

Bergische Universität Wuppertal

Fachbereich Mathematik und Naturwissenschaften

Institute of Mathematical Modelling, Analysis and Computational
Mathematics (IMACM)

Preprint BUW-IMACM 15/14

Christian Hendricks, Matthias Ehrhardt and Michael Günther

**High-Order-Compact ADI schemes for
diffusion equations with mixed derivatives
in the combination technique**

February 2015

<http://www.math.uni-wuppertal.de>

High-Order-Compact ADI schemes for diffusion equations with mixed derivatives in the combination technique

Christian Hendricks, Matthias Ehrhardt and Michael Günther

Abstract

In this article we combine the ideas of high order compact (HOC) and alternating direction implicit (ADI) schemes on sparse grids for diffusion equations with mixed derivatives. With the help of HOC and ADI schemes solutions, which are fourth order accurate in space and second order accurate in time can be computed. The computational effort in each leg of the ADI scheme just consists of solving tridiagonal linear systems. In order to reduce the number of grid points, we use the combination technique to construct a solution defined on the sparse grid. This approach allows to further reduce the computational effort and memory consumption.

Keywords: high order compact scheme, sparse grids, combination technique, alternating direction implicit method

1. Introduction

High dimensional problems arise in many fields of research and practice. In computational finance for example the pricing of financial derivatives requires to solve partial differential equations (PDEs) with several spatial dimensions. During the last decades both academics and industry have spent a great effort to derive techniques to solve these problems efficiently. One very important class of solvers is built up by operator splitting schemes, such as Alternating-Direction-Implicit (ADI) and Locally-One-Dimensional (LOD) schemes. These approaches rely on separating the underlying discretisation matrix to tridiagonal matrices, which can be solved in linear run-time. Thus the computational effort is significantly reduced. However if tensor based grids are employed, the exponential growing complexity in connection with memory constraints makes it very difficult to solve high dimensional problems. Therefore it is quite natural to ask for schemes, which are able to deliver highly accurate solutions with a very low number of grid points.

In this article we introduce schemes, which combine the ideas of ADI, HOC and sparse grid techniques to solve diffusion PDEs with mixed derivatives of the form

$$\frac{\partial u}{\partial t} = L u, \quad t > 0 \quad (1.1)$$

where L denotes an elliptic operator of the form

$$L u = \sum_{i=1}^d \sum_{j=1}^d q_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j}, \quad x = (x_1, \dots, x_d)^\top \in \Omega \subset \mathbb{R}^d.$$

The parabolicity of the problem implies that the matrix $Q = (q_{ij})$ is positive semi-definite.

ADI schemes decompose the discretisation matrix into simpler tridiagonal ones. Usually second order stencils are used to discretise the underlying PDE. HOC schemes have been employed to derive schemes with order four in space with compact stencils, such that solving the discrete system in general is not more expensive in terms of computation time than for second order schemes. In recent years HOC and ADI schemes have been combined to construct efficient solvers, e.g. by Düring et al. [1] and by Karaa and Zhang [2]. Nevertheless these schemes use a full tensor based grid, thus resulting in an exponential growing number of grid points. With the combination technique, the so called sparse grid solution, can be computed by linearly combining a sequence of sub-solutions.

Compared to a full grid with $\mathcal{O}(h^{-d})$ nodes, the sparse grid only consists of $\mathcal{O}(h^{-1} \log(h^{-1})^{d-1})$ grid points, but is able to maintain an approximation accuracy of $\mathcal{O}(h^4 \log(h^{-1})^{d-1})$ in case of order four schemes under suitable regularity assumptions. Hence the combination technique suffers from the curse of dimensionality to a much lower extent.

The outline of this article is as follows: In Section 2 we discuss four well known ADI schemes. Based on these schemes we derive HOC-ADI schemes and analyse their consistency and stability properties in Section 3 and 4. In Section 5 we give a brief discussion of HOC-ADI schemes within the combination technique. The theoretical results are illustrated by numerical examples in Section 6.

2. ADI schemes

We consider the semi-discretisation of our PDE (1.1)

$$\frac{\partial u}{\partial t} = F(u(t)), \quad t > 0,$$

with given initial and boundary data. The function F contains the spatial discretisation of the elliptic operator L . In many applications F is treated implicitly for stiffness and stability reasons. Especially in the high dimensional case the resulting problem can become unfeasible on now-a-days standard machines. Therefore it seems to be reasonable to decompose F into a simpler form, which can be solved sequentially

$$F(u) = F_0(u) + F_1(u) + \dots + F_d(u).$$

Here in case of equation (1.1) the term F_i , $i \geq 1$, takes the second-order derivative in the i -th coordinate direction, while F_0 stems from all mixed derivative terms. As F_0 will always be treated explicitly and the F_i s implicitly, only tridiagonal systems have to be solved if second-order finite difference schemes (FD) are employed. In the sequel we consider four well known ADI schemes.

Douglas scheme (DO) [3]:

$$\begin{cases} Y_0 & = u_n + \Delta_t F(u_n), \\ Y_i & = Y_{i-1} + \theta \Delta_t (F_i(Y_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ u_{n+1} & = Y_d. \end{cases} \quad (2.1)$$

Δ_t denotes the time step and u_n is the approximation at time level n , $u_n \sim u(n\Delta_t)$. In scheme (2.1) an explicit Euler step is followed by a stabilising correction step in each of the spatial directions. In the case $\theta = \frac{1}{2}$ the method is known as the Douglas [3] and Brian [4] scheme. The value $\theta = 1$ has been considered by Douglas in [5]. Without mixed derivative terms in (1.1) and $\theta = \frac{1}{2}$ the scheme is of order 2 in time and of order 1 otherwise. The scheme was initially developed to solve the heat equation in two or three dimensions, but as we are interested in equations with cross terms, the scheme (2.1) seems not well suited. Hence we turn our attention to more sophisticated schemes.

Craig-Sneyd scheme (CS) [6]:

$$\begin{cases} Y_0 & = u_n + \Delta_t F(u_n), \\ Y_i & = Y_{i-1} + \theta \Delta_t (F_i(Y_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ \tilde{Y}_0 & = Y_0 + \frac{1}{2} \Delta_t (F_0(Y_d) - F_0(u_n)) \\ \tilde{Y}_i & = \tilde{Y}_{i-1} + \theta \Delta_t (F_i(\tilde{Y}_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ u_{n+1} & = \tilde{Y}_d. \end{cases} \quad (2.2)$$

Modified Craig-Sneyd scheme (MCS) [7] :

$$\begin{cases} Y_0 &= u_n + \Delta_t F(u_n), \\ Y_i &= Y_{i-1} + \theta \Delta_t (F_i(Y_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ \hat{Y}_0 &= Y_0 + \theta \Delta_t (F_0(Y_d) - F_0(u_n)) \\ \tilde{Y}_0 &= \hat{Y}_0 + (\frac{1}{2} - \theta) \Delta_t (F(Y_d) - F(u_n)) \\ \tilde{Y}_i &= \tilde{Y}_{i-1} + \theta \Delta_t (F_i(\tilde{Y}_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ u_{n+1} &= \tilde{Y}_d. \end{cases} \quad (2.3)$$

The Craig-Sneyd scheme [6] was originally introduced as an extension of the Douglas scheme, where a second explicit step is followed by d implicit stabilising steps. It exhibits order 2 if $\theta = \frac{1}{2}$. The modified Craig-Sneyd scheme (2.3) can be seen as an extension of the iterated scheme in the article by Craig and Sneyd [6] and was defined by in't Hout and Welfert in [7]. This scheme has order 2 for arbitrary $\theta > 0$.

Hundsdorfer-Verwer scheme (HV) [8]:

$$\begin{cases} Y_0 &= u_n + \Delta_t F(u_n), \\ Y_i &= Y_{i-1} + \theta \Delta_t (F_i(Y_i) - F_i(u_n)) \text{ for } i = 1, \dots, d \\ \tilde{Y}_0 &= Y_0 + \frac{1}{2} \Delta_t (F(Y_d) - F(u_n)) \\ \tilde{Y}_i &= \tilde{Y}_{i-1} + \theta \Delta_t (F_i(\tilde{Y}_i) - F_i(Y_d)) \text{ for } i = 1, \dots, d \\ u_{n+1} &= \tilde{Y}_d. \end{cases} \quad (2.4)$$

The Hundsdorfer-Verwer scheme was derived in [8] and possesses like the modified Craig-Sneyd scheme order two for any $\theta > 0$.

