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Spurious solutions for the advection-diffusion equation using wide stencils for approximating the second derivative

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Abstract

A one dimensional steady-state advection-diffusion problem using summation-by-parts operators is investigated. For approximating the second derivative, a wide stencil is used, which simplifies implementation and stability proofs. However, it also introduces spurious, oscillating, modes for all mesh-sizes. We prove that the size of the spurious modes are equal to the size of the truncation error for a stable approximation and hence disappears with the convergence rate. The theoretical results are verified with numerical experiments.

Keywords: Summation-by-parts, spurious solutions, oscillating solutions.

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1. Introduction

Finite difference methods using central difference schemes often result in spurious modes, especially if second derivatives are computed using the first derivative operator twice. These modes, which are products of the discretization of the problem, have no connection to the continuous partial differential equation, and are therefore unwanted. One way to reduce these oscillations is by constructing appropriate boundary closures [1, 2]. Another way is to add artificial dissipation to the scheme [3, 4, 5]. The oscillations can also be reduced by using compact operators [6, 7] (operators with minimal stencil width). However, proving stability by energy methods and implementing fluxes when using compact operators can be cumbersome when mixed deriva-

tives together with second order ones exist, as in the compressible Navier-Stokes equations. These issues vanish when using the first derivative operator twice for the second derivatives. In this paper we ask the question: are the oscillating spurious modes a real problem, or can they be ignored?

Assuming that well-posed boundary conditions and a stable numerical scheme is in place, the spurious oscillations for the steady-state advection-diffusion problem will be analyzed. In particular, we will determine the rate with which these oscillations vanish during mesh refinement. We focus on finite difference operators with the Summation-By-Part (SBP) property, and weakly imposed boundary conditions. By using the SBP operators [8, 6], augmented with Simultaneous Approximation Terms (SAT) [9], a stable numerical scheme can be obtained when well-posed boundary conditions are available [7]. A comprehensive review of the SBP-SAT technique is given in [5].

The rest of this paper will proceed as follows. In Section 2, well-posed boundary conditions for the advection-diffusion equation in one space dimension are determined. Next, the SBP-SAT method is applied to the equation, and stable penalty parameters are derived. In Section 3, we will prove that the rate of convergence is two for the second order accurate scheme in the steady-state limit. The results from Section 3 are generalized to higher order stencils in Section 4. In Section 5, the theoretical results are tested in numerical experiments. Finally, in Section 6, we summarize the results of this work, and draw conclusions.

2. The advection-diffusion equation

Consider the advection-diffusion equation in the domain $x \in [0, 1]$ and $t \geq 0$,

$$\begin{aligned} u_t + au_x &= \epsilon u_{xx} \\ c_1 u(0, t) - \epsilon u_x(0, t) &= g_0(t) \\ c_2 u(1, t) - \epsilon u_x(1, t) &= g_1(t) \\ u(x, 0) &= f(x). \end{aligned} \tag{1}$$

In (1), $g_{0,1}(t)$ are the boundary data, $f(x)$ is the initial data, $c_{1,2}$ are constants to be determined such that (1) becomes well-posed and $\epsilon, a > 0$.

41 *2.1. Well-posedness*

42 By multiplying (1) with u and integrating over the domain, we obtain

43
$$\|u\|_t^2 + 2\|u_x\|^2 = [au^2 - 2\epsilon uu_x]_{x=0} - [au^2 - 2\epsilon uu_x]_{x=1}, \quad (2)$$

44 where $\|u\|^2 = \int_0^1 u^2 dx$. The boundary data does not influence the well-
 45 posedness of the problem, so we let $g_0 = g_1 = 0$ for simplicity [10]. Inserting
 46 the homogeneous boundary conditions from (1) into (2), yields

47
$$\|u\|_t^2 + 2\epsilon\|u_x\|^2 = u^2(0, t)(a - 2c_1) - u^2(1, t)(a - 2c_2) \quad (3)$$

48 and an energy estimate is obtained by choosing $c_1 \geq a/2$ and $c_2 \leq a/2$.
 49 With these choices of $c_{1,2}$, the solution u is bounded. The energy estimate
 50 (3) automatically lead to uniqueness, and existence is guaranteed since the
 51 right number of boundary conditions are used. We summarize the results in
 52 the following proposition.

53 **Proposition 1.** *Equation (1) is well-posed if $c_1 \geq a/2$ and $c_2 \leq a/2$.*

54 In the remainder of this paper, we use $c_1 = a$, $c_2 = 0$ and (1) is stated as

$$\begin{aligned} u_t + au_x &= \epsilon u_{xx} \\ au(0, t) - \epsilon u_x(0, t) &= g_0(t) \\ \epsilon u_x(1, t) &= g_1(t) \\ u(x, 0) &= f(x). \end{aligned} \quad (4)$$

56 *2.2. Stability*

57 When discretizing (4), we use the SBP operator $D = P^{-1}Q$, where $P =$
 58 $P^T > 0$ and proportional to the grid spacing h . The matrix Q satisfy the
 59 SBP property $Q + Q^T = \text{diag}(-1, 0, \dots, 0, 1)$. The operators P and Q are
 60 constructed such that the discrete energy estimate mimics the continuous
 61 one in (3). In this work, we consider SBP finite difference operators with
 62 diagonal P . The operators are of order $2s$ in the interior and s at a finite
 63 number of grid points within the boundary closures. The overall accuracy
 64 of the scheme becomes $s + 1$ [11]. We henceforth denote these operators as
 65 $SBP(2s, s)$.

