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PRESENTED BY Justin Hausauer

ACCEPTED BY THE DEPARTMENT OF Mathematical Sciences

Roy Nicolaides — MAJOR PROFESSOR — May 2015 — DATE

Thomas Bohman — DEPARTMENT HEAD — May 2015 — DATE

APPROVED BY THE COLLEGE COUNCIL

Frederick J. Gilman — DEAN — May 2015 — DATE

Sparse grid combination techniques for solving high-dimensional parabolic equations with an application to the LIBOR market model

Justin Hausauer
jhausaue@andrew.cmu.edu

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Abstract

In this thesis, we consider the use of the sparse grid combination technique with finite difference methods to solve parabolic partial differential equations. Convergence results are obtained in L^2 for arbitrary dimensions via Fourier analysis arguments under the assumption that the initial data lies in the Sobolev space H^4_{mix}. Numerical results are presented for model problems and for problems from the field of option pricing.

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I am very blessed to have the support of my parents. It is to them that I dedicate this thesis.

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Introduction

Since Black and Scholes [BS73] introduced a partial differential equation (PDE) governing the arbitrage-free price of a plain vanilla option in 1973, the numerical solution of PDE has become an important topic in mathematical finance. Arbitrage-free pricing soon expanded to include derivatives depending on the value of more than one underlying quantity. Among these derivatives are equity basket options on multiple stocks and interest rate derivatives.

For the particular case of interest rate derivatives, the underlying stochastic variable is not a single value, such as a stock price, or even a finite set of values but instead is a continuum of values in the form of a yield curve. Various methods are employed in practice to reduce the number of stochastic variables in the problem to a finite number n. We can then use standard martingale techniques to price derivatives with payoffs of the form $f(\vec{X}_t)$, where $\vec{X}_t$ is an n-dimensional stochastic state process and $f : \mathbb{R}^n \to \mathbb{R}$ is a function giving the dependence of the payoff on the state process. The martingale pricing formula gives the price V_t of the derivative paying off at time T as

$$V_t = \frac{1}{D_t}\tilde{E}_t[f(\vec{X}_T)D_T] \tag{1}$$

at time t, where D_t is the discount process.

Several means are available to the practitioner for calculating this quantity:

1. Analytical or semi-analytical methods
2. Monte Carlo

3. Numerical Solution of the partial differential equation obtained by the Feynman-Kac theorem using finite difference methods.

Analytical methods are available for only a handful of carefully chosen problems. For instance, the price of a simple caplet, under the assumption of lognormal forward rate dynamics, is given in closed form by Black's formula [Bla76]. More complex problems may only be solved by Monte Carlo methods or by numerical methods for PDE.

Each method has advantages and disadvantages. Monte Carlo methods are intuitive and applicable to a wide range of problems. They are, however, limited by their speed of convergence. The central limit theorem shows that we should expect a convergence rate of $O(\frac{1}{\sqrt{N}})$, where N is the number of sample paths.

On the other hand, finite difference methods for the solution of PDE are much quicker. When N is the number of grid points in a finite difference mesh in each coordinate direction, we should expect a convergence rate of $O(\frac{1}{N^2})$ in the L^2 norm. However, a serious disadvantage of numerical PDE methods is the so-called "curse of dimensionality," a term coined by Richard Bellman [Bel61]. Depending on computational resources, conventional finite difference methods are limited to problems of perhaps three or four dimensions. This is because the number of grid points in a finite difference discretization increases exponentially of order N^d. In five dimensions, if we choose a uniform discretization with $N = 2^7 = 128$ subdivisions in each coordinate direction, storing the values at each grid point in double-precision format requires 256 GB, far exceeding the amount of memory addressable on 32-bit hardware and even exceeding the 192 GB limit imposed by 64-bit Windows 7.

In the 1990s, a class of numerical methods called *sparse grid methods* were developed which mitigate the difficulties of solving high-dimensional PDE. The number of grid points in a sparse grid discretization increases at a rate of $O(N(\log N)^{d-1})$, a significant improvement over the $O(N^d)$ rate of conventional discretizations. Also, sparse grid methods are known to achieve a convergence rate of $O(\frac{1}{N^2}(\log N)^{d-1})$ in the L^2 norm. While this is a decrease in accuracy from the $O(\frac{1}{N^2})$ rate of conventional methods, it may be a necessary trade-off to bring a problem into the realm of tractability.

In this work, we focus on a particular implementation of sparse grid methods known as the *sparse grid combination technique*. The combination technique approximates the solution of a PDE by a linear combination of conventional finite difference (or finite element) solutions while retaining the complexity and accuracy of other sparse grid methods. Our principal aim is to clarify the convergence properties of the sparse grid combination technique applied to parabolic PDE, particularly when the technique is used in tandem with finite difference methods. In Chapter 2, we discuss different algorithms for solving parabolic PDE using the sparse grid combination technique and then, in Chapter 3, we prove convergence results for one of these algorithms.

The convergence proofs we give are attractive because of their familiarity. We use conventional Fourier analysis–based arguments to prove convergence in the L^2 norm. Existing proofs, which often depend on recursive arguments or Sobolev space techniques, are less intuitive. An interesting result of our approach is that the logarithmic factor $(\log N)^{d-1}$ from the $O(\frac{1}{N^2}(\log N)^{d-1})$ convergence rate disappears in the case of the heat equation without mixed derivatives, indicating that it is some artifact of alignment with the grid. Other published proofs do not reveal this.

Finally, in Chapter 4, we give some numerical results for the algorithms described in Chapter 2 applied to basic model problems with constant coefficients. In Chapter 5, we apply the combination technique to the pricing of derivative securities with multiple underlying sources of risk, culminating in an application to the LIBOR market model in Chapter 6.

Chapter 1

Parabolic equations and finite difference methods

Finite difference methods are techniques for the numerical solution of partial differential equations. We restrict attention to the study of *parabolic* equations, which are equations of the form

$$u_t = Lu, \tag{1.1}$$

where L is a negative-definite second-order elliptic operator.

The prototypical example of parabolic equations is the heat equation

$$u_t = u_{xx} + u_{yy}. \tag{1.2}$$

We usually know the value of u at some time t, often $t = 0$, and wish to find the solution at some time $T > 0$. In this case, we solve the initial value problem

$$\begin{aligned} &u_t = u_{xx} + u_{yy} && \mathbb{R}^2 \times [0, T] \\ &u(x, y, 0) = u_0(x, y). \end{aligned} \tag{1.3}$$

Because we are solving on a computer, we must also truncate $\mathbb{R}^2$ to a bounded domain $\Lambda := [-L, L]^2$ in the spatial variables, so that the problem we solve is

$$\begin{aligned} &\tilde{u}_t = \tilde{u}_{xx} + \tilde{u}_{yy} && \Lambda \times [0, T] \\ &\tilde{u}(x, y, t) = w(x, y, t) && \partial\Lambda \times [0, T] \\ &\tilde{u}(x, y, 0) = u_0(x, y). \end{aligned} \tag{1.4}$$

Finite difference methods proceed by discretizing space and time with a rectangular mesh over the domain and then replacing the derivatives in the equation by discrete difference quotients. A linear algebraic equation is thus obtained for each point in the mesh where the value of the PDE is unknown. Together, these equations form a system of equations, the solution of which gives an approximate solution to the continuous problem at each point in the mesh.

Let's establish some notation which we use throughout. For problems in two spatial dimensions we use the variables (x, y, t) and denote the mesh spacing in these directions by Δx, Δy, and Δt. For problems in d spatial dimensions we use the variables $(x_1, \ldots, x_d, t)$ and write $x = (x_1, \ldots, x_d)$ to refer to the vector of spatial variables. We denote the spatial mesh spacings by Δx_i. Often, the coordinates of the grid points are dyadic, in which case it is convenient to write the mesh spacings in terms of

$$h_i := 2^{-i}. \tag{1.5}$$

We use multi-index notation when referring to grids. When $\underline{l} = (l_1, \ldots, l_d)$, the grid $\Omega_{\underline{l}}$ is the grid with spacings $(2^{-l_1}, \ldots, 2^{-l_d})$ in each coordinate direction. When there is no chance of confusion, we sometimes write $(l_1, \ldots, l_d)$, rather than $\Omega_{\underline{l}}$ to refer to the corresponding grid $\Omega_{\underline{l}}$. Since we are dealing with parabolic equations, which have an additional time dimension, it is sometimes appropriate to use $(l_1, \ldots, l_d)$ to refer to a grid in space-time. In this case, the spatial spacings are $(2^{-l_1}, \ldots, 2^{-l_d})$ and the time spacing Δt is given separately.

1.1 Fourier transform

The initial value problem (1.3) may be solved analytically by Fourier analysis. Given a function $u : \mathbb{R}^d \times [0, T] \to \mathbb{R}$, we write $\hat{u}(\xi_1, \ldots, \xi_d, t)$ to denote the Fourier transform of u in the spatial variables:

$$\hat{u}(\xi_1, \ldots, \xi_d, t) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\xi\cdot x} u(x, t)\, dx. \tag{1.6}$$

Under this convention, the inverse transform is

$$u(x, t) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi\cdot x} \hat{u}(x, t)\, dx. \tag{1.7}$$

We write ξ to denote the vector $(\xi_1, \ldots, \xi_d)$, so that the Fourier transform is $\hat{u}(\xi, t)$. When u is the solution to (1.3), the following lemma states how $\hat{u}(\xi, t)$ evolves as a function of t.

Lemma 1. *Let $u : \mathbb{R}^2 \times [0, T] \to \mathbb{R}$ solve the initial value problem (1.3). Then the Fourier transform $\hat{u}$ of u satisfies*

$$\hat{u}(\xi, t) = e^{q(\xi)t}\hat{u}_0(\xi), \tag{1.8}$$

where $q(\xi) = -(\xi_1^2 + \xi_2^2)$.

Proof. We first take the Fourier transform of the partial differential equation (1.3) only in the spatial variables to get

$$\hat{u}_t = q(\xi)\hat{u}.$$

Solving the above equation gives

$$\hat{u}(\xi, t) = e^{q(\xi)t}\hat{u}_0(\xi).$$

□

1.1.1 Truncation and interpolation operators

One issue that arises with finite difference methods is how to compare functions defined on the grid with functions defined on the entire domain. Since a grid has Lebesgue measure 0 in $\mathbb{R}^2$, a function $u \in L^2(\mathbb{R}^2)$ cannot be simply be evaluated at the grid points. To this end, we define the truncation operator τ and the interpolation operator σ.

Definition 1. *Let $u \in L^2(\mathbb{R}^2)$. Then the truncation operator τ applied to u is*

$$\tau u(x) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta y}^{\pi/\Delta y} e^{ix\cdot\xi}\hat{u}(\xi)\, d\xi_2\, d\xi_1,$$

for every $x \in \Delta x\mathbb{Z} \times \Delta y\mathbb{Z}$, where $\hat{u}(\xi)$ is the Fourier transform of u.

The utility of the truncation operator is that it removes all Fourier modes from u which cannot be accurately resolved on the grid with spacings Δx and Δy.

For mapping functions on the grid to functions in $L^2(\mathbb{R}^2)$, we define the interpolation operator.

Definition 2. *Let $v \in L^2(\Delta x\mathbb{Z} \times \Delta y\mathbb{Z})$. Then the interpolation operator σ applied to v is*

$$\sigma v(x) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta y}^{\pi/\Delta y} e^{ix\cdot\xi} \hat{v}(\xi)\, d\xi_2\, d\xi_1,$$

for every $x \in \mathbb{R}^2$, where $\hat{v}(\xi)$ is the Fourier transform of v, that is,

$$\hat{v}(\xi) = \frac{1}{2\pi} \sum_{x \in \Delta x\mathbb{Z} \times \Delta y\mathbb{Z}} e^{-ix\cdot\xi} v(x) \Delta x \Delta y.$$

Thus, the interpolation operator allows us to compare a function $u \in L^2(\mathbb{R}^2)$ with a grid function $v \in L^2(\Delta x\mathbb{Z} \times \Delta y\mathbb{Z})$ in a natural two-part process. One part of the process entails comparing u with the extension σv of v to the plane, while the other part entails showing that the Fourier modes of u which are not resolved on the grid are sufficiently small.

1.2 Amplification factors

Consider an initial value problem

$$\begin{aligned} u_t &= Lu \qquad\qquad \mathbb{R}^d \times [0, T] \\ u(x, 0) &= u_0(x) \end{aligned} \tag{1.9}$$

for some second-order, constant-coefficient elliptic operator L. Let time be discretized into N steps of length Δt, so that $T = N\Delta t$. For $n = 0, \ldots, N$, let u^n denote a grid function that is the finite difference solution of (1.9) at time step n. Then $\hat{u}^n(\xi)$ denotes the Fourier transform of u^n at wave number ξ.

When a standard finite difference scheme is used, such as the fully implicit or Crank-Nicolson method, we find that evolution of the Fourier transform $\hat{u}^n(\xi)$ of the finite difference solution at wave number ξ is decoupled from other wave numbers. That is,

$$\hat{u}^{n+1}(\xi) = g(\xi)\hat{u}^n(\xi) \tag{1.10}$$

for some g which is called the *amplification factor*. Since the amplification factor depends on the discretization, we shall define

$$g_{\Delta x,\Delta y}(\xi) := \text{amplification factor for grid with spacings } \Delta x \text{ and } \Delta y, \tag{1.11a}$$

$$g_{i,j}(\xi) := g_{2^{-i},2^{-j}}(\xi) = \text{amplification factor for grid } \Omega_{i,j}, \tag{1.11b}$$

for finite difference grids in $\mathbb{R}^2$. It will be clear from the context, and by whether the subscripts are integers, which of the above two definitions is implied. For finite difference grids in $\mathbb{R}^d$, we write

$$g_{\underline{l}}(\xi) := \text{amplification factor for grid } \Omega_{\underline{l}}. \tag{1.12}$$

The amplification factor also implicitly depends on the chosen finite difference scheme. Although the choice of scheme is not indicated by the notation, we make it clear when necessary. We now present standard results for the amplification factor $g_{\Delta x,\Delta y}(\xi)$ when the chosen scheme is the fully implicit method.

1.2.1 Heat equation

First, we consider the heat equation

$$u_t = u_{xx} + u_{yy}. \tag{1.13}$$

To keep the notation simple, we restrict to two spatial dimensions. We denote the values of the finite difference solution of Equation (1.13) by $u_{i,j}^k$, where i, j, and k are the indices of the grid point in the x, y, and t directions. The discretization of Equation (1.13) by the fully implicit method is then

$$\frac{u_{i,j}^{k+1} - u_{i,j}^k}{\Delta t} = \frac{u_{i+1,j}^{k+1} - 2u_{i,j}^{k+1} + u_{i-1,j}^{k+1}}{\Delta x^2} + \frac{u_{i,j+1}^{k+1} - 2u_{i,j}^{k+1} + u_{i,j-1}^{k+1}}{\Delta y^2}. \tag{1.14}$$

By the Fourier inversion formula, with $I = \sqrt{-1}$,

$$u_{i,j}^k = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta y}^{\pi/\Delta y} e^{I(i\Delta x\xi_1 + j\Delta y\xi_2)} \hat{u}^k(\xi)\, d\xi_2\, d\xi_1. \tag{1.15}$$

Substituting Equation (1.15) into (1.14) gives

$$
\begin{aligned}
\frac{1}{2\pi} & \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta y}^{\pi/\Delta y} e^{I(i\Delta x \xi_1 + j\Delta y \xi_2)} \hat{u}^{k+1}(\xi)\, d\xi_2\, d\xi_1 \\
&= \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta y}^{\pi/\Delta y} e^{I(i\Delta x \xi_1 + j\Delta y \xi_2)} \hat{u}^{k}(\xi) \times \\
&\qquad \left(1 + \Delta t \frac{2\cos(\xi_1 \Delta x) - 2}{\Delta x^2} + \Delta t \frac{2\cos(\xi_2 \Delta_y) - 2}{\Delta y^2}\right) d\xi_2\, d\xi_1.
\end{aligned}
$$

Assuming $u \in L^2(\Delta x\mathbb{Z} \times \Delta y\mathbb{Z})$, uniqueness of the Fourier transform implies

$$
\hat{u}^{k+1}(\xi) = \hat{u}^{k}(\xi) \left(1 + \Delta t \left(\frac{2\cos(\xi_1 \Delta x) - 2}{\Delta x^2} + \frac{2\cos(\xi_2 \Delta y) - 2}{\Delta y^2}\right)\right). \tag{1.16}
$$

Therefore, the amplification factor $g_{\Delta x, \Delta y}(\xi)$ is

$$
g_{\Delta x, \Delta y}(\xi) = 1 + \Delta t \left(\frac{2\cos(\xi_1 \Delta x) - 2}{\Delta x^2} + \frac{2\cos(\xi_2 \Delta y) - 2}{\Delta y^2}\right). \tag{1.17}
$$

1.2.2 Heat equation with a mixed derivative term

We now introduce a mixed derivative term into the PDE and repeat the same analysis. Again, we restrict the exposition to two dimensions. We consider

$$
u_t = u_{xx} + u_{xy} + u_{yy}. \tag{1.18}
$$

We discretize Equation (1.18) using the fully implicit method and the four-point stencil for u_{xy}:

$$
\begin{aligned}
\frac{u_{i,j}^{k+1} - u_{i,j}^{k}}{\Delta t} = \frac{u_{i+1,j}^{k+1} - 2u_{i,j}^{k+1} + u_{i-1,j}^{k+1}}{\Delta x^2} &+ \frac{u_{i,j+1}^{k+1} - 2u_{i,j}^{k+1} + u_{i,j-1}^{k+1}}{\Delta y^2} \\
&+ \frac{u_{i+1,j+1}^{k+1} + u_{i-1,j-1}^{k+1} - u_{i+1,j-1}^{k+1} - u_{i-1,j+1}^{k+1}}{4\Delta x \Delta y}.
\end{aligned} \tag{1.19}
$$

Repeating the procedure from the last section, we obtain the amplification factor

$$\begin{aligned} g_{\Delta x,\Delta y}(\xi) = 1 + \Delta t \Bigg(& \frac{2\cos(\xi_1 \Delta x) - 2}{\Delta x^2} + \frac{2\cos(\xi_2 \Delta y) - 2}{\Delta y^2} \\ & - \frac{\sin(\xi_1 \Delta x)\sin(\xi_2 \Delta y)}{\Delta x \Delta y} \Bigg). \end{aligned} \tag{1.20}$$

1.2.3 Heat equation in d dimensions

For the heat equation

$$u_t = \sum_{i=1}^{d} u_{x_i x_i} \tag{1.21}$$

on $\mathbb{R}^d$, Equation (1.17) extends as one would expect. We have

$$g_{\Delta x_1,\ldots,\Delta x_d}(\xi) = 1 + \sum_{i=1}^{d} \Delta t \left(\frac{2\cos(\xi_i \Delta x_i) - 2}{\Delta x_i^2} \right). \tag{1.22}$$

Chapter 2

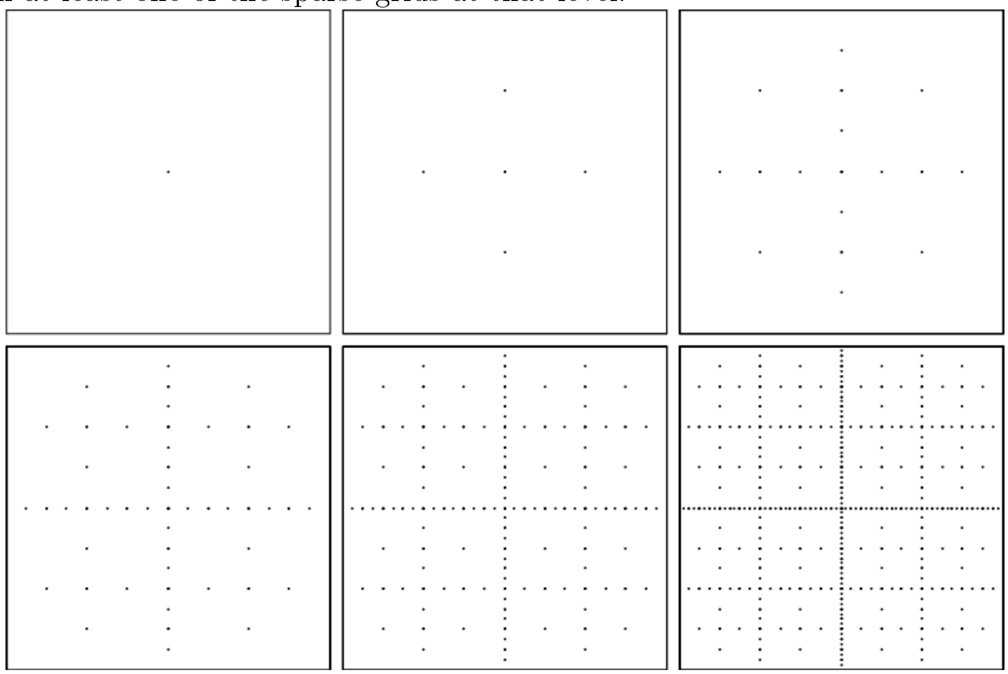
Sparse grid combination technique

Because of the curse of dimensionality, conventional finite difference methods are not suitable for the problem of pricing derivatives with high-dimensional underlying state processes. This problem may be partially tamed by a class of methods known as sparse grid methods. Sparse grids are useful tools for this purpose because they reduce the number of degrees of freedom of the problem while suffering only a small degradation in accuracy. To be precise, if N is the number of grid points in one coordinate direction, sparse grid discretizations include $O(N(\log N)^{d-1})$ grid points, whereas conventional discretizations include $O(N^d)$ grid points. Sparse grid methods converge at a rate of $O(N^{-2}(\log(N))^{d-1})$ in the L^2 norm, whereas conventional methods converge at a rate of $O(N^{-2})$ in the L^2 norm.

Sparse grids were originally introduced for the solution of partial differential equations by Zenger [Zen91] and Griebel [Gri91] in the early 1990s. An excellent overview of the field was produced by Bungartz and Griebel [BG04], and a succinct tutorial can be found in [Gar06].

Perhaps the most straightforward implementation of sparse grid methods for PDE is the *sparse grid combination technique*, proposed originally by Griebel, Schneider, and Zenger [GSZ90]. The combination technique involves solving the PDE on particular conventional finite difference (or finite element) grids and taking a well-chosen linear combination of these solutions as the solu-

Figure 2.1: These six plots show the points included in the sparse grid discretization at levels 2 through 7 for $d = 2$. Each of these points are included in at least one of the sparse grids at that level.



tion to the problem. This solution retains the advertised convergence rate of sparse grid methods. The constituent conventional grids are typically *anisotropic*, that is, the mesh spacing differs in each coordinate direction. The advantage of this method is that the problem can be solved on each of the constituent grids using standard solvers. The only novel operation in the sparse grid combination technique is the step of taking linear combinations of these solutions. In addition, the technique is parallelizable. Much of the literature pertaining to sparse grids focuses on this parallelizability property of the sparse grid combination technique [GT10, BHPS12, Dan11, Gri92].

Let us introduce some notation so that we may be more precise. We fix a multi-index $\underline{l} = (l_1, \dots, l_d) \in \mathbb{N}^d$ and consider, in the d-dimensional unit cube $[0, 1]^d$, an anisotropic but otherwise conventional grid $\Omega_{\underline{l}} = \Omega_{l_1,\dots,l_d}$ having uniform mesh spacing $h_i = 2^{-l_i}$ in each coordinate direction $i \in \{1, \dots, d\}$.

For each multi-index $\underline{l}$, we define the quantity

$$|\underline{l}|_1 := \sum_{i=1}^{d} l_i.$$

We consider an elliptic PDE on $[0,1]^d$ and define $u_{\underline{l}} : [0,1]^d \to \mathbb{R}$ to be the conventional finite difference solution to the PDE on grid $\Omega_{\underline{l}}$, extended to $[0,1]^d$ by interpolation. We define a positive integer n to be the *level* of the sparse grid solution, which we use as a proxy for mesh refinement. Increasing the level n should give a more accurate solution to the problem. Then the sparse grid combination solution is the following linear combination:

$$u_n^c := \sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1 = n-q} u_{\underline{l}}. \tag{2.1}$$

Figure 2 shows an illustration for $d = 2$ of the grid points which are included in the sparse grid discretization at levels 2 through 7.

Generalizations of the combination technique have since been developed [HGC07]. Sparse grid methods have been applied to option pricing problems in finance [BBNS12, Kra07, Bla04, Rei04, LO06, LO08, RW07].

2.1 Previous work

Theoretical error bounds for the sparse grid combination technique have been studied by a number of authors. In their seminal paper, Griebel, Scheieder, and Zenger [GSZ90] show that a sufficient condition for the two-dimensional sparse grid combination technique to achieve its advertised convergence rate is the existence of a so-called "error splitting" of the form

$$u_{\Delta x, \Delta y} - u = C_1(\Delta x)\Delta x^2 + C_2(\Delta y)\Delta y^2 + C(\Delta x, \Delta y)\Delta x^2 \Delta y^2 \tag{2.2}$$

at each point (x, y), where $|C_1(\Delta x)|$, $|C_2(\Delta y)|$, and $|C(\Delta x, \Delta y)|$ are bounded by some $B > 0$ independently of the grid spacings Δx and Δy. Assuming that Equation (2.2) holds, the pointwise error satisfies

$$u - u_n^c = u - \left(\sum_{i=1}^{n-1} u_{i,n-i} - \sum_{i=1}^{n-2} u_{i,n-i-1} \right)$$

$$
\begin{aligned}
&= \sum_{i=1}^{n-1}(u - u_{i,n-i}) - \sum_{i=1}^{n-2}(u - u_{i,n-i-1}) \\
&= \sum_{i=1}^{n-1} C_1(h_i)h_i^2 + C_2(h_{n-i})h_{n-i}^2 + C(h_i, h_{n-i})h_i^2 h_{n-i}^2 \\
&\qquad - \sum_{i=1}^{n-2} C_1(h_i)h_i^2 + C_2(h_{n-i-1})h_{n-i-1}^2 + C(h_i, h_{n-i-1})h_i^2 h_{n-i-1}^2,
\end{aligned}
$$

where C_1, C_2, and C depend on the point (x, y). We now find that most terms with C_1 and C_2 are canceled, while the terms with C accumulate:

$$
\begin{aligned}
&= C_1(h_{n-1})h_{n-1}^2 + C_2(h_{n-1})h_{n-1}^2 \\
&\qquad + \left(\sum_{i=1}^{n-1} C(h_i, h_{n-i})h_n^2 - \sum_{i=1}^{n-2} C(h_i, h_{n-i})h_{n-1}^2 \right) \\
&= h_n^2 \left(4C_1(h_{n-1}) + 4C_2(h_{n-1}) + \sum_{i=1}^{n-1} C(h_i, h_{n-i}) - \sum_{i=1}^{n-2} 4C(h_i, h_{n-i}) \right).
\end{aligned}
$$

Finally, using the fact that $|C_1(\Delta x)|$, $|C_2(\Delta y)|$, and $|C(\Delta x, \Delta y)|$ are uniformly bounded in $(\Delta x, \Delta y)$ by some $B > 0$,

$$
\begin{aligned}
|u - u_n^c| &\leq h_n^2 \left(4B + 4B + \sum_{i=1}^{n-1} B + \sum_{i=1}^{n-2} 4B \right) \\
&= h_n^2 \left(4B + 4B + (n-1)B + (n-2)4B \right) \\
&= h_n^2 \left(5n - 1 \right) B \\
&= h_n^2 \left(5 \log_2(h_n^{-1}) - 1 \right) B \\
&= O(h_n^2 \log_2(h_n^{-1})).
\end{aligned}
$$

The error splitting (2.2) depends on the particular equation being solved, and much of the subsequent work on the sparse grid combination technique has focused on establishing such error splittings for various model problems.

Bungartz et al. [BGRZ94] show the existence of an error splitting for the following boundary value problem for the Laplace equation

$$
\Delta u = 0 \qquad (x, y) \in \Omega := [0, 1] \times [0, 1]
$$

$$u = \begin{cases} g(x) & : (x,y) \in \partial\Omega,\ y = 0 \\ 0 & : (x,y) \in \partial\Omega,\ y > 0, \end{cases}$$

whenever g satisfies certain regularity assumptions.

Pflaum & Zhou [PZ99] prove the convergence of the combination technique for general elliptic equations in two dimensions and for the Poisson equation in higher dimensions under certain assumptions on the equation's coefficients. More recently, Reisinger [Rei13] provided a framework for the verification of the required error splitting for both elliptic and parabolic equations.

Two common features pervade earlier approaches. First, most authors invoke a discussion of hierarchical tensor-product bases and the "hierarchical surplus". This is certainly a useful framework for analyzing sparse grid methods, but it comes at the expense of being jargonistic and unfamiliar to researchers outside of the sparse grid community. We direct the reader to [BG04] to learn more about the hierarchical basis as it pertains to sparse grids.