In recent years huge effort has been spent on stability analysis of these ADI schemes, cf. [9, 7, 10, 11, 8]. There the ADI scheme is applied to the linear test equation

$$u'(t) = (\lambda_0 + \lambda_1 + \dots + \lambda_d) u(t),$$

with complex values λ_i for $i = 0, \dots, d$. This implies the assumption that all involved discretisation matrices are normal and commuting. Although this is often not the case in practice, it is common to neglect boundary conditions, freeze coefficients and apply von Neumann stability analysis. Let the stability matrix R of the scheme be given, such that

$$u_{n+1} = R u_n.$$

Then R reduces to the factor $r(z_0, z_1, \dots, z_d)$ if applied to the scalar test equation with $z_i = \Delta_t \lambda_i$ for all i . The numerical scheme is stable if

$$|r| \leq 1$$

holds. Defining $z = z_0 + z_1 + \dots + z_d$ and $p = (1 - \theta z_1) \cdot \dots \cdot (1 - \theta z_d)$, the stability functions of the ADI schemes (2.1), (2.2), (2.3), (2.4) are

$$\begin{aligned} r_{DO}(z_0, z_1, \dots, z_d) &= 1 + \frac{z}{p}, \\ r_{CS}(z_0, z_1, \dots, z_d) &= 1 + \frac{z}{p} + \frac{1}{2} \frac{z_0 z}{p^2}, \\ r_{MCS}(z_0, z_1, \dots, z_d) &= 1 + \frac{z}{p} + \theta \frac{z_0 z}{p^2} + (\frac{1}{2} - \theta) \frac{z^2}{p^2}, \\ r_{HV}(z_0, z_1, \dots, z_d) &= 1 + 2 \frac{z}{p} - \frac{z}{p^2} + \frac{1}{2} \frac{z^2}{p^2}. \end{aligned}$$

The single z_i can be derived by inserting Fourier modes into the discretisation of the derivatives. For more details we refer to in't Hout and Mishra [9]. In the literature the following lower bounds on θ ensuring unconditional stability have been derived: Douglas scheme $\theta \geq \frac{1}{2}$ if $d = 2$, $\theta \geq \frac{2}{3}$ if $d = 3$; Craig-Sneyd scheme $\theta \geq \frac{1}{2}$ if $d = 2, 3$; Modified Craig-Sneyd scheme $\theta \geq \frac{1}{3}$ if $d = 2$, $\theta \geq \frac{6}{13}$ if $d = 3$; Hundsdorfer-Verwer scheme $\theta \geq \frac{1}{2+\sqrt{2}}$ if $d = 2$, $\theta \geq \frac{3}{4+2\sqrt{3}}$ if $d = 3$. In't Hout [7] proved a condition on θ ensuring unconditional stability for scheme (2.4) with arbitrary dimensions. In case of the other three ADI schemes only necessary conditions have been derived and up to now it is unclear if these are sufficient if $d > 3$.

3. High Order Compact ADI schemes

In this Section we combine the ideas of ADI schemes with High-Order-Compact schemes. While high order finite difference schemes in general use broad stencils, HOC schemes exploit the structure of the underlying PDE to construct discretisation with order four, but maintain a compact stencils. Thus the resulting linear system can be solved efficiently and the introduction of ghost points at the domain's boundary is avoided.

HOC schemes have been used by Spatz in [12], while operator splitting schemes were employed by Karaa and Zhang [2], who introduced a D'Yakonov HOC scheme in 2-d for unsteady convection-diffusion equations. Düring et al. [1] were the first one, who applied a HOC-ADI schemes to PDEs with mixed derivative terms. However, as far as we know, there exists no detailed stability analysis for HOC-ADI schemes with mixed derivative terms in the literature.

3.1. Finite Difference Operators

The derivatives in (1.1) are discretised via finite differences, which can easily be derived by straightforward Taylor expansion. Let k, l denote the index of the grid node, then the standard difference operator approximating the second derivative in x_i direction is given by

$$\delta_{x_i}^2 u_{k,l} = \frac{u_{k+1,l} - 2u_{k,l} + u_{k-1,l}}{h_i^2},$$

This operator is of order two, i.e. $\frac{\partial^2 u(x_{k,l})}{\partial x_i^2} = \delta_{x_i}^2 u_{k,l} + \mathcal{O}(h_i^2)$. We will use it to construct fourth order discretisations with compact stencils, such that only the neighbouring grid nodes are involved. The mixed derivatives in the ADI schemes are always treated in an explicit fashion, thus we use broad stencils with order four

$$\delta_{x_i}^0 u_{k,l} = \frac{-u_{k+2,l} + 8u_{k+1,l} - 8u_{k-1,l} + u_{k-2,l}}{12h_i},$$

to obtain a fourth order approximation of the mixed derivative $\frac{\partial^2 u}{\partial x_i \partial x_j}$ for $i \neq j$

$$\delta_{x_i}^0 \delta_{x_j}^0 u_{k,l} = \frac{1}{144h_i h_j} \left[\begin{aligned} &64(u_{k+1,l+1} - u_{k-1,l+1} + u_{k-1,l-1} - u_{k+1,l-1}) \\ &+ 8(-u_{k+2,l+1} - u_{k+1,l+2} + u_{k-1,l+1} + u_{k-2,l+1} \\ &\quad - u_{k-2,l-1} - u_{k-1,l-2} + u_{k+1,l-2} + u_{k+2,l-1}) \\ &+ u_{k+2,l+2} - u_{k-2,l+2} + u_{k-2,l-2} - u_{k+2,l-2} \end{aligned} \right].$$

3.2. HOC scheme

In order to derive a high-order formulation of discrete L , we consider one-dimensional equations as a starting point

$$F_i(u) = q_{ii} \frac{\partial^2 u}{\partial x_i^2} = g, \quad i = 1, \dots, d, \quad (3.1)$$

where g is some arbitrary right hand side. Applying our discrete operators of the previous paragraph, we obtain

$$q_{ii} \frac{\partial^2 u}{\partial x_i^2} = q_{ii} \delta_{x_i}^2 u_k - q_{ii} \frac{h_i^2}{12} \frac{\partial^4 u}{\partial x_i^4} + \mathcal{O}(h_i^4) = g_k. \quad (3.2)$$

This is an order 2 approximation of equation (3.1) with a fourth derivative truncation error. In order to get a fourth order scheme, as the fourth derivative is multiplied by h_i^2 , a second order discretisation of $\frac{\partial^4 u}{\partial x_i^4}$ is needed. Differentiating equation (3.1) twice, yields

$$q_{ii} \frac{\partial^4 u}{\partial x_i^4} = \frac{\partial^2 g}{\partial x_i^2}. \quad (3.3)$$

Hence the fourth derivative can be expressed via the second derivative of the right hand side g . Replacing the truncation error in (3.2) by (3.3) and applying the second order difference operator, one obtains a one-dimensional fourth order scheme for equation (3.1)

$$q_{ii}\delta_{x_i}^2 u_k = g + \frac{h_i^2}{12}\delta_{x_i}^2 g_k + \mathcal{O}(h_i^4).$$

Thinking in terms of matrices or symbolic operators, we can write the scheme as

$$A_{x_i} u = B_{x_i} g,$$

where

$$A_{x_i} = q_{ii}\delta_{x_i}^2, \quad B_{x_i} = 1 + \frac{h_i^2}{12}\delta_{x_i}^2.$$

and vectors u, g . The mixed derivatives are approximated via standard fourth order stencils in an explicit fashion, such that we have $F_0(u_n) = \sum_{i \neq j} q_{ij}\delta_{x_i}^0 \delta_{x_j}^0 u_n$, or in matrix/symbolic notation $F_0 u_n = \sum_{i \neq j} A_{x_i, x_j} u_n$. The semi discrete scheme now reads

$$\frac{\partial u}{\partial t} = F_0(u) + B_{x_1}^{-1} A_{x_1} u + \dots + B_{x_d}^{-1} A_{x_d} u + \mathcal{O}(h_1^4) + \dots + \mathcal{O}(h_d^4) + \sum_{i,j} \mathcal{O}(h_i^4 h_j^4). \quad (3.4)$$