66 We have,

$$\begin{aligned} v_t + aP^{-1}Qv &= \epsilon(P^{-1}Q)v_x + \alpha_0 P^{-1}(av_0 - \epsilon(v_x)_0 - g_0)e_0 \\ &+ \alpha_1 P^{-1}(\epsilon(v_x)_N - g_1)e_N \\ v(0) &= f, \end{aligned} \quad (5)$$

where the notation $v_x = P^{-1}Qv$ is used, i.e a wide stencil approximates the second order derivative. In (5), $v = (v_0, v_1, \dots, v_N)^T$ is the semi-discrete approximation of u at each grid point. The penalty parameters $\alpha_{0,1}$ in the SAT's will be determined such that the approximation becomes stable. Also, $e_0 = [1, 0, \dots, 0]^T$ and $e_N = [0, \dots, 0, 1]^T$.

By multiplying (5) with $v^T P$ from the left, adding the transpose of the outcome to itself and using the SBP-property of Q , one arrives at

$$\begin{aligned} \frac{d}{dt}(\|v\|_P^2) + 2\epsilon\|v_x\|_P^2 &= v_0(av_0 - 2\epsilon(v_x)_0) - v_N(av_N - 2\epsilon(v_x)_N) \\ &\quad + 2\alpha_0 v_0(av_0 - \epsilon(v_x)_0) + 2\alpha_1 v_N(\epsilon(v_x)_N), \end{aligned} \quad (6)$$

where again zero boundary data is used. In (6), the norm is defined by $\|v\|_P^2 = v^T P v$. By choosing $\alpha_0 = \alpha_1 = -1$, (6) is reduced to

$$\frac{d}{dt}(\|v\|_P^2) + 2\epsilon\|v_x\|_P^2 = -av_0^2 - av_N^2 \leq 0. \quad (7)$$

In (7), we observe that the solution v is bounded, and the numerical scheme (5) is therefore stable. Note that, due to the SBP property of P and Q , (7) mimics (3) if $c_1 = a$ and $c_2 = 0$. For a more detailed discussion of well-posedness and stability, the reader is referred to [5]. We summarize the results of this section in the following proposition.

Proposition 2. *The semi-discrete formulation (5) is stable if $\alpha_0 = \alpha_1 = -1$.*

3. Spurious oscillations for the second order accurate case

The semi-discrete form of (4) in the steady-state limit (i.e. $v_t = 0$) is

$$aP^{-1}Qv = \epsilon(P^{-1}Q)v_x - P^{-1}(av - \epsilon(v_x)_0 - g_0)e_0 - P^{-1}(\epsilon(v_x)_N - g_1)e_N. \quad (8)$$

Since we are studying a steady-state problem, the boundary data $g_{0,1}$ are constants. We start by considering the second order SBP-stencil, where the internal discrete approximation is given by

$$a \frac{v_{i+1} - v_{i-1}}{2h} = \frac{\epsilon}{4h^2}(v_{i+2} - 2v_i + v_{i-2}) \quad (9)$$

for $2 \leq i \leq N-2$ and grid spacing h . Equation (9) can be solved by making the ansatz $v_i \sim K^i$ where K depends on h . Inserting the ansatz into (9) gives the relation

$$\frac{K^2 - 1}{2} \left(\frac{K^2 - 1}{2} - \theta K \right) K^{i-4} = 0 \quad (10)$$

96 where $\theta = ah/\epsilon$ is the so-called mesh Reynolds number.

97 The non-trivial solutions to (10) are

$$\begin{aligned}
K_1 &= 1 \\
K_2 &= \theta + \sqrt{1 + \theta^2} = 1 + \theta + \frac{\theta^2}{2} + \mathcal{O}(\theta^4) \\
K_3 &= -1 \\
K_4 &= \theta - \sqrt{1 + \theta^2} = -1 + \theta - \frac{\theta^2}{2} + \mathcal{O}(\theta^4).
\end{aligned}
\tag{11}$$

99 The spurious, or oscillating, modes are $K_{3,4}$, due to the negative sign. These
100 modes have no relevance to the physical problem and introduce errors in the
101 numerical solution.

102 The solution at each grid point i is a weighted sum of all modes and can
103 be written as

$$v_i = \sum_{k=1}^4 \sigma_k K_k^i.
\tag{12}$$

105 To determine the coefficients σ_{1-4} , we consider the boundary closures of the
106 scheme. These conditions are,

$$a\theta(v_1 - v_0) - a(v_2 - 2v_1 + v_0) + a\theta v_0 - a(v_1 - v_0) = \theta g_0,
\tag{13}$$

$$a\theta(v_2 - v_0) - \frac{a}{2}\left(\frac{1}{2}v_3 - \frac{3}{2}v_1 + v_0\right) = 0,
\tag{14}$$

$$a\theta(v_N - v_{N-2}) - \frac{a}{2}\left(\frac{1}{2}v_{N-3} - \frac{3}{2}v_{N-1} + v_N\right) = 0,
\tag{15}$$

$$a\theta(v_N - v_{N-1}) - a(v_N - 2v_{N-1} + v_{N-2}) - a(v_N - v_{N-1}) = \theta g_1.
\tag{16}$$

111 The equations (13)-(16) are obtained by considering the finite difference ap-
112 proximation at grid point 0, 1, $N - 1$ and N , respectively. At the first and
113 last grid point, SAT's have been applied.

