Journal of Computational Physics 360 (2018) 192–201

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

On pseudo-spectral time discretizations in summation-by-parts form

Andrea A. Ruggiu *, Jan Nordström

Department of Mathematics, Computational Mathematics, Linköping University, SE-581 83 Linköping, Sweden

ARTICLE INFO

Article history:
Received 4 December 2017
Received in revised form 22 January 2018
Accepted 23 January 2018
Available online xxxx

Keywords:
Time integration
Initial boundary value problem
Summation-by-parts operators
Pseudo-spectral methods
Eigenvalue problem

ABSTRACT

Fully-implicit discrete formulations in summation-by-parts form for initial-boundary value problems must be invertible in order to provide well functioning procedures. We prove that, under mild assumptions, pseudo-spectral collocation methods for the time derivative lead to invertible discrete systems when energy-stable spatial discretizations are used.

1. Introduction

Well-posedness of partial differential equations is a key concept in mathematical modeling. A well-posed problem has a unique solution which is bounded by the data of the problem [1,2]. Once initial and boundary conditions that lead to well-posedness are determined, a discrete approximation of the continuous problem can be formulated and solved, if it is stable. An additional requirement for fully-implicit discrete problems is the invertibility of the resulting system of equations. If this condition is not met, an iterative solver applied to such problems may converge to an erroneous solution [3].

Stable and high-order accurate discretizations for well-posed linear problems can be achieved in a straightforward way by combining Summation-By-Parts (SBP) operators [4,5] and weak boundary and initial procedures using Simultaneous-Approximation-Terms (SATs) [6–8]. For initial value problems, the dual-consistent [9] SBP–SAT formulations are A- and L-stable implicit Runge–Kutta schemes [10,11]. However, the invertibility of fully-discrete stable approximations have so far only been conjectured in this setting [7,11] (it does not follow from any known stability property). For further reading on these topics, see for example [12,13].

In this work, we focus on pseudo-spectral collocation methods on finite domains [14] for initial value problems. We prove that these discretizations, which can be recast as SBP–SAT schemes with diagonal norms [15,16], have eigenvalues with strictly positive real parts for specific choices of the penalty parameter. As a natural consequence, pseudo-spectral time discretizations combined with energy stable spatial approximations of initial-boundary value problems lead directly to invertible fully discrete approximations.

This paper is organized as follows. In section 2, the pseudo-spectral methods in SBP form are introduced for initial value problems. We also reformulate the invertibility issue in terms of the eigenvalues of the time discretization. In section 3,

* Corresponding author.
E-mail addresses: andrea.ruggiu@liu.se (A.A. Ruggiu), jan.nordstrom@liu.se (J. Nordström).

https://doi.org/10.1016/j.jcp.2018.01.043
0021-9991/

we show that pseudo-spectral SBP–SAT approximations yield discrete operators which can be easily studied through a coordinate transformation to Legendre polynomials. The eigenvalues of these matrices are analyzed in section 4, where the main result of the paper is stated and proved. Next, the properties of fully discrete systems with pseudo-spectral time discretizations are exemplified in section 5. Section 6 contains our conclusions.

2. Pseudo-spectral SBP–SAT time discretizations

The aim of this section is two-fold: firstly, we introduce the pseudo-spectral SBP–SAT discretizations for initial value problems [7]; secondly, we outline the main theoretical issue in this paper.

2.1. SBP operators

Consider a set of n nodes $\mathbf{x} = [x_1, \dots, x_n]^T \subset [\alpha, \beta]$ which may or may not include the endpoints of the interval. A Summation-By-Parts operator discretizing the first derivative on $\mathbf{x}$ can be defined as follows [16]:

Definition 2.1. A discrete operator D is a qth order accurate approximation of the first derivative with the Summation-By-Parts (SBP) property if

i) $D\mathbf{x}^j = P^{-1}Q\mathbf{x}^j = j\mathbf{x}^{j-1}$, $j \in [0, q]$,
ii) P is a symmetric positive definite matrix,
iii) $Q + Q^T = E$, where E is such that $(\mathbf{x}^i)^T E \mathbf{x}^j = \beta^{i+j} - \alpha^{i+j}$, $i, j = 0, \dots, r$, $r \geq q$.

Condition i) in Definition 2.1 implies that the operator D exactly mimics the first derivative for the grid monomials $\mathbf{x}^j = [x_1^j, \dots, x_n^j]^T$ up to the qth order. Condition ii) defines a discrete scalar product and a norm

$$(\mathbf{v}, \mathbf{w})_P = \mathbf{v}^T P \mathbf{w}, \qquad \|\mathbf{v}\|_P = \sqrt{(\mathbf{v}, \mathbf{v})_P}$$

which mimic the continuous L^2 counterparts. Furthermore, condition iii) implies that the integration-by-parts rule

$$\int_\alpha^\beta u v_x \mathrm{d}x = u(\beta)v(\beta) - u(\alpha)v(\alpha) - \int_\alpha^\beta u_x v \mathrm{d}x$$

is exactly mimicked for u and v being polynomials of at most order r. In particular,

$$(\mathbf{x}^i, D\mathbf{x}^j)_P = \beta^{i+j} - \alpha^{i+j} - (D\mathbf{x}^i, \mathbf{x}^j)_P, \quad i, j = 0, \dots, r. \tag{1}$$

The discrete operators that we consider in this paper are based on pseudo-spectral collocation methods with accuracy $q = n - 1$ that satisfy (1) with $r = n - 1$.

For pseudo-spectral methods on finite domains, the grid is usually a subset of the reference interval $[\alpha, \beta] = [-1, 1]$.

Example 2.2. Consider a 2nd order accurate SBP operator $D = P^{-1}Q$ based on the Legendre–Gauss–Radau quadrature. On the three-point grid $\mathbf{x} = [-1, (1-\sqrt{6})/5, (1+\sqrt{6})/5]^T$, the SBP operator is given by

$$P = \frac{1}{18}\begin{bmatrix} 4 & 0 & 0 \\ 0 & 16+\sqrt{6} & 0 \\ 0 & 0 & 16-\sqrt{6} \end{bmatrix}, \tag{2}$$

$$Q = \frac{1}{108}\begin{bmatrix} -48 & 24+14\sqrt{6} & 24-14\sqrt{6} \\ -12-32\sqrt{6} & 87-18\sqrt{6} & -75+50\sqrt{6} \\ -12+32\sqrt{6} & -75-50\sqrt{6} & 87+18\sqrt{6} \end{bmatrix}. \tag{3}$$

The matrix E in Definition 2.1 can be written in terms of boundary interpolants of degree r:

$$\mathbf{e}_\gamma^T \mathbf{x}^j = \gamma^j, \quad j \in 0, \dots, r, \quad \gamma \in \{\alpha, \beta\}, \tag{4}$$

where $\mathbf{e}_\gamma^T \mathbf{u} \approx u(\gamma)$. This gives rise to the relation $E = \mathbf{e}_1\mathbf{e}_1^T - \mathbf{e}_{-1}\mathbf{e}_{-1}^T$. In the example above, the interpolants are $\mathbf{e}_{-1} = [1, 0, 0]^T$ and $\mathbf{e}_1 = [1/3, (2-3\sqrt{6})/6, (2+3\sqrt{6})/6]^T$. The interpolation at $x = -1$ is exact, since this point is included in $\mathbf{x}$. At $x = 1$ the interpolation is exact only for 2nd order polynomials.

Remark 2.3. Pseudo-spectral collocation methods typically involve only a few nodes and, hence, are suitable for multi-stage discretizations in time.