Please note that the scheme exhibits order 4 in all single coordinate directions. It is also possible to construct HOC schemes by taking into account the full PDE, which leads to a different truncation error. We illustrate this approach by a simple example. For simplicity let equation (1.1) be given without cross derivatives and $d = 2$, then we have a problem of the form

$$q_{11} \frac{\partial^2 u}{\partial x_1^2} + q_{22} \frac{\partial^2 u}{\partial x_2^2} = f.$$

Discretisation leads to

$$q_{11}\delta_{x_1}^2 u_{kl} - \frac{h_1^2}{12} \frac{\partial^4 u}{\partial x_1^4} + q_{22} \frac{\partial^2 u}{\partial x_2^2} - \frac{h_2^2}{12} \frac{\partial^4 u}{\partial x_2^4} = f_{kl}.$$

Again we approximate the truncation error with second order stencils and obtain after some straightforward calculations

$$\begin{aligned} & q_{11}\delta_{x_1}^2 u_{kl} + q_{22}\delta_{x_2}^2 u_{kl} + \frac{h_1^2}{12} (q_{22}\delta_{x_1}^2 \delta_{x_2}^2 u_{kl} + \mathcal{O}(h_1^2) + \mathcal{O}(h_2^2) + \mathcal{O}(h_1^2 h_2^2)) \\ & + \frac{h_2^2}{12} (q_{11}\delta_{x_1}^2 \delta_{x_2}^2 u_{kl} + \mathcal{O}(h_1^2) + \mathcal{O}(h_2^2) + \mathcal{O}(h_1^2 h_2^2)) \\ & = \left(1 + \frac{h_1^2}{12} \delta_{x_1}^2 + \frac{h_2^2}{12} \delta_{x_2}^2 \right) f_{kl}. \end{aligned}$$

The semi-discrete scheme is

$$\left(1 + \frac{h_1^2}{12} \delta_{x_1}^2 + \frac{h_2^2}{12} \delta_{x_2}^2 \right) \frac{\partial u}{\partial t} = q_{11}\delta_{x_1}^2 u_{kl} + q_{22}\delta_{x_2}^2 u_{kl} + \frac{h_1^2}{12} q_{22}\delta_{x_1}^2 \delta_{x_2}^2 u_{kl} + \frac{h_2^2}{12} q_{11}\delta_{x_1}^2 \delta_{x_2}^2 u_{kl} + \mathcal{O}(h_1^2 h_2^2) \quad (3.5)$$

This scheme has a leading error term of order $\mathcal{O}(h_1^2 h_2^2)$. Thus we can only expect order 4 if $h_1 = ch_2$ holds for some constant c . Therefore this scheme will not exhibit an asymptotic order of $\mathcal{O}(h^4 \log(h^{-1})^{d-1})$ in the combination technique, c.f. Section 5.

3.3. HOC-ADI schemes

We now apply the time discretisation given in Section 2 to the semi-discrete HOC formulation (3.4).

HOC Douglas scheme (HDO):

$$\begin{cases} Y_0 & = u_n + \Delta_t (F_0(u_n) + B_{x_1}^{-1} A_{x_1} u_n + \dots + B_{x_d}^{-1} A_{x_d} u_n), \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Y_i & = B_{x_i} Y_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ u_{n+1} & = Y_d. \end{cases} \quad (3.6)$$

HOC Craig-Sneyd scheme (HCS):

$$\begin{cases} Y_0 & = u_n + \Delta_t (F_0(u_n) + B_{x_1}^{-1} A_{x_1} u_n + \dots + B_{x_d}^{-1} A_{x_d} u_n), \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Y_i & = B_{x_i} Y_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ \tilde{Y}_0 & = Y_0 + \frac{1}{2} \Delta_t (F_0(Y_d) - F_0(u_n)) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Y}_i & = B_{x_i} \tilde{Y}_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ u_{n+1} & = \tilde{Y}_d. \end{cases} \quad (3.7)$$

HOC modified Craig-Sneyd scheme (HMCS):

$$\begin{cases} Y_0 & = u_n + \Delta_t (F_0(u_n) + B_{x_1}^{-1} A_{x_1} u_n + \dots + B_{x_d}^{-1} A_{x_d} u_n), \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Y_i & = B_{x_i} Y_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ \hat{Y}_0 & = Y_0 + \theta \Delta_t (F_0(Y_d) - F_0(u_n)) \\ \tilde{Y}_0 & = \hat{Y}_0 + (\frac{1}{2} - \theta) \Delta_t (F(Y_d) - F(u_n)) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Y}_i & = B_{x_i} \tilde{Y}_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ u_{n+1} & = \tilde{Y}_d. \end{cases} \quad (3.8)$$

HOC Hundsdorfer-Verwer scheme (HHV):

$$\begin{cases} Y_0 & = u_n + \Delta_t (F_0(u_n) + B_{x_1}^{-1} A_{x_1} u_n + \dots + B_{x_d}^{-1} A_{x_d} u_n), \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Y_i & = B_{x_i} Y_{i-1} - \theta \Delta_t A_{x_i} u_n \text{ for } i = 1, \dots, d \\ \tilde{Y}_0 & = Y_0 + \frac{1}{2} \Delta_t (F(Y_d) - F(u_n)) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Y}_i & = B_{x_i} \tilde{Y}_{i-1} - \theta \Delta_t A_{x_i} Y_d \text{ for } i = 1, \dots, d \\ u_{n+1} & = \tilde{Y}_d. \end{cases} \quad (3.9)$$

In order to avoid the inverse of the operators B_{x_i} for $i = 1, \dots, d$ one can rewrite the schemes. Please note that we assume B_{x_i}, A_{x_i} to be commuting for all i , which is reasonable since they are only one-directional with constant coefficients.

HOC Douglas scheme (HDO):

$$\begin{cases} Z_0 & = \prod_{j=1}^d B_{x_j} u_n + \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(u_n) + \sum_{i=1}^d \prod_{\substack{j=1 \\ j \neq i}}^d B_{x_j} A_{x_i} u_n \right) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Z_i & = Z_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} u_n \text{ for } i = 1, \dots, d \\ u_{n+1} & = Z_d, \end{cases} \quad (3.10)$$

HOC Craig-Sneyd scheme (HCS):

$$\begin{cases} Z_0 & = \prod_{j=1}^d B_{x_j} u_n + \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(u_n) + \sum_{i=1}^d \prod_{\substack{j=1 \\ j \neq i}}^d B_{x_j} A_{x_i} u_n \right) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Z_i & = Z_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} u_n \text{ for } i = 1, \dots, d \\ \tilde{Z}_0 & = Z_0 + \frac{1}{2} \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(Z_d) - \prod_{j=1}^d B_{x_j} F_0(u_n) \right) \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Z}_i & = \tilde{Z}_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} u_n \text{ for } i = 1, \dots, d \\ u_{n+1} & = \tilde{Z}_d. \end{cases} \quad (3.11)$$

HOC modified Craig-Sneyd scheme (HMCS):

$$\left\{ \begin{array}{l} Z_0 \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Z_i \\ \hat{Z}_0 \\ \tilde{Z}_0 \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Z}_i \\ u_{n+1} \end{array} \right. = \begin{array}{l} \prod_{j=1}^d B_{x_j} u_n + \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(u_n) + \sum_{i=1}^d \prod_{\substack{j=1 \\ j \neq i}}^d B_{x_j} A_{x_i} u_n \right) \\ Z_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} u_n \text{ for } i = 1, \dots, d \\ Z_0 + \theta \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(Z_d) - \prod_{j=1}^d B_{x_j} F_0(u_n) \right) \\ \hat{Z}_0 + \left(\frac{1}{2} - \theta\right) \Delta_t \left(\prod_{j=1}^d B_{x_j} F(Z_d) - \prod_{j=1}^d B_{x_j} F(u_n) \right) \\ \tilde{Z}_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} u_n \text{ for } i = 1, \dots, d \\ \tilde{Z}_d. \end{array} \quad (3.12)$$