114 It can be shown that (13)-(16) uniquely determine the coefficients σ_{1-4} . In
115 fact, the coefficients are determined uniquely as long as well-posed boundary
116 conditions and stability are guaranteed. If (13)-(16) had several solutions, the
117 numerical solution v would not be unique. Since stability implies convergence
118 to the analytic solution, the continuous problem would also have several
119 solutions, which contradicts well-posedness. This is shown in [11].

120 In this paper, we are not interested in the exact values of σ_{1-4} , and will
121 instead use (14)-(15) to determine the order of magnitudes of $\sigma_{3,4}$. Inserting

122 (12) into (14) yields

$$123 \quad \sum_{k=1}^4 \left(\theta(K_k^2 - 1) - \frac{a}{2}(K_k - 1)^2(K_k + \frac{1}{2}) \right) \sigma_k = \sum_{k=1}^4 \tau_k \sigma_k = 0 \quad (17)$$

124 where

$$125 \quad \tau_k = a\theta(K_k^2 - 1) - \frac{a}{2}(K_k - 1)^2(K_k + \frac{1}{2}). \quad (18)$$

126 Since we are only interested in the order of magnitude, it suffice to consider
127 the order of magnitudes of the τ_k 's. By using K_k , given by (11), in (18) one
128 can conclude that

$$129 \quad \tau_1 = 0, \quad \tau_2 = \mathcal{O}(h^2), \quad \tau_3 = a, \quad \tau_4 = a - 2a\theta + \mathcal{O}(h^2).$$

130 Inserting this result in (17) yields

$$131 \quad a\sigma_3 + a(1 - 3\theta + \mathcal{O}(h^2))\sigma_4 = -\tau_2\sigma_2 = \mathcal{O}(h^2), \quad (19)$$

132 if σ_2 is bounded, which is necessary for a stable scheme. Inserting (12) into
133 (15) yields

$$134 \quad \sum_{k=1}^4 \left(\theta(K_k^2 - 1)K_k^{N-2} - \frac{a}{2}K_k^{N-3}(K_k - 1)^2(K_k + \frac{1}{2}) \right) \sigma_k = \sum_{k=1}^4 \kappa_k \sigma_k = 0, \quad (20)$$

135 where

$$136 \quad \kappa_k = \theta(K_k^2 - 1)K_k^{N-2} - \frac{a}{2}K_k^{N-3}(K_k - 1)^2(K_k + \frac{1}{2}).$$

137 With the values of K_k , given by (11), inserted into (20) for large values of
138 N , one obtains

$$139 \quad a(-1)^{N-2}\sigma_3 + ae^{-a/\epsilon}(-1)^{N-2}(1 - 2\theta + \mathcal{O}(h^2))\sigma_4 = -\kappa_2\sigma_2 = \mathcal{O}(h^2) \quad (21)$$

140 where the approximation $|K_4|^N = e^{-a/\epsilon} + \mathcal{O}(h^2)$ is used and

$$141 \quad \kappa_2 = a\theta(K_2^2 - 1)K_2^{N-2} - \frac{aK_2^{N-3}}{2}(K_2 - 1)^2(K_2 + \frac{1}{2}) = \mathcal{O}(h^2).$$

142 Equations (19) and (21) can be written as

$$143 \quad \begin{bmatrix} a & a - 3a\theta + \mathcal{O}(h^2) \\ a(-1)^{N-2} & ae^{-a/\epsilon}(-1)^{N-2}(1 + 2\theta) + \mathcal{O}(h^2) \end{bmatrix} \begin{bmatrix} \sigma_3 \\ \sigma_4 \end{bmatrix} = \mathcal{O}(h^2). \quad (22)$$

144 It is easy to show that the matrix in (22) is non-singular for any h . Therefore,
 145 the coefficients $\sigma_{3,4}$ must be of order $\mathcal{O}(h^2)$. Hence, the oscillatory modes
 146 only contribute with second order terms.

147 We summarize the conclusions obtained so far in the following proposi-
 148 tion.

149 **Proposition 3.** *For the second order semi-discrete approximation (8), the*
 150 *spurious modes in (12) contribute with $\mathcal{O}(h^2)$ terms.*

151 **Remark.** *Neither the boundary terms nor the penalty parameters enter the*
 152 *derivation above, which means that the spurious part contributes with $\mathcal{O}(h^2)$*
 153 *terms for all stable boundary procedures. Note also that if $\sigma_2 = 0$, equations*
 154 *(19) and (21) demand that both σ_3 and σ_4 must be zero, which shows that*
 155 *constant solutions are approximated exactly.*

156 4. Generalization to higher order schemes

157 In the previous section, we demonstrated how a stable boundary proce-
 158 dure automatically makes the spurious modes vanish when second order SBP
 159 operators are used. A similar phenomena is actually valid for any stable high
 160 order finite difference scheme, as we will show in this section.