Second, earlier papers have the common feature that semi-discretizations of the original problem are used as an intermediate step in the analysis. Such constructs do not arise in our arguments.

Instead, we use Fourier analysis to obtain convergence estimates in the L^2 norm. Combinatorial arguments are needed to manipulate the terms comprising the L^2 error, but we bypass any discussion of the "hierarchical surplus" or semi-discretized problems.

2.2 A derivation of the sparse grid combination weights

We now give a derivation of the weights used to linearly combine the solutions $u_{\underline{l}}$ in Equation (2.1). We sometimes abuse terminology slightly by speaking of the weight on a grid $\Omega_{\underline{l}}$, in which case we mean the weight used to combine the corresponding *solution* $u_{\underline{l}}$. To motivate the following argument, suppose we are taking a linear combination of two solutions u_1 and u_2, both of which approximate the exact solution u of some problem, with weights a_1 and

a_2:

$$a_1u_1 + a_2u_2.$$

Since each of u_1 and u_2 approximate u, it would be unreasonable to expect an arbitrary linear combination, such as $3u_1 + 2u_2$, to approximate u as well. Naturally, this particular linear combination would better approximate $5u$. Thus, it seems reasonable to impose the requirement

$$a_1 + a_2 = 1.$$

We may use this argument to derive the weights used in the sparse grid combination technique. We base our derivation on the following principle.

Principle 1 (Pointwise sum of weights is one)**.** *If a point x belongs to at least one sparse grid $\Omega_{\underline{l}}$, the sum of the weights on all grids which include x must be one.*

This principle may be considered an extension of a result presented by Reisinger [Rei13, p. 561], which states that a necessary condition for consistency of the combination technique is that the sum of all the weights is one. However, whereas Reisinger's condition provides one linear constraint on the weights of the combination technique, Principle 1 fixes all the weights uniquely. To show this, it will help to find a rule for characterizing when a grid point belongs to a grid $\Omega_{\underline{m}}$.

Lemma 2. *For each grid point x which belongs to at least one sparse grid, there is a multi-index $\underline{l}^{\min}$ such that $x \in \Omega_{\underline{m}}$ if and only if $\underline{m} \geq \underline{l}^{\min}$.*

Proof. First note that the coordinates of a point x belonging to a grid $\Omega_{\underline{l}}$ on $[0,1]^d$ must satisfy

$$x_i = \frac{k_i}{2^{l_i}} \text{ for some } k_i = 0, \ldots, 2^{l_i},$$

for each $i \in \{1, \ldots, d\}$. If k_i has a power of 2, say 2^{α_i}, in its prime factorization, we can cancel it from both the numerator and the denominator to show that

$$x_i = \frac{k_i}{2^{l_i}} = \frac{k_i' 2^{\alpha_i}}{2^{l_i^{\min}} 2^{\alpha_i}} = \frac{k_i'}{2^{l_i^{\min}}}$$

for some k_i' and some index $l_i^{\min} := l_i - \alpha_i$ for each $i \in \{1, \ldots, d\}$. Thus, there is a coarsest grid $\Omega_{\underline{l}^{\min}}$ in $\{\Omega_{\underline{l}} : \underline{l} \in \mathbb{N}^d\}$ which contains x. A grid which is coarser than $\Omega_{\underline{l}^{\min}}$ in any coordinate direction does not contain the point x. That is, if $m_i < l_i^{\min}$ for some $i \in \{1, \ldots, d\}$ then $x \notin \Omega_{\underline{m}}$.

We now show that if $\underline{m} \geq \underline{l}^{\min}$ then $x \in \Omega_{\underline{m}}$. In that case, we have $\underline{m} = \underline{l}^{\min} + (p_1, \ldots, p_d)$ for some integers $p_i \geq 0$ and so

$$x_i = \frac{k_i'}{2^{l_i^{\min}}} = \frac{k_i' 2^{p_i}}{2^{l_i^{\min}} 2^{p_i}} = \frac{k_i' 2^{p_i}}{2^{m_i}}$$

for each $i \in \{1, \ldots, d\}$. Therefore, $x \in \Omega_{\underline{m}}$. □

2.2.1 The case $d = 2$

We now have the tools to derive the weights of the sparse grid combination technique. Let's first consider the case $d = 2$. We now show that the weight on the grid $\Omega_{\underline{l}}$ is $+1$ when $|\underline{l}|_1 = \ell$ and -1 when $|\underline{l}|_1 = \ell - 1$.

First, the weight on a grid $\Omega_{\underline{l}}$ must be $+1$ when $|\underline{l}|_1 = \ell$ because we can find a point in $\Omega_{\underline{l}}$ for which $\Omega_{\underline{l}}$ is the coarsest grid containing x. Since any grid with $|\underline{l}|_1 = \ell - 1$ is coarser and does not contain x, $\Omega_{\underline{l}}$ is the only grid in the combination technique which contains x. Principle 1 thus requires that the weight on $\Omega_{\underline{l}}$ be $+1$.

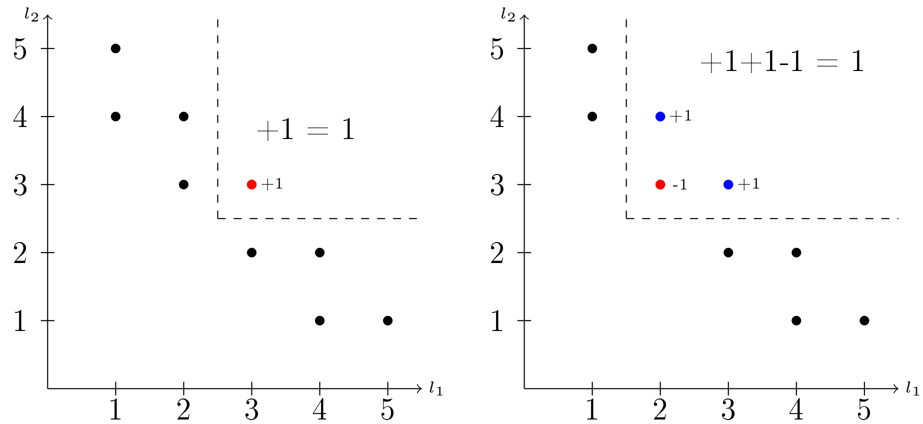
When $|\underline{l}|_1 = \ell - 1$, we can again find a point x for which $\Omega_{\underline{l}}$ is the coarsest grid containing x. This time, however, the grids with multi-indices $(l_1, l_2 + 1)$ and $(l_1 + 1, l_2)$ also contain x and are included in the combination solution. We have already determined that these grids must have a weight of $+1$. Therefore, Principle 1 requires that $\Omega_{\underline{l}}$ have a weight of -1. See Figure 2.2.1 for an illustration of the two-dimensional case.

2.2.2 The case $d > 2$

We can use Principle 1 to derive the weights of the sparse grid combination technique when $d > 2$ as well, but it is a bit more involved, since the geometry is more complex. Recall from Equation (2.1) that, for a fixed dimension d and level n, the weight on a grid $\Omega_{\underline{l}}$ with $|\underline{l}|_1 = n - q$ is

$$(-1)^q \binom{d-1}{q},$$

Figure 2.2: Each dot represents a grid Ω_{l_1,l_2} in the sparse grid combination technique for $d = 2$. For any grid, we can find x such that the grid is the coarsest grid containing x. By Lemma 2, grids containing x lie outside of an L-shaped boundary. Principle 1 requires that the sum of the weights on these grids be one.



which is a function of the integer q.

Theorem 3. *Assume that Principle 1 holds. Then the weight used on grid $\Omega_{\underline{l}}$ in the level-n sparse grid combination technique is*

$$(-1)^q \binom{d-1}{q},$$

where q is such that $|\underline{l}|_1 = n - q$.

Proof. We prove this formula by induction on q. First, the formula is true when $q = 0$ because we can find a point x on a grid $\Omega_{\underline{l}}$ with $|\underline{l}|_1 = n$ such that $\Omega_{\underline{l}}$ is the only grid in the level-n combination solution which contains x. By Principle 1, the weight must be $1 = (-1)^0 \binom{d-1}{0}$.

Now we prove that the formula is true for $q = k$, assuming that it holds when $q < k$. That is, we wish to prove that the weight w on a grid $\Omega_{\underline{l}}$ with $|\underline{l}|_1 = n - k$ is

$$w = (-1)^k \binom{d-1}{k}.$$

We know there exists a grid point $x \in \Omega_{\underline{l}}$ such that $\Omega_{\underline{l}}$ is the coarsest grid containing x. By Principle 1, the sum of the weights on grids which contain

x is one:

$$1 = w + \sum_{q=0}^{k-1} (\text{weight on } \Omega_{\underline{m}},\ |\underline{m}|_1 = n - q) \left(\sum_{\substack{\Omega_{\underline{m}} \text{ containing } x \\ |\underline{m}|_1 = n-q}} 1 \right).$$

To find the second factor inside the summation, recall that any grid $\Omega_{\underline{m}}$ which contains x has

$$\underline{m} = \underline{l} + (p_1, \ldots, p_d),$$

where $p_i \geq 0$. Therefore,

$$\begin{aligned} |\underline{m}|_1 &= |\underline{l}|_1 + |(p_1, \ldots, p_d)|_1 \\ (n - q) &= (n - k) + |(p_1, \ldots, p_d)|_1 \\ |(p_1, \ldots, p_d)|_1 &= k - q \\ p_1 + \ldots + p_d &= k - q. \end{aligned}$$

Thus, the second factor inside the summation is given by the answer to the question "How many ways can one place $k - q$ balls into d bins?". This is a familiar problem from combinatorics which has the answer $\binom{(d-1)+k-q}{k-q}$. Therefore,

$$\begin{aligned} 1 &= w + \sum_{q=0}^{k-1} \left((-1)^q \binom{d-1}{q} \right) \binom{(d-1)+k-q}{k-q} \\ w &= 1 - \sum_{q=0}^{k-1} (-1)^q \binom{d-1}{q} \binom{d-1+k-q}{k-q}. \end{aligned}$$

Now, we wish to show

$$w = (-1)^k \binom{d-1}{k}.$$

But this is equivalent to showing

$$\begin{aligned} 1 &= \sum_{q=0}^{k} (-1)^q \binom{d-1}{q} \binom{d-1+k-q}{k-q} \\ 1 &= \sum_{q=0}^{k} (-1)^q \binom{y}{q} \binom{y+k-q}{k-q} \qquad (y := d-1). \end{aligned}$$

This is the statement of Lemma 15 in the appendix. This completes the proof by induction. □

2.3 Three methods for the solution of parabolic equations

The sparse grid combination technique, while initially formulated for elliptic PDE, has also been applied to parabolic PDE [BRSZ94, Rei04, Rei13]. One of the contributions of this section is to clarify some of the subtleties involved in the implementation of the sparse grid combination technique for parabolic equations. There are at least three distinct algorithms, which we now describe.

2.3.1 Elliptic method

The sparse grid combination technique has its roots in the solution of elliptic partial differential equations, such as Laplace's and Poisson's equation. Therefore, one may apply Rothe's method to solve a parabolic equation, discretizing first in time and then in space with the sparse grid combination technique. To be precise, consider an initial value problem consisting of Equation (1.1) with an initial condition at $t = 0$:

$$\begin{aligned} &u_t = Lu && \mathbb{R}^d \times [0, T] \\ &u(x, 0) = u_0(x). && \end{aligned} \tag{2.3}$$

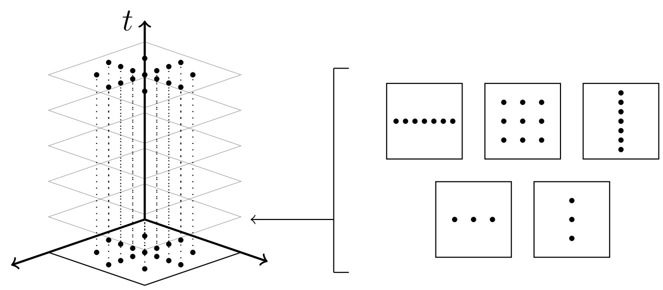
Discretizing the preceding problem in time by, say, the fully implicit method with time step Δt yields a sequence of elliptic problems

$$\frac{u^{n+1} - u^n}{\Delta t} = Lu^{n+1}, \tag{2.4}$$

where $u^n : \mathbb{R}^d \to \mathbb{R}$ approximates the exact solution $u(., t_n)$ at time $t = t_n = n\Delta t$. For each of the above problems, u^{n+1} is unknown and u^n is data. An approximate solution to Equation (2.3) may then be obtained by solving the sequence of problems in Equation (2.4) by the sparse grid combination technique at some level ℓ.

We shall call the preceding method the *elliptic method* or the *elliptic sparse grid combination technique*, since it involves solving an elliptic problem by the sparse grid combination technique at each time step.

Figure 2.3: Diagram of the elliptic method, level 4. An elliptic problem in the spatial coordinates is solved at each time step using the sparse grid combination technique.



2.3.2 Parabolic method

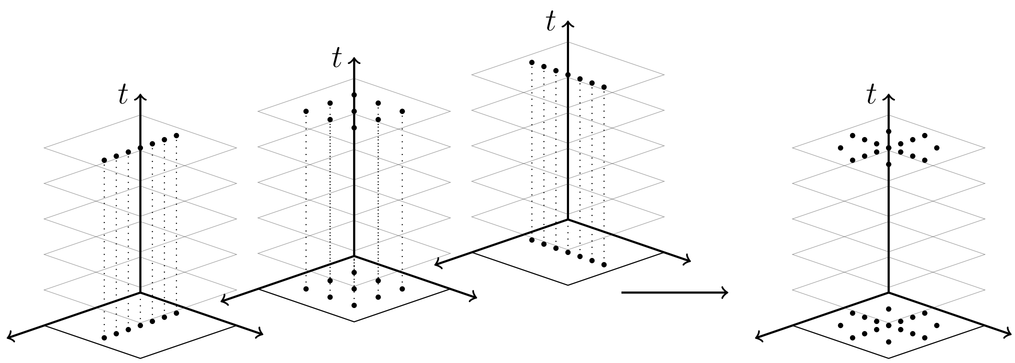
We can also solve the Equation (2.3) by another permutation of the above steps. Fix some sparse grid level ℓ and temporal mesh spacing Δt. Define $u_{\underline{l}}$ to be the conventional finite difference solution of Equation (2.3) on a grid with spatial mesh spacings $\Delta x_i = 2^{-l_i}$ for $i \in \{1, \ldots, d\}$ and temporal mesh spacing Δt. An approximate solution to Equation (2.3) may be obtained by combining the solutions $u_{\underline{l}}$ according to Equation (2.1).

We shall call the preceding method the *parabolic method* or the *parabolic sparse grid combination technique*. While it appears that the parabolic method is only a small permutation of the elliptic method, the consequences on the run time of the algorithm are significant. Recall that the solutions $u_{\underline{l}}$ in each step of the elliptic method are interpolated at points in $[0,1]^d$ which are not contained in $\Omega_{\underline{l}}$. Consequently, at each time step of the elliptic method, a non-negligible amount of interpolation must be performed.

On the other hand, calculating the solution u_ℓ^c by the parabolic method for a given $x \in \mathbb{R}^d$ at $t = T$ requires interpolation from grid values at $t = T$ but not at intermediate time steps prior to $t = T$. Thus, when the solution is only needed at the final time, which is frequently the case in finance, the parabolic method offers an advantage.

[2] Grids $\Omega_{\underline{l}}$ with $\underline{l} = (1,2)$ and $(2,1)$ are also included in this combination but are omitted to not clutter the diagram.

Figure 2.4: Diagram of the parabolic method, level 4. The parabolic equation is solved on each sparse grid and combined at the end. [2]



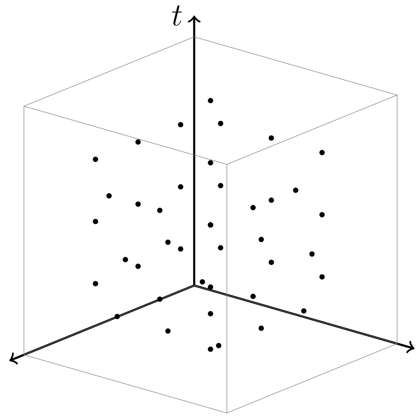
2.3.3 Space-time method

Finally, a parabolic equation can be solved by the sparse grid combination technique using a "space-time" approach where the temporal dimension is included along with the spatial dimensions in the sparse grid discretization. This is the approach of Reisinger in [Rei13, p. 556]. Reisinger notes that this approach is not viable for use with explicit schemes, since the sparse grid combination technique imposes relationships between the temporal and spatial grid spacings which violate the stability constraint associated with such schemes.

2.3.4 Summary of the three methods

We have presented three methods for the solution of parabolic PDE using a sparse grid combination technique. It is sometimes the case that authors are not explicit about which of the above methods they use, perhaps because they are unaware of the alternatives. Furthermore, it is not evident that there is a single canonical method which stands out as being *the* sparse grid combination technique. On the one hand, the sparse grid combination technique arose as a method for the solution of elliptic PDE, and much of the theory that exists has been developed for elliptic PDE, suggesting that the elliptic method is the natural approach. Although it is not always explicit, some authors seem to indicate that they are using the simpler-to-implement

Figure 2.5: Diagram of the space-time method. Time is treated no differently from the spatial coordinates and is included in the sparse grid discretization.



parabolic method. To complicate the matter further, other authors, e.g. Reisinger [Rei13], choose to combine time and space into a space-time discretization.

Henceforth, we set aside the space-time method and focus on the parabolic method and the elliptic method, both of which treat the temporal and spatial dimensions separately.

Chapter 3

Convergence of the elliptic sparse grid combination technique

This chapter culminates in a proof that the level-ℓ elliptic sparse grid combination solution converges to the exact solution u of the d-dimensional heat equation at a rate of $O(h_\ell^2 \log(h_\ell^{-1})^{d-1})$ in the L^2 norm, given that the initial condition u_0 has enough regularity (a notion which we shall make precise). We first consider the Cauchy problem for the heat equation in two spatial dimensions:

$$\begin{aligned} u_t &= u_{xx} + u_{yy} \qquad && \mathbb{R}^2 \times [0, T] \\ u(x, y, 0) &= u_0(x, y). && \end{aligned} \tag{3.1}$$

We then extend this result to the heat equation with a mixed derivative term and to the heat equation on a bounded domain with periodic boundary conditions. Finally, we prove the result for the Cauchy problem for the heat equation on $\mathbb{R}^d$ for $d \geq 2$.

We assume that the constituent sparse grid problems are solved by the fully implicit finite difference method. Recall that the sparse grid combination solution is a linear combination of solutions $u_{\underline{l}}$ with $|\underline{l}|_1 = \ell - q$ for $q \in \{0, \ldots, d-1\}$. Each of these grids are rectangular with spacings $\Delta x_i = h_{l_i} = 2^{-l_i}$ in the spatial dimensions and Δt in the temporal dimension. Across all such grids, Δt is fixed to be

$$\Delta t = \rho 2^{-2(\ell-1)},$$

for some $\rho > 0$. All equations considered in this section will be well-posed in the forward direction, so that the data is given at time $t = 0$. We consider the solution at time $t_n = n\Delta t$ where $0 < t_n \leq T$ for some time horizon $T > 0$.

3.1 Preliminaries

First, we give some preliminary definitions.

3.1.1 Function spaces

We use multi-index notation for partial derivatives. If $\underline{k} = (k_1, \dots, k_d)$, then partial derivatives are denoted by

$$D^{\underline{k}}u = \frac{\partial^{|\underline{k}|_1} u}{\partial x_1^{k_1} \dots \partial x_d^{k_d}}.$$

We measure the order of a partial derivative by the following quantities:

$$|\underline{k}|_1 = \sum_{i=1}^{d} k_i,$$
$$|\underline{k}|_\infty = \max_{i \in \{1,\dots,d\}} k_i.$$

The Sobolev space H^s is defined as follows:

$$\|u\|_{H^s}^2 := \sum_{|\underline{k}|_1 \leq s} \left|D^{\underline{k}}u\right|_2^2 := \sum_{|\underline{k}|_1 \leq s} \int_{\mathbb{R}^2} \left|D^{\underline{k}}u\right|^2 \, dx,$$
$$H^s := \{u : \mathbb{R}^2 \to \mathbb{R} : \|u\|_{H^s} < \infty\}.$$

Furthermore, the Sobolev space H^s_{mix} is defined as follows:

$$\|u\|_{H^s_{\text{mix}}}^2 := \sum_{|\underline{k}|_\infty \leq s} \left|D^{\underline{k}}u\right|_2^2 = \sum_{|\underline{k}|_\infty \leq s} \int_{\mathbb{R}^2} \left|D^{\underline{k}}u\right|^2 \, dx,$$

$$H^s_{\text{mix}} := \{u : \mathbb{R}^2 \to \mathbb{R} : \|u\|_{H^s_{\text{mix}}} < \infty\}.$$

For example, if $u \in H^1_{\text{mix}}$ then $\frac{\partial^2 u}{\partial x \partial y}$ is in L^2, but if $u \in H^1$ then $\frac{\partial^2 u}{\partial x \partial y}$ is not necessarily in L^2.

3.1.2 Partitioning of the frequency domain

Since the following proofs involve integration in the frequency domain

$$\{(\xi_1, \dots, \xi_d) \in \mathbb{R}^d\},$$

we find it useful to notate particular subsets of $\mathbb{R}^d$. In $\mathbb{R}^2$, we define

$$A_{i,j} := [0, 2^i\pi] \times [0, 2^j\pi] \tag{3.2a}$$

$$B_{i,j} := A_{i,j} \setminus \left(\left(\bigcup_{m=1}^{i-1} A_{m,j} \right) \bigcup \left(\bigcup_{n=1}^{j-1} A_{i,n} \right) \right) \tag{3.2b}$$

$$A_\ell := \bigcup_{i=1}^{\ell-1} A_{i,\ell-i} = \bigcup_{i=1}^{\ell-1} \left(\bigcup_{j=1}^{\ell-i} B_{i,j} \right). \tag{3.2c}$$

See Figures 3.1, 3.2, and 3.3. More generally, in $\mathbb{R}^d$, we define

$$A_{\underline{l}} := [0, 2^{l_1}\pi] \times \dots \times [0, 2^{l_d}\pi] \tag{3.3a}$$

$$B_{\underline{l}} := A_{\underline{l}} \setminus \left(\bigcup_{\substack{\underline{m} \text{ s.t. } m_i \leq l_i \text{ and} \\ m_i < l_i \text{ for some } i}} A_{\underline{m}} \right) \tag{3.3b}$$

$$A_\ell := \bigcup_{|\underline{l}|_1 = \ell} A_{\underline{l}} = \bigcup_{|\underline{l}|_1 \leq \ell} B_{\underline{l}}, \tag{3.3c}$$

where $\underline{l} = (l_1, \dots, l_d)$ is a multi-index.

Figure 3.1: The sets $A_{i,j} \subset \mathbb{R}^2$

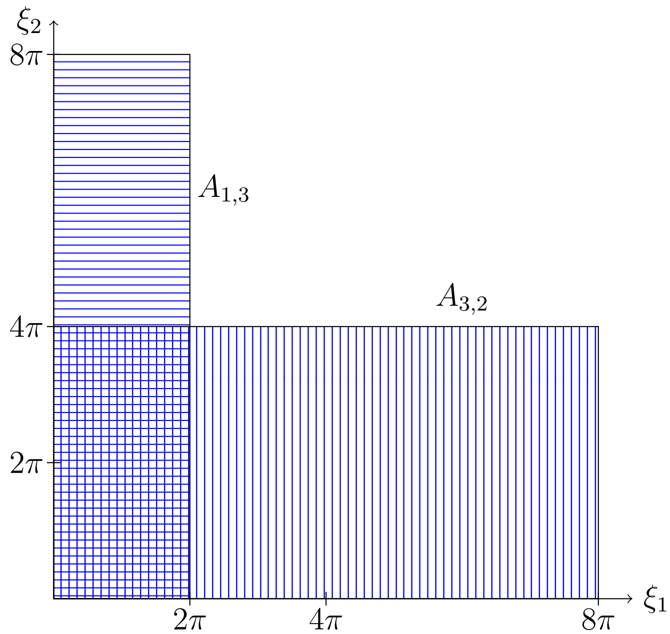


Figure 3.2: The sets $B_{i,j} \subset \mathbb{R}^2$

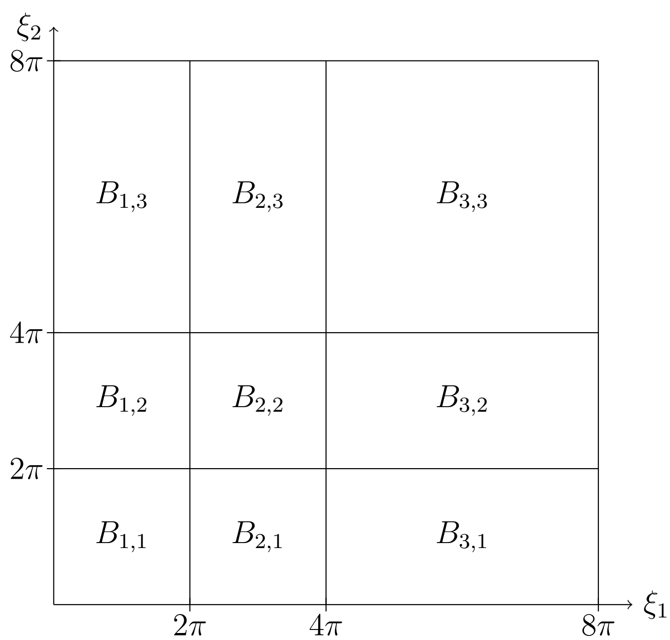
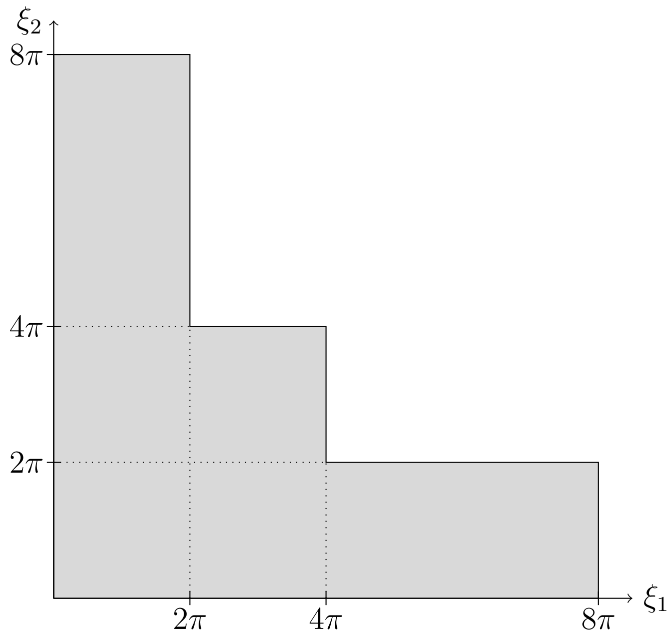


Figure 3.3: The set $A_\ell \subset \mathbb{R}^2$ when $\ell = 4$



3.2 Heat equation on $\mathbb{R}^2$

In the following theorem, we write v_{t_n} to denote the grid function which is the elliptic sparse grid combination solution of (3.4).

Theorem 4. *If the initial value problem*

$$\begin{aligned} u_t &= u_{xx} + u_{yy} \qquad \mathbb{R}^2 \times [0, T] \\ u(x, y, 0) &= u_0(x, y) \end{aligned} \tag{3.4}$$

is approximated by the elliptic sparse grid combination technique at level ℓ, in which the constituent sparse grids are solved by the fully implicit method, and the initial function is τu_0, then for each time T there exists a constant C_T independent of u_0 such that

$$\|u(t_n, \cdot) - (\sigma v_{t_n})(.)\|_2 \leq C_T h_\ell^2 \|u_0\|_{H^4_{mix}(\mathbb{R}^2)} \tag{3.5}$$

for each $t_n = n\Delta t$ with $0 < t_n \leq T$, where σ is the interpolation operator.

Note that the time t_n is fixed here and the . is a placeholder for the spatial variables x and y. We postpone the proof of the theorem until we establish two preliminary lemmas.