HOC Hundsdorfer-Verwer scheme (HHV):

$$\left\{ \begin{array}{l} Z_0 \\ (B_{x_i} - \theta \Delta_t A_{x_i}) Z_i \\ \tilde{Z}_0 \\ (B_{x_i} - \theta \Delta_t A_{x_i}) \tilde{Z}_i \\ u_{n+1} \end{array} \right. = \begin{array}{l} \prod_{j=1}^d B_{x_j} u_n + \Delta_t \left(\prod_{j=1}^d B_{x_j} F_0(u_n) + \sum_{i=1}^d \prod_{\substack{j=1 \\ j \neq i}}^d B_{x_j} A_{x_i} u_n \right) \\ Z_{i-1} - \theta \Delta_t \prod_{j=i+1}^d A_{x_i} u_n \text{ for } i = 1, \dots, d \\ Z_0 + \frac{1}{2} \Delta_t \left(\prod_{j=1}^d B_{x_j} F(Z_d) - \prod_{j=1}^d B_{x_j} F(u_n) \right) \\ \tilde{Z}_{i-1} - \theta \Delta_t \prod_{j=i+1}^d B_{x_j} A_{x_i} Z_d \text{ for } i = 1, \dots, d \\ \tilde{Z}_d. \end{array} \quad (3.13)$$

The new variables are defined as $Z_i := \prod_{j=i+1}^d B_{x_j} Y_i$ and \hat{Z}_i, \tilde{Z}_i in an analogue way. Each implicit step during the stabilising procedure just requires one LU -decomposition. If the matrices are not time-dependent the d decomposition can be performed only once during the start-up phase, which significantly reduces the run-time.

4. Stability of HOC-ADI schemes

In a first step we rewrite our schemes to one step schemes of the form

$$u_{n+1} = R u_n.$$

Stability requires that $\|R\| \leq 1$ holds. For a shorthand writing we introduce the following notation $Z_0 = \Delta_t \sum_{i \neq j} A_{x_i, x_j}$, $Z = Z_0 + \Delta_t B_{x_1}^{-1} A_{x_1} + \dots + \Delta_t B_{x_d}^{-1} A_{x_d}$, $Q_i = B_{x_i} - \theta \Delta_t A_{x_i}$ for $i = 1, \dots, d$ and $P = \prod_{i=1}^d Q_{x_i}^{-1} B_{x_i}$.

HDO scheme:

The first Euler step is

$$Y_0 - u_n = Z u_n$$

and the stabilising steps are of the form

$$Y_i - u_n = Q_{x_i}^{-1} B_{x_i} (Y_{i-1} - u_n) \quad \text{for } i = 1, \dots, d.$$

This leads to a stability matrix of the form

$$R_{HDO} = I + P Z.$$

HCS scheme:

The stability matrix for the HOC Craig-Sneyd scheme can be derived in a similar fashion with two Euler and stabilising steps. We have for the explicit steps

$$Y_0 - u_n = Z u_n, \quad \tilde{Y}_0 = Y_0 + \frac{1}{2} Z_0 (Y_d - u_n).$$

And for the intermediate values

$$Y_i - u_n = Q_{x_i}^{-1} B_{x_i} (Y_{i-1} - u_n), \quad \tilde{Y}_i - u_n = Q_{x_i}^{-1} B_{x_i} (\tilde{Y}_{i-1} - u_n).$$

Recursive insertion we obtain the stability matrix

$$R_{HCS} = I + PZ + \frac{1}{2}PZ_0Z.$$

HMCS scheme:

In the modified Craig-Sneyd scheme one additional Euler step is performed, thus we have

$$Y_0 - u_n = Zu_n, \quad \hat{Y}_0 = Y_0 + \theta Z_0(Y_d - u_n), \quad \tilde{Y}_0 = (\frac{1}{2} - \theta)Z(Y_d - u_n).$$

The intermediate values are given by

$$Y_i - u_n = Q_{x_i}^{-1}B_{x_i}(Y_{i-1} - u_n), \quad \tilde{Y}_i - u_n = Q_{x_i}^{-1}B_{x_i}(\tilde{Y}_0 - u_n).$$

This leads to the following stability matrix

$$R_{HMCS} = I + PZ + \theta P^2 Z_0 Z + (\frac{1}{2} - \theta)P^2 Z^2.$$

HHV scheme:

The two explicit steps are given by

$$Y_0 - u_n = Zu_n, \quad \hat{Y}_0 = Y_0 + \frac{1}{2}Z_0(Y_d - u_n).$$

The intermediate values are given by

$$Y_i - u_n = Q_{x_i}^{-1}B_{x_i}(Y_{i-1} - u_n), \quad \tilde{Y}_i - Y_d = Q_{x_i}^{-1}B_{x_i}(\tilde{Y}_0 - Y_d).$$

Inserting the values for the second stabilising step, we obtain

$$u_{n+1} = \tilde{Y}_d = (I + PZ)Y_d + P(I + \frac{1}{2}Z)(u_n - Y_d).$$

From the HDO scheme we know that $Y_d = u_n + PZu_n$, thus

$$u_{n+1} = (I + PZ)(I + PZ)u_n - P(I + \frac{1}{2}Z)PZu_n$$

and

$$R_{HHV} = I + 2PZ - P^2Z + \frac{1}{2}P^2Z^2.$$

In the following we perform a von Neumann stability analysis. Inserting Fourier modes into the discretisation operators we obtain the eigenvalues

$$\begin{aligned} \tilde{z}_i &= -2q_{ii}\frac{1}{h_i^2}(1 - \cos \phi_i) && \text{for } i = 1, \dots, d, \\ \bar{z}_i &= 1 - \frac{1}{6}(1 - \cos \phi_i) && \text{for } i = 1, \dots, d, \\ z_0 &= -\sum_{i \neq j} q_{ij}\frac{4}{144}\frac{\Delta_t}{h_i h_j}(8 \sin \phi_i - \sin 2\phi_i)(8 \sin \phi_j - \sin 2\phi_j) && . \end{aligned} \quad (4.1)$$

The eigenvalues \tilde{z}_i stem from $q_{ii}\delta_{x_i}^2$, A_{x_i} respectively, \bar{z}_i from $1 + \frac{h_i^2}{12}\delta_{x_i}^2$, B_{x_i} respectively, and z_0 from all mixed derivatives. The angles ϕ_i are integer multipliers of $2\pi/m_i$ with m_i the dimension of the grid in x_i -direction for $i = 1, \dots, d$. Hence we have the scalar factor

$$\begin{aligned} p &= \prod_i \frac{\tilde{z}_i}{\bar{z}_i - \theta \Delta_t \tilde{z}_i} \\ z &= z_0 + \Delta_t \sum_i \frac{\tilde{z}_i}{\bar{z}_i}. \end{aligned}$$

Since $\bar{z}_i \neq 0$ we can rewrite p

$$p = \prod_i \frac{1}{1 - \theta \Delta_t \tilde{z}_i / \bar{z}_i}.$$

Defining

$$z_i := \Delta_t \tilde{z}_i / \bar{z}_i \quad (4.2)$$

one obtains

$$p = \prod_i \frac{1}{1 - \theta z_i},$$

$$z = z_0 + z_1 + \dots + z_d.$$

The stability matrices reduce to the following stability functions

$$\begin{aligned} r_{HDO}(z_0, z_1, \dots, z_d) &= 1 + p z, \\ r_{HCS}(z_0, z_1, \dots, z_d) &= 1 + p z + \frac{1}{2} p z_0 z, \\ r_{HMCS}(z_0, z_1, \dots, z_d) &= 1 + p z + \theta p^2 z_0 z + \left(\frac{1}{2} - \theta\right) p^2 z^2, \\ r_{HHV}(z_0, z_1, \dots, z_d) &= 1 + 2p z - p^2 z + \frac{1}{2} p^2 z^2. \end{aligned}$$

Please note that the stability functions of the HOC-ADI schemes have the same structure as for the 'standard' ADI schemes. This gives rise to the assumption that both approaches have the same stability properties. Nevertheless the eigenvalues z_i for $i = 0, 1, \dots, d$ stem from different discretisations compared to the ones in the literature. In the following we want to use the results from the literature as far as possible, c.f. [7, 9]. Therefore we formulate a Lemma, which states some properties regarding the eigenvalues, which will be used later on in the proofs.