161 To ease the derivations, we restrict ourselves to diagonal matrices P . The
 162 following propositions and theorem are also true for a general symmetric
 163 matrix P , but the treatment of such operators will obscure the main points
 164 of the derivations. We start by stating

165 **Proposition 4.** *Consider the approximation (8) with a SBP operator $P^{-1}Q$*
 166 *of internal order $2m$ and a diagonal matrix P . The ansatz*

$$167 \quad v_i(h) \sim K^i(h), \quad (23)$$

where h is the grid spacing and i the grid point index, inserted into (8) leads
 to

$$\lim_{h \rightarrow 0} K_j(h) = K_{j0}.$$

168 That is, all $K_j, j = 1, \dots, 4m$, approach finite values as $h \rightarrow 0$.

169 *Proof.* Let $D = P^{-1}Q$ be a finite difference operator of order $2m$ in the
 170 internal domain that approximates the first and second derivatives as $v_x \approx$

171 Dv , $v_{xx} \approx D^2v$. A SBP finite difference operator of internal order $2m$ uses
 172 the grid points $i - m, \dots, i + m$ to approximate the derivative at i , so we have

$$\begin{aligned}
 (Dv)_i &= (P^{-1}Qv)_i = \frac{1}{h} \sum_{j=i-m}^{i+m} Q_{i,j} v_j = \frac{1}{h} \sum_{j=i-m}^{i+m} Q_{i,j} K^j \\
 &= \frac{1}{h} \left(\sum_{j=0}^{2m} Q_{i,j+i-m} K^j \right) K^{i-m} = \frac{1}{h} \mathcal{P}_{2m}(K) K^{i-m},
 \end{aligned} \tag{24}$$

174 where $\mathcal{P}_{2m}(K) = \sum_{j=0}^{2m} Q_{i,j+i-m} K^j$ is a polynomial of order $2m$, independent
 175 of h . In (24), Q is the matrix with the SBP-property in (8) and the index
 176 i denotes an internal grid point. For example, in the fourth order case, we
 177 have

$$\begin{aligned}
 (Dv)_i &= \frac{1}{h} \left(\frac{1}{12} v_{i-2} - \frac{2}{3} v_{i-1} + \frac{2}{3} v_{i+1} - \frac{1}{12} v_{i+2} \right) \Rightarrow \\
 \frac{1}{h} P_4(K) K^{i-2} &= \frac{1}{h} \left(\frac{1}{12} - \frac{2}{3} K + \frac{2}{3} K^3 - \frac{1}{12} K^4 \right) K^{i-2}.
 \end{aligned}$$

179 Similarly, for the second derivative approximation, one obtains

$$(D^2v)_i = D \frac{1}{h} \mathcal{P}_{2m}(K) K^{i-m} = \frac{1}{h^2} \mathcal{P}_{2m}^2(K) K^{i-2m}. \tag{25}$$

181 We now use the results above to solve for the modes K in (8). Inserting
 182 (24) and (25) into (8) at an internal grid point yields

$$a(Dv)_i - \epsilon(D^2v)_i = \frac{a}{h} \mathcal{P}_{2m}(K) K^{i-m} - \frac{\epsilon}{h^2} \mathcal{P}_{2m}^2(K) K^{i-2m} = 0. \tag{26}$$

184 By multiplying both sides of (26) with $h^2 K^m / \epsilon$, one arrives at

$$\mathcal{P}_{2m}(K) (\mathcal{P}_{2m}(K) - K^m \theta) K^{i-m} = 0. \tag{27}$$

186 Note that (10) is a special case of (27), where $P_2(K) = (K^2 - 1)/2$.
 187 According to (27), all $4m$ modes are determined by

$$\mathcal{P}_{2m}(K) = 0 \tag{28}$$

$$\mathcal{P}_{2m}(K) = \theta K^m. \tag{29}$$

190 Note that (28) has $2m$ solutions, all independent of h , that is $K_j = K_{0j} =$
 191 *constant* for $j = 1, \dots, 2m$.

Equation (29) is similar to (28), with a perturbation of magnitude h at the right hand side. Since $\mathcal{P}_{2m}$ is a polynomial, the solutions to (29) must therefore be close to the ones of (28), that is $K_{jp} = K_{j0} + \mathcal{O}(h)$ where the index p denotes the perturbed solutions to (29). Hence, for any solution to (27), we have $\lim_{h \rightarrow 0} K_j(h) = K_{j0} = \text{constant}$. $\square$

With all modes obtained from (27), the final form of the solution is

$$v_k = \sum_j \sigma_j K_j^k, \quad (30)$$

where the modes K are the solutions to (27) and σ_j are constants to be determined by the boundary conditions. We state the following lemma and proposition.

Lemma 1. *Let the numerical solution at grid point k be given by (30), such that the solution at every grid point can be written $v = \hat{K}\tilde{\sigma}$, where $\tilde{\sigma}$ is a $4m \times 1$ vector containing the coefficients σ_j and $\hat{K}$ is a $N \times 4m$ matrix with $\hat{K}_{ij} = K_j^{i-1}$, where all K_j are distinct. The rank of $\hat{K}$ is then $4m$ and, consequently, $\hat{K}^* \hat{K}$ is non-singular.*

Proof. See Appendix A. $\square$

Proposition 5. *Let the numerical solution to (8) be given by (30) where k denotes the grid point and the modes K_j are distinct. If v approximates the analytic solution, u , with an accuracy $\mathcal{O}(h^{m+1})$, then all σ_j converges to fixed values.*

