SAT) method [4]. (The SAT method was originally developed for pseudo-spectral approximations [9,10]. Examples of the pseudo-spectral penalty approach can be found in [16,48].) Examples of the SBP–SAT approach can be found in [36–38,30,33,34,39,29,45,24,8,32,18,17,20,27,2].

An added benefit of the SBP–SAT method is that it naturally extends to multi-block geometries while retaining the essential single-block properties: strict stability, accuracy, and conservation [7]. Thus, problems involving complex domains or non-smooth geometries are easily amenable to the approach. Refs. [29,33,19] report applications of the SBP–SAT method to problems involving nontrivial geometries.

A wide variety of numerical methods may be expressed as summation-by-parts operators; examples include finite difference operators, spectral collocation [6,5], and some finite volume methods [46]. Herein we focus exclusively on finite difference operators.

http://dx.doi.org/10.1016/j.jcp.2014.06.027
0021-9991/

The SBP–SAT approach has so far been developed for problems involving first and second derivatives in space. However, there are many problems where higher order derivatives are present. Some examples include the Korteweg–de Vries and the Boussinesq equations (describing nonlinear water waves), soliton models in neuroscience [41], the Euler–Lagrange equation for beams, and the Cahn–Hilliard equation which describes the process of phase separation.

The main focus in the present study is to construct high-order accurate explicit (i.e., do not require solving any equation system to obtain the difference approximation) narrow-stencil SBP operators for third and fourth derivatives. One option to approximate higher order derivatives is a successive application of the existing first-derivative SBP operators. However, that leads to very wide difference stencils and loss of convergence due to the lowered accuracy at the boundaries (which will be demonstrated in Section 7 in the present study). Since many problems involve various orders of derivatives (the Korteweg–de Vries equation involves first and third derivatives, while Boussinesq equations involve second and fourth derivatives) it is necessary to build the various orders of SBP operators (having the same internal order of accuracy) using the same norm, and that the boundary derivative operators involved do not change between the various operators. In the present study we have derived completely new SBP operators for the first, second, third and fourth derivatives, based on the same norm (the energy method relies on this).

In Section 2 the SBP–SAT method is introduced starting with the previous SBP definitions for the first and second derivatives and then introducing the novel SBP definitions for the third and fourth derivatives. Details of the necessary steps to derive the SBP operators are presented in Section 3. In Section 4 we analyse a non-linear dispersive wave equation and a system of dispersive wave equations. A higher order wave equation is analysed in Section 5 where we focus on the dynamic beam equation. Time integration is analysed and discussed in Section 6. In Section 7 the accuracy and stability properties of the newly developed SBP operators are verified by performing numerical simulations. Section 8 summarises the work. The SBP operators are presented in Appendix A.

2. The finite difference method

SBP operators are essentially central finite difference stencils closed at the boundaries with a careful choice of one-sided difference stencils, to mimic the underlying integration-by-parts formula in a discrete norm. In the present paper we address the SBP operators by the accuracy of the central scheme and the type of norm which they are based on.

First- and second-derivative SBP operators have been derived in earlier papers (see for example [22,30,35,26,27]), and will be referred to as *traditional*. These operators use a minimal number of non-central boundary stencils. The focus in the present study is the derivation of SBP operators for higher order derivatives, up to fourth order. When combining SBP operators of various derivative orders it is necessary to build them using the same norm. The norms that are used in the construction of traditional first- and second-derivative SBP operators cannot be used to construct third- and fourth-derivative SBP operators since there are simply not enough free parameters to fulfil all the necessary SBP requirements. Hence, we must extend the number of free parameters by introducing more boundary points, i.e., using norms with additional boundary points (compared to the traditional first- and second-derivative SBP operators).

2.1. Definitions

The following definitions are needed later in the present study. Let $\mathbf{u},\mathbf{v} \in L^2[l,r]$ where $\mathbf{u}^T = [u^{(1)}, u^{(2)}, \dots, u^{(k)}]$ and $\mathbf{v}^T = [v^{(1)}, v^{(2)}, \dots, v^{(k)}]$ are real-valued vector functions with k components. Let the inner product be defined by $(\mathbf{u}, \mathbf{A}\mathbf{v}) = \int_l^r \mathbf{u}^T \mathbf{A}(x)\mathbf{v}\,dx$, $\mathbf{A}(x) = \mathbf{A}^T(x) > 0$, and let the corresponding norm be $\|\mathbf{u}\|_A^2 = (\mathbf{u}, \mathbf{A}\mathbf{u})$. We introduce the notation $\mathbf{u}_l = \mathbf{u}(l,t)$ and $\mathbf{u}_r = \mathbf{u}(r,t)$, i.e., referring to the boundary values (at the left and right boundary).

The domain ($l \le x \le r$) is discretized using m grid points:

$$\mathbf{x} = [x_1, x_2, \dots, x_{m-1}, x_m]^T,$$

i.e., $\mathbf{x}$ denotes a vector holding the grid-points, where

$$x_i = (i-1)h, \quad i = 1, 2, \dots, m, \; h = \frac{r-l}{m-1}.$$

In the present study we make use of the Kronecker product:

$$C \otimes D = \begin{bmatrix} c_{0,0}\,D & \cdots & c_{0,q-1}\,D \\ \vdots & & \vdots \\ c_{p-1,0}\,D & \cdots & c_{p-1,q-1}\,D \end{bmatrix},$$

where C is a $p \times q$ matrix and D is an $m \times n$ matrix. Two useful rules for the Kronecker product are $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$ and $(A \otimes B)^T = A^T \otimes B^T$.

The approximate solution vector is given by $v^T = [v^{(1)}, v^{(2)}, \dots, v^{(k)}]$, where $v^{(j)} = [v_1^{(j)}, v_2^{(j)}, \dots, v_m^{(j)}]^T$ is the discrete solution vector of the jth component. Similarly, we define an inner product for discrete real-valued vector functions $u, v \in \mathbf{R}^{k \times m}$ by $(u, Av) = u^T H_k A\, v$, where $H_k = I_k \otimes H$ is positive definite (H is a symmetric positive definite $m \times m$ matrix) and A is the projection of $\mathbf{A}(x)$ onto the block diagonals. If $\mathbf{A}(x)$ is a diagonal $k \times k$ matrix, A is a diagonal $(km) \times (km)$ matrix. I_k denotes the unit matrix of size $k \times k$. The corresponding norm is $\|v\|_{H_A}^2 = v^T H_k A\, v$.