Maximum Norm Regularity of Implicit Difference Methods for Parabolic Equations

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Dissertation submitted in partial fulfillment of the requirements for the degree of
Doctor of Philosophy in the Department of Mathematics
in the Graduate School of Duke University
2011

Abstract
(Mathematics)

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Abstract

We prove maximum norm regularity properties of L-stable finite difference methods for linear-second order parabolic equations with coefficients independent of time, valid for large time steps. These results are almost sharp; the regularity property for first differences of the numerical solution is of the same form as that of the continuous problem, and the regularity property for second differences is the same as the continuous problem except for logarithmic factors. This generalizes results proved by Beale valid for the constant-coefficient diffusion equation, and is in the spirit of work by Aronson, Widlund and Thomeé.

To prove maximum norm regularity properties for the homogeneous problem, we introduce a semi-discrete problem (discrete in space, continuous in time). We estimate the semi-discrete evolution operator and its spatial differences on a sector of the complex plan by constructing a fundamental solution. The semidiscrete fundamental solution is obtained from the fundamental solution to the frozen coefficient problem by adding a correction term found through an iterative process. From the bounds obtained on the evolution operator and its spatial differences, we find bounds on the resolvent of the discrete elliptic operator and its differences through the Laplace transform representation of the resolvent. Using the resolvent estimates and the assumed stability properties of the time-stepping method in the Cauchy integral representation of the fully discrete solution operator yields the homogeneous regularity result.

Maximum norm regularity results for the inhomogeneous problem follow from the homogeneous results using Duhamel's principle. The results for the inhomogeneous problem imply that when the time step is taken proportional to the grid spacing, the rate of convergence of the numerical solution and its differences is controlled by the maximum norm of the local truncation error.

As an application of the theory, we prove almost sharp maximum norm resolvent estimates for divergence form elliptic operators on spatially periodic grid functions. Such operators are invertible, with inverses and their first differences bounded in maximum norm, uniformly in the grid spacing. Second differences of the inverse operator are bounded except for logarithmic factors.

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Symbols

$\mathbb{R}_h^d$	The set of all grid points with grid spacing h.
$L^\infty(\mathbb{R}_h^d)$	The set of bounded (possibly complex-valued) grid functions.
e_j	The jth standard basis vector for $\mathbb{R}^d$.
$\hat{f}$	The discrete Fourier transform of f.
S_j^+	The forward shift operator in the x_j direction.
S_j^-	The backward shift operator in the x_j direction.
S_h^γ	The composition of shift operators $\left(S_1^+\right)^{\gamma_1} \cdots \left(S_d^+\right)^{\gamma_d}$.
D_j^+	The forward (divided) difference in the x_j direction.
D_j^-	The backward (divided) difference in the x_j direction.
D_h^γ	The composition of difference operators $\left(D_1^+\right)^{\gamma_1} \cdots \left(D_d^+\right)^{\gamma_d}$.
$\lfloor n \rfloor$	The floor function; the greatest integer less than or equal to n.

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1

Introduction

Parabolic partial differential equations possess the characteristic property that solutions to the Cauchy problem exhibit greater spatial regularity than the initial data in L^p or Sobolev norms. For instance, solutions to the linear parabolic problem

$$u_t = Au \tag{1.1}$$

$$u(x,0) = u_0(x) \tag{1.2}$$

on $\mathbb{R}^d \times [0,T)$ satisfy regularity estimates such as

$$||D^\gamma u(x,\cdot)||_{L^\infty(\mathbb{R}^d)} \leq C_T t^{-|\gamma|/2} \, ||u_0||_{L^\infty(R^d)}\,, \qquad |\gamma| \leq 2 \tag{1.3}$$

when A is a second-order uniformly elliptic operator with smooth bounded coefficients and continuous u_0. Likewise, for the inhomogeneous problem

$$u_t = Au + f \tag{1.4}$$

$$u(x,0) = 0 \tag{1.5}$$

with Hölder continuous f, we have

$$||D_h^\gamma u||_{L^\infty(\mathbb{R}^d)} \leq C_T \sup_{t \leq T} ||f(x,t)||_{L^\infty(\mathbb{R}^d)} \qquad |\gamma| \leq 2. \tag{1.6}$$

It is desirable that numerical methods for solving parabolic problems reflect such qualitative behavior, particularly in strong norms such as the maximum norm, which give control over the exact solution by truncation errors. Unfortunately, explicit finite difference methods require that the time step k and spatial grid spacing h satisfy $k = ch^2$ for some fixed constant c, a significant constraint for practical computation. With implicit methods, it is often possible to allow large time steps, such as $k = ch$, and it is profitable to know if any regularity properties are retained. Early work on maximum norm estimates was done by Aronson (1963) and Widlund (1966), who proved stability and regularity properties under the small time step restriction $k = ch^2$.