Proof. The vector v , which represents the solution at every grid point, can be written as

$$v = \hat{K}\tilde{\sigma}, \quad (31)$$

where v , $\tilde{\sigma}$ and $\hat{K}$ are the vectors and matrices defined in Lemma 1. If the overall accuracy of the scheme is $\mathcal{O}(h^{m+1})$, the numerical solution approximates the analytic one, u , as

$$v - u = \hat{K}\tilde{\sigma} - u = \mathcal{O}(h^{m+1}). \quad (32)$$

By multiplying (32) with $(\hat{K}^* \hat{K})^{-1} \hat{K}^*$ from the left, one obtains the coefficients $\tilde{\sigma}$,

$$\tilde{\sigma} = (\hat{K}^* \hat{K})^{-1} \hat{K}^* u + \mathcal{O}(h^{m+1}), \quad (33)$$

222 and we observe that $\lim_{h \rightarrow 0} \tilde{\sigma} = (\hat{K}^* \hat{K})^{-1} \hat{K}^* u$. Since the matrix $(\hat{K}^* \hat{K})^{-1}$ is
 223 non-singular (as stated in Lemma 1) and converges to a constant matrix, $\tilde{\sigma}$ is
 224 uniquely determined by $\hat{K}^* u$, which means that every σ_j converges towards
 225 fixed values according to (33). $\square$

226 **Remark.** *It can be shown that (28) has distinct roots for all SBP schemes*
 227 *with up to, at least, eight order accuracy in the interior. Proposition 5 is*
 228 *therefore valid for all such schemes.*

229 The numerical solution at any grid point k can be divided into positive
 230 and negative (spurious) modes, such that

$$231 \quad v_k = (v_k)_+ + (v_k)_- = \sum_{j+} \sigma_{j+} K_{j+}^k + \sum_{j-} \sigma_{j-} K_{j-}^k. \quad (34)$$

232 In (34), the spurious modes are denoted by $K_{j-} < 0$ and the converging
 233 modes by $K_{j+} > 0$. We are now ready to state the main result of this paper.

234 **Theorem 1.** *If $v = v_+ + v_-$ in (34) is approximated with the $m + 1$ order*
 235 *accurate scheme (8) and $u(x)$ is the analytic solution to (1) in the steady-*
 236 *state limit, then*

$$237 \quad v_+ - u(x) = \mathcal{O}(h^{m+1}), \quad v_- = \mathcal{O}(h^{m+1}).$$

238 *Proof.* Assuming that well-posed boundary conditions and a stable and ac-
 239 curate numerical approximation exist, then

$$240 \quad \|v - u\|_P^2 = \|v_+ - u\|_P^2 + \|v_-\|_P^2 + 2v_-^T P(v_+ - u) = \mathcal{O}(h^{2m+2}), \quad (35)$$

241 since the overall accuracy of the scheme is $\|v - u\|_P = \mathcal{O}(h^{m+1})$.

242 For (35) to be valid, the left hand side needs to be of the same order of
 243 magnitude as the right-hand side. From Proposition 4 and 5 we know that
 244 v_+ approaches a function $\hat{v}_+(x)$, and therefore

$$245 \quad \lim_{h \rightarrow 0} \|v_+(h)\|_P^2 = \int_0^1 \hat{v}_+^2 dx,$$

246 since both $\sigma_{j+}(h)$ and $K_{j+}(h) > 0$ approach finite values and the weight
 247 matrix P is a discrete integration operator of order $m + 1$ [12]. Similarly, the
 248 norm of the spurious part also approaches some finite value,

$$249 \quad \lim_{h \rightarrow 0} \|v_-(h)\|_P^2 = \int_0^1 \hat{v}_-^2 dx.$$

Equation (35) can be written as

$$v_-^T P(v_+ - u) = -\frac{\|v_+ - u\|_P^2 + \|v_-\|_P^2}{2} + \mathcal{O}(h^{2m+2}). \quad (36)$$

The left-hand side of (36) can be written as

$$\begin{aligned} v_-^T P(v_+ - u) &= \sum_{i=0}^N P_{ii}(v_-)_i(v_+ - u)_i = \sum_{i=0}^N \sum_{j_-} P_{ii}(v_+ - u)_i \sigma_{j_-} K_{j_-}^i = \\ &= \sum_{i=0}^N P_{ii} \sigma_{1-} K_{1-}^i (v_+ - u)_i + \sum_{i=0}^N P_{ii} \sigma_{2-} K_{2-}^i (v_+ - u)_i + \dots, \end{aligned} \quad (37)$$

where we have used $(v_-)_i = \sum_{j_-} \sigma_{j_-} K_{j_-}^i$. All K_{j_-} are negative and converge to fixed values. For sufficiently small h , a limit-value of (37) does not exist unless $\sigma_{j_-} \rightarrow 0$ or $(v_+ - u)_i \rightarrow 0$. We can thus conclude that both of the norms $\|v_+ - u\|_P$ and $\|v_-\|_P$ must approach zero during mesh refinement, since (36) and (37) would yield a contradiction otherwise. If none of them converge, (36) can not be satisfied since the limit on the left-hand side does not exist; if only one of the norms converges, the limit on the left-hand side exists and is zero, which is then inconsistent with the right-hand side. Hence, both norms must approach zero with a rate $\mathcal{O}(h^{m+1})$. $\square$