Lemma 1. *Let z_0, z_1, \dots, z_d be given by (4.1), (4.2) respectively. Further let Q be positive semi-definite, then*

$$\text{all } z_i \text{ are real,} \quad (4.3)$$

$$z_i \leq 0 \text{ for all } i \quad (4.4)$$

$$z \leq 0, \quad (4.5)$$

$$|z_0| \leq \sum_{i \neq j} \sqrt{z_i z_j}. \quad (4.6)$$

Proof. The properties (4.3), (4.4) are clear. It remains to prove (4.5), (4.6). In order to show that $z \leq 0$ holds, we show the equivalent condition $-z \geq 0$:

$$\sum_i 2q_{ii} \frac{\Delta_t}{h_i^2} \frac{1 - \cos \phi_i}{1 - \frac{1}{6}(1 - \cos \phi_i)} + \sum_{i \neq j} q_{ij} \frac{4}{144} \frac{\Delta_t}{h_i h_j} (8 \sin \phi_i - \sin 2\phi_i) (8 \sin \phi_j - \sin 2\phi_j) \geq 0$$

Defining $x_i := \frac{2}{12} \frac{\sqrt{\Delta_t}}{h_i} (8 \sin \phi_i - \sin 2\phi_i)$, we rewrite the condition to

$$x^T Q x + \sum_i q_{ii} 4 \frac{\Delta_t}{h_i^2} \sin^6 \frac{1}{2} \phi_i \left(\frac{55 - \cos 2\phi_i}{\cos \phi_i + 5} \right) \geq 0,$$

which is fulfilled since Q is positive semi-definite.

By the definiteness of Q it follows $|q_{ij}| \leq \sqrt{q_{ii} q_{jj}}$. Further it holds

$$\frac{4}{144} \left| (8 \sin \phi_i - \sin 2\phi_i) (8 \sin \phi_j - \sin 2\phi_j) \right| \leq \sqrt{\frac{2(1 - \cos \phi_i)}{1 - \frac{1}{6}(1 - \cos \phi_i)} \frac{2(1 - \cos \phi_j)}{1 - \frac{1}{6}(1 - \cos \phi_j)}}. \quad (4.7)$$

Applying the Cauchy-Schwarz and the triangle inequality we have

$$\begin{aligned} |z_0| &\leq \sum_{i \neq j} |q_{ij}| \frac{4}{144} \frac{\Delta_t}{h_i h_j} \left| (8 \sin \phi_i - \sin 2\phi_i) (8 \sin \phi_j - \sin 2\phi_j) \right| \\ &\leq \sum_{i \neq j} \sqrt{q_{ii} q_{jj}} \frac{4}{144} \frac{\Delta_t}{h_i h_j} \left| (8 \sin \phi_i - \sin 2\phi_i) (8 \sin \phi_j - \sin 2\phi_j) \right| \end{aligned}$$

Using (4.7) we conclude $|z_0| \leq \sum_{i \neq j} \sqrt{z_i z_j}$. □

4.1. Stability in 2 or 3 dimensions

Theorem 2.3 in [9] states the parameters for θ such that the ADI schemes (2.1) - (2.4) using second order central finite difference stencils are unconditionally stable when applied to the PDE (1.1). Since only the conditions in Lemma 1 are used in the proof, the same stability conditions also hold for the HOC-ADI schemes:

Theorem 1. *Consider diffusion equation (1.1) with periodic boundary condition and positive semi-definite coefficient matrix Q in two or three spatial dimensions, then the HOC - ADI schemes (3.6) - (3.9) derived in Section 3 are unconditionally stable with the following lower bound on θ :*

HOC Douglas scheme (3.6)

$$\theta \geq \frac{1}{2} \text{ if } d = 2 \qquad \theta \geq \frac{2}{3} \text{ if } d = 3$$

HOC Craig-Sneyd scheme (3.7)

$$\theta \geq \frac{1}{2} \text{ if } d = 2, 3$$

HOC modified Craig-Sneyd scheme (3.8)

$$\theta \geq \frac{1}{3} \text{ if } d = 2 \qquad \theta \geq \frac{6}{13} \text{ if } d = 3$$

HOC Hundsdorfer-Verwer scheme (3.9)

$$\theta \geq \frac{1}{2 + \sqrt{2}} \text{ if } d = 2 \qquad \theta \geq \frac{3}{4 + 2\sqrt{3}} \text{ if } d = 3$$

Proof. The proof follows directly from Lemma 1 and the analogue steps as in Theorem 2.3 in [9]. \square

4.2. Stability for arbitrary dimensions

In this Section we want to derive necessary conditions on θ for our HOC-ADI schemes. The stability condition $|r| \leq 1$ can be rewritten to

HOC Douglas scheme (3.6)

$$2p^{-1} + z \geq 0, \qquad z \leq 0, \qquad (4.8)$$

HOC Craig-Sneyd scheme (3.7)

$$p^{-1} + \frac{1}{2}z_0 \geq 0, \qquad 2p^{-2} + p^{-1}z + \frac{1}{2}z_0 z \geq 0, \qquad (4.9)$$

HOC modified Craig-Sneyd scheme (3.8)

$$p^{-1} - \theta(z - z_0) + \frac{1}{2}z \geq 0, \qquad 2p^{-2} + p^{-1}z + \theta z_0 z + (\frac{1}{2} - \theta)z^2 \geq 0, \qquad (4.10)$$

HOC Hundsdorfer-Verwer scheme (3.9)

$$2p^{-1} - 1 + \frac{1}{2}z \geq 0, \qquad 2p^{-2} + (2p^{-1} - 1)z + \frac{1}{2}z^2 \geq 0. \qquad (4.11)$$

Theorem 2. *Let $d \geq 2$ be given. Then any HOC-ADI scheme (1.1) derived in Section 3 applied to diffusion equations (1.1) with positive semi-definite coefficient matrix Q and periodic boundary conditions needs to fulfill the following lower bound on θ for unconditionally stability:*

HOC Douglas scheme (3.6)

$$\theta \geq \frac{1}{2}d(1 - \frac{1}{d})^{d-1},$$

HOC Craig-Sneyd scheme (3.7)

$$\theta \geq \max \left\{ \frac{1}{2}, \frac{1}{2}d(1 - \frac{1}{d})^d \right\},$$

HOC modified Craig-Sneyd scheme (3.8)

$$\theta \geq \frac{1}{2} \frac{d}{1 + (\frac{d}{d-1})^{d-1}},$$

HOC Hundsdorfer-Verwer scheme (3.9)

$$\theta \geq \frac{1}{2} da_k$$

where a_k is the unique solution $a \in (0, \frac{1}{2})$ of $2a \left(1 + \frac{1-a}{d-1}\right)^{d-1} - 1 = 0$.

Proof. We consider a coefficient matrix Q with $q_{ij} = 1$ for $1 \leq i, j \leq d$. Please note that for this choice Q is positive semi-definite. In the following we assume equal step sizes in all coordinate directions $h = h_1 = \dots = h_d$ and choose equal angles $\phi = \phi_1 = \dots = \phi_d$ for all z_i . Hence the eigenvalues are given by

$$\begin{aligned} z - z_0 &= -2d \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)} \\ z_0 &= -d(d-1) \frac{4}{144} \frac{\Delta_t}{h^2} (8 \sin \phi - \sin 2\phi)^2. \end{aligned}$$

The stability conditions (4.8)-(4.11) yield

$$(4.8) : \theta \geq -\theta \frac{z}{2p^{-1}} = \frac{1}{2} \frac{d(d-1) \theta \frac{4}{144} \frac{\Delta_t}{h^2} (8 \sin \phi - \sin 2\phi)^2 + 2d\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}}{2 \left(1 + 2\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}\right)^d}$$

$$(4.9) : \theta \geq -\frac{1}{2}\theta \frac{z_0}{p^{-1}} = \frac{1}{2} \frac{d(d-1) \theta \frac{4}{144} \frac{\Delta_t}{h^2} (8 \sin \phi - \sin 2\phi)^2}{\left(1 + 2\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}\right)^d}$$

$$(4.10) : \theta \geq -\frac{1}{2}\theta \frac{z}{p^{-1} - \theta(z - z_0)} = \frac{1}{2} \frac{d(d-1) \theta \frac{4}{144} \frac{\Delta_t}{h^2} (8 \sin \phi - \sin 2\phi)^2 + 2d\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}}{\left(1 + 2\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}\right)^d + 2d\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}}$$

$$(4.11) : \theta \geq -\frac{1}{2}\theta \frac{z}{2p^{-1} - 1} = \frac{1}{2} \frac{d(d-1) \theta \frac{4}{144} \frac{\Delta_t}{h^2} (8 \sin \phi - \sin 2\phi)^2 + 2d\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}}{2 \left(1 + 2\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}\right)^d - 1}$$