Lemma 5. *When the heat equation is solved by the fully implicit method, the amplification factor $g_{\Delta x, \Delta y}(\xi)$, as defined in Equation (1.11a), satisfies*

$$\begin{aligned} &e^{\Delta t q(\xi)} - g_{\Delta x, \Delta y}(\xi) \\ &= \Delta t \left(\frac{1}{2} \Delta t \mu_t |\xi|^4 - \frac{1}{12} \xi_1^4 \Delta x^2 \alpha(\xi_1, \Delta x) - \frac{1}{12} \xi_2^4 \Delta y^2 \alpha(\xi_2, \Delta y) \right), \end{aligned} \tag{3.6}$$

at every point $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$, where

$$\alpha(., .) \in (-1, 1), \quad \mu_t \in (0, 1)$$

and

$$q(\xi) = -(\xi_1^2 + \xi_2^2).$$

Proof. By Taylor's theorem, we can write $e^{-\Delta t |\xi|^2}$ as

$$e^{-\Delta t |\xi|^2} =: f(\Delta t) = f(0) + f'(0)\Delta t + \frac{1}{2} f''(\eta) \Delta t^2$$

for some $\eta \in (0, \Delta t)$ where

$$f'(\Delta t) = -|\xi|^2 e^{-\Delta t|\xi|^2},$$
$$f''(\Delta t) = |\xi|^4 e^{-\Delta t|\xi|^2}.$$

Therefore,

$$e^{-\Delta t|\xi|^2} = 1 - \Delta t|\xi|^2 + \frac{1}{2}\Delta t^2|\xi|^4 e^{-\eta|\xi|^2}.$$

If we take $\mu_t := e^{-\eta|\xi|^2} \in (0,1)$,

$$e^{-\Delta t|\xi|^2} = 1 - \Delta t|\xi|^2 + \frac{1}{2}\Delta t^2|\xi|^4 \mu_t. \tag{3.7}$$

We can write $\cos(\xi_1 \Delta x)$ as

$$\begin{aligned}\cos(\xi_1\Delta x) &=: f(\Delta x) \\ &= f(0) + f'(0)\Delta x + \frac{1}{2}f''(0)\Delta x^2 + \frac{1}{6}f'''(0)\Delta x^3 + \frac{1}{24}f''''(\eta)\Delta x^4\end{aligned}$$

for some $\eta \in (0, \Delta x)$, where

$$\begin{aligned}f'(\Delta x) &= -\xi_1 \sin(\xi_1\Delta x) \\ f''(\Delta x) &= -\xi_1^2 \cos(\xi_1\Delta x) \\ f'''(\Delta x) &= \xi_1^3 \sin(\xi_1\Delta x) \\ f''''(\Delta x) &= \xi_1^4 \cos(\xi_1\Delta x).\end{aligned}$$

Therefore,

$$\begin{aligned}\cos(\xi_1\Delta x) &= 1 - \frac{1}{2}\xi_1^2\Delta x^2 + \frac{1}{24}\cos(\xi_1\eta)\xi_1^4\Delta x^4 \\ 2\cos(\xi_1\Delta x) - 2 &= -\xi_1^2\Delta x^2 + \frac{1}{12}\cos(\xi_1\eta)\xi_1^4\Delta x^4.\end{aligned}$$

For some $\alpha(.,.) \in (-1,1)$,

$$\frac{2\cos(\xi_1\Delta x) - 2}{\Delta x^2} = -\xi_1^2 + \frac{1}{12}\xi_1^4\Delta x^2\alpha(\xi_1, \Delta x). \tag{3.8}$$

The amplification factor $g_{\Delta x,\Delta y}$ is then

$$g_{\Delta x,\Delta y} = 1 + \Delta t\left(\frac{2\cos(\xi_1\Delta x) - 2}{\Delta x^2} + \frac{2\cos(\xi_2\Delta y) - 2}{\Delta y^2}\right) \tag{3.9}$$

$$= 1 + \Delta t \left(-\xi_1^2 + \frac{1}{12}\xi_1^4 \Delta x^2 \alpha(\xi_1, \Delta x) - \xi_2^2 + \frac{1}{12}\xi_2^4 \Delta y^2 \alpha(\xi_2, \Delta y) \right). \tag{3.10}$$

Subtracting Equations (3.7) and (3.9) gives

$$\begin{aligned} &e^{\Delta t q(\xi)} - g_{\Delta x, \Delta y}(\xi) \\ &= \Delta t \left(\frac{1}{2}\Delta t \mu_t |\xi|^4 - \frac{1}{12}\xi_1^4 \Delta x^2 \alpha(\xi_1, \Delta x) - \frac{1}{12}\xi_2^4 \Delta y^2 \alpha(\xi_2, \Delta y) \right). \end{aligned} \tag{3.11}$$

□

Lemma 6. *The bound*

$$\left| \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{i=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi) \right| \leq 1 + 8\Delta t \tag{3.12}$$

holds for all $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$.

Proof. Denote

$$b(\xi) = \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{i=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} g_{i,\ell-i-1}(\xi).$$

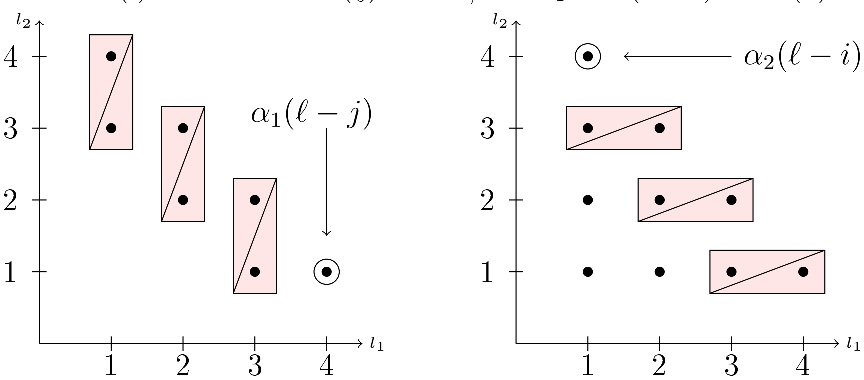
Since

$$g_{i,j}(\xi) = 1 + \Delta t \left(\frac{2\cos(\xi_1 2^{-i}) - 2}{2^{-2i}} + \frac{2\cos(\xi_2 2^{-j}) - 2}{2^{-2j}} \right),$$

we can write

$$\begin{aligned} b(\xi) = \mathbf{1}_{A_\ell} &+ \Delta t \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \left(\frac{2\cos(\xi_1 2^{-i}) - 2}{2^{-2i}} + \frac{2\cos(\xi_2 2^{-(\ell-i)}) - 2}{2^{-2(\ell-i)}} \right) \\ &- \Delta t \sum_{i=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \left(\frac{2\cos(\xi_1 2^{-i}) - 2}{2^{-2i}} + \frac{2\cos(\xi_2 2^{-(\ell-i-1)}) - 2}{2^{-2(\ell-i-1)}} \right) \\ = \mathbf{1}_{A_\ell} &+ \Delta t \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \left(\alpha_1(i) + \alpha_2(\ell - i) \right) \\ &- \Delta t \sum_{i=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \left(\alpha_1(i) + \alpha_2(\ell - i - 1) \right), \end{aligned}$$

Figure 3.4: Each black dot represents a grid Ω_{l_1,l_2} in the sparse grid combination at level 5. Each grid introduces a term $\alpha_1(.)$ and a term $\alpha_2(.)$. **Left:** All terms $\alpha_1(.)$ cancel from $b(\xi)$ on $B_{1,1}$ except $\alpha_1(\ell - j) = \alpha_1(4)$. **Right:** All terms $\alpha_2(.)$ cancel from $b(\xi)$ on $B_{1,1}$ except $\alpha_2(\ell - i) = \alpha_2(4)$.



where

$$\alpha_j(i) := \frac{2\cos(\xi_j 2^{-i}) - 2}{2^{-2i}}.$$

We can re-express $b(\xi)$ using the mutually disjoint sets $B_{i,j}$. Recall that $B_{k,l} \subset A_{i,j}$ if and only if $k \le i$ and $l \le j$. We see that all terms $\alpha_{\cdot}(.)$ from the above summations cancel except for two. See Figure 3.2 for an illustration of this cancellation. This leaves

$$b(\xi) = \mathbf{1}_{A_\ell} + \Delta t \sum_{i=1}^{\ell-i} \sum_{j=1}^{i-1} \mathbf{1}_{B_{i,j}} \left(\alpha_1(\ell - j) + \alpha_2(\ell - i)\right).$$

Due to the indicator functions, we have $b(\xi) = 0$ outside of A_ℓ. For $\xi \in A_\ell$, $b(\xi)$ is 1 plus a negative quantity inside the summation, so $b(\xi) < 1$. Furthermore, $b(\xi)$ cannot be too negative. The quantity $\alpha_1(\ell - j) + \alpha_2(\ell - i)$ can be no less than -8. So $|b(\xi)| \le 1 + 8\Delta t$. $\square$

We now present the proof of Theorem 4. We use the definition

$$\Delta_{ij} := e^{q(\xi)\Delta t} - g_{i,j}(\xi). \tag{3.13}$$

Proof of Theorem 4. To estimate the norm $\|u(x, t_n) - \sigma v_{t_n}(x)\|_2$, we must first derive an expression for $u(x, t_n) - \sigma v_{t_n}(x)$. For each time $t_n \in [0, T]$, we may express the exact solution of the heat equation as the inverse of its Fourier transform, given by Equation (1.8). That is,

$$u(x,t_n) = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{ix\cdot\xi} e^{q(\xi)t_n} \hat{u_0}(\xi)\,d\xi, \tag{3.14}$$

where $q(\xi) = -(\xi_1^2 + \xi_2^2)$.

The elliptic sparse grid solution, extended to $\mathbb{R}^2$ by the interpolation operator, is

$$(\sigma v_{t_n})(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{ix\xi}\left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi)\right)^n \hat{u_0}(\xi)\,d\xi. \tag{3.15}$$

By subtracting Equations (3.14) and (3.15), we obtain

$$\begin{aligned}
&u(x,t_n) - (\sigma v_{t_n})(x) \\
&= \frac{1}{2\pi}\int_{\mathbb{R}^2} e^{ix\xi}\left(e^{q(\xi)t_n} - \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi)\right)^n\right) \hat{u_0}(\xi)\,d\xi.
\end{aligned}$$

By Parseval's theorem,

$$\begin{aligned}
&\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2^2 \\
&= \int_{\mathbb{R}^2} \left| e^{q(\xi)t_n} - \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi)\right)^n \right|^2 \hat{u_0}(\xi)^2\,d\xi.
\end{aligned}$$

We now show that if we take $a := e^{q(\xi)\Delta t}$ and

$$b := \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{i=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} g_{i,\ell-i-1}(\xi),$$

we have

$$|a^n - b^n| \le n|a-b|e^{8t_n}. \tag{3.16}$$

This holds because

$$a^n - b^n = (a-b)\sum_{i=0}^{n-1} a^{n-i-1} b^i$$

$$|a^n - b^n| = |a-b| \left| \sum_{i=0}^{n-1} a^{n-i-1} b^i \right|.$$

Since $|a| \leq 1$ and Equation (3.12) holds, we can bound the summation by

$$\begin{aligned}
\left| \sum_{i=0}^{n-1} a^{n-i-1} b^i \right| &\leq \sum_{i=0}^{n-1} |a|^{n-i-1} |b|^i \\
&\leq n(1+8\Delta t)^n \\
&= n\left(1 + \frac{8t_n}{n}\right)^n \\
&\leq n e^{8t_n}.
\end{aligned}$$

Now using the relation $|a^n - b^n| \leq n|a-b|e^{8t_n}$,

$$\begin{aligned}
&\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2^2 \\
&= \int_{A_\ell} \left| e^{q(\xi)t_n} - \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi) \right)^n \right|^2 \hat{u}_0(\xi)^2 \, d\xi \\
&\qquad + \int_{\mathbb{R}^2 \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2 \, d\xi \\
&\leq \Omega_1(h_\ell) + \Omega_2(h_\ell),
\end{aligned}$$

where

$$\begin{aligned}
\Gamma(\xi) &:= \left| \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} (e^{q(\xi)\Delta t} - g_{i,\ell-i}(\xi)) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} (e^{q(\xi)\Delta t} - g_{j,\ell-j-1}(\xi)) \right|^2 \\
\Omega_1(h_\ell) &:= e^{16t_n} n^2 \int_{A_\ell} \Gamma(\xi) \hat{u_0}(\xi)^2 \, d\xi \\
\Omega_2(h_\ell) &:= \int_{\mathbb{R}^2 \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2 \, d\xi.
\end{aligned}$$

In order to show that $\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2 = O(h_\ell^2)$, we prove the equivalent statement $\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2^2 = O(h_\ell^4)$. Now we look at the rate of convergence of the terms $\Omega_1(h_\ell)$ and $\Omega_2(h_\ell)$.

3.2.1 Rate of convergence of $\Omega_1(h_\ell)$

The quantity $\Gamma(\xi)$, which is found in the integrand of Ω_1, contains six distinct terms, which have as a factor one of the following polynomials in ξ_1 and ξ_2:

1. ξ_1^8
2. ξ_2^8
3. $|\xi|^4\xi_1^4$
4. $|\xi|^4\xi_2^4$
5. $\xi_1^4\xi_2^4$
6. $|\xi|^8$

We shall denote each of these six terms $\Gamma_{\xi_1^8}$, $\Gamma_{\xi_2^8}$, $\Gamma_{|\xi|^4\xi_1^4}$, $\Gamma_{|\xi|^4\xi_2^4}$, $\Gamma_{\xi_1^4\xi_2^4}$, and $\Gamma_{|\xi|^8}$. We need only calculate $\Gamma_{\xi_1^8}$, $\Gamma_{|\xi|^4\xi_1^4}$, $\Gamma_{\xi_1^4\xi_2^4}$, and $\Gamma_{|\xi|^8}$—analysis of $\Gamma_{\xi_2^8}$ and $\Gamma_{|\xi|^4\xi_2^4}$ follow by symmetry. The quantity $\Gamma(\xi)$, as the square of a difference of two terms, may be expressed as

$$\begin{aligned}\Gamma(\xi) = {} & \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \Delta_{i,\ell-i}\right)^2 + \left(\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} \Delta_{j,\ell-j-1}\right)^2 \\ & - 2\left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \Delta_{i,\ell-i}\right)\left(\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} \Delta_{i,\ell-j-1}\right) \\ = {} & \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \Delta_{i,\ell-i}\Delta_{j,\ell-j} \\ & + \sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \Delta_{i,\ell-i-1}\Delta_{j,\ell-j-1} \\ & - 2\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \Delta_{i,\ell-i}\Delta_{j,\ell-j-1}.\end{aligned} \tag{3.17}$$

Note that each of the above terms contains the product of two factors which are defined in Equation (3.13). For the sake of more concise notation, we define

$$\alpha_{i,j} := \alpha(\xi_i, h_j). \tag{3.18}$$

When we multiply two such factors for arbitrary grids of multi-index (i, j) and (m, n) we get

$$
\begin{aligned}
\Delta_{i,j}\Delta_{m,n} &= (e^{q(\xi)\Delta t} - g_{i,j}(\xi))(e^{q(\xi)\Delta t} - g_{m,n}(\xi)) \\
&= \Delta t^2 \left(\frac{1}{2}\rho h_{\ell-1}^2 \mu_t |\xi|^4 - \frac{1}{12}\xi_1^4 h_i^2 \alpha(\xi_1, h_i) - \frac{1}{12}\xi_2^4 h_j^2 \alpha(\xi_2, h_j) \right) \\
&\quad \times \left(\frac{1}{2}\rho h_{\ell-1}^2 \mu_t |\xi|^4 - \frac{1}{12}\xi_1^4 h_m^2 \alpha(\xi_1, h_m) - \frac{1}{12}\xi_2^4 h_n^2 \alpha(\xi_2, h_n) \right) \\
&= \Delta t^2 \left(\frac{1}{144}(\xi_1^8 \alpha_{1,i}\alpha_{1,m} h_{i+m}^2 \right. \\
&\qquad + \xi_1^4\xi_2^4(\alpha_{1,i}\alpha_{2,n} h_{i+n}^2 \\
&\qquad + \alpha_{1,m}\alpha_{2,j} h_{j+m}^2) + \xi_2^8 \alpha_{2,j}\alpha_{2,n} h_{j+n}^8) \\
&\quad - \frac{1}{24}\mu_t \rho h_{\ell-1}^2 |\xi|^4 (\xi_1^4 \alpha_{1,i} h_i^2 + \xi_2^4 \alpha_{2,j} h_j^2) \\
&\quad - \frac{1}{24}\mu_t \rho h_{\ell-1}^2 |\xi|^4 (\xi_1^4 \alpha_{1,m} h_m^2 + \xi_1^4 \alpha_{1,n} h_n^2) \\
&\quad \left. + \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \right).
\end{aligned}
\tag{3.19}
$$

Now we substitute this expression into the formula for $\Gamma(\xi)$ and then substitute $\Gamma(\xi)$ into the formula for $\Omega_1(h_\ell)$. Note the presence of the terms $\Gamma_{\xi_1^8}$, $\Gamma_{\xi_2^8}$, $\Gamma_{|\xi|^4\xi_1^4}$, $\Gamma_{|\xi|^4\xi_2^4}$, $\Gamma_{\xi_1^4\xi_2^4}$, and $\Gamma_{|\xi|^8}$ in Equation (3.19). Now we can write

$$
\begin{aligned}
\Omega_1(h_\ell) &= e^{16t_n} n^2 \Delta t^2 \int_{A_\ell} \left(\Gamma_{\xi_1^8} + \Gamma_{\xi_2^8} + \Gamma_{|\xi|^4\xi_1^4} + \Gamma_{|\xi|^4\xi_2^4} + \Gamma_{\xi_1^4\xi_2^4} + \Gamma_{|\xi|^8} \right) \hat{u_0}(\xi)^2 \, d\xi \\
&= e^{16t_n} t_n^2 \int_{A_\ell} \left(\Gamma_{\xi_1^8} + \Gamma_{\xi_2^8} + \Gamma_{|\xi|^4\xi_1^4} + \Gamma_{|\xi|^4\xi_2^4} + \Gamma_{\xi_1^4\xi_2^4} + \Gamma_{|\xi|^8} \right) \hat{u_0}(\xi)^2 \, d\xi \\
&\le e^{16t_n} t_n^2 \int_{A_\ell} \left(|\Gamma_{\xi_1^8}| + |\Gamma_{\xi_2^8}| + |\Gamma_{|\xi|^4\xi_1^4}| + |\Gamma_{|\xi|^4\xi_2^4}| + |\Gamma_{\xi_1^4\xi_2^4}| + |\Gamma_{|\xi|^8}| \right) \hat{u_0}(\xi)^2 \, d\xi,
\end{aligned}
$$

where we have used the fact that $t_n = n\Delta t$.

We now show that $\Omega_1(h_\ell) = O(h_\ell^4)$. In the following subsections, we use the fact that if $\xi \in B_{i,j}$ then $\xi_1 \in [2^{i-1}\pi, 2^i\pi]$ for $i > 1$ and $\xi_2 \in [2^{j-1}\pi, 2^j\pi]$ for $j > 1$. Therefore,

$$
2^i \le \frac{2}{\pi}\xi_1
$$

$$2^j \leq \frac{2}{\pi}\xi_2,$$

when $i, j > 1$ so that

$$\begin{aligned} 2^i &\leq 2(1 + \frac{1}{\pi}\xi_1) \\ 2^j &\leq 2(1 + \frac{1}{\pi}\xi_2), \end{aligned}$$

for $i, j \geq 1$.

Terms of type ξ_i^8

First, we examine terms of type ξ_1^8:

$$\begin{aligned} \Gamma_{\xi_1^8} &= \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}}\mathbf{1}_{A_{j,\ell-j}}\frac{1}{144}\xi_1^8\alpha_{1,i}\alpha_{1,j}h_{i+j}^2 \\ &\quad + \sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}}\mathbf{1}_{A_{j,\ell-j-1}}\frac{1}{144}\xi_1^8\alpha_{1,i}\alpha_{1,j}h_{i+j}^2 \\ &\quad - 2\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}}\mathbf{1}_{A_{j,\ell-j-1}}\frac{1}{144}\xi_1^8\alpha_{1,i}\alpha_{1,j}h_{i+j}^2 \\ &= \frac{1}{144}\xi_1^8\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i}\mathbf{1}_{B_{i,j}}h_{2\ell-2j}^2\alpha_{1,\ell-j}^2 \\ &= \frac{1}{144}h_\ell^4\xi_1^8\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i}\mathbf{1}_{B_{i,j}}2^{4j}\alpha_{1,\ell-j}^2 \\ &\leq \frac{1}{144}h_\ell^4\xi_1^8(1 + \frac{1}{\pi}\xi_2)^4. \end{aligned}$$

Therefore, for some constant C_1,

$$\begin{aligned} \int_{A_\ell} |\Gamma_{\xi_1^8}|\hat{u_0}(\xi)^2\,d\xi &\leq \int_{A_\ell}\frac{1}{144}h_\ell^4\xi_1^8(1 + \frac{1}{\pi}\xi_2)^4\hat{u_0}(\xi)^2\,d\xi \\ &\leq \frac{1}{144}h_\ell^4\int_{A_\ell}\xi_1^8(1 + \frac{1}{\pi}\xi_2)^4\hat{u_0}(\xi)^2\,d\xi \end{aligned}$$

$$\leq \frac{1}{144}C_1 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^2)}.$$

Due to the symmetry of the problem, the above argument may be repeated, with ξ_1 replaced with ξ_2 and C_1 replaced with some constant C_2, to show

$$\int_{A_\ell} |\Gamma_{\xi_2^8}| \hat{u_0}(\xi)^2 \, d\xi \leq \frac{1}{144}C_2 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^2)}.$$

Terms of type $|\xi|^4\xi_i^4$

Next, we examine terms of type $|\xi|^4\xi_1^4$:

$$\begin{aligned}
\Gamma_{|\xi|^4\xi_1^4} &= -\frac{1}{24}\rho h_{\ell-1}^2 \mu_t \left(\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} (h_j^2 \alpha_{1,j} |\xi|^4 \xi_1^4 + h_i^2 \alpha_{1,i} |\xi|^4 \xi_1^4) \right. \\
&\qquad + \sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} (h_j^2 \alpha_{1,j} |\xi|^4 \xi_1^4 + h_i^2 \alpha_{1,i} |\xi|^4 \xi_1^4) \\
&\qquad \left. -2 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} (h_j^2 \alpha_{1,j} |\xi|^4 \xi_1^4 + h_i^2 \alpha_{1,i} |\xi|^4 \xi_1^4) \right) \\
&= -\frac{1}{24}\rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_1^4 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}} 2 h_{\ell-j}^2 \alpha_{1,\ell-j} \\
&= -\frac{1}{12}\rho h_{\ell-1}^2 h_\ell^2 \mu_t |\xi|^4 \xi_1^4 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}} 2^{2j} \alpha_{1,\ell-j} \\
&= -\frac{1}{3}\rho h_\ell^4 \mu_t |\xi|^4 \xi_1^4 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}} 2^{2j} \alpha_{1,\ell-j} \\
|\Gamma_{|\xi|^4\xi_1^4}| &\leq \frac{1}{3}\rho h_\ell^4 \mu_t |\xi|^4 \xi_1^4 (1 + \frac{1}{\pi}\xi_2)^2.
\end{aligned}$$

Therefore, for some constant C_3,

$$\int_{A_\ell} |\Gamma_{|\xi|^4\xi_1^4}| \hat{u_0}(\xi)^2 \, d\xi \leq \int_{A_\ell} \frac{1}{3}\rho h_\ell^4 \mu_t |\xi|^4 \xi_1^4 (1 + \frac{1}{\pi}\xi_2)^2 \hat{u_0}(\xi)^2 \, d\xi$$

$$= \frac{1}{3}\rho h_\ell^4 \mu_t \int_{A_\ell} |\xi|^4 \xi_1^4 (1 + \frac{1}{\pi}\xi_2)^2 \hat{u_0}(\xi)^2 \, d\xi$$
$$\le \frac{1}{3}\rho h_\ell^4 \mu_t C_3 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)}.$$

Similarly, for some constant C_4,

$$\int_{A_\ell} |\Gamma_{|\xi|^4\xi_2^4}| \hat{u_0}(\xi)^2 \, d\xi \le \frac{1}{3}\rho h_\ell^4 \mu_t C_4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)}.$$

Terms of type $\xi_1^4\xi_2^4$

Next, we examine terms of type $\xi_1^4\xi_2^4$:

$$\begin{aligned}
\Gamma_{\xi_1^4\xi_2^4} = & \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \frac{1}{144} (h^2_{i+\ell-j} \alpha_{1,i}\alpha_{2,\ell-j}\xi_1^4\xi_2^4 + h^2_{\ell-i+j}\alpha_{2,\ell-i}\alpha_{1,j}\xi_1^4\xi_2^4) \\
& + \sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \frac{1}{144} (h^2_{i+\ell-j-1} \alpha_{1,i}\alpha_{2,\ell-j-1}\xi_1^4\xi_2^4 \\
& \qquad + h^2_{\ell-i-1+j}\alpha_{2,\ell-i-1}\alpha_{1,j}\xi_1^4\xi_2^4) \\
& - 2\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \frac{1}{144} (h^2_{i+\ell-j-1} \alpha_{1,i}\alpha_{2,\ell-j-1}\xi_1^4\xi_2^4 \\
& \qquad + h^2_{\ell-i+j}\alpha_{2,\ell-i}\alpha_{1,j}\xi_1^4\xi_2^4) \\
= & \frac{1}{144}\xi_1^4\xi_2^4 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}} h^2_{2\ell-i-j}\alpha_{1,\ell-i}\alpha_{2,\ell-j} \\
= & \frac{1}{144} h_\ell^4 \xi_1^4\xi_2^4 \sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}} 2^{2(i+j)}\alpha_{1,\ell-i}\alpha_{2,\ell-j} \\
|\Gamma_{\xi_1^4\xi_2^4}| \le & \frac{1}{144} h_\ell^4 \xi_1^4\xi_2^4 (1 + \frac{1}{\pi}\xi_1)^2 (1 + \frac{1}{\pi}\xi_2)^2.
\end{aligned}$$

Therefore, for some constant C_5,

$$\int_{A_\ell} |\Gamma_{\xi_1^4\xi_2^4}| \hat{u_0}(\xi)^2 \, d\xi \le \int_{A_\ell} \frac{1}{144} h_\ell^4 \xi_1^4\xi_2^4 (1 + \frac{1}{\pi}\xi_1)^2 (1 + \frac{1}{\pi}\xi_2)^2 \hat{u_0}(\xi)^2 \, d\xi$$

$$
\begin{aligned}
&= \frac{1}{144} h_\ell^4 \int_{A_\ell} \xi_1^4 \xi_2^4 (1 + \frac{1}{\pi}\xi_1)^2 (1 + \frac{1}{\pi}\xi_2)^2 \hat{u_0}(\xi)^2 \, d\xi \\
&\leq \frac{1}{144} h_\ell^4 C_5 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^2)}.
\end{aligned}
$$

Terms of type $|\xi|^8$

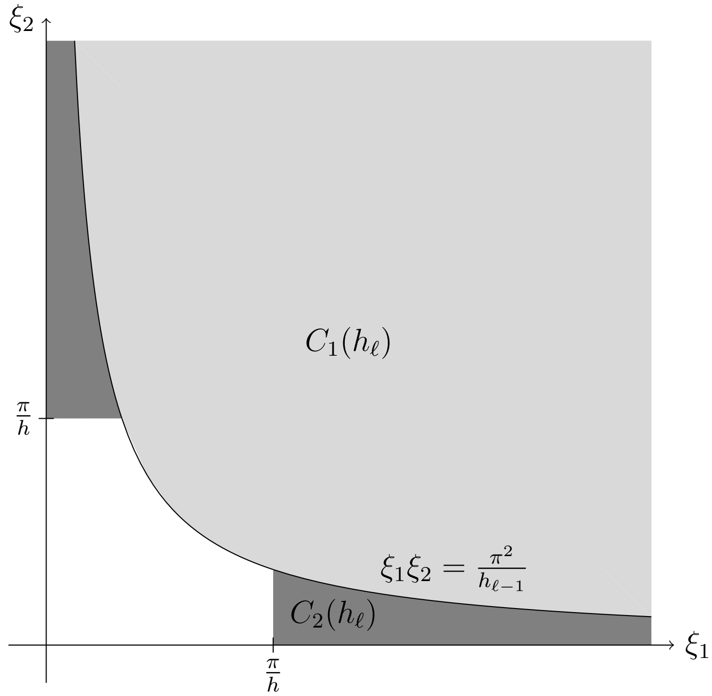
Finally, we examine terms of type $|\xi|^8$:

$$
\begin{aligned}
\Gamma_{|\xi|^8} &= \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \\
&\quad + \sum_{i=1}^{\ell-2} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \\
&\quad - 2 \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \\
&= \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \Bigg(\sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \\
&\quad + \sum_{i=1}^{\ell-2} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \\
&\quad -2 \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \Bigg) \\
&= 4 \rho^2 h_\ell^4 \mu_t^2 |\xi|^8 \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-i} \mathbf{1}_{B_{i,j}}.
\end{aligned}
$$

Therefore, for some constant C_6,

$$
\begin{aligned}
\int_{A_\ell} |\Gamma_{|\xi|^8}| \hat{u_0}(\xi)^2 \, d\xi &\leq \int_{A_\ell} 4 \rho^2 h_\ell^4 \mu_t^2 |\xi|^8 \hat{u_0}(\xi)^2 \, d\xi \\
&= 4 \rho^2 h_\ell^4 \mu_t^2 \int_{A_\ell} |\xi|^8 \hat{u_0}(\xi)^2 \, d\xi \\
&\leq 4 \rho^2 h_\ell^4 \mu_t^2 C_6 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^2)}.
\end{aligned}
$$

Figure 3.5: The sets $C_1(h_\ell)$ and $C_2(h_\ell)$.