Next, we exemplify the theoretical results in the second order case, where all details are known. First, note that two of the solutions to (10), given by (11), are constant (± 1) and the other two are identical, with a perturbation $\mathcal{O}(h)$. Hence, Proposition 4 is, at least, true for the second order case. To determine the coefficients σ_j , we need the analytic solution $u(x)$. In our case, we can easily invent one; $u(x) = 1 + e^{a/\epsilon x}$ satisfies (1) in the steady-state limit and with the boundary data chosen accordingly. In our test-case, $a = 1$ and $\epsilon = 0.1$. The numerical solution is identical to the analytic one if $\sigma_{1,2} = 1$ and $\sigma_{3,4} = 0$ in the limit $N \rightarrow \infty$. According to Proposition 5, we have

$$\tilde{\sigma} = (\hat{K}^* \hat{K})^{-1} \hat{K}^* u + \mathcal{O}(h^{m+1}) \quad (38)$$

where u is the exact solution injected at the grid points and the vector $\tilde{\sigma} = [\sigma_1, \sigma_2, \sigma_3, \sigma_4]^T$. Equation (38) implies that $(\hat{K}^* \hat{K})^{-1} \hat{K}^* u \rightarrow \tilde{\sigma}_0 = [1, 1, 0, 0]^T$, which are the coefficients for the exact solution. In Table 1, we show how

Table 1: Rate of convergence of the coefficients σ_j during mesh-refinement.

Number of grid points	$\ (\hat{K}^* \hat{K})^{-1} \hat{K}^* u - \tilde{\sigma}_0\ _2$	Rate of convergence
10	$3.8 \cdot 10^{-3}$	-
20	$9.6 \cdot 10^{-4}$	1.98
40	$2.4 \cdot 10^{-4}$	2.00
80	$6.0 \cdot 10^{-5}$	2.00
160	$1.5 \cdot 10^{-5}$	2.00

276 $(\hat{K}^* \hat{K})^{-1} \hat{K}^* u$ converges to $\tilde{\sigma}_0$ during mesh-refinement, thus showing the va-
 277 lidity of Proposition 5. The rate of convergence is two, as Theorem 1 indi-
 278 cates. We can then conclude that

$$279 \quad \|v_-\|_P = |\sigma_3 \sum_i P_{i,i} K_3^i + \sigma_4 \sum_i P_{i,i} K_4^i| = \mathcal{O}(h^2)$$

280 and

$$281 \quad \|v_+ - u\|_P = \sqrt{\sum_i P_{ii} [(\sigma_1 - 1) + (\sigma_2 K_2^i - e^{a/\epsilon x})]^2} = \mathcal{O}(h^2),$$

282 since $K_2^i = e^{a/\epsilon x} + \mathcal{O}(h^2)$. This exemplifies the validity of Proposition 4,
 283 Proposition 5 and Theorem 1 for the second order scheme.

284 5. Numerical results

285 **We exemplify the theoretical results in one and two space dimensions.**

286 5.1. **One dimensional experiments**

287 Numerical experiments have been performed on problem (5) with $a = 1$,
 288 $\epsilon = 0.1$, the boundary data $g_0 = 1$, $g_1 = -1$ and the initial condition
 289 $f(x) = 0$. The exact solution is then $u(x) = 1 - \exp(10(x - 1))$. The
 290 *SBP*(2, 1) scheme (a scheme with second order accuracy in the interior and
 291 first order at the boundaries) is integrated in time using the classical explicit
 292 Runge-Kutta of fourth order accuracy until the system have reached the
 293 steady-state solution. The domain considered is $x \in [0, 1]$.

294 Figure 1-3 show how the oscillations vanish as the grid is refined. The
 295 rate of convergence and error levels are displayed for $\epsilon = 0.1$ in Table 2-4, and
 296 one can see that the rates of convergence approach the design order of the

Figure 1: The solution as a function of x at steady-state for different meshes. An $SBP(2, 1)$ scheme is used and $a = 1, \epsilon = 0.1$.

297 scheme. Moreover, increasing the order of accuracy of the scheme drastically
 298 reduce the errors from the spurious modes.

299 As one can see in Figure 1-3, the oscillations are only problematic if one
 300 uses a coarse mesh and scheme of low order. When increasing the order
 301 of the scheme or the number of grid points, the oscillations vanish rapidly.
 302 Consequently, using wide stencils does not cause any real problems.

303 5.2. *Two dimensional experiments*

304 To exemplify that the one-dimensional analysis hold also in multiple di-

Table 2: Error and convergence rate for different meshes and $a = 1, \epsilon = 0.1$. An $SBP(2, 1)$ scheme is used.

Number of grid points	Error at steady-state	Rate of convergence
10	0.20	-
20	0.08	1.32
40	0.025	1.68
80	0.007	1.84
160	0.002	1.81
320	0.00051	1.99

Figure 2: The solution as a function of x at steady-state for different meshes. An $SBP(4,2)$ scheme is used and $a = 1, \epsilon = 0.1$.

Figure 3: The solution as a function of x at steady-state for different meshes. An $SBP(6,3)$ scheme is used and $a = 1, \epsilon = 0.1$.

Table 3: Error and convergence rate for different meshes and $a = 1, \epsilon = 0.1$. An $SBP(4, 2)$ scheme is used.

Number of grid points	Error at steady-state	Rate of convergence
20	1.3×10^{-2}	-
40	2.3×10^{-3}	2.5
80	3.3×10^{-4}	2.8
160	4.4×10^{-5}	2.9
320	5.7×10^{-6}	2.9

Table 4: Error and convergence rate for different meshes and $a = 1, \epsilon = 0.1$. An $SBP(6, 3)$ scheme is used.