Defining $\alpha := 2\theta \frac{\Delta_t}{h^2} \frac{1 - \cos \phi}{1 - \frac{1}{6}(1 - \cos \phi)}$ we obtain

$$(4.8) : \theta \geq \frac{\alpha d (d-1) \left(\frac{1}{216}(5 + \cos \phi)(\cos \frac{3}{2}\phi - 7 \cos \frac{1}{2}\phi)^2\right) + 1}{(1 + \alpha)^d}$$

$$(4.9) : \theta \geq \frac{\alpha d (d-1) \left(\frac{1}{216}(5 + \cos \phi)(\cos \frac{3}{2}\phi - 7 \cos \frac{1}{2}\phi)^2\right)}{(1 + \alpha)^d}$$

$$(4.10) : \theta \geq \frac{\alpha d (d-1) \left(\frac{1}{216}(5 + \cos \phi)(\cos \frac{3}{2}\phi - 7 \cos \frac{1}{2}\phi)^2\right) + 1}{(1 + \alpha)^d + d\alpha}$$

$$(4.11) : \theta \geq \frac{\alpha d (d-1) \left(\frac{1}{216}(5 + \cos \phi)(\cos \frac{3}{2}\phi - 7 \cos \frac{1}{2}\phi)^2\right) + 1}{2(1 + \alpha)^d - 1}.$$

Please note that $\frac{1}{216}(5 + \cos \phi)(\cos \frac{3}{2}\phi - 7 \cos \frac{1}{2}\phi)^2 \leq 1$ holds for all ϕ . Taking the supremum over ϕ one obtains

$$(4.8) : \theta \geq \frac{\alpha d^2}{2(1 + \alpha)^d}$$

$$(4.9) : \theta \geq \frac{\alpha d(d-1)}{(1 + \alpha)^d}$$

$$(4.10) : \theta \geq \frac{d}{2} \frac{d\alpha}{(1 + \alpha)^d + d\alpha}$$

$$(4.11) : \theta \geq \frac{d}{2} \frac{d\alpha}{2(1 + \alpha)^d - 1}.$$

Maximization regarding the parameter $\alpha > 0$ completes the proof.

In case of the HOC Craig-Sneyd scheme we also consider the case $\phi_i = 0$ for all $i > 1$, such that $z_2 = \dots = z_d = 0$ and $z_0 = 0$. The stability criterion (4.9) reduces to

$$2(1 - \theta z_1)^2 + (1 - \theta z_1) z_1 \geq 0 \quad \Leftrightarrow \quad 2 + (1 - 2\theta) z_1 \geq 0.$$

This leads to the lower bound $\theta \geq \frac{1}{2}$. □

We see that the necessary condition on θ coincides with the sufficient condition in two or three spatial dimensions.

5. Combination technique

Solving high dimensional equations like (1.1) on a full tensor based grid with $\mathcal{O}(h^{-d})$ grid points is an extensive work. Although ADI or HOC-ADI schemes can reduce the computationally workload significantly, there will be a limit on the number of nodes as the available memory is finite.

The sparse grid approach, developed by Bungartz and Griebel in [13] and Zenger in [14], reduces the number of grid points to $\mathcal{O}(h^{-1} \log(h^{-1})^{d-1})$ by splitting the full grid to a sequence of sub-grids. These grids can be efficiently constructed with help of the combination technique, which solves the problem on a sequence of anisotropic grids. As the sub-problems can be computed independently, the method is embarrassingly parallel and can easily be used on a cluster of computers or on GPUs [15].

$$u_n^s = \sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\mathbf{l}|_1 = n-q} u_{\mathbf{l}},$$

The sparse grid solution on refinement level n is denoted by u_n^s . The numerical sub-solution $u_{\mathbf{l}}$ is computed on a grid with step sizes $\mathbf{h} = (h_1, h_2, \dots, h_d) = (2^{-l_1} \cdot c_1, 2^{-l_2} \cdot c_2, \dots, 2^{-l_d} \cdot c_d)$, with multi-index $\mathbf{l} = (l_1, l_2, \dots, l_d)$ and grid length c_i in coordinate direction i for $i = 1, \dots, d$. The sum of \mathbf{l} is defined by $|\mathbf{l}|_1 = \sum_i l_i$.

Figure 1 shows the sub-grids on level 5 and 4 in the two dimensional case. The sub-solutions on level four are subtracted from level five solutions to construct the sparse grid solution. The combination technique exploits the error splitting structure of the numerical sub-solution, such that low order terms cancel out. In the case of a scheme with a rate of convergence p , the error is assumed to be of the form

$$u(\mathbf{x}_{\mathbf{h}}) - u_{\mathbf{l}} = \sum_{k=1}^d \sum_{\substack{\{j_1, \dots, j_k\} \\ \subseteq \{1, \dots, d\}}} w_{j_1, \dots, j_k}(\cdot; h_{j_1}, \dots, h_{j_k}) h_{j_1}^p \cdots h_{j_k}^p,$$

where $u(\mathbf{x}_{\mathbf{h}})$ is the analytical solution on the discrete grid $\mathbf{x}_{\mathbf{h}}$. The coefficient functions w are assumed to be bounded by some constant K , such that $|w| \leq K$. Then we can expect under suitable regularity assumptions a pointwise rate of convergence $\mathcal{O}(h^p \log_2(h^{-1})^{d-1})$. Bungartz et

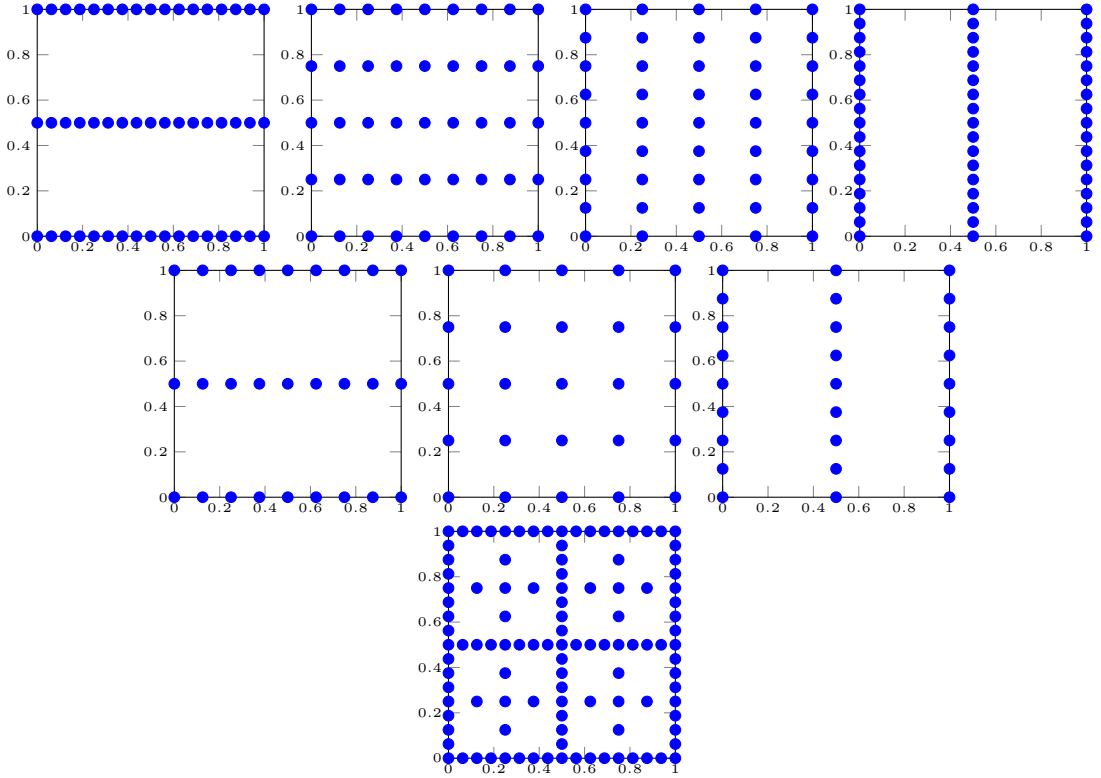


Figure 1: Sub-grids on level 5, 4 and combined grid.

al. [16] proved with help of Fourier series of discrete and semi-discrete solutions for the 2-d Laplace equation that a second order central difference scheme exhibits this error structure. Reisinger [17] recently extended the framework to a wider class of equations and linear finite difference schemes. He notes the following key properties, which have to be fulfilled:

1. The scheme has a truncation error of the form

$$(L - L_h)u(\mathbf{x}_h) = \sum_{k=1}^d \sum_{\substack{\{j_1, \dots, j_k\} \\ \subseteq \{1, \dots, d\}}} \tau_{j_1, \dots, j_k}(\cdot; h_{j_1}, \dots, h_{j_k}) h_{j_1}^p \cdots h_{j_k}^p,$$

where L is the elliptic operator of equation (1.1) and L_h its discrete approximation from Section 3.