Conclusion

In summary,

$$
\begin{aligned}
\Omega_1(h_\ell) &\leq e^{16t_n} t_n^2 \int_{A_\ell} \left(|\Gamma_{\xi_1^8}| + |\Gamma_{\xi_2^8}| + |\Gamma_{|\xi|^4\xi_1^4}| + |\Gamma_{|\xi|^4\xi_2^4}| + |\Gamma_{|\xi|^4\xi_1^4}| + |\Gamma_{|\xi|^8}| \right) \hat{u_0}(\xi)^2 \, d\xi \\
&= e^{16t_n} t_n^2 \Bigg(\frac{1}{144} C_1 h_\ell^4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} + \frac{1}{144} C_2 h_\ell^4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} + \frac{1}{3} \rho h_\ell^4 \mu_t C_3 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} \\
&\qquad + \frac{1}{3} \rho h_\ell^4 \mu_t C_4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} + \frac{1}{144} h_\ell^4 C_5 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} + 4\rho^2 h_\ell^4 \mu_t^2 C_6 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^2)} \Bigg).
\end{aligned}
$$

Therefore, $\Omega_1(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\mathrm{mix}}(\mathbb{R}^2)$.

3.2.2 Rate of convergence of $\Omega_2(h_\ell)$

Define $C_1(h_\ell) := \{(\xi_1, \xi_2) : \xi_1\xi_2 \geq \frac{\pi^2}{h_{\ell-1}}\}$ and $C_2(h_\ell) := \mathbb{R}^2 \setminus C_1(h_\ell) \setminus A_\ell$. Then $\mathbb{R}^2 \setminus A_\ell \subset C_1(h_\ell) \cup C_2(h_\ell)$. See Figure 3.5.

Since $|e^{q(\xi)t_n}| \leq 1$, we have

$$\begin{aligned}\Omega_2(h_\ell) &= \int_{\mathbb{R}^2\setminus A_\ell} |e^{q(\xi)t_n}\hat{u_0}(\xi)|^2\, d\xi \\ &\leq \int_{\mathbb{R}^2\setminus A_\ell} |\hat{u_0}(\xi)|^2\, d\xi \\ &\leq \int_{C_1(h_\ell)} |\hat{u_0}(\xi)|^2\, d\xi + \int_{C_2(h_\ell)} |\hat{u_0}(\xi)|^2\, d\xi.\end{aligned}$$

On the domain $C_1(h_\ell)$ we have $1 \leq \frac{\xi_1\xi_2 h_{\ell-1}}{\pi^2}$ and thus $1 \leq \frac{\xi_1^4\xi_2^4 h_{\ell-1}^4}{\pi^8}$. Therefore, we have for the first term:

$$\begin{aligned}\int_{C_1(h_\ell)} |\hat{u_0}(\xi)|^2\, d\xi &\leq \frac{1}{\pi^8} h_{\ell-1}^4 \int_{C_1(h_\ell)} \xi_1^4\xi_2^4 |\hat{u_0}(\xi)|^2\, d\xi \\ &\leq \frac{16}{\pi^8} h_\ell^4 \left\|\frac{\partial^4 u_0}{\partial x^2 \partial y^2}\right\|_2^2.\end{aligned}$$

For the second term, we have $\xi_1 \geq \frac{\pi}{h_\ell}$ or $1 \leq \frac{\xi_1 h_\ell}{\pi}$ and thus $1 \leq \frac{\xi_1^4 h_\ell^4}{\pi^4}$ and, similarly, $1 \leq \frac{\xi_2^4 h_\ell^4}{\pi^4}$:

$$\begin{aligned}&\int_{C_2(h_\ell)} |\hat{u_0}(\xi)|^2\, d\xi \\ &= \int_{\pi/h_\ell}^{\infty} \int_0^{\pi^2/h_\ell \xi_1} |\hat{u_0}(\xi)|^2\, d\xi_2\, d\xi_1 + \int_{\pi/h_\ell}^{\infty} \int_0^{\pi^2/h_\ell \xi_2} |\hat{u_0}(\xi)|^2\, d\xi_1\, d\xi_2 \\ &\leq \frac{1}{\pi^4} h_\ell^4 \left(\int_{\pi/h_\ell}^{\infty} \int_0^{\pi^2/h_\ell \xi_1} \xi_1^4 |\hat{u_0}(\xi)|^2\, d\xi_2\, d\xi_1 + \int_{\pi/h_\ell}^{\infty} \int_0^{\pi^2/h_\ell \xi_2} \xi_2^4 |\hat{u_0}(\xi)|^2\, d\xi_1\, d\xi_2 \right) \\ &\leq \frac{1}{\pi^4} h_\ell^4 \left(\left\|\frac{\partial^2 u_0}{\partial x^2}\right\|_2^2 + \left\|\frac{\partial^2 u_0}{\partial y^2}\right\|_2^2 \right).\end{aligned}$$

Adding the two parts of $\Omega(h_\ell)$ then gives

$$\begin{aligned}\Omega_2(h_\ell) &\leq \int_{C_1(h_\ell)} |\hat{u}_0(\xi)|^2\, d\xi + \int_{C_2(h_\ell)} |\hat{u}_0(\xi)|^2\, d\xi \\ &\leq h_\ell^4 \left(\frac{16}{\pi^8} \left\| \frac{\partial^4 u_0}{\partial x^2 \partial y^2} \right\|_2^2 + \frac{1}{\pi^4} \left\| \frac{\partial^2 u_0}{\partial x^2} \right\|_2^2 + \frac{1}{\pi^4} \left\| \frac{\partial^2 u_0}{\partial y^2} \right\|_2^2 \right).\end{aligned}$$

In summary, $\Omega_2(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^2)$. Thus,

$$\begin{aligned}\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2^2 &= \Omega_1(h_\ell) + \Omega_2(h_\ell) \\ &= O(h_\ell^4) + O(h_\ell^4) \\ &= O(h_\ell^4)\end{aligned}$$

when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^2)$ and so $\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2 = O(h_\ell^2)$.

$\square$

3.3 Heat equation with mixed derivatives on $\mathbb{R}^2$

We now repeat the preceding analysis for the Cauchy problem for the heat equation with a mixed derivative term:

$$\begin{aligned} &u_t = u_{xx} + u_{xy} + u_{yy} \quad \mathbb{R}^2 \times [0,T] \\ &u(x,y,0) = u_0(x,y). \end{aligned} \tag{3.20}$$

We choose this equation because it is representative of the class of well-scaled parabolic equations. We must repeat Lemma 5, this time for Equation (3.20).

Lemma 7. *When the heat equation is solved by the fully implicit method, the amplification factor $g_{\Delta x,\Delta y}(\xi)$, as defined in Equation (1.11b), satisfies*

$$\begin{aligned} e^{\Delta t q(\xi)} - g_{\Delta x,\Delta y}(\xi) = \Delta t \Bigg(&\frac{1}{2}\Delta t \mu_t (|\xi|^2 + \xi_1\xi_2)^2 + \frac{1}{36}\xi_1^3\xi_2^3\beta(\xi_1,\Delta x)\beta(\xi_2,\Delta y)\Delta x^2\Delta y^2 \\ &-\Delta x^2 (\frac{1}{6}\xi_2\xi_1^3\beta(\xi_1,\Delta x) + \frac{1}{12}\xi_1^4\alpha(\xi_1,\Delta x)) \\ &-\Delta y^2 (\frac{1}{12}\xi_2^4\alpha(\xi_2,\Delta y) + \frac{1}{6}\xi_1\xi_2^3\beta(\xi_2,\Delta y)) \Bigg) \end{aligned} \tag{3.21}$$

at every point $\xi = (\xi_1,\xi_2) \in \mathbb{R}^2$, where

$$\alpha(.,.) \in (-1,1), \quad \beta(.,.) \in (-1,1), \quad \mu_t \in (0,1)$$

and

$$q(\xi) = -(\xi_1^2 + \xi_2^2 + \xi_1\xi_2).$$

Proof. By Taylor's theorem, we can write $e^{\Delta t q(\xi)}$ as

$$e^{-\Delta t(|\xi|^2+\xi_1\xi_2)} =: f(\Delta t) = f(0) + f'(0)\Delta t + \frac{1}{2}f''(\eta)\Delta t^2$$

for some $\eta \in (0,\Delta t)$ where

$$\begin{aligned} f'(\Delta t) &= -(|\xi|^2 + \xi_1\xi_2)e^{-\Delta t(|\xi|^2+\xi_1\xi_2)}, \\ f''(\Delta t) &= (|\xi|^2 + \xi_1\xi_2)^2 e^{-\Delta t(|\xi|^2+\xi_1\xi_2)}. \end{aligned}$$

Therefore,

$$e^{-\Delta t(|\xi|^2+\xi_1\xi_2)} = 1 - \Delta t(|\xi|^2 + \xi_1\xi_2) + \frac{1}{2}\Delta t^2(|\xi|^2 + \xi_1\xi_2)^2 e^{-\eta(|\xi|^2+\xi_1\xi_2)}.$$

If we take $\mu_t := e^{-\eta(|\xi|^2+\xi_1\xi_2)} \in (0, 1)$,

$$e^{-\Delta t(|\xi|^2+\xi_1\xi_2)} = 1 - \Delta t(|\xi|^2 + \xi_1\xi_2) + \frac{1}{2}\Delta t^2(|\xi|^2 + \xi_1\xi_2)^2 \mu_t. \tag{3.22}$$

From Equation 3.8 we have

$$\frac{2\cos(\xi_1\Delta x) - 2}{\Delta x^2} = -\xi_1^2 + \frac{1}{12}\xi_1^4 \Delta x^2 \alpha(\xi_1, \Delta x). \tag{3.23}$$

By Taylor's theorem, we can write $\sin(\xi_1\Delta x)$ as

$$\sin(\xi_1\Delta x) =: f(x) = f(0) + f'(0)\Delta x + \frac{1}{2}f''(0)\Delta x^2 + \frac{1}{6}f'''(\eta)\Delta x^3$$

for some $\eta \in (0, \Delta x)$, where

$$\begin{aligned} f'(\Delta x) &= \xi_1 \cos(\xi_1\Delta x) \\ f''(\Delta x) &= -\xi_1^2 \sin(\xi_1\Delta x) \\ f'''(\Delta x) &= -\xi_1^3 \cos(\xi_1\Delta x). \end{aligned}$$

Therefore, for some $\beta(.,.) \in (-1, 1)$,

$$\begin{aligned} \sin(\xi_1\Delta x) &= \xi_1\Delta x - \frac{1}{6}\xi_1^3 \cos(\xi_1\eta)\Delta x^3 \\ \frac{\sin(\xi_1\Delta x)}{\Delta x} &= \xi_1 - \frac{1}{6}\xi_1^3 \cos(\xi_1\eta)\Delta x^2 \\ \frac{\sin(\xi_1\Delta x)}{\Delta x} &= \xi_1 - \frac{1}{6}\xi_1^3 \beta(\xi_1, \Delta x)\Delta x^2. \end{aligned}$$

Multiplying two such factors gives

$$\begin{aligned} \frac{\sin(\xi_1\Delta x)\sin(\xi_2\Delta y)}{\Delta x\Delta y} &= (\xi_1 - \frac{1}{6}\xi_1^3\beta(\xi_1, \Delta x)\Delta x^2)(\xi_2 - \frac{1}{6}\xi_2^3\beta(\xi_2, \Delta y)\Delta y^2) \\ &= \xi_1\xi_2 - \frac{1}{6}\xi_2\xi_1^3\beta(\xi_1, \Delta x)\Delta x^2 - \frac{1}{6}\xi_1\xi_2^3\beta(\xi_2, \Delta y)\Delta y^2 \end{aligned}$$

$$+\frac{1}{36}\xi_1^3\xi_2^3\beta(\xi_1,\Delta x)\beta(\xi_2,\Delta y)\Delta x^2\Delta y^2.$$

The amplification factor $g_{\Delta x,\Delta y}$ is then

$$\begin{aligned}
g_{\Delta x,\Delta y}(\xi) &= 1+\Delta t\left(\frac{2\cos(\xi_1\Delta x)-2}{\Delta x^2}+\frac{2\cos(\xi_2\Delta y)-2}{\Delta y^2}-\frac{\sin(\xi_1\Delta x)\sin(\xi_2\Delta y)}{\Delta x\Delta y}\right)\\
&= 1+\Delta t\left(-\xi_1^2+\frac{1}{12}\xi_1^4\Delta x^2\alpha(\xi_1,\Delta x)-\xi_2^2+\frac{1}{12}\xi_2^4\Delta y^2\alpha(\xi_2,\Delta y)\right.\\
&\qquad -\xi_1\xi_2+\frac{1}{6}\xi_2\xi_1^3\beta(\xi_1,\Delta x)\Delta x^2+\frac{1}{6}\xi_1\xi_2^3\beta(\xi_2,\Delta y)\Delta y^2\\
&\qquad \left.-\frac{1}{36}\xi_1^3\xi_2^3\beta(\xi_1,\Delta x)\beta(\xi_2,\Delta y)\Delta x^2\Delta y^2\right).
\end{aligned} \tag{3.24}$$

Subtracting Equations (3.22) and (3.24) gives

$$\begin{aligned}
e^{\Delta t q(\xi)}-g_{\Delta x,\Delta y}(\xi) &= \Delta t\left(\frac{1}{2}\Delta t\mu_t(|\xi|^2+\xi_1\xi_2)^2\right.\\
&\qquad +\frac{1}{36}\xi_1^3\xi_2^3\beta(\xi_1,\Delta x)\beta(\xi_2,\Delta y)\Delta x^2\Delta y^2\\
&\qquad -\Delta x^2\left(\frac{1}{6}\xi_2\xi_1^3\beta(\xi_1,\Delta x)+\frac{1}{12}\xi_1^4\alpha(\xi_1,\Delta x)\right)\\
&\qquad \left.-\Delta y^2\left(\frac{1}{12}\xi_2^4\alpha(\xi_2,\Delta y)+\frac{1}{6}\xi_1\xi_2^3\beta(\xi_2,\Delta y)\right)\right) \qquad (3.25)\\
&=: \Delta t\,\big(\Phi_1\Delta t\\
&\qquad +\Phi_2(\Delta x)\Delta x^2+\Phi_3(\Delta y)\Delta y^2\\
&\qquad +\Phi_4(\Delta x,\Delta y)\Delta x^2\Delta y^2\big),
\end{aligned}$$

□

where we have defined Φ_i, $i\in\{1,2,3,4\}$, for convenience of notation.

Now we state the convergence theorem for the heat equation with mixed derivatives.

Theorem 8. *If the initial value problem*

$$\begin{aligned}
&u_t = u_{xx}+u_{xy}+u_{yy} \quad \mathbb{R}^2\times[0,T]\\
&u(x,y,0)=u_0(x,y)
\end{aligned} \tag{3.26}$$

is approximated by the elliptic sparse grid combination technique at level ℓ, in which the constituent sparse grids are solved by the fully implicit method, and the initial function is τu_0, then for each time T there exists a constant C_T independent of u_0 such that

$$\|u(t_n,\cdot)-(\sigma v_{t_n})(.)\|_2 \le C_T h_\ell^2 \log_2(h_\ell^{-1})\|u_0\|_{H^4_{mix}(\mathbb{R}^2)} \tag{3.27}$$

for each $t_n = n\Delta t$ with $0 < t_n \le T$.

Proof. As in Theorem 4, we can write

$$\|u(x,t_n)-(\sigma v_{t_n})(x)\|_2^2 = \Omega_1(h_\ell)+\Omega_2(h_\ell),$$

where $\Omega_1(h_\ell)$ and $\Omega_2(h_\ell)$ have the same definition. Since the domain has the same geometry, $\Omega_2(h_\ell)$ still has the convergence rate of $O(h_\ell^4)$ when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^2)$. The equation-specific part is $\Omega_1(h_\ell)$, which we proceed to analyze. As before, the term $\Gamma(\xi)$ inside $\Omega(h_\ell)$ can be expanded to

$$\begin{aligned}\Gamma(\xi) = &\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1}\mathbf{1}_{A_{i,\ell-i}}\mathbf{1}_{A_{j,\ell-j}}(e^{q(\xi)n\Delta t}-g^n_{i,\ell-i}(\xi))(e^{q(\xi)n\Delta t}-g^n_{j,\ell-j}(\xi))\\ &+\sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2}\mathbf{1}_{A_{i,\ell-i-1}}\mathbf{1}_{A_{j,\ell-j-1}}(e^{q(\xi)n\Delta t}-g^n_{i,\ell-i-1}(\xi))(e^{q(\xi)n\Delta t}-g^n_{j,\ell-j-1}(\xi))\\ &-2\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2}\mathbf{1}_{A_{i,\ell-i}}\mathbf{1}_{A_{j,\ell-j-1}}(e^{q(\xi)n\Delta t}-g^n_{i,\ell-i}(\xi))(e^{q(\xi)n\Delta t}-g^n_{j,\ell-j-1}(\xi)).\end{aligned}$$

For the heat equation with mixed derivatives, the analogue of Equation (3.19) is

$$
\begin{aligned}
&(e^{q(\xi)\Delta t} - g_{i,j}(\xi))(e^{q(\xi)\Delta t} - g_{m,n}(\xi)) \\
&= \Delta t^2 \left(\Phi_1 \rho h_{\ell-1}^2 + \Phi_2(i) h_i^2 + \Phi_3(j) h_j^2 + \Phi_4(i,j) h_{i+j}^2\right) \times \\
&\qquad \left(\Phi_1 \rho h_{\ell-1}^2 + \Phi_2(m) h_m^2 + \Phi_3(n) h_n^2 + \Phi_4(m,n) h_{m+n}^2\right) \\
&= \Delta t^2 \left(\Phi_1^2 \rho^2 h_{\ell-1}^4 + \Phi_2(i)\Phi_2(m) h_{i+m}^2\right. \\
&\qquad + \Phi_3(j)\Phi_3(n) h_{j+n}^2 + \Phi_4(i,j)\Phi_4(m,n) h_{i+j+m+n}^2 \\
&\qquad + \Phi_1 \rho h_{\ell-1}^2 (\Phi_2(i) h_i^2 + \Phi_2(m) h_m^2) + \Phi_1 \rho h_{\ell-1}^2 (\Phi_3(j) h_j^2 + \Phi_3(n) h_n^2) \\
&\qquad + \Phi_1 \rho h_{\ell-1}^2 (\Phi_4(m,n) h_{m+n}^2 + \Phi_4(i,j) h_{i+j}^2) \\
&\qquad + \Phi_2(i)\Phi_3(n) h_{i+n}^2 + \Phi_2(m)\Phi_3(j) h_{j+m}^2 + \Phi_2(i)\Phi_4(m,n) h_{i+m+n}^2 \\
&\qquad \left. + \Phi_2(m)\Phi_4(i,j) h_{m+i+j}^2 + \Phi_3(j)\Phi_4(m,n) h_{j+m+n}^2 + \Phi_3(n)\Phi_4(i,j) h_{n+i+j}^2\right).
\end{aligned} \tag{3.28}
$$

Now we substitute this expression into the formula for $\Gamma(\xi)$ and then substitute $\Gamma(\xi)$ into the formula for $\Omega_1(h_\ell)$. After this, our work entails determining the convergence rate of each of the terms which comprise $\Omega_1(h_\ell)$. We have

$$
\begin{aligned}
\Omega_1(h_\ell) &= e^{16t_n} n^2 \Delta t^2 \int_{A_\ell} (\Gamma_1 + \Gamma_2 + \ldots)\, \hat{u_0}(\xi)^2 \, d\xi \\
&= e^{16t_n} t_n^2 \int_{A_\ell} (\Gamma_1 + \Gamma_2 + \ldots)\, \hat{u_0}(\xi)^2 \, d\xi \\
&\leq e^{16t_n} t_n^2 \int_{A_\ell} (|\Gamma_1| + |\Gamma_2| + \ldots)\, \hat{u_0}(\xi)^2 \, d\xi.
\end{aligned}
$$

Since the terms are quite similar to those in the proof for the heat equation, we focus only on the novel terms:

$$
\begin{aligned}
\Gamma_1 = &\sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \Phi_2(i) \Phi_4(j, \ell-j) h_{\ell+i}^2 \\
&+ \sum_{i=1}^{\ell-2} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \Phi_2(i) \Phi_4(j, \ell-j-1) h_{\ell+i-1}^2 \\
&- 2 \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \Phi_2(i) \Phi_4(j, \ell-j-1) h_{\ell+i-1}^2
\end{aligned}
$$

$$
\begin{aligned}
\Gamma_2 = &\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j}} \Phi_4(i,\ell-i)\Phi_4(j,\ell-j)h_{2\ell}^2 \\
&+ \sum_{i=1}^{\ell-2}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i-1}} \mathbf{1}_{A_{j,\ell-j-1}} \Phi_4(i,\ell-i-1)\Phi_4(j,\ell-j-1)h_{2\ell-2}^2 \\
&- 2\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-2} \mathbf{1}_{A_{i,\ell-i}} \mathbf{1}_{A_{j,\ell-j-1}} \Phi_4(i,\ell-i)\Phi_4(j,\ell-j-1)h_{2\ell-1}^2
\end{aligned}
$$

Convergence of Γ_1

The summation is over pairs of grids $(\Omega_{i,j}, \Omega_{m,n})$. For each pair (m,n), all terms $\Phi_2(i)\Phi_4(m,n)h_{i+m+n}^2$ cancel except for one due to offsetting of adjacent grids. The term which remains in each case has $i = \ell - 1$. Figure 3.2 again provides a good visualization. Hence, the number of terms grows like the number of combined grids, which is $2\ell - 3 = 2\log_2(h_\ell^{-1}) - 3 = O(\log_2(h_\ell^{-1}))$, and so we have

$$\int_{A_\ell} |\Gamma_1| \hat{u_0}(\xi)^2 \, d\xi = O(h_\ell^4 \log_2(h_\ell^{-1})).$$

Convergence of Γ_2

The summation is over pairs of grids $(\Omega_{i,j}, \Omega_{m,n})$. Each term $\Phi_4(i,j)\Phi_4(m,n)$ is distinct and not canceled out by any other term. Hence, the number of terms grows like the square of the number of combined grids, which is $(2\ell-3)^2 = O(\log_2(h_\ell^{-1})^2)$, and so we have

$$\int_{A_\ell} |\Gamma_2| \hat{u_0}(\xi)^2 \, d\xi = O(h_\ell^4 \log_2(h_\ell^{-1})^2).$$

Conclusion

The convergence rate of $\Omega_1(h_\ell)$ is now limited by the last term. We have $\Omega_1(h_\ell) = O(h_\ell^4 \log(h_\ell^{-1})^2)$ when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^2)$, and so we have the result

$$\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2 = O(h_\ell^2 \log(h_\ell^{-1}))$$

when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^2)$ for the heat equation with a mixed derivative term. $\square$

3.4 Heat equation on a periodic domain in $\mathbb{R}^2$

We now give a proof of the convergence of the elliptic sparse grid combination technique for an initial-boundary value problem for the heat equation with periodic boundary conditions. We need some notation for Fourier series which, being tangential to the main course of this work, can be found in the appendix.

Theorem 9. *If the initial-boundary value problem*

$$\begin{aligned} &u_t = u_{xx} + u_{yy} && [-\pi,\pi]^2 \times [0,T] \\ &u(x,y,0) = u_0(x,y) && \\ &u(-\pi,y,t) = u(\pi,y,t) && \\ &u(x,-\pi,t) = u(x,\pi,t) && \end{aligned} \tag{3.29}$$

is approximated by the elliptic sparse grid combination technique at level ℓ, in which the constituent sparse grids are solved by the fully implicit method, and the initial function is τu_0, then for each time T there exists a constant C_T independent of u_0 such that

$$\|u(t_n,.) - (\sigma v_{t_n})(.)\|_2 \leq C_T h_\ell^2 \|u_0\|_{H^4_{mix}([-\pi,\pi]^2)} \tag{3.30}$$

for each $t_n = n\Delta t$ with $0 < t_n \leq T$.

Proof. Let $\{\hat{u}(\xi,t_n)\}_{\xi_1,\xi_2=-\infty}^{\infty}$ denote the Fourier coefficients of $u(x,t_n)$. For each time $t_n \in [0,T]$, we may write the exact solution of the heat equation by inverting its Fourier transform. That is,

$$\begin{aligned} u(x,t_n) &= \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} e^{ix\cdot\xi} \hat{u}(\xi,t_n) \\ &= \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} e^{ix\cdot\xi} e^{t_n q(\xi)} \hat{u}_0(\xi), \end{aligned} \tag{3.31}$$

where $q(\xi) = -(\xi_1^2 + \xi_2^2)$.

The elliptic sparse grid solution, extended to $[-\pi,\pi]^2$ by the interpolation operator σ, is

$$(\sigma v_{t_n})(x) = \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} e^{ix\cdot\xi} \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi) \right)^n \hat{u}_0(\xi). \tag{3.32}$$

By subtracting Equations (3.31) and (3.32), we obtain

$$u(x,t_n) - (\sigma v_{t_n})(x) =$$
$$\sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} e^{ix\cdot\xi} \left(e^{t_n q(\xi)} - \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi) \right)^n \right) \hat{u}_0(\xi).$$

By Parseval's theorem, and the discrete analogue of Lemma 6,

$$\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2 =$$
$$\sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \left| e^{t_n q(\xi)} - \left(\sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} g_{i,\ell-i}(\xi) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} g_{j,\ell-j-1}(\xi) \right)^n \right|^2 \hat{u}_0(\xi)$$
$$\leq e^{16t_n} n^2 \Omega_1(h_\ell) + \Omega_2(h_\ell)$$

where

$$\Gamma(\xi) := \left| \sum_{i=1}^{\ell-1} \mathbf{1}_{A_{i,\ell-i}} (e^{q(\xi)\Delta t} - g_{i,\ell-i}(\xi)) - \sum_{j=1}^{\ell-2} \mathbf{1}_{A_{j,\ell-j-1}} (e^{q(\xi)\Delta t} - g_{j,\ell-j-1}(\xi)) \right|^2$$
$$\Omega_1(h_\ell) := \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \Gamma(\xi) \hat{u}_0(\xi)$$
$$\Omega_2(h_\ell) := \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \mathbf{1}_{\mathbb{R}^2 \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2.$$

Again, we have defined $\Gamma(\xi)$ to be the factor inside the summation which multiplies $\hat{u}_0(\xi)^2$. Now we look at the rate of convergence of the terms $\Omega_1(h_\ell)$ and $\Omega_2(h_\ell)$.

3.4.1 Rate of convergence of $\Omega_1(h_\ell)$

Since Equations (3.17) and (3.19) still hold, the quantity $\Gamma(\xi)$ is notationally the same as in Theorem 4, aside from the different definitions of the sets $A_{i,j}$. Therefore, we still have

$$\begin{aligned}
|\Gamma_{\xi_1^8}| &\leq \frac{1}{144} h_\ell^4 \xi_1^8 (1+\xi_2)^4 \\
|\Gamma_{\xi_2^8}| &\leq \frac{1}{144} h_\ell^4 \xi_2^8 (1+\xi_1)^4 \\
|\Gamma_{|\xi|^4\xi_1^4}| &\leq \frac{1}{3} \rho h_\ell^4 \mu_t |\xi|^4 \xi_1^4 (1+\xi_2)^2 \\
|\Gamma_{|\xi|^4\xi_2^4}| &\leq \frac{1}{3} \rho h_\ell^4 \mu_t |\xi|^4 \xi_2^4 (1+\xi_1)^2 \\
|\Gamma_{\xi_1^4\xi_2^4}| &\leq \frac{1}{144} h_\ell^4 \xi_1^4 \xi_2^4 (1+\xi_1)^2 (1+\xi_2)^2 \\
|\Gamma_{|\xi|^8}| &\leq 4\rho^2 h_\ell^4 \mu_t^2 |\xi|^8.
\end{aligned} \tag{3.33}$$

There are only two considerations which differ from Theorem 4. First, the polynomials in ξ_1 and ξ_2 at the end of each line of Equation (3.33) are slightly different. This is because we now have if $\xi \in B_{i,j}$ then $\xi_1 \in \{2^{i-1}, \ldots, 2^i\}$ for $i > 1$ and $\xi_2 \in \{2^{j-1}, \ldots, 2^j\}$ for $j > 1$. Therefore,

$$\begin{aligned}
2^i &\leq 2\xi_1 \\
2^j &\leq 2\xi_2
\end{aligned}$$

when $i, j > 1$ so that

$$\begin{aligned}
2^i &\leq 2(1+\xi_1) \\
2^j &\leq 2(1+\xi_2)
\end{aligned}$$

for $i, j \geq 1$. Hence, the factor of $\frac{1}{\pi}$ has disappeared.