Number of grid points	Error at steady-state	Rate of convergence
20	7.9×10^{-3}	-
40	6.2×10^{-4}	3.7
80	3.5×10^{-5}	4.1
160	1.8×10^{-6}	4.3
320	8.8×10^{-8}	4.4

305 mensions, consider the problem,

$$\begin{aligned}
u_t + u_x + u_y &= \epsilon(u_{xx} + u_{yy}), \quad x, y \in [0, 1], t \geq 0 \\
u(0, y, t) - \epsilon u_x(0, y, t) &= g_{0,x}(y, t), \quad y \in [0, 1], t \geq 0 \\
\epsilon u_x(1, y, t) &= g_{1,x}(y, t), \quad y \in [0, 1], t \geq 0 \\
u(x, 0, t) - \epsilon u_y(x, 0, t) &= g_{0,y}(x, t), \quad x \in [0, 1], t \geq 0 \\
\epsilon u_y(x, 1, t) &= g_{1,y}(x, t), \quad x \in [0, 1], t \geq 0 \\
u(x, y, 0) &= f(x, y).
\end{aligned} \tag{39}$$

306 We choose the initial data $f(x, y) = 0$, $\epsilon = 0.1$, the steady state solution
307 to be $u_{SS} = 1 - \exp((x + y - 2)/\epsilon)$ and the boundary data accordingly. An
308 $SBP(4, 2)$ operator is used for the spatial discretization and a fourth order
309 Runge-Kutta method is used to integrate in time until the system have
310 reached steady state.

311 In Figure 4-6, the solution at steady state is displayed when using
312 $N = 10, 20, 40$ grid points in each space direction. The spurious modes can
313 best be seen close to the line $x = 1$, and we observe that they vanish during

Figure 4: The solution to (39) at steady state when using $N = 10$ points in each space direction.

314 mesh refinement, in the same way as for the one-dimensional case. It can also
 315 be shown that the convergence is similar.

316 6. Conclusions

317 We have shown that the spurious modes, for the advection-diffusion equa-
 318 tion, are of the same order of magnitude as the truncation error when using
 319 wide operators for approximating the second derivative. The theoretical re-
 320 sults are consistent with the numerical experiments.

321 The results derived in this work are independent of the boundary pro-
 322 cedure or the numerical scheme. Consequently, the spurious modes vanish
 323 with a rate equal to the order of the scheme for any numerical method as
 324 long as it is stable.

325 As the spurious modes only contribute with errors of the same magnitude
 326 as the order of the scheme, the oscillations can always be removed by choosing
 327 a scheme of high order or using a fine mesh. Since the oscillations converge
 328 with the same rate as the scheme, no real problems exist for wide operators.

Figure 5: The solution to (39) at steady state when using $N = 20$ points in each space direction.

Figure 6: The solution to (39) at steady state when using $N = 40$ points in each space direction.

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333 Appendix A

334 We will in this appendix prove that the $N - by - 4m$ matrix $\hat{K}$ in (31) has
 335 rank $4m$ and, consequently, $\hat{K}^* \hat{K}$ is non-singular. First, we note that there
 336 are $2m$ solutions to (28) and $2m$ similar solutions to (29) with a perturbation
 337 $\mathcal{O}(h)$. It can be shown that the $2m$ solutions to (28) are distinct for all
 338 SBP operators with up to eighth order internal accuracy; consequently, all
 339 solutions to (28) and (29) are distinct with a perturbation of at least $\mathcal{O}(h)$.
 340 We have

$$341 \quad \hat{K} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ K_1 & K_2 & \cdots & K_{4m} \\ K_1^2 & K_2^2 & \cdots & K_{4m}^2 \\ \vdots & \vdots & \vdots & \vdots \\ K_1^N & K_2^N & \cdots & K_{4m}^N \end{bmatrix}.$$

342 The matrix $\hat{K}$ has rank $4m$ if one can find $4m$ linearly independent row-
 343 vectors.

344 We choose $4m$ rows from $\hat{K}$ and put them as column vectors in a ma-
 345 trix that we call $\tilde{K}$. As first column, we choose the row vector $\tilde{K}_1 =$
 346 $[K_1^{N/4m}, K_2^{N/4m}, \dots, K_{4m}^{N/4m}]$, the second as $\tilde{K}_2 = [K_1^{2N/4m}, K_2^{2N/4m}, \dots, K_{4m}^{2N/4m}]$
 347 and so forth. Then, we have

$$348 \quad \tilde{K} = \begin{bmatrix} \tilde{K}_1 & \tilde{K}_1^2 & \cdots & \tilde{K}_1^{4m} \\ \tilde{K}_2 & \tilde{K}_2^2 & \cdots & \tilde{K}_2^{4m} \\ \vdots & \vdots & \vdots & \vdots \\ \tilde{K}_{4m} & \tilde{K}_{4m}^2 & \cdots & \tilde{K}_{4m}^{4m} \end{bmatrix}, \quad (\text{A-1})$$

349 where $\tilde{K}_j = K_j^{N/4m}$. If these $4m$ rows are linearly independent, i.e $\tilde{K}$ is
 350 non-singular, then the matrix $\hat{K}$ has rank $4m$.

351 **Remark.** In (A-1), we have chosen $\tilde{K}_i = K_i^{N/4m}$ for simplicity. However,
 352 one can also choose $\tilde{K}_i = K_i^{N/k}$ for any integer $N \gg k > 1$, and the
 353 following arguments would still be valid.