2. Stability of the discretisation scheme.
3. Sufficiently smooth initial data and compatible boundary data, such that the mixed derivatives of required order are bounded.

In Section 3 and 4 we have already seen that the semi-discretisation has an truncation error of the form, c.f. (3.4)

$$(L - L_h)u(\mathbf{x}_h) = h_1^4 \tau_1(\mathbf{x}_h, h_1) + \dots + h_d^4 \tau_d(\mathbf{x}_h, h_d) + \sum_{i \neq j} h_i^4 h_j^4 \tau_{i,j}(\mathbf{x}_h, h_i, h_j).$$

Please note that the second approach (3.5) does not have this error structure, hence the error cancellation is disturbed and leads to a lower rate of convergence.

Since we have already derived bounds on θ to ensure unconditional stability, we can expect a pointwise rate of convergence $\mathcal{O}(h^4 \log_2(h^{-1})^{d-1})$ for sufficiently smooth initial data. However this result is only valid for all points which are not affected by the interpolation technique. Since there is only one interior point, which belongs to all sub-grids, this result seems to be rather limiting. It was shown in [18] that if a suitable interpolation technique is applied, the convergence result can be extended to the entire domain. Following [18] we use multivariate cubic spline interpolation.

6. Numerical example

In this Section we validate our theoretical results with numerical experiments. We consider the 2-d diffusion equation on the unit cube $\Omega = [0, 1]^2$, which was also used as a test example in [9, 19]. The coefficient matrix Q is given by

$$Q = 0.025 \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}.$$

The initial value is chosen to be

$$u(x_1, x_2, 0) = e^{-4(\sin^2(\pi x_1) + \cos^2(\pi x_2))}.$$

We apply periodic boundary conditions, such that

$$u(x_1 \pm 1, x_2 \pm 1, t) = u(x_1, x_2, t)$$

holds. Figure 2 shows the initial value and the solution at $t = 1$. In a first experiment we

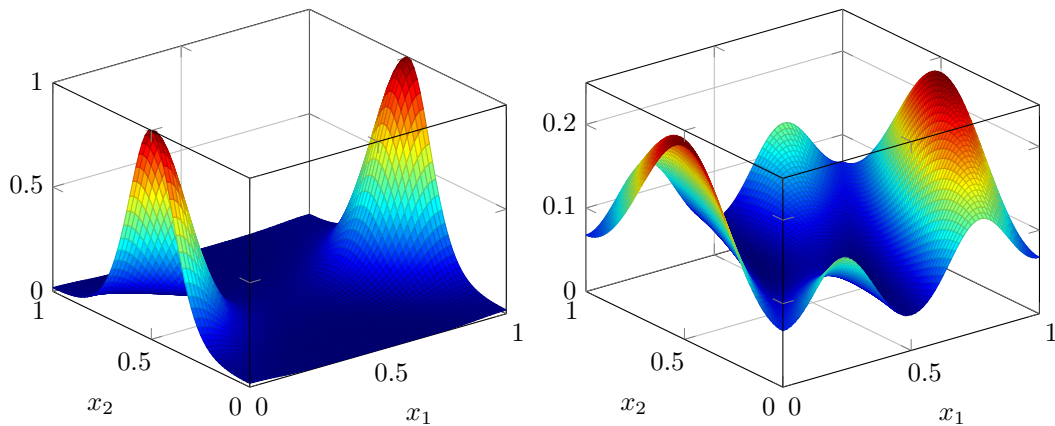


Figure 2: Initial condition and solution at $t = 1$.

numerically evaluate the order of convergence in time of our four HOC-ADI schemes. The space step sizes are fixed at $h_1 = h_2 = 2^{-5}$. In order to measure the error, we use the ℓ_2 vector norm and compute

$$\text{err}_{\ell_2}^t = \|u(1) - u_h\|_{\ell_2},$$

where $u(1)$ is the exact solution of the semi-discrete system $u'(t) = Fu(t)$, given in terms of the propagator via $u(t) = e^{tF}u(0)$. The simulation results in Figure 3 are in line with the theoretical

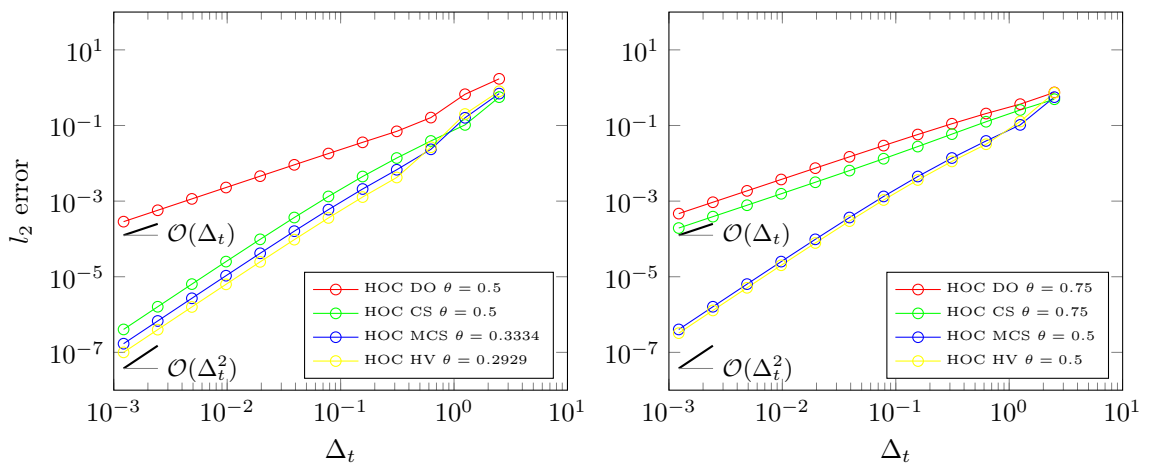


Figure 3: ℓ_2 error for $\Delta_t \rightarrow 0$.

results. On the left hand plot the θ value has been set to its lower bound. The HOC DO scheme

exhibits order one in time, while the other three schemes are of order two. All schemes show a stable behaviour. If θ is chosen to be larger the accuracy is slightly reduced due to damping effects. Here the HOC Craig-Sneyd scheme only exhibits order one since $\theta \neq \frac{1}{2}$. In the next experiment

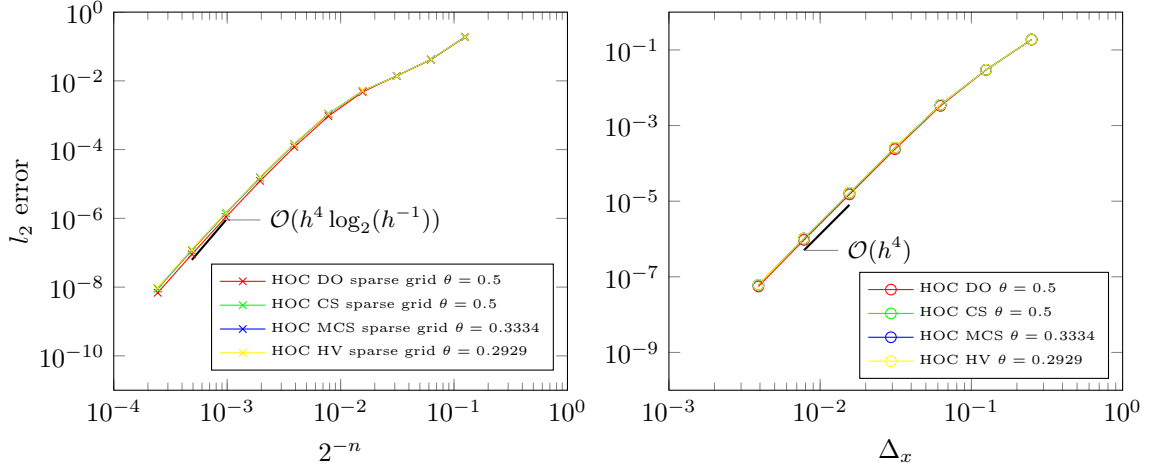


Figure 4: l_2 error for $n \rightarrow \infty$, $h \rightarrow 0$ respectively.