Second, the sets $B_{i,j}$ now overlap, but counting the same point multiple times only adds to the right-hand side of the expressions in Equation (3.33), so the inequality is preserved. Now we finish showing that each term of $\Omega_1(h_\ell)$ converges to zero at the desired rate.

Terms of type ξ_i^8

For some constants C_1 and C_2,

$$\begin{aligned}\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{\xi_1^8}|\hat{u}_0(\xi)^2 &\leq \sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\left(\frac{1}{144}h_\ell^4\xi_1^8(1+\xi_2)^4\right)\hat{u}_0(\xi)^2\\ &= \frac{1}{144}h_\ell^4\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\xi_1^8(1+\xi_2)^4\hat{u}_0(\xi)^2\\ &\leq \frac{1}{144}C_1h_\ell^4\|u_0\|^2_{H^4_{\text{mix}}([-\pi,\pi]^2)}\end{aligned}$$

and

$$\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{\xi_2^8}|\hat{u}_0(\xi)^2 \leq \frac{1}{144}C_2h_\ell^4\|u_0\|^2_{H^4_{\text{mix}}([-\pi,\pi]^2)}.$$

Terms of type $|\xi|^4\xi_i^4$

For some constants C_3 and C_4,

$$\begin{aligned}\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{|\xi|^4\xi_1^4}|\hat{u}_0(\xi)^2 &\leq \sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\left(\frac{1}{3}\rho h_\ell^4\mu_t|\xi|^4\xi_1^4(1+\xi_2)^2\right)\hat{u}_0(\xi)^2\\ &= \frac{1}{3}\rho h_\ell^4\mu_t\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\xi|^4\xi_1^4(1+\xi_2)^2\hat{u}_0(\xi)^2\\ &\leq \frac{1}{3}\rho h_\ell^4\mu_tC_3\|u_0\|^2_{H^4_{\text{mix}}([-\pi,\pi]^2)}\end{aligned}$$

and

$$\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{|\xi|^4\xi_2^4}|\hat{u}_0(\xi)^2 \leq \frac{1}{3}\rho h_\ell^4\mu_tC_4\|u_0\|^2_{H^4_{\text{mix}}([-\pi,\pi]^2)}.$$

Terms of type $\xi_1^4\xi_2^4$

For some constant C_5,

$$\begin{aligned}
\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{\xi_1^4\xi_2^4}|\hat{u}_0(\xi)^2 &\le \sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\left(\frac{1}{144}h_\ell^4\xi_1^4\xi_2^4(1+\xi_1)^2(1+\xi_2)^2\right)\hat{u}_0(\xi)^2 \\
&= \frac{1}{144}h_\ell^4\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\xi_1^4\xi_2^4(1+\xi_1)^2(1+\xi_2)^2\hat{u}_0(\xi)^2 \\
&\le \frac{1}{144}h_\ell^4 C_5\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}.
\end{aligned}$$

Terms of type $|\xi|^8$

Finally, for some constant C_6,

$$\begin{aligned}
\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\Gamma_{|\xi|^8}|\hat{u}_0(\xi)^2 &\le \sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\left(4\rho^2h_\ell^4\mu_t^2|\xi|^8\right)\hat{u}_0(\xi)^2 \\
&= 4\rho^2h_\ell^4\mu_t^2\sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}|\xi|^8\hat{u}_0(\xi)^2 \\
&\le 4\rho^2h_\ell^4\mu_t^2C_6\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}.
\end{aligned}$$

Conclusion

In summary,

$$\begin{aligned}
\Omega_1(h_\ell) \le& \sum_{\xi_1=-\infty}^{\infty}\sum_{\xi_2=-\infty}^{\infty}\left(|\Gamma_{\xi_1^8}|+|\Gamma_{\xi_2^8}|+|\Gamma_{|\xi|^4\xi_1^4}|+|\Gamma_{|\xi|^4\xi_2^4}|+|\Gamma_{|\xi|^4\xi_1^4}|+|\Gamma_{|\xi|^8}|\right)\hat{u_0}(\xi)^2 \\
&\le h_\ell^4\left(\frac{1}{144}C_1\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}+\frac{1}{144}C_2\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}\right. \\
&\quad +\frac{1}{3}\rho\mu_tC_3\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}+\frac{1}{3}\rho\mu_tC_4\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)} \\
&\quad \left.+\frac{1}{144}C_5\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}+4\rho^2\mu_t^2C_6\|u_0\|^2_{H^4_{\mathrm{mix}}([-\pi,\pi]^2)}\right).
\end{aligned}$$

Therefore, $\Omega_1(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\mathrm{mix}}([-\pi,\pi]^2)$.

3.4.2 Rate of convergence of $\Omega_2(h_\ell)$

Define $C(h_\ell) := \{(\xi_1, \xi_2) \in \mathbb{Z}^2 : \xi_1 \xi_2 \geq \frac{1}{h_{\ell-1}}\}$. Then $\mathbb{R}^2 \setminus A_\ell \subset C(h_\ell)$.

Since $|e^{q(\xi)t_n}| \leq 1$, we have

$$\begin{aligned}
\Omega_2(h_\ell) &:= \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \mathbf{1}_{\mathbb{R}^2 \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2 \\
&\leq \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \mathbf{1}_{\mathbb{R}^2 \setminus A_\ell} |\hat{u}_0(\xi)|^2 \\
&\leq \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \mathbf{1}_{C(h_\ell)} |\hat{u}_0(\xi)|^2.
\end{aligned}$$

On the domain $C(h_\ell)$ we have $1 \leq \xi_1 \xi_2 h_{\ell-1}$ and thus $1 \leq \xi_1^4 \xi_2^4 h_{\ell-1}^4$. Therefore,

$$\begin{aligned}
\Omega_2(h_\ell) &\leq h_{\ell-1}^4 \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} \mathbf{1}_{C(h_\ell)} \xi_1^4 \xi_2^4 |\hat{u}_0(\xi)|^2 \\
&\leq 16 h_\ell^4 \left\| \frac{\partial^4 u_0}{\partial^2 x \partial^2 y} \right\|_2^2 .
\end{aligned}$$

So we have $\Omega_2(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\text{mix}}([-\pi, \pi]^2)$. Thus,

$$\begin{aligned}
\|u(x, t_n) - (\sigma v_{t_n})(x)\|_2^2 &= \Omega_1(h_\ell) + \Omega_2(h_\ell) \\
&= O(h_\ell^4) + O(h_\ell^4) \\
&= O(h_\ell^4)
\end{aligned}$$

when $u_0 \in H^4_{\text{mix}}([-\pi, \pi]^2)$ and so $\|u(x, t_n) - (\sigma v_{t_n})(x)\|_2 = O(h_\ell^2)$.

$\square$

3.5 Heat equation on $\mathbb{R}^d$, $d \geq 2$

We now repeat Theorem 4 for the Cauchy problem for the d-dimensional heat equation:

$$\begin{aligned} u_t &= \sum_{i=1}^{d} u_{x_i x_i} \qquad \mathbb{R}^d \times [0,T] \\ u(x,0) &= u_0(x) \end{aligned} \tag{3.34}$$

The proof of the theorem depends on the following two lemmas, which are the d-dimensional analogues of Lemma 5 and Lemma 6.

Lemma 10. *When the heat equation is solved by the fully implicit method, the amplification factor $g_{\underline{\ell}}(\xi)$, as defined in Equation (1.12), satisfies*

$$e^{\Delta t q(\xi)} - g_{\underline{\ell}}(\xi) = \Delta t \left(\frac{1}{2} \Delta t \mu_t |\xi|^4 - \frac{1}{12} \sum_{i=1}^{d} \xi_i^4 \Delta x_i^2 \alpha(\xi_i, \Delta x_i) \right) \tag{3.35}$$

at every point $\xi = (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d$, where

$$\alpha(.,.) \in (-1,1), \quad \mu_t \in (0,1)$$

and

$$q(\xi) = -\sum_{i=1}^{d} \xi_i^2.$$

Lemma 11. *The bound*

$$\left| \sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1 = \ell - q} \mathbf{1}_{A_{\underline{l}}} g_{\underline{l}}(\xi) \right| \leq 1 + 4d\Delta t \tag{3.36}$$

holds for all $\xi = (\xi_1, \xi_2) \in \mathbb{R}^d$.

Now we state and prove the convergence theorem for the d-dimensional heat equation.

Theorem 12. *If the initial value problem*

$$\begin{aligned} u_t &= \sum_{i=1}^{d} u_{x_i x_i} \qquad \mathbb{R}^d \times [0,T] \\ u(x,0) &= u_0(x) \end{aligned} \tag{3.37}$$

is approximated by the elliptic sparse grid combination technique at level ℓ, in which the constituent sparse grids are solved by the fully implicit method, and the initial function is τu_0, then for each time T there exists a constant $C = C(T,d)$ independent of u_0 such that

$$\|u(t_n,\cdot) - (\sigma v_{t_n})(.)\|_2 \leq C h_\ell^4 \|u_0\|_{H^4_{mix}(\mathbb{R}^d)} \tag{3.38}$$

for each $t_n = n\Delta t$ with $0 < t_n \leq T$.

Proof. For each time $t_n \in [0,T]$, we may express the exact solution of the heat equation as the inverse of its Fourier transform, that is

$$u(x,t_n) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{ix\cdot\xi} e^{q(\xi)t_n} \hat{u}_0(\xi)\, d\xi, \tag{3.39}$$

where $q(\xi) = -\sum_{i=1}^{d} \xi_i^2 = -|\xi|^2$.

By linearity, we have for the sparse grid solution:

$$(\sigma v_{t_n})(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{ix\cdot\xi} \left(\sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1 = \ell - q} \mathbf{1}_{A_{\underline{l}}} g_{\underline{l}}(\xi) \right)^n \hat{u_0}(\xi)\, d\xi \tag{3.40}$$

By subtracting Equations (3.39) and (3.40), we obtain

$$\begin{aligned} &u(x,t_n) - (\sigma v_{t_n})(x) \\ &= \frac{1}{(2\pi)^{d/2}} \int_{A_\ell} e^{ix\cdot\xi} \left(e^{q(\xi)t_n} - \left(\sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1 = \ell - q} \mathbf{1}_{A_{\underline{l}}} g_{\underline{l}}(\xi) \right)^n \right) \hat{u_0}(\xi)\, d\xi \\ &\qquad + \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d \setminus A_\ell} e^{ix\cdot\xi} e^{q(\xi)t_n} \hat{u_0}(\xi)\, d\xi. \end{aligned}$$

In order to show that $\|u(x,t_n)-(\sigma v_{t_n})(x)\|_2 = O(h_\ell^2)$, we prove the equivalent statement $\|u(x,t_n)-(\sigma v_{t_n})(x)\|_2^2 = O(h_\ell^4)$. By Parseval's theorem,

$$\begin{aligned}
&\|u(x,t_n)-(\sigma v_{t_n})(x)\|_2^2 \\
&= \int_{A_\ell} \left| e^{q(\xi)t_n} - \left(\sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1=\ell-q} \mathbf{1}_{A_{\underline{l}}} g_{\underline{l}}(\xi) \right)^n \right|^2 \hat{u}_0(\xi)\, d\xi \\
&\qquad + \int_{\mathbb{R}^d \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2\, d\xi \\
&\leq \Omega_1(h_\ell) + \Omega_2(h_\ell),
\end{aligned}$$

where

$$\begin{aligned}
\Omega_1(h_\ell) &:= e^{8dt_n} n^2 \int_{A_\ell} \left(\sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{|\underline{l}|_1=\ell-q} \mathbf{1}_{A_{\underline{l}}} (e^{q(\xi)\Delta t} - g_{\underline{l}}(\xi)) \right)^2 \hat{u}_0(\xi)\, d\xi \\
&=: e^{8dt_n} n^2 \int_{A_\ell} \Gamma(\xi) \hat{u}_0(\xi)^2\, d\xi \\
\Omega_2(h_\ell) &:= \int_{\mathbb{R}^d \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2\, d\xi.
\end{aligned}$$

As we did in the proof of Theorem 4, we have defined $\Gamma(\xi)$ to be the factor in the integrand of $\Omega_1(h_\ell)$ which multiplies $\hat{u}_0(\xi)^2$. Now we look at the rate of convergence of the terms $\Omega_1(h_\ell)$ and $\Omega_2(h_\ell)$.

3.5.1 Rate of convergence of $\Omega_1(h_\ell)$

First, we expand $\Gamma(\xi)$:

$$\begin{aligned}\Gamma(\xi) &= \left(\sum_{q=0}^{d-1}(-1)^q\binom{d-1}{q}\sum_{|\underline{l}|_1=\ell-q}\mathbf{1}_{A_{\underline{l}}}(e^{q(\xi)\Delta t}-g_{\underline{l}}(\xi))\right)^2\\ &= \sum_{p=0}^{d-1}\sum_{q=0}^{d-1}(-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}\times\\ &\qquad \sum_{|\underline{k}|_1=\ell-p}\mathbf{1}_{A_{\underline{k}}}(e^{q(\xi)\Delta t}-g_{\underline{k}}(\xi))\sum_{|\underline{l}|_1=\ell-q}\mathbf{1}_{A_{\underline{l}}}(e^{q(\xi)\Delta t}-g_{\underline{l}}(\xi))\\ &= \sum_{p=0}^{d-1}\sum_{|\underline{k}|_1=\ell-p}\sum_{q=0}^{d-1}\sum_{|\underline{l}|_1=\ell-q}(-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}\times\\ &\qquad \mathbf{1}_{A_{\underline{k}}}\mathbf{1}_{A_{\underline{l}}}(e^{q(\xi)\Delta t}-g_{\underline{k}}(\xi))(e^{q(\xi)\Delta t}-g_{\underline{l}}(\xi))\end{aligned} \tag{3.41}$$

The four consecutive summation symbols look intimidating, but they simply iterate over all pairs $(\Omega_{\underline{k}}, \Omega_{\underline{l}})$ of sparse grids which are combined in the sparse grid combination technique at level ℓ. Each of the terms inside the summation contains the product of two factors which are given in Equation (3.35). When we multiply two such factors for arbitrary grids of multi-index $\underline{k} = (k_1, \dots, k_d)$ and $\underline{l} = (l_1, \dots, l_d)$ we get

$$\begin{aligned}&\left(e^{\Delta t q(\xi)}-g_{\underline{k}}(\xi)\right)\left(e^{\Delta t q(\xi)}-g_{\underline{l}}(\xi)\right)\\ &= \Delta t\left(\frac{1}{2}\rho h_{\ell-1}^2\mu_t|\xi|^4-\frac{1}{12}\sum_{i=1}^d \xi_i^4 h_{k_i}^2\alpha_{i,k_i}\right)\times\\ &\qquad \Delta t\left(\frac{1}{2}\rho h_{\ell-1}^2\mu_t|\xi|^4-\frac{1}{12}\sum_{i=1}^d \xi_i^4 h_{l_i}^2\alpha_{i,l_i}\right)\\ &= \frac{1}{144}\Big(\sum_{i=1}^d \xi_i^4 h_{k_i}^2\alpha_{i,k_i}\Big)\Big(\sum_{i=1}^d \xi_i^4 h_{l_i}^2\alpha_{i,l_i}\Big)\\ &\qquad -\frac{1}{24}\rho h_{\ell-1}^2\mu_t|\xi|^4\left(\sum_{i=1}^d \xi_i^4 h_{k_i}^2\alpha_{i,k_i}+\sum_{i=1}^d \xi_i^4 h_{l_i}^2\alpha_{i,l_i}\right)\\ &\qquad +\frac{1}{4}\rho^2 h_{\ell-1}^4\mu_t^2|\xi|^8\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=1}^{d} \frac{1}{144} \xi_i^8 h_{k_i+l_i}^2 \alpha_{i,k_i} \alpha_{i,l_i} \\
&\quad + \sum_{i=1}^{d} \sum_{j=1}^{i-1} \frac{1}{72} \xi_i^4 \xi_j^4 (h_{k_i+l_j}^2 \alpha_{i,k_i} \alpha_{j,l_j} + h_{k_j+l_i}^2 \alpha_{j,k_j} \alpha_{i,l_i}) \\
&\quad - \sum_{i=1}^{d} \frac{1}{24} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \left(h_{k_i}^2 \alpha_{i,k_i} + h_{l_i}^2 \alpha_{i,l_i} \right) \\
&\quad + \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8.
\end{aligned}
$$

From the last equality, we see that $\Gamma(\xi)$ contains four types of terms in its expansion. These are terms of the following types:

1. ξ_i^8 for $i \in \{1, \dots, d\}$
2. $\xi_i^4 \xi_j^4$ for $i, j \in \{1, \dots, d\}$ with $j < i$
3. $|\xi|^4 \xi_i^4$ for $i \in \{1, \dots, d\}$
4. $|\xi|^8$

We label these terms $\Gamma_{\xi_i^8}$, $\Gamma_{\xi_i^4 \xi_j^4}$, $\Gamma_{|\xi|^4 \xi_i^4}$, and $\Gamma_{|\xi|^8}$. Therefore, we can write

$$
\begin{aligned}
\Omega_1(h_\ell) &= \int_{A_\ell} \left(\sum_{i=1}^{d} \Gamma_{\xi_i^8} + \sum_{i=1}^{d} \sum_{j=1}^{i-1} \Gamma_{\xi_i^4 \xi_j^4} + \sum_{i=1}^{d} \Gamma_{|\xi|^4 \xi_i^4} + \Gamma_{|\xi^8|} \right) d\xi \\
&\le \int_{A_\ell} \left(\sum_{i=1}^{d} |\Gamma_{\xi_i^8}| + \sum_{i=1}^{d} \sum_{j=1}^{i-1} |\Gamma_{\xi_i^4 \xi_j^4}| + \sum_{i=1}^{d} |\Gamma_{|\xi|^4 \xi_i^4}| + |\Gamma_{|\xi^8|}| \right) d\xi.
\end{aligned}
$$

We look at the terms $\Gamma_{\xi_i^8}$, $\Gamma_{\xi_i^4 \xi_j^4}$, $\Gamma_{|\xi|^4 \xi_i^4}$, and $\Gamma_{|\xi|^8}$ as piecewise functions of ξ due to the presence of the indicator $\mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}}$ in Equation (3.41). Therefore, throughout the following analysis, we fix a set $B_{\underline{m}} \subset \mathbb{R}^d$. Then the only terms from Equation (3.41) which are nonzero on $B_{\underline{m}}$ are those for which

$$
\underline{m} \le \underline{k} \wedge \underline{l}.
$$

In the following subsections, we use the fact that if $\xi \in B_{\underline{m}}$ then $\xi_i \in [2^{m_i - 1}\pi, 2^{m_i}\pi]$ for $m_i > 1$. Therefore,

$$
2^{m_i} \le \frac{2}{\pi} \xi_i
$$

for $m_i > 1$. And so

$$2^{m_i} \leq 2(1 + \frac{1}{\pi}\xi_i)$$

for $m_i \geq 1$.

We now show that $\Omega_1(h_\ell) = O(h_\ell^4)$.

Terms of type ξ_i^8

First, we look at $\Gamma_{\xi_i^8}$, that is, terms of type ξ_i^8 for $i \in \{1, \ldots, d\}$. These terms are

$$\begin{aligned}
\Gamma_{\xi_i^8} &= \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \frac{1}{144} \xi_i^8 h_{k_i+l_i}^2 \alpha_{i,k_i} \alpha_{i,l_i} \\
&= \frac{1}{144} \xi_i^8 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} h_{k_i+l_i}^2 \alpha_{i,k_i} \alpha_{i,l_i}.
\end{aligned}$$

Again, note that the four summations iterate over all pairs $(\Omega_{\underline{k}}, \Omega_{\underline{l}})$ of sparse grids which are combined in the sparse grid combination technique at level ℓ and that, on the set $B_{\underline{m}}$, only those terms above for which $\underline{m} \leq \underline{k} \wedge \underline{l}$ are nonzero. To deduce the value of $\Gamma_{\xi_i^8}$ on $B_{\underline{m}}$, our work now entails counting the terms $h_{k_i+l_i}^2 \alpha_{i,k_i} \alpha_{i,l_i}$. We shall see that the coefficient $(-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}$ is chosen precisely so that all except one of the terms cancel.

Now, we proceed to calculate the coefficient of $h_{k_i+l_i}^2 \alpha_{i,k_i} \alpha_{i,l_i}$ on $B_{\underline{m}}$ for all possible values of k_i and l_i. We momentarily ignore all factors before the four summations since they are constant across all sets $B_{\underline{m}}$, but we will bring them back into our analysis at the end. We fix $r, s \in \mathbb{N}$ and count the terms $h_{r+s}^2 \alpha_{i,r} \alpha_{i,s}$. Then the coefficient of $h_{r+s}^2 \alpha_{i,r} \alpha_{i,s}$ on $B_{\underline{m}}$ must be

$$\sum_{\substack{\text{Pairs of grids } (\Omega_{\underline{k}}, \Omega_{\underline{l}}) \\ \text{with } \underline{m} \leq \underline{k} \wedge \underline{l}, \\ k_i = r,\ l_i = s}} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q},$$

where p and q satisfy $|\underline{k}|_1 = \ell - p$ and $|\underline{l}|_1 = \ell - q$. Now we must enumerate the grids in the above summation. We can expand this as

$$\sum_{p=0}^{d-1}(\#\text{ of grids }\Omega_{\underline{k}}\text{ with }|\underline{k}|_1 = \ell - p\text{ and }k_i = r)\times$$
$$\sum_{q=0}^{d-1}(\#\text{ of grids }\Omega_{\underline{l}}\text{ with }|\underline{l}|_1 = \ell - q\text{ and }l_i = s)(-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}.$$

The first summation symbol above represents iteration over $\Omega_{\underline{k}}$. We only iterate over grids having $k_i = r$. We count the number of such grids and then multiply this by the number of grids $\Omega_{\underline{l}}$ having $l_i = s$.

Finally, to get a useful expression, we must make sense of the two factors which represent the number of grids. Note that $\underline{m} \leq \underline{k}$ so we must have

$$\underline{k} = \underline{m} + (p_1, \ldots, p_d),$$

where $p_i \geq 0$. Therefore,

$$\begin{aligned} |\underline{k}|_1 &= |\underline{m}|_1 + |(p_1, \ldots, p_d)|_1 \\ \ell - p &= |\underline{m}|_1 + |(p_1, \ldots, p_d)|_1 \\ |(p_1, \ldots, p_d)|_1 &= \ell - p - |\underline{m}|_1 \\ \sum_{i=1}^{d} p_i &= \ell - p - |\underline{m}|_1. \end{aligned}$$

But we have fixed $k_i = r$ so $p_i = r - m_i$. Subtracting p_i from both sides gives

$$\sum_{\substack{j=1 \\ j\neq i}}^{d} p_j = \ell - p - |\underline{m}|_1 - (r - m_i).$$

Thus, the number of grids $\Omega_{\underline{k}}$ with $|\underline{k}|_1 = \ell - p$ and $k_i = r$ is given by the answer to the question "How many ways can one place $\ell - p - |\underline{m}|_1 - (r - m_i)$ balls into $d - 1$ bins?". By a similar argument, the number of grids $\Omega_{\underline{l}}$ with $|\underline{l}|_1 = \ell - q$ and $l_i = s$ is given by the answer to the question "How many ways can one place $\ell - p - |\underline{m}|_1 - (s - m_i)$ balls into $d - 1$ bins?". Both quantities can be written with a binomial coefficient as

$$
\begin{aligned}
&= \sum_{p=0}^{d-1} \binom{(d-2) + (\ell - p - |\underline{m}|_1 - (r - m_i))}{\ell - p - |\underline{m}|_1 - (r - m_i)} \times \\
&\quad \sum_{q=0}^{d-1} \binom{(d-2) + (\ell - q - |\underline{m}|_1 - (s - m_i))}{\ell - q - |\underline{m}|_1 - (s - m_i)} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \\
&= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{K_i - p - r} \times \\
&\quad \sum_{q=0}^{d-1} \binom{(K_i + d - 2) - q - s}{K_i - q - s} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q},
\end{aligned}
$$

where we have defined

$$K_i := \ell - |\underline{m}|_1 + m_i$$

to simplify the notation.

It remains to determine the value of this sum. We use Equation (A.7) twice. The above double sum is then

$$
\begin{aligned}
&= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{d-2} \times \\
&\quad \sum_{q=0}^{d-1} \binom{(K_i + d - 2) - q - s}{d-2} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \\
&= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{d-2} \binom{d-1}{p} (-1)^p \times \\
&\quad \sum_{q=0}^{d-1} (-1)^q \binom{(K_i + d - 2) - q - s}{d-2} \binom{d-1}{q} \\
&= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{d-2} \binom{d-1}{p} (-1)^p \binom{K_i - s - 1}{-1},
\end{aligned}
$$

where we have used Equation (A.7) to reduce the sum over q to a single binomial coefficient. Since

$$\binom{K_i - s - 1}{-1} = \begin{cases} 1 : K_i - s - 1 = -1 \\ 0 : \text{otherwise}, \end{cases}$$

we must have $s = K_i$ for the quantity to be nonzero. Henceforth, fix $s = K_i$. In that case, the quantity reduces to

$$\begin{aligned}
&= \sum_{p=0}^{d-1} (-1)^p \binom{d-1}{p} \binom{(K_i + d - 2) - p - r}{d-2} \\
&= \sum_{p=0}^{d-1} (-1)^p \binom{d-1}{p} \binom{(K_i + d - 2 - r) - p}{d-2} \\
&= \binom{K_i - r - 1}{-1},
\end{aligned}$$

where we have used Equation (A.7) to reduce the sum over p to a single binomial coefficient. Since

$$\binom{K_i - r - 1}{-1} = \begin{cases} 1 : K_i - r - 1 = -1 \\ 0 : \text{otherwise}, \end{cases}$$

we conclude that $h_{r+s}^2 \alpha_{i,r} \alpha_{i,s}$ has a coefficient of 0 except when $r = s = K_i$. In this case, the term is $h_{2K_i}^2 \alpha_{i,K_i}^2$. Therefore, we can write

$$\begin{aligned}
\Gamma_{\xi_i^8} &= \frac{1}{144} \xi_i^8 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h_{2K_i}^2 \alpha_{i,K_i}^2 \\
&= \frac{1}{144} \xi_i^8 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h_{2(\ell - |\underline{m}|_1 + m_i)}^2 \alpha_{i,K_i}^2 \\
&= \frac{1}{144} h_\ell^4 \xi_i^8 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h_{2(-|\underline{m}|_1 + m_i)}^2 \alpha_{i,K_i}^2 \\
&= \frac{1}{144} h_\ell^4 \xi_i^8 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} \prod_{\substack{j=1 \\ j \neq i}}^{d} 2^{4m_i} \alpha_{i,K_i}^2
\end{aligned}$$

$$\leq \frac{1}{144} h_\ell^4 \xi_i^8 \prod_{\substack{j=1 \\ j\neq i}}^{d} 16(1+\frac{1}{\pi}\xi_i)^4,$$

where we have used the fact that $0 \leq \alpha_{i,K_i}^2 \leq 1$.