354 We note that (A-1) is a $4m - by - 4m$ Vandermonde matrix and its
 355 determinant is

$$356 \quad \det(\tilde{K}) = \prod_i \tilde{K}_i \prod_{1 \leq i < j \leq 4m} (\tilde{K}_j - \tilde{K}_i)$$

357 where $\tilde{K}_i = K_i^{N/4m}$. Note that if all $\tilde{K}_i$ in (A-1) are distinct and does not
 358 approach each other as $N \rightarrow \infty$, then $\tilde{K}$ is non-singular. By Proposition 4,
 359 there exist $2m$ constant K and $2m$ identical K 's with a perturbation $\mathcal{O}(h)$.
 360 We denote these modes as K_c and K_p according to

$$361 \quad \begin{aligned} K_c &= K_0 \\ K_p &= K_0 + \Delta K h + \mathcal{O}(h^2) \end{aligned}$$

362 where $\Delta K \neq 0$. For large N , we have

$$363 \quad \tilde{K}_p = K_p^{N/4m} \approx (K_0 + \Delta K h)^{N/4m} \approx K_0^{N/4m} e^{4m \Delta K / K_0} \neq \tilde{K}_c$$

364 and all $\tilde{K}$ are thus distinct in (A-1). Consequently, $\tilde{K}$ is non-singular. For
 365 the second order accurate scheme, $K_c = \pm 1$, and all K_j are therefore distinct
 366 for all h . One can therefore conclude that Lemma 1 is true for the second
 367 order scheme.

368 For higher order schemes, however, there exist modes that vanish inside
 369 the domain, that is $|K_j|^i \rightarrow 0$ for some index j and grid points i . In this
 370 case, $\tilde{K}$ will be singular (some rows will contain only zeros), and we need to
 371 choose other rows from $\hat{K}$ to form a linearly independent set of dimension
 372 $4m$. First, we note that the vanishing modes always occur in pairs: one which
 373 is constant, and another one with a perturbation $\mathcal{O}(h)$. For the moment, let
 374 us assume that there exist two vanishing modes, which is the case for the
 375 SBP 42 scheme, and denote them as $K_{1,2}$. The structure of the matrix $\hat{K}$ is
 376 then

$$377 \quad \hat{K} = \begin{bmatrix} V & W \\ \delta V & A \end{bmatrix},$$

378 where the matrix

$$379 \quad A = \begin{bmatrix} K_3^{N/4m-2} & K_4^{N/4m-2} & \cdots & K_{4m}^{N/4m-2} \\ K_3^{N/4m-1} & K_4^{N/4m-1} & \cdots & K_{4m}^{N/4m-1} \\ \vdots & \vdots & \vdots & \vdots \\ K_3^N & K_4^N & \cdots & K_{4m}^N \end{bmatrix},$$

380

381

382

383

384 and

385

$$V = \begin{bmatrix} 1 & 1 \\ K_1 & K_2 \\ \vdots & \vdots \\ K_1^{N/4m-3} & K_2^{N/4m-3} \end{bmatrix},$$

$$W = \begin{bmatrix} 1 & \cdots & 1 \\ K_3 & \cdots & K_{4m} \\ \vdots & \vdots & \vdots \\ K_3^{N/4m-3} & \cdots & K_{4m}^{N/4m-3} \end{bmatrix},$$

$$\delta V = \begin{bmatrix} K_1^{N/4m-2} & K_2^{N/4m-2} \\ \vdots & \vdots \\ K_1^N & K_2^N \end{bmatrix} \approx 0,$$

386 since $|K_{1,2}| < 0$ and N is large. The matrix A has full rank since none of the
 387 modes $K_{3\dots 4m}$ vanish, as concluded earlier in this section. Consequently, $\hat{K}$
 388 will have full rank if the column vectors of V are linearly independent, since
 389 we, in that case, have found $4m$ linearly independent column vectors. We
 390 know that $K_2 = K_1 + \Delta K h + \mathcal{O}(h^2)$ where $\Delta K \neq 0$, so

$$V \approx \begin{bmatrix} 1 & 1 \\ K_1 & K_1 + \Delta K h \\ K_1^2 & K_1^2(1 + \frac{\Delta K}{K_1}h)^2 \\ \vdots & \vdots \\ K_1^{N/4m-3} & K_1^{N/4m-3}(1 + \frac{\Delta K}{K_1}h)^{N/4m-3} \end{bmatrix}$$

392 by neglecting higher order terms. Since

$$\lim_{k \rightarrow \infty} \left(1 + \frac{\Delta K}{K_1}h\right)^k = e^{\frac{\Delta K}{K_1}kh} \neq 1,$$

394 the column vectors are linearly independent and $\hat{K}$ has therefore full rank.
 395 Sylvester's rank inequality states that

$$\text{rank}(AB) \geq \text{rank}(A) + \text{rank}(B) - k,$$

396

397 if A is a $l - by - k$ matrix and B is $k - by - n$ for any integers l and n . Using
398 $k = 4m$, $A = \hat{K}^*$ and $B = \hat{K}$, one arrives at

$$399 \quad \text{rank}(\hat{K}^* \hat{K}) \geq \text{rank}(\hat{K}^*) + \text{rank}(\hat{K}) - 4m = 4m + 4m - 4m = 4m$$

400 and the matrix $\hat{K}^* \hat{K}$ must have rank $4m$ and is therefore non-singular. This
401 concludes the proof of Lemma 1.

402 **Remark.** *If more than two vanishing modes exist, the procedure above is*
403 *repeated by adding additional columns in the matrix V . The proof would*
404 *therefore be similar.*

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