we test the rate of convergence of the spatial discretisation. The time step is fixed at $\Delta_t = 1/100$ and the space error is

$$\text{err}_{l_2}^s = \frac{\|u_{ref} - u_h\|_{l_2}}{\|u_h\|_{l_2}},$$

where u_{ref} is a highly accurate reference solution at time level $t = 1$ with step sizes $\Delta_t = 1/100$, $h_1 = h_2 = 2^{-11}$. The left plot shows the numerical solution u_h of the sparse grid solution, while the second plot shows the solution computed with the HOC-ADI schemes. As all schemes use the same spatial discretisation, the errors are almost identical. The order of convergence is in line with the theoretical order of $\mathcal{O}(h^4 \log_2(h^{-1}))$, $\mathcal{O}(h^4)$ respectively. In Section 5 it was motivated

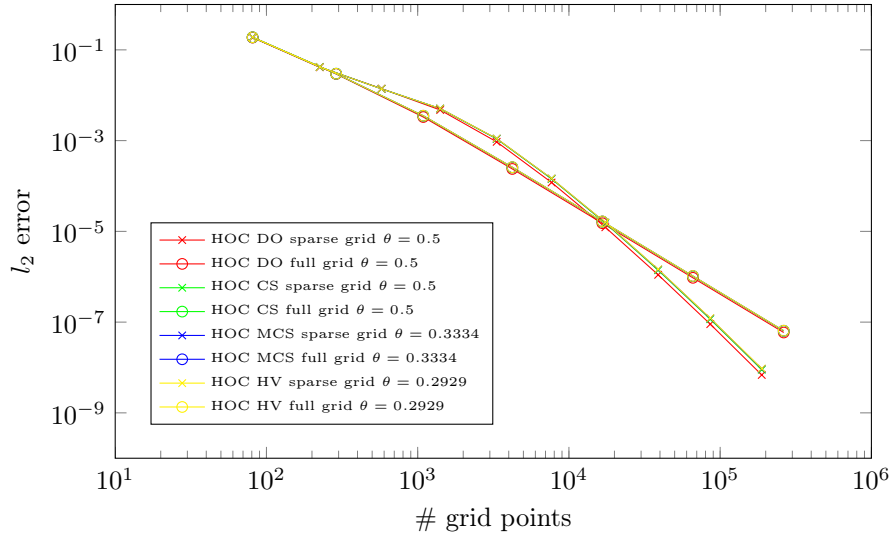


Figure 5: Number of grid points versus accuracy in logarithmic scale.

that the number of grid points can be significantly reduced with the help of sparse grids and the combination technique. In Figure 5 we compare the number of grid points to the obtained accuracy. If we take them as a measure of memory consumption and computation time, the sparse grid solution outperforms the standard full grid approach for sufficiently high level. The workload can be further reduced by not only considering space sparse grids, but by constructing time-space sparse grids. Since all schemes are unconditionally stable for appropriate chosen θ , one can simply consider time as an additional variable.

7. Conclusion and outlook

In this article we derived HOC-ADI schemes for diffusion equations. We were able to prove that the stability of the schemes coincides with their second order central differences counterpart. In the case of two and three spatial dimensions conditions guaranteeing unconditional stability could be found. For arbitrary dimensions necessary conditions on θ were given. Furthermore we showed that HOC schemes derived from one-dimensional problems have an error structure, which fits into the framework of the combination technique. With the help of sparse grids the memory consumption and computational workload could be reduced. Based on our theoretical findings we validated our results and tested the constructed schemes for a 2-d diffusion problem.

In the next step we plan to use these schemes for convection-diffusion problems arising in computational finance.

Acknowledgement

The work of the authors was partially supported by the European Union in the FP7-PEOPLE-2012-ITN Programme under Grant Agreement Number 304617 (FP7 Marie Curie Action, Project Multi-ITN STRIKE – Novel Methods in Computational Finance).

Further the authors acknowledge partial support from the bilateral German-Spanish Project HiPeCa – High Performance Calibration and Computation in Finance, Programme Acciones Conjuntas Hispano-Alemanas financed by DAAD.

8. References

- [1] B. Düring, M. Fournié, A. Rigal, High-Order ADI Schemes for Convection-Diffusion Equations with Mixed Derivative Terms, in: Spectral and High Order Methods for Partial Differential Equations - ICOSAHOM 2012, Vol. 95, Springer International Publishing, 2014, pp. 217–226.
- [2] S. Karaa, J. Zhang, High-order ADI method for solving unsteady convection-diffusion problems, *J. Comput. Phys.* 198 (1) (2004) 1–9.
- [3] J. Douglas, Jim, Alternating direction methods for three space variables, *Numerische Mathematik* 4 (1) (1962) 41–63.
- [4] P. Brian, A finite-difference method of high-order accuracy for the solution of threedimensional transient heat conduction problems, *AIChE Journal* 7 (1961) 367–370.
- [5] J. Douglas, H. Rachford, On the numerical solution of heat conduction problems in two and three space variables, *Trans. Amer. Math. Soc.* 82 (1956) 421–439.
- [6] I.J.D. Craig and A.D. Sneddy, An alternating-direction implicit scheme for parabolic equations with mixed derivatives, *Comput. & Math. Appl.* 16 (4) (1988) 341–350.
- [7] K. J. in't Hout, B. Welfert, Unconditional stability of second-order ADI schemes applied to multi-dimensional diffusion equations with mixed derivative terms, *Appl. Numer. Math.* 59 (3-4) (2009) 677–692.
- [8] W. Hundsdorfer, Accuracy and stability of splitting with stabilizing corrections., *Appl. Numer. Math.* 42 (1-3) (2002) 213–233.
- [9] K. J. in't Hout, C. Mishra, Stability of ADI schemes for multidimensional diffusion equations with mixed derivative terms, *Appl. Numer. Math.* 74 (2013) 83–94.
- [10] W. Hundsdorfer, A note on stability of the Douglas splitting method, *Math. Comput.* 67 (221) (1998) 183–190.
- [11] W. Hundsdorfer, Stability of Approximate Factorization with θ -Methods, *BIT Numer. Math.* 39 (3) (1999) 473–483.

- [12] W. Spitz, High Compact Finite Difference Schemes for Computational Mechanics, Ph.D. thesis, University of Texas, Austin (1995).
- [13] H. Bungartz, M. Griebel, Sparse grids, Cambridge University Press (2004) 1–123.
- [14] C. Zenger, Sparse Grids, Tech. rep., Institut für Informatik, Technische Universität München (Oct. 1990).
- [15] A. Gaikwad, I. M. Toke, GPU Based Sparse Grid Technique for Solving Multidimensional Options Pricing PDEs, in: Proceedings of the 2nd Workshop on High Performance Computational Finance, WHPCF '09, ACM, New York, NY, USA, 2009, pp. 6:1–6:9.
- [16] H.-J. Bungartz, M. Griebel, D. Röschke, C. Zenger, Pointwise Convergence of the Combination Technique for Laplace's Equation, East-West J. Numer. Math. 2 (1994) 21–45.
- [17] C. Reisinger, Analysis of Linear Difference Schemes in Sparse Grid Combination Technique, IMA J. Numer. Anal. 33 (2) (2013) 544–581.
- [18] C. Hendricks, M. Ehrhardt, M. Günther, High order tensor product interpolation in the Combination Technique, Preprint 14/25.
- [19] K. J. in't Hout, B. D. Welfert, Stability of ADI Schemes Applied to Convection-Diffusion Equations with Mixed Derivative Terms, Appl. Numer. Math. 57 (1) (2007) 19–35.