Therefore, for some constant C_1,

$$\begin{aligned}
\int_{A_\ell} |\Gamma_{\xi_i^8}| \hat{u}_0(\xi)^2 \, d\xi &\leq \int_{A_\ell} \frac{1}{144} h_\ell^4 \xi_i^8 \prod_{\substack{j=1 \\ j\neq i}}^{d} 16(1+\frac{1}{\pi}\xi_i)^4 \hat{u}_0(\xi)^2 \, d\xi \\
&\leq \frac{1}{144} h_\ell^4 \int_{A_\ell} \xi_i^8 \prod_{\substack{j=1 \\ j\neq i}}^{d} 16(1+\frac{1}{\pi}\xi_i)^4 \hat{u}_0(\xi)^2 \, d\xi \\
&= \frac{1}{144} C_1 h_\ell^4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^d)}.
\end{aligned}$$

Terms of type $\xi_i^4 \xi_j^4$

Next, we look at $\Gamma_{\xi_i^4\xi_j^4}$, that is, terms of type $\xi_i^4\xi_j^4$ for $i, j \in \{1, \ldots, d\}$ with $i \neq j$. These terms are

$$\begin{aligned}
\Gamma_{\xi_i^4\xi_j^4} &= \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \\
&\quad \times \frac{1}{72} \xi_i^4 \xi_j^4 (h_{k_i+l_j}^2 \alpha_{i,k_i} \alpha_{j,l_j} + h_{k_j+l_i}^2 \alpha_{j,k_j} \alpha_{i,l_i}) \\
&= \frac{1}{72} \xi_i^4 \xi_j^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \\
&\quad \times (h_{k_i+l_j}^2 \alpha_{i,k_i} \alpha_{j,l_j} + h_{k_j+l_i}^2 \alpha_{j,k_j} \alpha_{i,l_i}).
\end{aligned}$$

Our work now entails counting the terms $h_{k_i+l_j}^2$ and $h_{k_j+l_i}^2$ which are part of the sum on $B_{\underline{m}}$. By symmetry, we can immediately halve our work and write

$$= \frac{1}{36} \xi_i^4 \xi_j^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} h_{k_i+l_j}^2 \alpha_{i,k_i} \alpha_{j,l_j}.$$

We fix $r, s \in \mathbb{N}$ and count the terms $h_{r+s}^2 \alpha_{i,r}\alpha_{j,s}$. The coefficient of $h_{r+s}^2 \alpha_{i,r}\alpha_{j,s}$ on $B_{\underline{m}}$ must be

$$\sum_{\substack{\text{Pairs of grids } (\Omega_{\underline{k}},\Omega_{\underline{l}}) \\ \text{with } \underline{m}\leq \underline{k}\wedge \underline{l} \\ k_i=s,\ l_j=r}} (-1)^{p+q} \binom{d-1}{p}\binom{d-1}{q},$$

where p and q satisfy $|\underline{k}|_1 = \ell - p$ and $|\underline{l}|_2 = \ell - q$. We may expand this as

$$\sum_{p=0}^{d-1} (\#\text{ of grids } \Omega_{\underline{k}} \text{ such that } |\underline{k}|_1 = \ell - p \text{ and } k_i = r) \times$$
$$\sum_{q=0}^{d-1} (\#\text{ of grids } \Omega_{\underline{l}} \text{ such that } |\underline{l}|_1 = \ell - q \text{ and } l_j = s)(-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}$$
$$= \sum_{p=0}^{d-1} \binom{(d-2) + (\ell - p - |\underline{m}|_1 - (r - m_i))}{\ell - p - |\underline{m}|_1 - (r - m_i)} \times$$
$$\sum_{q=0}^{d-1} \binom{(d-2) + (\ell - q - |\underline{m}|_1 - (s - m_j))}{\ell - q - |\underline{m}|_1 - (s - m_j)} (-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}$$
$$= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{K_i - p - r} \times$$
$$\sum_{q=0}^{d-1} \binom{(K_j + d - 2) - q - s}{K_j - q - s} (-1)^{p+q}\binom{d-1}{p}\binom{d-1}{q}.$$

It remains to determine the value of this sum. Applying Equation (A.7) twice gives

$$= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{d-2}\binom{d-1}{p}(-1)^p \times$$
$$\sum_{q=0}^{d-1} (-1)^q \binom{(K_j + d - 2) - q - s}{d-2}\binom{d-1}{q}$$
$$= \sum_{p=0}^{d-1} \binom{(K_i + d - 2) - p - r}{d-2}\binom{d-1}{p}(-1)^p \binom{K_j - s - 1}{-1}$$

$$
\begin{aligned}
&= \binom{K_j - s - 1}{-1} \sum_{p=0}^{d-1} (-1)^p \binom{d-1}{p} \binom{(K_i + d - 2) - p - r}{d-2} \\
&= \binom{K_j - s - 1}{-1} \binom{K_i - r - 1}{-1} \\
&= \begin{cases} 1 : K_j - s - 1 = -1 \text{ and } K_i - r - 1 = -1 \\ 0 : \text{otherwise}, \end{cases} \\
&= \begin{cases} 1 : s = K_j, r = K_i \\ 0 : \text{otherwise}, \end{cases}
\end{aligned}
$$

Thus, we have found that $h^2_{r+s}\alpha_{i,r}\alpha_{j,s}$ has a coefficient of 0 except when $r = K_i$ and $s = K_j$. Now we can write

$$
\begin{aligned}
\Gamma_{\xi_i^4 \xi_j^4} &= \frac{1}{36} \xi_i^4 \xi_j^4 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h^2_{K_i + K_j} \alpha_{i,K_i} \alpha_{j,K_j} \\
&= \frac{1}{36} \xi_i^4 \xi_j^4 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h^2_{2(\ell - |\underline{m}|_1) + m_i + m_j} \alpha_{i,K_i} \alpha_{j,K_j} \\
&= \frac{1}{36} h_\ell^4 \xi_i^4 \xi_j^4 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} h^2_{-2|\underline{m}|_1 + m_i + m_j} \alpha_{i,K_i} \alpha_{j,K_j} \\
&= \frac{1}{36} h_\ell^4 \xi_i^4 \xi_j^4 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}} \prod_{\substack{k=1 \\ k \neq i,j}}^{d} 2^{4m_k} \alpha_{i,K_i} \alpha_{j,K_j} \\
|\Gamma_{\xi_i^4 \xi_j^4}| &\leq \frac{1}{36} h_\ell^4 \xi_i^4 \xi_j^4 \prod_{\substack{k=1 \\ k \neq i,j}}^{d} 16(1 + \frac{1}{\pi} \xi_k)^4.
\end{aligned}
$$

Therefore, for some constant C_2,

$$
\begin{aligned}
\int_{A_\ell} |\Gamma_{\xi_i^4 \xi_j^4}| \hat{u}_0(\xi)^2 \, d\xi &= \int_{A_\ell} \frac{1}{36} h_\ell^4 \xi_i^4 \xi_j^4 \prod_{\substack{k=1 \\ k \neq i,j}}^{d} 16(1 + \frac{1}{\pi} \xi_k)^4 \hat{u}_0(\xi)^2 \, d\xi \\
&= \frac{1}{36} h_\ell^4 \int_{A_\ell} \xi_i^4 \xi_j^4 \prod_{\substack{k=1 \\ k \neq i,j}}^{d} 16(1 + \frac{1}{\pi} \xi_k)^4 \hat{u}_0(\xi)^2 \, d\xi
\end{aligned}
$$

$$\leq \frac{1}{36} C_2 h_\ell^4 \|u_0\|^2_{H^4_{\mathrm{mix}}(\mathbb{R}^d)}.$$

Terms of type $|\xi|^4 \xi_i^4$

Next, we look at $\Gamma_{|\xi|^4\xi_i^4}$, that is, terms of type $|\xi|^4\xi_i^4$ for $i \in \{1, \dots, d\}$. These terms are

$$\begin{aligned}
\Gamma_{|\xi|^4\xi_i^4} &= \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \times \\
&\quad \binom{d-1}{p}\binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \frac{1}{24} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \left(h_{k_i}^2 \alpha_{i,k_i} + h_{l_i}^2 \alpha_{i,l_i} \right) \\
&= \frac{1}{24} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \times \\
&\quad \binom{d-1}{p}\binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \left(h_{k_i}^2 \alpha_{i,k_i} + h_{l_i}^2 \alpha_{i,l_i} \right) \\
&= \frac{1}{12} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p}\binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} h_{k_i}^2 \alpha_{i,k_i} \\
&= \frac{1}{12} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} (-1)^{p} \binom{d-1}{p} \mathbf{1}_{A_{\underline{k}}} h_{k_i}^2 \alpha_{i,k_i} \\
&\quad \times \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{q} \binom{d-1}{q} \mathbf{1}_{A_{\underline{l}}} \\
&= \frac{1}{12} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} (-1)^{p} \binom{d-1}{p} \mathbf{1}_{A_{\underline{k}}} h_{k_i}^2 \alpha_{i,k_i}.
\end{aligned}$$

We prove the last equality in the following lemma, which we shall recall again in the next subsection.

Lemma 13. *For all $d \geq 2$,*

$$\sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{q} \binom{d-1}{q} \mathbf{1}_{A_{\underline{l}}} = \mathbf{1}_{A_\ell}. \tag{3.42}$$

Proof. Fix a multi-index $\underline{m}$. Due to the definition of the sets $A_{\underline{l}}$ and A_ℓ, each side of the equality is 0 whenever $x \in B_{\underline{m}}$ and $|\underline{m}|_1 > \ell$. Otherwise, the problem reduces again to the counting of grids. By Equation (A.7),

$$
\begin{aligned}
&\sum_{\substack{\text{Grids } \Omega_{\underline{l}} \\ \text{with } \underline{m} \le \underline{l}}} (-1)^q \binom{d-1}{q} \\
&= \sum_{q=0}^{d-1} (\#\text{ of grids } \Omega_{\underline{l}} \text{ with } |\underline{l}|_1 = \ell - q)(-1)^q \binom{d-1}{q} \\
&= \sum_{q=0}^{d-1} \binom{(d-1) + (\ell - q - |\underline{m}|_1)}{\ell - q - |\underline{m}|_1} (-1)^q \binom{d-1}{q} \\
&= \sum_{q=0}^{d-1} \binom{(d-1) + (\ell - q - |\underline{m}|_1)}{d-1} (-1)^q \binom{d-1}{q} \\
&= \binom{\ell - |\underline{m}|_1}{0} \\
&= 1.
\end{aligned}
$$

$\square$

Our work now entails counting the terms $h_{k_i}^2 \alpha_{i,k_i}$ which are part of the sum on $B_{\underline{m}}$. Fix a multi-index $\underline{m}$ and $n \in \mathbb{N}$. The coefficient of $h_n^2 \alpha_{i,n}$ on $B_{\underline{m}}$ must be

$$
\sum_{\substack{\text{Grids } \Omega_{\underline{k}} \\ \text{with } \underline{m} \le \underline{k} \\ \text{and } k_i = n}} (-1)^p \binom{d-1}{p},
$$

where p and q satisfy $|\underline{k}|_1 = \ell - p$ and $|\underline{l}|_1 = \ell - q$. We can expand this as

$$
\begin{aligned}
&\sum_{p=0}^{d-1} (\#\text{ of grids } \Omega_{\underline{k}} \text{ with } |\underline{k}|_1 = \ell - p \text{ and } k_i = n)(-1)^p \binom{d-1}{p} \\
&= \sum_{p=0}^{d-1} (-1)^p \binom{(d-2) + (\ell - p - |\underline{m}|_1 - (n - m_i))}{\ell - p - |\underline{m}|_1 - (n - m_i)} \binom{d-1}{p}
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{p=0}^{d-1} (-1)^p \binom{(K_i + d - 2) - p - n}{d-2} \binom{d-1}{p} \\
&= \binom{K_i - n - 1}{-1} \\
&= 1
\end{aligned}
$$

when $n = K_i$ and 0 otherwise. Therefore,

$$
\begin{aligned}
\Gamma_{|\xi|^4 \xi_i^4} &= \frac{1}{12} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \\
&\qquad \times \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1 = \ell - p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1 = \ell - q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} h_{k_i}^2 \alpha_{i,k_i} \\
&= \frac{1}{12} h_{K_i}^2 \alpha_{i,K_i} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \\
&= \frac{1}{12} h_{\ell - |\underline{m}|_1 + m_i}^2 \alpha_{i,K_i} \rho h_{\ell-1}^2 \mu_t |\xi|^4 \xi_i^4 \\
&= \frac{1}{3} h_{-|\underline{m}|_1 + m_i}^2 \alpha_{i,K_i} \rho h_\ell^4 \mu_t |\xi|^4 \xi_i^4 \\
&= \frac{1}{3} \prod_{\substack{j=1 \\ j \neq i}}^{d} 2^{4 m_j} \alpha_{i,K_i} \rho h_\ell^4 \mu_t |\xi|^4 \xi_i^4 .
\end{aligned}
$$

Taking the absolute value,

$$
\begin{aligned}
|\Gamma_{|\xi|^4 \xi_i^4}| &\leq \frac{1}{3} \prod_{\substack{j=1 \\ j \neq i}}^{d} 2^{4 m_j} \rho h_\ell^4 \mu_t |\xi|^4 \xi_i^4 \\
&\leq \frac{1}{3} \prod_{\substack{j=1 \\ j \neq i}}^{d} 16 (1 + \frac{1}{\pi} \xi_j)^4 \rho h_\ell^4 \mu_t |\xi|^4 \xi_i^4 .
\end{aligned}
$$

Therefore, for some constant C_3,

$$
\int_{A_\ell} |\Gamma_{|\xi|^4 \xi_i^4}| \hat{u}_0(\xi)^2 \, d\xi \leq \int_{A_\ell} \frac{1}{3} \prod_{\substack{j=1 \\ j \neq i}}^{d} 16 (1 + \frac{1}{\pi} \xi_j)^4 \rho h_\ell^4 \mu_t |\xi|^4 \xi_i^4 \hat{u}_0(\xi)^2 \, d\xi
$$

$$
\begin{aligned}
&\leq \frac{1}{3}\rho h_\ell^4 \mu_t \int_{A_\ell} \prod_{\substack{j=1 \\ j\neq i}}^{d} 16(1+\frac{1}{\pi}\xi_j)^4 |\xi|^4 \xi_i^4 \hat{u}_0(\xi)^2 \, d\xi \\
&\leq \frac{1}{3}\rho h_\ell^4 \mu_t C_3 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)}.
\end{aligned}
$$

Terms of type $|\xi|^8$

Finally, we look at $\Gamma_{|\xi|^8}$, that is, terms of type $|\xi|^8$. These terms are

$$
\begin{aligned}
\Gamma_{|\xi|^8} &= \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \\
&= \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} \sum_{q=0}^{d-1} \sum_{|\underline{l}|_1=\ell-q} (-1)^{p+q} \binom{d-1}{p} \binom{d-1}{q} \mathbf{1}_{A_{\underline{k}}} \mathbf{1}_{A_{\underline{l}}} \\
&= \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \left(\sum_{p=0}^{d-1} \sum_{|\underline{k}|_1=\ell-p} (-1)^{p} \binom{d-1}{p} \mathbf{1}_{A_{\underline{k}}} \right)^2 \\
&= \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \sum_{|\underline{m}|_1 \leq \ell} \mathbf{1}_{B_{\underline{m}}}.
\end{aligned}
$$

Taking the absolute value,

$$
|\Gamma_{|\xi|^8}| \leq \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8.
$$

Therefore, for some constant C_4,

$$
\begin{aligned}
\int_{A_\ell} |\Gamma_{|\xi|^8}| \hat{u}_0(\xi)^2 \, d\xi &\leq \int_{A_\ell} \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 |\xi|^8 \hat{u}_0(\xi)^2 \, d\xi \\
&\leq \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 \int_{A_\ell} |\xi|^8 \hat{u}_0(\xi)^2 \, d\xi \\
&\leq \frac{1}{4}\rho^2 h_{\ell-1}^4 \mu_t^2 C_4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)}.
\end{aligned}
$$

Conclusion

In summary,

$$\begin{aligned}
\Omega_1(h_\ell) &\leq \int_{A_\ell} \left(\sum_{i=1}^{d} |\Gamma_{\xi_i^8}| + \sum_{i=1}^{d} \sum_{j=1}^{i-1} |\Gamma_{\xi_i^4 \xi_j^4}| + \sum_{i=1}^{d} |\Gamma_{|\xi|^4 \xi_i^4}| + |\Gamma_{|\xi^8|}| \right) d\xi \\
&\leq \sum_{i=1}^{d} \frac{1}{144} C_1 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \sum_{i=1}^{d} \sum_{j=1}^{i-1} \frac{1}{36} C_2 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \\
&\quad \sum_{i=1}^{d} \frac{1}{3} \rho h_\ell^4 \mu_t C_3 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 C_4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} \\
&= d \frac{1}{144} C_1 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \frac{d(d-1)}{2} \frac{1}{36} C_2 h_\ell^4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \\
&\quad d \frac{1}{3} \rho h_\ell^4 \mu_t C_3 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)} + \frac{1}{4} \rho^2 h_{\ell-1}^4 \mu_t^2 C_4 \|u_0\|^2_{H^4_{\text{mix}}(\mathbb{R}^d)}.
\end{aligned}$$

Therefore, $\Omega_1(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^d)$.

3.5.2 Rate of convergence of $\Omega_2(h_\ell)$

Define $C_1(h_\ell) = \{(\xi_1, \ldots, \xi_d) : \xi_1 \xi_2 \ldots \xi_d \geq \frac{\pi^d}{h_{\ell-d}}\}$ and $C_2(h_\ell) = \mathbb{R}^d \setminus C_1(h_\ell) \setminus A_\ell$. It is clear by definition of $C_1(h_\ell)$ and $C_2(h_\ell)$ that $\mathbb{R}^d \setminus A_\ell \subset C_1(h_\ell) \cup C_2(h_\ell)$.

Since $|e^{q(\xi)t_n}| \leq 1$, we have

$$\begin{aligned}
\Omega_2(h_\ell) &= \int_{\mathbb{R}^d \setminus A_\ell} |e^{q(\xi)t_n} \hat{u}_0(\xi)|^2 \, d\xi \\
&\leq \int_{\mathbb{R}^d \setminus A_\ell} |\hat{u}_0(\xi)|^2 \, d\xi \\
&\leq \int_{C_1(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi + \int_{C_2(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi.
\end{aligned}$$

On the domain $C_1(h_\ell)$ we have $1 \leq \frac{(\xi_1 \xi_2 \ldots \xi_d) h_{\ell-d}}{\pi^d}$ and thus $1 \leq \frac{(\xi_1^4 \xi_2^4 \ldots \xi_d^4) h_{\ell-d}^4}{\pi^{4d}}$.

Therefore, we have for the first term:

$$\begin{aligned}\int_{C_1(h_\ell)} |\hat{u}_0(\xi)|^2\, d\xi &\le \frac{1}{\pi^{4d}} h_{\ell-d}^4 \int_{C_1(h_\ell)} (\xi_1^4\xi_2^4 \dots \xi_d^4)|\hat{u}_0(\xi)|^2\, d\xi \\ &\le \left(\frac{2}{\pi}\right)^{4d} h_\ell^4 \left\| \frac{\partial^{2d} u_0}{\partial x_1^2 \partial x_2^2 \dots \partial x_d^2} \right\|_2^2\end{aligned}$$

Now we look at the second term. The structure of the set $C_2(h_\ell)$ is less clear in d dimensions than it was in 2 dimensions. Let's define the auxiliary sets

$$C_{2,i}(h_\ell) := \{(\xi_1, \dots, \xi_d) : \xi_i \ge \frac{\pi}{h_\ell}\}.$$

Then following lemma gives us enough information about $C_2(h_\ell)$ to finish the proof of the theorem.

Lemma 14. *If $\xi = (\xi_1, \dots, \xi_d) \in C_2(h_\ell)$ then $\xi \in C_{2,i}(h_\ell)$ for some $i \in \{1, \dots, d\}$. That is,*

$$C_2(h_\ell) \subset \bigcup_{i=1}^{d} C_{2,i}(h_\ell).$$

Proof. Fix $\xi \in C_2(h_\ell)$. Suppose, for the sake of contradiction, that $\xi_i < \frac{\pi}{h_\ell}$ for all $i \in \{1, \dots, d\}$. We proceed by showing that ξ must lie in A_ℓ, thus contradicting $\xi \in C_2(h_\ell)$. To show this, it is sufficient to find one $A_{\underline{l}} \subset A_\ell$ such that $\xi \in A_{\underline{l}}$.

Since $\xi \in C_2(h_\ell)$ we must have that $\xi \notin C_1(h_\ell)$. Therefore, $\xi_1\xi_2 \dots \xi_d < \frac{\pi^d}{h_{\ell-d}}$. Also, since $\xi_i < \frac{\pi}{h_\ell}$ for all $i \in \{1, \dots, d\}$, we have $\xi \in A_{(\ell-1,\dots,\ell-1)}$. Furthermore, there must be some $A_{\underline{l}} \subset A_{(\ell-1,\dots,\ell-1)}$ which contains ξ and is smallest in the sense that if $k = (k_1, \dots, k_d)$ has $k_i < l_i$ for at least one i, then $\xi \notin A_{\underline{k}}$. Then we can also say $\xi \in B_{\underline{l}}$.

Now, it is sufficient to show that $|\underline{l}|_1 \le \ell$. This implies that $\xi \in B_{\underline{l}} \subset A_\ell$ and then we are done. Since $\xi \in B_{\underline{l}}$ we have, for each coordinate, $2^{l_i-1}\pi \le \xi_i$. Taking the product over all i,

$$\prod_{i=1}^{d} 2^{l_i-1}\pi = 2^{|\underline{l}|_1-d}\pi^d$$

$$
\begin{aligned}
&\le \xi_1 \dots \xi_d \\
&\le \frac{\pi^d}{h_{\ell-d}} \\
&\le \pi^d 2^{\ell-d}.
\end{aligned}
$$

Stringing the inequalities together gives $2^{|\underline{l}|_1-d}\pi^d \le \pi^d 2^{\ell-d}$ and so $|\underline{l}|_1 \le \ell$.

$\square$

Now, by the preceding lemma, we have the inequality

$$
\begin{aligned}
\int_{C_2(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi &\le \sum_{i=1}^{d} \int_{C_{2,i}(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi \\
&\le \frac{1}{\pi^4} h_\ell^4 \sum_{i=1}^{d} \int_{C_{2,i}(h_\ell)} \xi_i^4 |\hat{u}_0(\xi)|^2 \, d\xi \\
&\le \frac{1}{\pi^4} h_\ell^4 \sum_{i=1}^{d} \left\| \frac{\partial^2 u_0}{\partial x_i^2} \right\|_2^2.
\end{aligned}
$$

Adding the two parts of $\Omega_2(h_\ell)$ then gives

$$
\begin{aligned}
\Omega_2(h_\ell) &\le \int_{C_1(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi + \int_{C_2(h_\ell)} |\hat{u}_0(\xi)|^2 \, d\xi \\
&\le h_\ell^4 \left(\left(\frac{2}{\pi}\right)^{4d} \left\| \frac{\partial^{2d} u_0}{\partial x_1^2 \partial x_2^2 \dots \partial x_d^2} \right\|_2^2 + \frac{1}{\pi^4} \sum_{i=1}^{d} \left\| \frac{\partial^2 u_0}{\partial x_i^2} \right\|_2^2 \right).
\end{aligned}
$$

In summary $\Omega_2(h_\ell) = O(h_\ell^4)$ when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^d)$. Thus,

$$
\begin{aligned}
\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2^2 &= \Omega_1(h_\ell) + \Omega_2(h_\ell) \\
&= O(h_\ell^4) + O(h_\ell^4) \\
&= O(h_\ell^4)
\end{aligned}
$$

when $u_0 \in H^4_{\text{mix}}(\mathbb{R}^d)$ and so $\|u(x,t_n) - (\sigma v_{t_n})(x)\|_2 = O(h_\ell^2)$. $\square$

Chapter 4

Numerical results for constant-coefficient equations

We now present some numerical results for the parabolic method applied to the solution of constant-coefficient equations of the form

$$u_t + \sum_{i,j=1}^{d} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i \frac{\partial u}{\partial x_i} = 0 \tag{4.1}$$

in d-dimensional space, where (a_{ij}) is a real, positive definite $d \times d$ matrix and (b_i) is a real d-vector. Constant-coefficient equations make useful test cases because analytic solutions are available by means of Fourier analysis. Note that Equation (4.1) is now of *backward* parabolic type, so that the problem is only well-posed when solved backwards from some terminal time $t = T$. We choose this convention to be consistent with option-pricing problems from finance, which are naturally backward parabolic.

We begin with the simplest example of (4.1), the heat equation in $\mathbb{R}^d$. We then allow $a_{ij} \neq 0$ for $i \neq j$ and later $b_i \neq 0$ to show that the presence of cross-derivative and drift terms in the PDE does not hamper the convergence of the parabolic method.

Our goal is to compare the parabolic method with both its sparse grid counterpart, the elliptic method, and the conventional Crank-Nicolson method. We look at the rate of convergence of the error at the midpoint of the mesh

Level	Error	Ratio	Mean ratio
1	1.0		
2	0.5	2	2
3	0.1	5	$\sqrt{2 \times 5} \approx 3.16$

Table 4.1: Example of mean ratio

and the run time of the methods. We define the spatial mesh spacing for the level-ℓ Crank-Nicolson solution to be $2^{-(\ell-(d-1))}$ in each coordinate direction, which is the smallest among the mesh spacings of all sparse grids at level ℓ. Thus, it is the coarsest conventional mesh which contains all sparse grids in the level-ℓ combination.

We present results for dimensions 2, 4, and 6. The results for each dimension are presented in order of increasing mesh refinement. We give the percent error in the approximate solution at the midpoint of the mesh. To assess the rate of convergence, we calculate the running mean error ratio. This is the geometric mean of the ratios of the errors at successive mesh refinement levels. In table headings, we call this quantity the *mean ratio*. For example, suppose approximate solutions are calculated at levels 1 through 3, with respective errors 1.0, 0.5, 0.1. Table 4.1 demonstrates the calculation of the mean ratio. The mean ratio serves as a device to evaluate the rate of convergence. When quadratic convergence is observed, the mean ratio should converge to 4. When linear convergence is observed, the mean ratio should converge to 2.

Throughout this chapter, we take

$$[0, 2\pi]^d \times [0, 1]$$

as the domain and

$$u(x_1, \ldots, x_d, T) = \cos(x_1 + \ldots x_d)$$

as the terminal condition. The boundary conditions are set to be 2π-periodic so that the exact solution can be recovered by the inverse Fourier transform.

4.1 Implementation details

The following results were obtained using a code written in C++. Although sparse grid methods are popular for their ease of parallelization, discussion of load balancing is beyond the intent of this work, and our results were obtained by single-threaded execution.

We use the Crank-Nicolson method for time discretization and fix the time step

$$\Delta t = 2\Delta x_{min},$$

where Δx_{min} is the smallest spatial mesh spacing used in the sparse grid discretization. The ratio 2 was chosen to avoid Crank-Nicolson oscillations (see [Smi85, p. 122]).

Systems of equations were solved by the iterative Biconjugate Gradient Stabilized (BiCGSTAB) method, except when the matrix is tridiagonal, in which case we use the Thomas algorithm. For each system of equations $Ax = b$, the stopping criterion used for the BiCGSTAB algorithm was to stop when $\|Ax - b\|_\infty < 5 \times 10^{-11}$. We refer the reader to [Saa03, p. 244] for details on the BiCGSTAB algorithm. Note that the matrix is tridiagonal for two-dimensional sparse grids $\Omega_{\underline{l}}$ when either $l_1 = 1$ or $l_2 = 1$. These are the same grids which are the most time-consuming for the iterative solver, since the mesh spacing in the other coordinate direction must consequently be very fine. Matrices were stored in compressed sparse row format [Saa03, p. 92].

4.2 Heat equation

The simplest example of Equation (4.1) is the heat equation:

$$u_t + \frac{\partial^2 u}{\partial x_1^2} + \ldots + \frac{\partial^2 u}{\partial x_d^2} = 0. \tag{4.2}$$

Table 4.2 presents a comparison of the results of the parabolic method and the conventional Crank-Nicolson method. Table 4.3 presents a comparison of the results of the parabolic method and the elliptic method.

			Parabolic method			Crank-Nicolson method		
d	$\max_i N_i$	Level	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)
2	2	2	45.542300		0.00	45.542300		0.00
2	4	3	7.974991	5.71	0.02	10.438467	4.36	0.01
2	8	4	1.181201	6.21	0.08	2.548872	4.23	0.05
2	16	5	0.095842	7.80	0.34	0.633407	4.16	0.37
2	32	6	0.025662	6.49	1.54	0.158113	4.12	4.41
2	64	7	0.018806	4.75	7.14	0.039513	4.10	40.83
2	128	8	0.007798	4.24	32.16	0.009877	4.08	478.39
2	256	9	0.002724	4.01	147.15			
2	512	10	0.000874	3.89	646.50			
4	2	4	107.272117		0.06	107.272117		0.06
4	4	5	1.109096	96.72	0.84	20.919431	5.13	0.62
4	8	6	3.602137	5.46	8.88	4.909603	4.67	20.44
4	16	7	1.362523	4.29	66.86	1.208130	4.46	1496.61
4	32	8	0.352762	4.18	389.21			
4	64	9	0.070389	4.33	1942.78			
6	2	6	182.122227		1.31	182.122227		1.32
6	4	7	36.188627	5.03	26.59	30.100689	6.05	36.00
6	8	8	13.470628	3.68	294.75			

Table 4.2: Comparison of parabolic and Crank-Nicolson methods, heat equation (4.2).

			Parabolic method			Elliptic method		
d	$\max_i N_i$	Level	Pct. error at $(\pi,\ldots,\pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi,\ldots,\pi)$	Mean ratio	Total time (s)
2	2	2	45.542300		0.00	45.542300		0.00
2	4	3	7.974991	5.71	0.02	13.574913	3.35	0.02
2	8	4	1.181201	6.21	0.07	4.581978	3.15	0.09
2	16	5	0.095842	7.80	0.33	1.500749	3.12	0.43
2	32	6	0.025662	6.49	1.54	0.470608	3.14	2.42
2	64	7	0.018806	4.75	7.11	0.142169	3.17	16.58
2	128	8	0.007798	4.24	36.55	0.041728	3.21	121.58
2	256	9	0.002724	4.01	168.26	0.011982	3.25	789.90
2	512	10	0.000874	3.89	694.63			
4	2	4	107.272117		0.06	107.272117		0.06
4	4	5	1.109096	96.72	0.87	39.906062	2.69	1.07
4	8	6	3.602137	5.46	8.19	17.422180	2.48	20.87
4	16	7	1.362523	4.29	64.19	7.402381	2.44	772.02
4	32	8	0.352762	4.18	381.58			
4	64	9	0.070389	4.33	1804.27			
6	2	6	182.122227		1.32	182.122227		1.44
6	4	7	36.188627	5.03	30.32	79.294021	2.30	56.02
6	8	8	13.470628	3.68	329.56	39.382476	2.15	6524.34

Table 4.3: Comparison of parabolic and elliptic methods, heat equation (4.2).

4.3 Diffusion equation with unit diagonal

Next, we present results for the diffusion equation

$$u_t + \sum_{i,j=1}^{d} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} = 0, \tag{4.3}$$

which is precisely Equation (4.1) with the drift coefficients b_i set to 0. We take

$$(a_{ij}) = \begin{pmatrix} 1 & -0.06 & -0.02 & -0.02 & -0.06 & -0.02 \\ -0.07 & 1 & -0.01 & -0.02 & 0.00 & -0.06 \\ -0.02 & -0.01 & 1 & 0.11 & 0.13 & -0.13 \\ -0.02 & -0.01 & 0.12 & 1 & -0.02 & -0.09 \\ -0.07 & 0.00 & 0.15 & -0.02 & 1 & -0.05 \\ -0.03 & -0.06 & -0.13 & -0.09 & -0.05 & 1 \end{pmatrix},$$

which was randomly generated so that its eigenvalues lie in $[0.5, 1.5]$ and its diagonal elements a_{ii} are 1. The elements of the preceding matrix have been rounded to the second decimal place for presentation in this paper.

Table 4.4 presents a comparison of the results of the parabolic method and the conventional Crank-Nicolson method. Table 4.5 presents a comparison of the results of the parabolic method and the elliptic method.

4.4 Heat equation with non-zero drift

Next, we present results for the equation

$$u_t + \frac{\partial^2 u}{\partial x_1^2} + \ldots + \frac{\partial^2 u}{\partial x_d^2} + \sum_{i=1}^{d} b_i \frac{\partial u}{\partial x_i} = 0, \tag{4.4}$$

which is precisely Equation (4.1) with diagonal diffusion matrix (a_{ij}). We take

$$b = \begin{pmatrix} -0.11 \\ 0.15 \\ -0.10 \\ -0.15 \\ 0.05 \\ -0.09 \end{pmatrix},$$

			Parabolic method			Crank-Nicolson method		
d	$\max_i N_i$	Level	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)
2	2	2	34.574188		0.00	34.574188		0.00
2	4	3	5.097704	6.78	0.02	7.729290	4.47	0.01
2	8	4	0.416154	9.11	0.08	1.875116	4.29	0.05
2	16	5	0.108418	6.83	0.34	0.465210	4.20	0.37
2	32	6	0.080125	4.56	1.55	0.116080	4.15	4.33
2	64	7	0.033284	4.01	7.54	0.029006	4.12	51.62
2	128	8	0.011634	3.79	36.86	0.007251	4.10	532.04
2	256	9	0.003737	3.69	168.80			
2	512	10	0.001141	3.63	700.40			
4	2	4	102.665044		0.07	102.665044		0.07
4	4	5	1.516067	67.72	0.86	20.074562	5.11	0.61
4	8	6	2.986756	5.86	8.10	4.715660	4.67	17.37
4	16	7	1.040094	4.62	60.64	1.160690	4.46	1489.16
4	32	8	0.221544	4.64	371.96			
4	64	9	0.023604	5.34	1939.62			
6	2	6	97.414360		1.31	97.414360		1.32
6	4	7	14.574647	6.68	26.38	16.671662	5.84	36.30
6	8	8	4.648685	4.58	293.79			

Table 4.4: Comparison of parabolic and Crank-Nicolson methods, diffusion equation with unit diagonal (4.3).

			Parabolic method			Elliptic method		
d	$\max_i$ N_i	Level	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)
2	2	2	34.574188		0.00	34.574188		0.00
2	4	3	5.097704	6.78	0.02	9.360147	3.69	0.02
2	8	4	0.416154	9.11	0.08	2.389173	3.80	0.09
2	16	5	0.108418	6.83	0.33	0.023611	11.36	0.42
2	32	6	0.080125	4.56	1.52	0.635800	2.72	2.56
2	64	7	0.033284	4.01	7.42	0.620680	2.23	17.98
2	128	8	0.011634	3.79	37.52	0.456587	2.06	123.52
2	256	9	0.003737	3.69	173.48	0.299811	1.97	804.04
2	512	10	0.001141	3.63	723.87			
4	2	4	102.665044		0.06	102.665044		0.07
4	4	5	1.516067	67.72	0.85	38.237027	2.68	1.06
4	8	6	2.986756	5.86	8.14	13.180542	2.79	19.92
4	16	7	1.040094	4.62	61.71	1.176185	4.44	778.40
4	32	8	0.221544	4.64	376.67			
4	64	9	0.023604	5.34	1796.32			
6	2	6	97.414360		1.36	97.414360		1.39
6	4	7	14.574647	6.68	29.12	41.343939	2.36	56.40
6	8	8	4.648685	4.58	320.27			

Table 4.5: Comparison of parabolic and elliptic methods, diffusion equation with unit diagonal (4.3).

where the elements have b have been randomly generated and rounded to the second decimal place for presentation in this paper. Table 4.6 presents a comparison of the results of the parabolic method and the conventional Crank-Nicolson method. Table 4.7 presents a comparison of the results of the parabolic method and the elliptic method.

			Parabolic method			Crank-Nicolson method		
d	$\max_i$ N_i	Level	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)
2	2	2	45.601829		0.00	45.601829		0.00
2	4	3	7.829846	5.82	0.02	10.452772	4.36	0.01
2	8	4	1.091988	6.46	0.08	2.552396	4.23	0.05
2	16	5	0.059489	9.15	0.35	0.634284	4.16	0.37
2	32	6	0.038316	5.87	1.62	0.158332	4.12	4.60
2	64	7	0.022865	4.57	7.92	0.039568	4.10	48.03
2	128	8	0.009037	4.14	38.05	0.009891	4.08	524.48
2	256	9	0.003089	3.94	170.64			
2	512	10	0.000980	3.83	691.53			
4	2	4	110.061682		0.06	110.061682		0.06
4	4	5	0.584260	188.38	0.89	21.419973	5.14	0.62
4	8	6	3.902218	5.31	8.23	5.023601	4.68	17.49
4	16	7	1.437905	4.25	62.77	1.235955	4.47	1474.96
4	32	8	0.362881	4.17	381.44			
4	64	9	0.069148	4.37	1916.44			
6	2	6	187.193572		1.26	187.193572		1.29
6	4	7	38.730570	4.83	27.07	30.781708	6.08	36.43
6	8	8	14.112716	3.64	296.93			

Table 4.6: Comparison of parabolic and Crank-Nicolson methods, heat equation with drift (4.4).

			Parabolic method			Elliptic method		
d	$\max_i$ N_i	Level	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)	Pct. error at $(\pi, \ldots, \pi)$	Mean ratio	Total time (s)
2	2	2	45.601829		0.00	45.601829		0.00
2	4	3	7.829846	5.82	0.02	14.436439	3.16	0.02
2	8	4	1.091988	6.46	0.08	5.767463	2.81	0.10
2	16	5	0.059489	9.15	0.35	2.551510	2.61	0.43
2	32	6	0.038316	5.87	1.59	1.252419	2.46	2.56
2	64	7	0.022865	4.57	7.38	0.669192	2.33	17.26
2	128	8	0.009037	4.14	39.37	0.375170	2.23	125.30
2	256	9	0.003089	3.94	180.09	0.214132	2.15	799.39
2	512	10	0.000980	3.83	717.01			
4	2	4	110.061682		0.06	110.061682		0.06
4	4	5	0.584260	188.38	0.90	42.451481	2.59	1.08
4	8	6	3.902218	5.31	8.21	19.842669	2.36	20.92
4	16	7	1.437905	4.25	64.21	9.515864	2.26	783.39
4	32	8	0.362881	4.17	386.02			
4	64	9	0.069148	4.37	1858.70			
6	2	6	187.193572		1.27	187.193572		1.34
6	4	7	38.730570	4.83	26.57	84.616034	2.21	50.06
6	8	8	14.112716	3.64	289.43			

Table 4.7: Comparison of parabolic and elliptic methods, heat equation with drift (4.4).

Chapter 5

Applications to option pricing: Black-Scholes model

We now apply the techniques of the previous chapter to the pricing of options on multiple risky assets under the multidimensional Black-Scholes model. Let $\{S_t^{(i)}\}_{i=1}^d$ be a collection of d risky assets satisfying

$$dS_t^{(i)} = rS_t^{(i)}\,dt + \sigma_i S_t^{(i)}\,dW_t^{(i)}, \qquad i \in \{1, \ldots, d\}, \tag{5.1}$$

where W is Brownian motion under the risk-neutral measure $\tilde{\mathbb{P}}$ with correlation matrix ρ. Given a payoff function $p : \mathbb{R}^d \to \mathbb{R}$, the price V of a derivative security paying $p(S_T)$ at time T satisfies the problem

$$\begin{aligned} &\frac{\partial V}{\partial t} + \frac{1}{2}\sum_{i,j=1}^d \rho_{ij}\sigma_i\sigma_j s_i s_j \frac{\partial^2 V}{\partial s_i \partial s_j} + \sum_{i=1}^d r s_i \frac{\partial V}{\partial s_i} - rV = 0, \qquad (0,\infty)^d \times (0,T), \\ &V(\mathbf{s}, T) = p(\mathbf{s}). \end{aligned} \tag{5.2}$$

By Fichera theory, no boundary condition is required on the near boundary. Since we are solving on a computer, we must impose an artificial boundary condition on a far boundary. Choice of the location and data for the artificial boundary have been considered for the multidimensional Black-Scholes equation by Kangro and Nicolaides [KN00], who found that imposing $V(\mathbf{s}, t) = p(\mathbf{s})$ on an artificial boundary which is 4 times the strike price produces reasonable results.

We consider a model with risk-free interest rate $r = 0.09$ and 5 risky assets having the following volatilities σ and correlations ρ. The correlation matrix ρ was taken to be the identity matrix since we have already shown that the introduction of correlation does not degrade the convergence of the parabolic method.

$$\sigma = \begin{pmatrix} 0.318 \\ 0.243 \\ 0.212 \\ 0.180 \\ 0.130 \end{pmatrix} \qquad \rho = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{5.3}$$

5.1 Monte Carlo simulation

Having previously established the benefits of the parabolic method over the elliptic and full grid methods, we compare the parabolic method to Monte Carlo simulation, which is the only practical alternative for high-dimensional problems. For the multidimensional Black-Scholes model, the risk-neutral distribution of the underlying asset prices at time T is known explicitly; it is not needed to discretize the stochastic differential equation (SDE) (5.1) to perform a Monte Carlo simulation. However, it is usually the case that if the distribution of the asset prices is known explicitly, Monte Carlo simulation or PDE methods are not needed to determine the price anyway. Thus, we believe the most just comparison is made by discretizing the SDEs in the Monte Carlo simulation by Euler's method, since that would have to be done in realistic situations.

5.1.1 Choice of Δt

We must choose a suitable time step Δt for the discretization of the SDEs. An unnecessarily small time step yields a small time discretization error but makes the method of simulation seem slower than it need be. A balance must be struck. We choose the time step Δt so that the time discretization error is of the same order of magnitude as the standard error of the simulation.

Note that Δt should be a function of the number N of simulation paths. When increasing N, we must increase the number of time steps so that the time discretization error remains of the same order as the standard error of the simulation. Monte Carlo theory suggests that Δt should be proportional to $\frac{1}{\sqrt{N}}$. Therefore, for a simulation with N paths, we take

$$\Delta t = \kappa \frac{1}{\sqrt{N}} \tag{5.4}$$

for some constant of proportionality κ.

To choose κ we priced an at-the-money European call option expiring at $T = 1$ on an asset S_t which satisfies

$$dS_t = \sigma(t) S_t \, dW_t, \quad S_0 = 1,$$

for various choices of $\sigma : [0,1] \to [0,1]$. We priced each option with a continuous-time simulation having $N = 1{,}000{,}000$ paths, using a single random draw for each path, and observed the standard error of the simulation. Then we priced each option with a discrete-time simulation having $N = 1{,}000{,}000$ paths and various numbers of time steps. Thus, we could ascertain the number of time steps needed so that the error of the discrete-time simulation is near the standard error of the continuous-time simulation. We found that 500 time steps were needed to cover several reasonable choices of σ. Therefore, κ must be 2:

$$\Delta t = \frac{1}{500} \sqrt{\frac{1{,}000{,}000}{N}} = \frac{2}{\sqrt{N}}. \tag{5.5}$$

5.2 A note about non-smooth data

It is well known that non-smooth data degrades the rate of convergence of numerical methods for PDE. This is true even for conventional methods, but is more pronounced in the case of sparse grid methods. In option-pricing problems, the data is rarely, if ever, a smooth function. Instead, the data usually has a discontinuous derivative (e.g., standard call and put options) or is discontinuous itself (e.g., digital options).

Rates of convergence of the Crank-Nicolson method for one- and two-dimensional problems with non-smooth data have been reviewed by Pooley, Vetzal, and

Forsyth [PVF03], who found that—denoting the spatial mesh spacing by h—$O(h^2)$ convergence can be obtained when the Crank-Nicolson method is augmented in two ways. First, one of several smoothing techniques is applied to the data. Second, the time-stepping method of Rannacher [Ran84] is employed, by which Crank-Nicolson steps are preceded by a small number of steps of the fully implicit method. Among the smoothing techniques discussed by the authors is one introduced by Tavella and Randall [TR00], who propose that the grid be constructed so that any discontinuities in the data (or its derivatives) lie midway between adjacent grid points. Another of the smoothing techniques discussed is a technique of Heston and Zhou [HZ00] by which the data is averaged in some neighborhood of the grid point, instead of simply evaluated at the grid point.

It has been recognized that the same difficulties persist for the sparse grid combination technique when the data are not smooth. For the case of the basket call option, Leentvaar and Oosterlee [LO08] propose coordinate transformations by which the grid is aligned with the points of non-differentiability in the payoff $\max(\sum_{i=1}^{d} \mu_i S_i - K, 0)$. The proposed transformations take advantage of the structure of this particular payoff function by setting the first transformed variable to $x_1 = \sum_{i=1}^{d} \mu_i S_i$, so that all points of non-differentiability are aligned with the grid. The method is not extensible to arbitrary payoffs.

5.3 Portfolio of European call options

We price a portfolio of d European call options on assets $\{S_t^{(i)}\}_{i=1}^{d}$ having strikes $\{K_i\}_{i=1}^{d}$ for $d = 2, 3, 4, 5$. Each option is weighted in the portfolio by a weight μ_i. Thus, the payoff is

$$p(S_T^{(1)}, \ldots, S_T^{(d)}) = \mu_1 \max(S_T^{(1)} - K_1, 0) + \ldots + \mu_d \max(S_T^{(d)} - K_d, 0). \quad (5.6)$$

We take $(K_i) = (1, 2, 1, 1, 1.25)$, $(\mu_i) = (1, 2, 1, 3, 2)$, and $(S_0^{(i)}) = (1, 1, 1, 1, 1)$. See Figure 5.1.

This example has a few advantages. First, we can easily compute the exact solution by the Black-Scholes formula. Second, it is typical of many examples of options in that it has a piecewise linear payoff and is continuous but

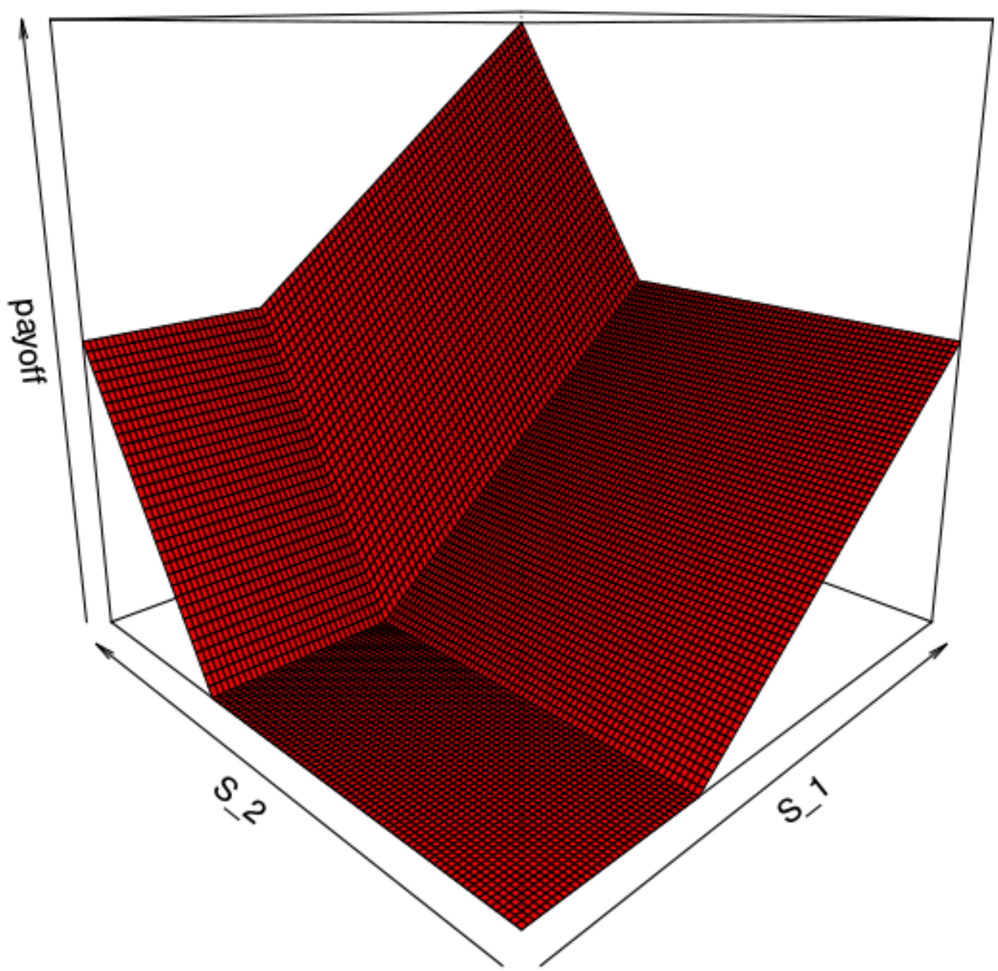


Figure 5.1: The payoff (5.6) for $d = 2$.

not differentiable. Third, it is interesting from a practical viewpoint. The points of nonsmoothness of its payoff are not constrained to a single hyperplane.

Tables 5.1, 5.2, 5.3, and 5.4 compare the percent error of the parabolic method with the percent error of simulation for dimensions $d = 2, 3, 4,$ and 5 respectively. For each dimension we calculate the parabolic method results up through level 12. We see that the accuracy of the parabolic method surpasses that of simulation by level 12 for dimensions $d = 2, 3, 4$. Simulation is more accurate than the level 12 solution for $d = 5$, but, given the observed convergence rate of the parabolic method, it can be seen that the parabolic method will surpass simulation at a subsequent level. Calculating further levels should be easier with the superior hardware that would be used in practice.

We observe that the level at which the accuracy of the parabolic method surpasses simulation increases with increasing dimension. This limits the practicality of the method for very high dimensional problems. For dimensions $d = 2, 3, 4,$ and 5 the method appears to provide a useful alternative to simulation. The parabolic method has the advantage that all levels lower than a given level can be computed with a fraction of additional effort. This shows which digit the sequence of approximate solutions has stabilized at. Since the result from Monte Carlo simulation is random, it does not share this quality.

Monte Carlo results	
Paths	50,000
Run time (s)	155
Pct. Error	0.1144

d	$\max_i N_i$	Level	Percent error	Ratio of errors	Total time (s)
2	2	2	100.1986		0.01
2	4	3	134.7256	0.74	0.03
2	8	4	33.2592	4.05	0.08
2	16	5	13.3117	2.50	0.22
2	32	6	2.9543	4.51	0.61
2	64	7	0.5872	5.03	1.69
2	128	8	0.1428	4.11	4.72
2	256	9	0.0354	4.04	13.21
2	512	10	0.0088	4.04	44.19
2	1024	11	0.0022	4.05	154.13

Table 5.1: Portfolio of call options, $d = 2$ (Equation (5.6)). Left: Monte Carlo simulation results. Right: Parabolic method results.

Monte Carlo results	
Paths	190,000
Run time (s)	1352
Pct. Error	0.5202

d	$\max_i N_i$	Level	Percent error	Ratio of errors	Total time (s)
3	2	3	1.3504		0.02
3	4	4	118.8457	0.01	0.07
3	8	5	46.7422	2.54	0.32
3	16	6	30.1112	1.55	1.24
3	32	7	11.5237	2.61	4.11
3	64	8	3.0355	3.80	12.91
3	128	9	0.6037	5.03	39.82
3	256	10	0.1432	4.21	125.06
3	512	11	0.0353	4.06	398.51
3	1024	12	0.0090	3.94	1346.78

Table 5.2: Portfolio of call options, $d = 3$ (Equation (5.6)). Left: Monte Carlo simulation results. Right: Parabolic method results.

Monte Carlo results	
Paths	180,000
Run time (s)	1164
Pct. Error	0.2619

d	$\max_i N_i$	Level	Percent error	Ratio of errors	Total time (s)
4	2	4	45.9008		0.03
4	4	5	69.8628	0.66	0.12
4	8	6	89.4865	0.78	0.50
4	16	7	4.4726	20.01	2.15
4	32	8	26.9241	0.17	8.42
4	64	9	9.9436	2.71	29.40
4	128	10	2.7260	3.65	103.79
4	256	11	0.5151	5.29	365.00
4	512	12	0.1189	4.33	1273.92

Table 5.3: Portfolio of call options, $d = 4$ (Equation (5.6)). Left: Monte Carlo simulation results. Right: Parabolic method results.

Monte Carlo results	
Paths	380,000
Run time (s)	3853
Pct. Error	0.2327

d	$\max_i N_i$	Level	Percent error	Ratio of errors	Total time (s)
5	2	5	63.5985		0.08
5	4	6	61.1610	1.04	0.41
5	8	7	157.5310	0.39	2.45
5	16	8	99.8259	1.58	11.47
5	32	9	3.2644	30.58	49.43
5	64	10	14.7043	0.22	196.22
5	128	11	2.7305	5.39	822.05
5	256	12	0.5541	4.93	3755.25

Table 5.4: Portfolio of call options, $d = 5$ (Equation (5.6)). Left: Monte Carlo simulation results. Right: Parabolic method results.

Chapter 6

Applications to option pricing: LIBOR market model

Market models are a class of interest rate models whose distinguishing feature is that they directly describe market-observable interest rates. This is in contrast to earlier models which give the evolution of an instantaneous short rate or a collection of instantaneous forward rates, both of which are not quoted in the market. Among the class of market models are the LIBOR market model (LMM), introduced in 1997 separately by Brace, Gatą̧rek, and Musiela [BGM97] and by Miltersen, Sandmann, and Sondermann [MSS97], and the swap market model of Jamshidian [Jam97].

In this chapter we apply the sparse grid combination technique to the solution of a partial differential equation for the pricing of interest rate derivatives under the LMM. The number of spatial dimensions of the PDE is exactly the number of forward LIBOR rates upon which the payoff of the derivative depends. We look at the *ratchet caplet*, a caplet whose strike is a functional of LIBOR rates which have already reset.

6.1 Setup

Let $T_0 < \ldots < T_{N+1} \leq T$ indicate a set of dates with fixed tenor $\delta = T_{n+1} - T_n$ 0 before a finite trading horizon T. We denote by $B(t, T)$ the price at time t

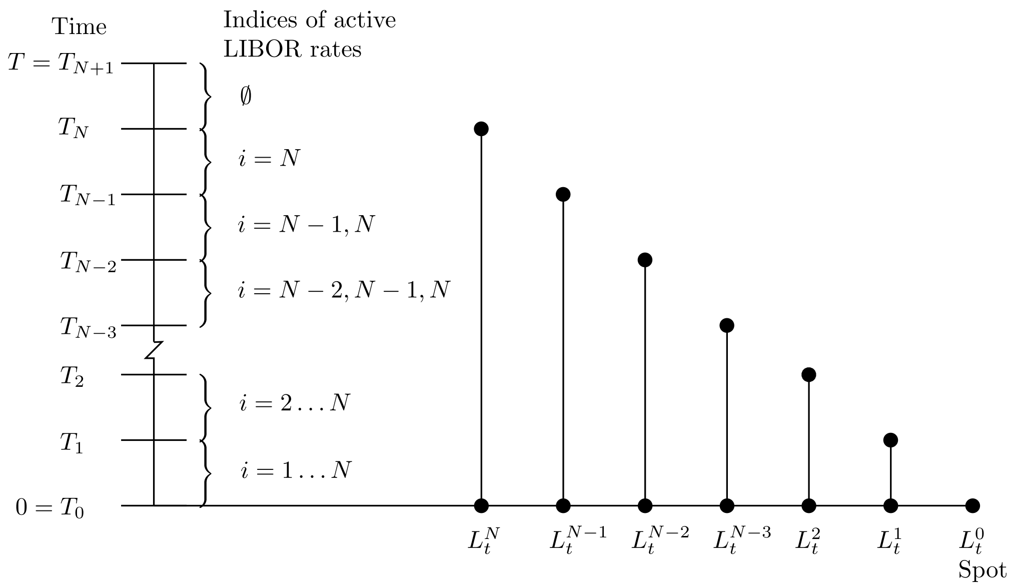


Figure 6.1: The tenor structure of the LIBOR market model.

of a zero-coupon bond which pays 1 at time T. We denote by $L(t, T_n, T_{n+1})$ the simple rate of interest which can be locked in at time t for borrowing over the interval $[T_n, T_{n+1}]$ by trading in zero-coupon bonds maturing at times T_n and T_{n+1}. The absence of arbitrage implies (see [Shr04, p. 436]) that

$$1 + \delta L(t, T_n, T_{n+1}) = \frac{B(t, T_n)}{B(t, T_{n+1})}. \tag{6.1}$$

We can unambiguously write $L_t^n := L(t, T_n, T_{n+1})$. Figure 6.1 illustrates this setup.

Let $\mathbb{P}^{T_{n+1}}$ denote the T_{n+1}-forward measure, i.e., the risk-neutral measure corresponding to the numéraire $B(t, T_{n+1})$. By definition, asset prices discounted by the numéraire are martingales. Therefore, Equation 6.1 demands that L_t^n be a martingale under the T_{n+1}-forward measure. We assume that L_t^n has lognormal dynamics under the T_{n+1}-forward measure. If W^{n+1} is Brownian motion under $\mathbb{P}^{T_{n+1}}$ and $\sigma_n(t) : [0, T_n] \to [0, \infty)$ is a deterministic volatility function, then we assume

$$dL_t^n = L_t^n \sigma_n(t)\, dW_t^{n+1}, \quad 0 \leq t \leq T_n.$$

In order to price more complicated securities which depend on multiple forward rates we need to consider all LIBOR rates under a single measure. For this purpose, we model all rates under the terminal measure $\mathbb{P}^{T_{N+1}}$, the forward measure associated with the final maturity. The terminal measure is the natural forward measure for the given time horizon since rates of *all* maturities can be modeled. However, only the LIBOR rate $L(t, T_N, T_{N+1})$ is a martingale under this measure. The forward rates which reset prior to T_N have nonzero drifts under the terminal measure. An application of Girsanov's theorem gives the drifts in explicit form, as a functional of the LIBOR rates. We have

$$\frac{dL_t^n}{L_t^n} = -\sum_{k=n+1}^{N} \frac{\delta\sigma_k(t) L_t^k}{1+\delta L_t^k}\sigma_n(t)\, dt + \sigma_n(t)\, dW_t, \qquad 0 \le t \le T_n, \tag{6.2}$$

where $W_t = (W_t^1, \ldots, W_t^{N+1})$ is a Brownian motion under $\mathbb{P}^{T_{N+1}}$. The calculation of the drifts is detailed in the appendix.

6.2 Ratchet caplets

A ratchet caplet is a special kind of caplet for which the strike depends on the values of already-reset forward LIBOR rates. To be concrete, let T_0 be the reset date of the first caplet so that $T_1, ..., T_N$ are the payment dates. Then the payment of a ratchet caplet with notional P at time T_{N+1} is

$$P\delta(L_{T_N}^N - K_N)^+,$$

where

$$\begin{aligned} K_N &= \beta(aL_{T_{N-1}}^{N-1} + bK_{N-1} + c)^+, \\ K_1 &= 0, \end{aligned}$$

for constants $\beta, a, b, c \in \mathbb{R}$ fixed by the contract.

We will call a ratchet caplet for which the strike depends on a single previously-reset LIBOR rate a *simple ratchet caplet*. A simple ratchet caplet with notional P on the interval $[T_N, T_{N+1}]$ pays

$$P\delta(L_{T_N}^N - \beta(aL_{T_{N-1}}^{N-1} + c)^+)^+$$

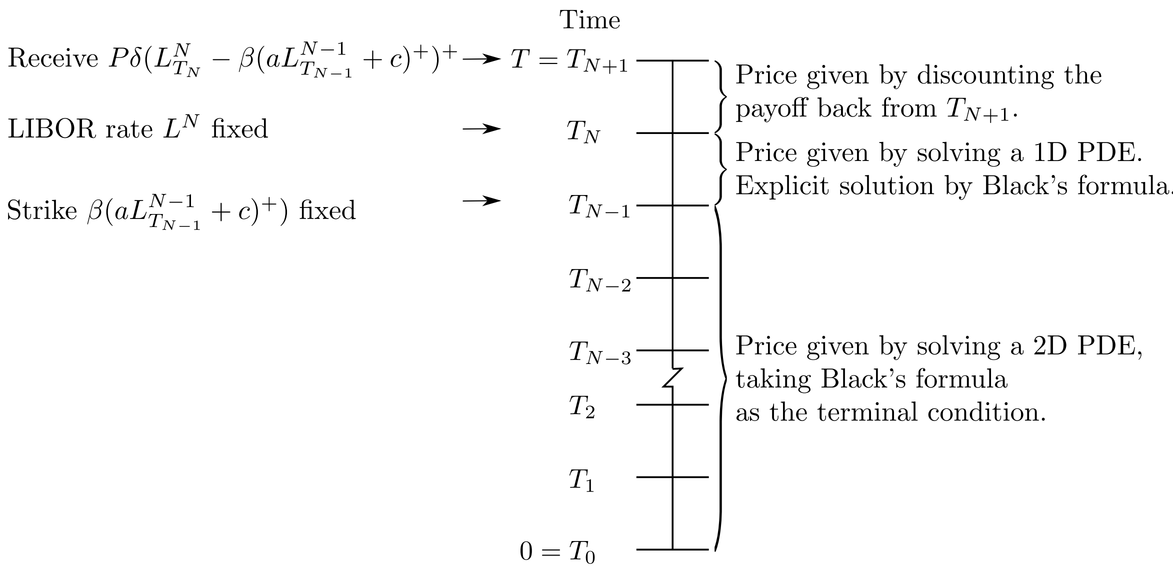


Figure 6.2: Payoff structure and pricing of a simple ratchet caplet.

at time T_{N+1}, which is precisely a ratchet caplet with $b = 0$. Figure 6.2 shows the payoff in the context of the tenor structure described earlier. Note that the ratchet caplet lacks the closed-form pricing formula of a regular caplet.

6.3 The LIBOR market model PDE

There is scant literature covering implementations of the LIBOR market model using partial differential equations. One of the first papers to appear on the topic was by Pietersz in 2002 [Pie02]. Pietersz invokes the Feynman-Kac theorem to derive one- and two-dimensional PDEs for pricing caplets and simple ratchet caplets. The paper did not discuss numerical methods. In 2004, Blackham applied sparse grid methods to the solution of the LIBOR market model PDE with success for three- and four-dimensional products. More recently in 2011, two papers by Pascucci, Suárez-Taboada, and Vázquez [PSTV11] and Suárez-Taboada and Vázquez [STV12] give a numerical method for the solution of the ratchet cap problem by means of PDE.

6.3.1 Derivation

We now derive the partial differential equation governing the price of a derivative security under the LIBOR market model. Consider an interest rate derivative with price C_t at time t whose payoff C_T at time T is a functional of the LIBOR rates $\{L_T^i\}_{i=0}^N$. As a tradable asset, its price discounted by the zero-coupon bond expiring at time T must be a martingale under the terminal measure $\mathbb{P}^T$:

$$\Pi_t \triangleq \frac{C_t}{B(t,T)} = E^T[C_T|\mathcal{F}_t]$$

By the Markov property, we can write

$$\Pi_t = u(L_t^1, \ldots, L_t^N, t)$$

for some function u. Upon taking the differential of Π_t and using the fact that Π_t must have zero drift, we see that u must satisfy

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sum_{i,j=1}^{N} \rho_{ij}(t)\sigma_i(t)\sigma_j(t)L_iL_j\frac{\partial^2 u}{\partial L_i \partial L_j} + \sum_{i=1}^{N} \mu_i(t)L_i\frac{\partial u}{\partial L_i} = 0, \qquad (6.3)$$

where

$$\mu_i(t) = -\left(\sum_{k=i+1}^{N} \frac{\delta L_k(t)}{1+\delta L_k(t)}\rho_{ik}(t)\sigma_k(t)\right)\sigma_i(t).$$

See the appendix for a discussion of how to impose boundary conditions so that the problem is well-posed.

6.4 Results

We now present results for the pricing of ratchet caplets by solution of Equation (6.3). We consider a setup of $N+1$ quarterly ($\delta = 0.25$) LIBOR rates $\{L(t, T_i, T_{i+1})\}_{i=0}^N$. We take $T_0 = 0.25$.

We now detail our choice of volatility and correlation structure. For the volatility $\sigma_n(t)$ of the forward LIBOR rate $L(t, T_n, T_{n+1})$ we use parametric linear-exponential volatilities (see [Reb12, p. 167]). That is,

$$\sigma_n(t) = \begin{cases} (a + b(T_n - t))\exp(-c(T_n - t)) + d & 0 \le t < T_n, \\ 0 & t \ge T_n, \end{cases}$$

for which we take

$$\begin{aligned} a &= 0.2, & b &= 0.05, \\ c &= 2, & d &= 0.18. \end{aligned}$$

For the instantaneous correlations $\rho_{ij}(t)$ we choose the constant-in-time parametric form

$$\rho_{ij}(t) = \exp(-\beta|T_i - T_j|),$$

for which we take $\beta = 0.2$ (see [Reb12, p. 177]).

We use the following parameters for the ratchet caplet payoff:

$$\begin{aligned} K_a &= 0.09 \\ K_b &= 1 \\ K_c &= 0.03 \\ K_\beta &= 0.3 \end{aligned}$$

We now present results for the pricing of a ratchet caplet by solution of Equation (6.3). Tables 6.1, 6.2, 6.3, and 6.4 present the results of Monte Carlo simulation and the parabolic method side-by-side for dimensions $d = 2, 3, 4,$ and 5 respectively. The superior relative performance of the parabolic method can be seen for lower dimensions. For $d = 2$ we observe that 4 digits have stabilized in the parabolic method results in 1154 seconds, while simulation still has a standard error of approximately 0.0005 after nearly two hours. Furthermore, the standard error is only a probabilistic estimate and cannot be interpreted in the same way as the stabilization of digits in the parabolic method results. On the other hand, it appears that the mesh refinement level at which the accuracy of the parabolic method surpasses that of simulation is again increasing with increasing dimension. From the sequence of parabolic method, results it appears that simulation and the parabolic method are likely comparable in accuracy during the given time frame for $d = 4$. We expect the accuracy of the parabolic method to surpass simulation with further run time. For $d = 5$ it appears that simulation is likely more accurate during the given time frame. With further run time we expect the

Monte Carlo results	
Paths	20,000
Run time (s)	1092
Price	0.687634
Standard error	0.001769

d	$\max_i N_i$	Level	Price	Total time (s)
2	2	2	0.972359	0.0
2	4	3	0.698168	0.1
2	8	4	0.697712	0.2
2	16	5	0.676337	0.5
2	32	6	0.687294	1.4
2	64	7	0.687744	3.5
2	128	8	0.687844	9.9
2	256	9	0.687841	27.5
2	512	10	0.687681	86.6
2	1024	11	0.687615	296.4
2	2048	12	0.687602	1154.6

Table 6.1: Ratchet caplet, $d = 2$. Left: Monte Carlo simulation results. Right: Parabolic method results.

parabolic method to be comparable to simulation, with the additional advantage that it produces a sequence of deterministic approximations rather than a standard error with a probabilistic interpretation.

Monte Carlo results	
Paths	50,000
Run time (s)	4861
Price	0.518863
Standard error	0.001213

d	$\max_i N_i$	Level	Price	Total time (s)
3	2	3	0.887213	0.1
3	4	4	0.532552	0.2
3	8	5	0.539096	0.8
3	16	6	0.536725	2.8
3	32	7	0.512493	9.4
3	64	8	0.513775	29.9
3	128	9	0.516846	95.1
3	256	10	0.517044	312.5
3	512	11	0.518271	1155.1
3	1024	12	0.518913	4865.1

Table 6.2: Ratchet caplet, $d = 3$. Left: Monte Carlo simulation results. Right: Parabolic method results.

Monte Carlo results	
Paths	57,000
Run time (s)	7561
Price	0.471529
Standard error	0.001199

d	$\max_i N_i$	Level	Price	Total time (s)
4	2	4	0.860781	0.1
4	4	5	0.479322	0.6
4	8	6	0.489794	2.8
4	16	7	0.494195	11.5
4	32	8	0.481053	42.0
4	64	9	0.465453	145.7
4	128	10	0.464663	523.3
4	256	11	0.465955	1878.2
4	512	12	0.466705	7654.6

Table 6.3: Ratchet caplet, $d = 4$. Left: Monte Carlo simulation results. Right: Parabolic method results.

Monte Carlo results	
Paths	32,000
Run time (s)	3406
Price	0.457042
Standard error	0.001663

d	$\max_i$ N_i	Level	Price	Total time (s)
5	2	5	0.852376	0.4
5	4	6	0.461833	2.9
5	8	7	0.467954	16.0
5	16	8	0.480882	68.9
5	32	9	0.474478	267.3
5	64	10	0.459596	990.1
5	128	11	0.450715	3511.1

Table 6.4: Ratchet caplet, $d = 5$. Left: Monte Carlo simulation results. Right: Parabolic method results.

Appendices

Appendix A

Combinatorial identities

Since the weight in the sparse grid combination technique includes a binomial coefficient, we require a few identities involving binomial coefficients. These are frequently called combinatorial identities. A useful tabulation of such identities is [Gou72].

Recall that the binomial coefficient is defined as

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}, \tag{A.1}$$

for non-negative integers n and $k \leq n$. Some of our arguments make use of the fact that binomial coefficients can be extended to arbitrary complex numbers $x, y \in \mathbb{C}$ in a natural way. The binomial coefficient is then defined as

$$\binom{x}{y} = \frac{\Gamma(x+1)}{\Gamma(y+1)\Gamma(x-y+1)}, \tag{A.2}$$

where Γ is the gamma function.

A consequence of allowing non-integer arguments is that

$$\binom{x}{-1} = \begin{cases} 1 : x = -1 \\ 0 : \text{otherwise.} \end{cases} \tag{A.3}$$

One of the most basic identities for the binomial coefficient is the symmetry formula

$$\binom{n}{k} = \binom{n}{n-k}, \tag{A.4}$$

which we frequently invoke without explicit mention. Another basic identity is

$$\binom{-x}{n} = (-1)^n \binom{x+n-1}{n}. \tag{A.5}$$

There are also a variety of summation formulas which we need. The Chu-Vandemonde convolution formula is

$$\binom{s+t}{n} = \sum_{k=0}^{n} \binom{s}{k} \binom{t}{n-k}, \tag{A.6}$$

which holds for all $s, t \in \mathbb{C}$ and non-negative integers n. We also need

$$\sum_{k=0}^{n} (-1)^k \binom{n}{k} \binom{x-k}{r} = \binom{x-n}{r-n}. \tag{A.7}$$

The following identity arises in the heuristic derivation of the sparse grid combination weights.

Lemma 15. *For all integers $y \geq 1$ and $0 \leq k \leq y$,*

$$1 = \sum_{q=0}^{k} (-1)^q \binom{y}{q} \binom{y+k-q}{k-q}. \tag{A.8}$$

Proof. We have

$$\binom{-x}{n} = (-1)^n \binom{x+n-1}{n}$$

and the Chu-Vandermonde identity

$$\binom{s+t}{n} = \sum_{k=0}^{n} \binom{s}{k} \binom{t}{n-k},$$

which holds for all $s, t \in \mathbb{C}$ and non-negative integers n. Applying the first identity with $n = k - q$ and $x = y + 1$ shows that

$$\binom{y+k-q}{k-q} = (-1)^{k-q} \binom{-y-1}{k-q}.$$

Therefore, the sum becomes

$$
\begin{aligned}
&\sum_{q=0}^{k}(-1)^q\binom{y}{q}\binom{y+k-q}{k-q} \\
&= (-1)^k\sum_{q=0}^{k}\binom{y}{q}\binom{-y-1}{k-q} \\
&= (-1)^k\binom{-1}{k} \\
&= (-1)^k(-1)^k \\
&= 1,
\end{aligned}
$$

where we have used the Chu-Vandermonde identity to reduce the sum to $\binom{-1}{k}$. $\square$

Appendix B

Fourier series

While the Fourier transform is the appropriate tool for studying initial value problems (on an unbounded domain), we turn to Fourier series for studying problems on a bounded domain $[-\pi, \pi]^2 \subset \mathbb{R}^2$. We try our best to make sure that the notation for Fourier series parallels that which we have defined for the Fourier transform on $\mathbb{R}^2$. To this end, we use ξ_1 and ξ_2 to represent integers.

The Fourier coefficients of a 2π-periodic function $u : \mathbb{R}^2 \to \mathbb{R}$ are defined as

$$\hat{u}(\xi_1, \xi_2) := \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{-i(\xi_1 x + \xi_2 y)} u(x, y)\, dx\, dy$$

for all $\xi_1, \xi_2 \in \mathbb{Z}$. The inverse transformation is then

$$u(x, y) = \sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} e^{i(\xi_1 x + \xi_2 y)} \hat{u}(\xi_1, \xi_2).$$

Integration by parts implies that the Fourier coefficients of $\frac{\partial u}{\partial x}$ are:

$$\begin{aligned}
\widehat{\frac{\partial u}{\partial x}}(\xi_1, \xi_2) &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{-i(\xi_1 x + \xi_2 y)} u_x(x, y)\, dx\, dy \\
&= i\xi_1 \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{-i(\xi_1 x + \xi_2 y)} u(x, y)\, dx\, dy + e^{-i(\xi_1 x + \xi_2 y)} u(x, y)|_{x=-\pi}^{x=\pi}
\end{aligned}$$

$$= i\xi_1 \hat{u}(\xi_1, \xi_2)$$

Furthermore, we still have Parseval's theorem:

$$\sum_{\xi_1=-\infty}^{\infty} \sum_{\xi_2=-\infty}^{\infty} |\hat{u}(\xi_1, \xi_2)|^2 = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} u(x, y)\, dx\, dy$$

B.1 Truncation and interpolation operators

We now define the analogue of truncation and interpolation operators for Fourier series.

Definition 3. *Let $u \in L^2([-\pi, \pi]^2)$. Then the truncation operator τ applied to u is*

$$\tau u(x) = \sum_{\xi_1=-\pi/\Delta x}^{\pi/\Delta x} \sum_{\xi_2=-\pi/\Delta y}^{\pi/\Delta y} e^{i(\xi_1 x + \xi_2 y)} \hat{u}(\xi_1, \xi_2)$$

for every $x \in \Delta x\mathbb{Z} \times \Delta y\mathbb{Z}$, where $\hat{u}(\xi)$ is the Fourier transform of u.

Definition 4. *Let $v \in L^2(\Delta x\mathbb{Z} \times \Delta y\mathbb{Z})$. Then the interpolation operator σ applied to v is*

$$\sigma v(x) = \sum_{\xi_1=-\pi/\Delta x}^{\pi/\Delta x} \sum_{\xi_2=-\pi/\Delta y}^{\pi/\Delta y} e^{i(\xi_1 x + \xi_2 y)} \hat{v}(\xi_1, \xi_2)$$

for every $x \in \mathbb{R}^2$, where $\hat{v}(\xi_1, \xi_2)$ is the Fourier transform of v.

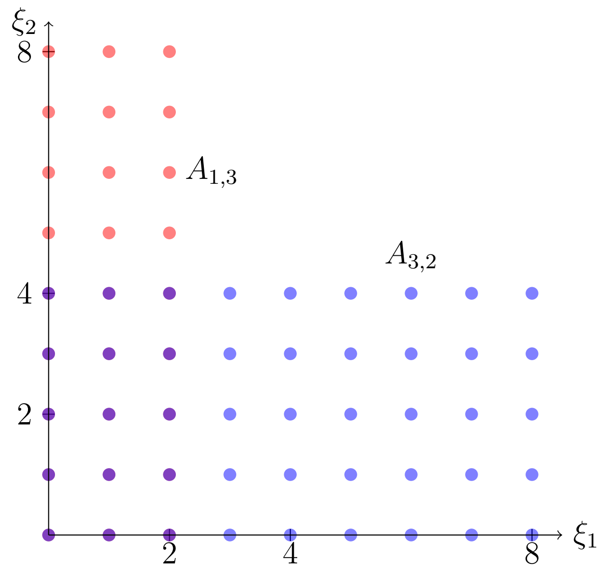
B.2 Partitioning of the frequency domain

We find it useful to notate particular subsets of the frequency domain $\mathbb{Z}^2$, as we did for $\mathbb{R}^2$. We define

$$A_{i,j} := \{0, \ldots, 2^i\} \times \{0, \ldots, 2^j\} \tag{B.1a}$$

$$b_i := \begin{cases} \{0, 1, 2\} & i = 1 \\ \{2^{i-1}, \ldots, 2^i\} & i \geq 2 \end{cases} \tag{B.1b}$$

Figure B.1: The sets $A_{i,j} \subset \mathbb{Z}^2$. Purple dots indicate overlap of the sets $A_{1,3}$ and $A_{3,2}$.



$$B_{i,j} := b_i \times b_j \tag{B.1c}$$

$$A_\ell := \bigcup_{i=1}^{\ell-1} A_{i,\ell-i} = \bigcup_{i=1}^{\ell-1} \left(\bigcup_{j=1}^{\ell-i} B_{i,j} \right). \tag{B.1d}$$

The sets B_{ij} are no longer disjoint, but instead share boundary values with adjacent sets. See Figures B.1, B.2, and B.3.

Figure B.2: The sets $B_{i,j} \subset \mathbb{Z}^2$ are no longer disjoint.

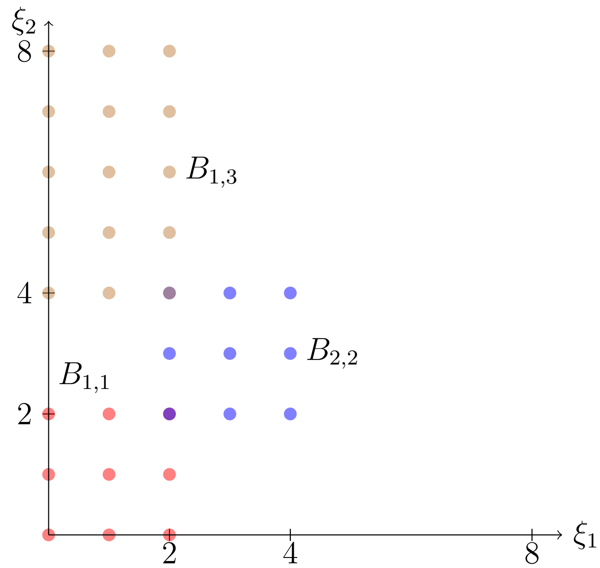
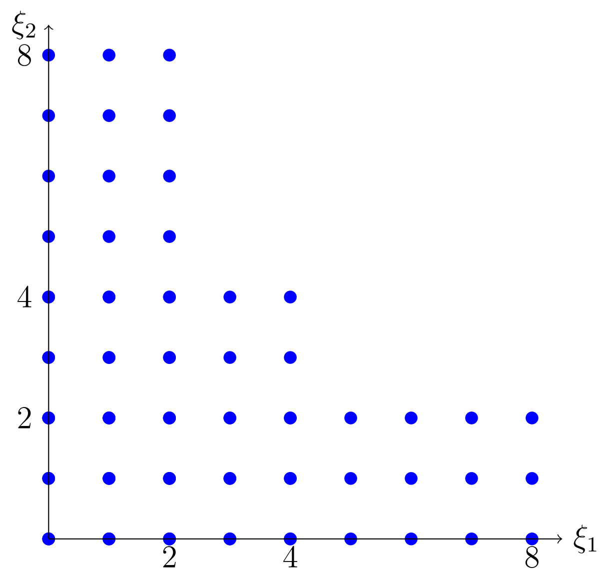


Figure B.3: The set $A_\ell \subset \mathbb{Z}^2$ when $\ell = 4$.



Appendix C

LIBOR market model

In this appendix we present some calculations pertaining to the LIBOR market model.

C.1 Calculation of drifts under the terminal measure

We know that the LIBOR rate L_t^n is driftless under the forward measure $\mathbb{P}^{T_{n+1}}$ associated with the time T_{n+1}. We would also like to calculate the drift of L_t^n under other forward measures, especially the terminal measure. We proceed by calculating the Radon-Nikodym derivative $\frac{d\mathbb{P}^{i+1}}{d\mathbb{P}^i}$ which relates adjacent forward measures.

The forward measures are defined by the fact that discounted asset prices are martingales. That is, for an asset A, we have

$$\frac{A_0}{B_i(0)} = E^i[\frac{A_t}{B_i(t)}|\mathcal{F}_0]$$

and

$$\frac{A_0}{B_{i+1}(0)} = E^{i+1}[\frac{A_t}{B_{i+1}(t)}|\mathcal{F}_0].$$

Multiplying the first equation by $\frac{B_i(0)}{B_{i+1}(0)}$ and multiplying the right hand side by $\frac{B_{i+1}(t)}{B_{i+1}(t)}$ gives

$$\frac{A_0}{B_{i+1}(0)} = E^i[\frac{B_i(0)}{B_{i+1}(0)}\frac{B_{i+1}(t)}{B_i(t)}\frac{A_t}{B_{i+1}(t)}|\mathcal{F}_0].$$

Comparing this with the second equation, we find that the Radon-Nikodym derivative process is

$$Z_t = \frac{B_i(0)}{B_{i+1}(0)}\frac{B_{i+1}(t)}{B_i(t)} = \frac{B_i(0)}{B_{i+1}(0)}(1+\delta L_t^i).$$

Taking the differential of Z_t, we get

$$dZ_t = \frac{B_i(0)}{B_{i+1}(0)}\delta dL_t^i = \frac{B_i(0)}{B_{i+1}(0)}\delta\sigma_i(t)L_t^i dW^{i+1}(t) = \frac{Z_t}{1+\delta L_t^i}\delta\sigma_i(t)L_t^i dW^{i+1}(t).$$

Therefore, Girsanov's theorem gives the following relationship between Brownian motions under $\mathbb{P}^{T_i}$ and $\mathbb{P}^{T_{i+1}}$:

$$dW^i(t) = dW^{i+1}(t) - \frac{\delta\sigma_i(t)L_t^i}{1+\delta L_t^i}\,dt.$$

Iterating this process, we get

$$\frac{dL_t^i}{L_t^i} = -\sum_{k=i+1}^{N}\frac{\delta\sigma_k(t)L_t^k}{1+\delta L_t^k}\sigma_i(t)\,dt + \sigma_i(t)\,dW_i^{N+1}(t),$$

where $W^{N+1}(t)$ is a correlated N-dimensional Brownian motion under the terminal measure.

C.2 Boundary conditions which guarantee well-posedness for the LIBOR market model PDE

We now discuss how to impose boundary conditions so that the problem is well-posed. We turn to Fichera theory to answer this question [Ole71].

Consider second-order linear equations of the following general form:

$$\sum_{i,j=1}^{m} a_{ij}(y)u_{y_i y_j} + \sum_{i=1}^{m} b_i(y)u_{y_i} + c(y)u = f(y).$$

Working within this framework, we take $m = N + 1$ and make the identification

$$(L^1, \ldots, L^N, t) = (y_1, \ldots, y_N, y_{N+1}).$$

Let n be the inward-oriented normal to $\partial\Omega$. Let Σ_3 be the portion of $\partial\Omega$ where $n^T An > 0$. On $\partial\Omega \setminus \Sigma_3$, we define the Fichera function:

$$h(y) = \sum_{i=1}^{m} \left[b_i(y) - \sum_{j=1}^{m} (a_{ij}(y))_{y_j} \right] n_i$$

For Equation 6.3, the Fichera function becomes

$$h(y) = \sum_{i=1}^{N} \left[y_i \mu_i(y_{N+1}) - \sum_{j=1}^{m} \rho_{ij}(t)\sigma_i(t)\sigma_j(t) y_i \right] n_i + n_{N+1} \tag{C.1}$$

$$= \sum_{i=1}^{N} [< \text{negative number} >] \, y_i n_i + n_{N+1}. \tag{C.2}$$

Now consider the domain $\Omega = [0, T] \times [0, M]^N$. Its boundary $\partial\Omega$ may be viewed as a collection of hyperplanes $\{y_i = 0\}$ for $i = 1 \ldots N+1$ and $\{Y_{N+1} = T\}$ and $\{y_i = M\}$ for $i = 1 \ldots N$. The boundary can also be decomposed as $\partial\Omega = \Sigma_0 \cup \Sigma_1 \cup \Sigma_2 \cup \Sigma_3$, where

$$\begin{aligned} \Sigma_0 &= \{y : h(y) = 0\} \\ \Sigma_1 &= \{y : h(y) > 0\} \\ \Sigma_2 &= \{y : h(y) < 0\}. \end{aligned}$$

Fichera theory dictates that we impose an exogenous boundary condition on $\Sigma_2 \cup \Sigma_3$. We proceed to identify which hyperplanes of $\partial\Omega$ belong to $\Sigma_2 \cup \Sigma_3$.

Consider first the hyperplanes $\{y_i = 0\}$ for $i = 1 \dots N+1$. The inward-oriented normal on the surface is $\mathbf{e}_i$. We have that $\mathbf{e}_i^T A \mathbf{e}_i = 0$ on $\{y_i = 0\}$ so it belongs to $\partial\Omega \setminus \Sigma_3$. The Fichera function is non-negative on these hyperplanes, so no exogenous boundary 0 need be imposed.

Now consider the hyperplanes $\{y_i = M\}$ for $i = 1 \dots N$. The inward-oriented normal on the surface is $-\mathbf{e}_i$. On this hyperplane, $(-\mathbf{e}_i)^T A(-\mathbf{e}_i)$ does not vanish, so it belongs to Σ_3. Thus, we impose a far boundary condition $g : \Sigma_3 \to \mathbb{R}$ on these hyperplanes.

Now consider the hyperplane $\{y_{N+1} = T\}$. The inward-oriented normal is $-\mathbf{e}_{N+1}$. Since the equation is parabolic, $\mathbf{e}_{N+1}^T A \mathbf{e}_{N+1} = 0$ here. Furthermore, the Fichera function is negative so the hyperplane belongs to Σ_2. Thus, we impose a terminal condition here.

In summary, the three-rate ratchet caplet pricing problem can be written as follows:

Find $u : [0, M]^3 \times [0, T] \to \mathbb{R}$ such that

$$
\begin{aligned}
0 &= \frac{\partial u}{\partial t} + \frac{1}{2} \sum_{i,j=1}^{3} \rho_{ij}(t)\sigma_i(t)\sigma_j(t) L_i L_j \frac{\partial^2 u}{\partial L_i \partial L_j} \\
&\quad - \sum_{i=1}^{3} \left(\sum_{k=i+1}^{3} \frac{\delta L_k(t)}{1 + \delta L_k(t)} \rho_{ik}(t)\sigma_k(t) \right) \sigma_i(t) L_i \frac{\partial u}{\partial L_i} \\
u(L^1, L^2, L^3, T) &= (L^3 - K_3(L^1, L^2))^+ \\
u = g &\qquad \text{on } \Sigma_3
\end{aligned}
$$

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