In this dissertation, we show that certain implicit L-stable methods possess almost sharp maximum norm discrete regularity properties similar to (1.3) and (1.6), valid for large time steps. We derive discrete regularity estimates analogous to the continuous case for first spatial differences, and for second spatial differences with the exception of a $\log h$ factor. Our results extend those that Beale (2009) proved for the constant-coefficient diffusion equation to a more general class of parabolic equations with time-independent coefficients.

From the inhomogeneous regularity theorem, we derive a convergence result for the inhomogeneous problem. For a sufficiently smooth solution to the exact problem, the rate of convergence of the solution and its first differences is controlled by the maximum norm of the local truncation error. The rate of convergence of second differences is also controlled by the maximum norm of the local truncation error, but contains logarithmic factors in the rate of convergence. As a consequence, if the local truncation error of the scheme is $O(h^2+k^2)$, and $k = ch$, then the rate of convergence of the numerical solution and its first difference to the true solution and its derivative is $O(h^2)$, and the rate of convergence of second differences is $O(h^2|\log h|^2)$.

Beale (2009) showed that the class of time-stepping methods that satisfy the hypotheses of our regularity theorems include second-order methods such as the modified form of Crank-Nicolson due to Twizell et al. (1996), known as TGA, a second-order singly diagonally implicit Runge-Kutta method (SDIRK2), as well as the well-known first-order implicit Euler method. Our results also apply to multi-step methods, including the second-order backward difference formula (BDF2).

We examine the problem of obtaining maximum norm discrete regularity properties from the perspective of analytic semigroup theory, influenced by the approach to semi-discrete finite element problems taken by Thomée (2006). Our argument proceeds in three stages. We begin by introducing the semi-discrete problem (discrete in space, continuous in time)

$$u_t = A_h u \tag{1.7}$$

by replacing the elliptic spatial operator by an elliptic difference operator that depends upon the grid spacing h as a parameter. We construct a solution to the semi-discrete problem to obtain maximum norm bounds on $D_h^\gamma e^{A_h t}$, valid for complex t in a wedge about the real axis. In the second stage of our argument, we use analytic semigroup theory to transform our maximum norm bounds on the evolution operator into maximum norm bounds on spatial differences of the resolvent operator $(z - A_h)^{-1}$. In the final stage, we use the resolvent estimates in conjunction with the L-stability assumption on the time-stepping method to obtain maximum norm regularity bounds on the fully discrete solution.

To find maximum norm bounds on $D_h^\gamma e^{A_h t}$ for complex t in a sector about the real axis, we solve the semi-discrete problem by constructing a semi-discrete fundamental solution. The fundamental solution is obtained through a parametrix construction. Aronson (1963) and Widlund (1966) used a fully discrete parametrix construction for proving stability of difference methods for parabolic systems with small time steps. Friedman (1964) provides a valuable introduction to the technique for the exact problem. Our semi-discrete version of the parametrix requires some additional subtlety due to its incorporation of complex time.

In the parametrix construction, the fundamental solution Γ_h of the semi-discrete problem is expressed as the sum of the fundamental solution G_h of the frozen coefficient problem and a correction term Φ_h. Because G_h solves a constant-coefficient problem, we can estimate G_h by examining its Fourier transform. Deforming the contour of integration for the inverse transform into the complex plane allows us to find pointwise bounds on G_h and its spatial differences. This technique can be used to show that G_h exhibits exponential decay like $\exp(-|x|/\sqrt{|t|})$. (We might expect exponential decay like $e^{-|x|^2/t}$ in analogy with the heat kernel, but in Appendix B we explain why this cannot be obtained.)

The correction term Φ_h must satisfy an integral equation involving G_h. The integral equation for Φ_h can be solved by an infinite series expansion. Each term of the series has a bound less singular for small time than its predecessor. The first finitely many terms of the series may have bounds that are singular in time, although each is less singular than the bound for G_h. The remainder of the terms in the series exhibit increasing temporal regularity, and possess rapidly decaying coefficients. Every term in the expansion exhibits a uniform rate of decay in $\exp(-|x|/\sqrt{|t|})$. These facts enable us to show that the series for Φ_h converges, and has better temporal regularity than G_h.

The pointwise bounds on G_h and Φ_h lead directly to pointwise bounds on $D_h^\gamma \Gamma_h$. These are easily leveraged to find maximum norm bounds on $D_h^\gamma e^{A_h t}$.

Adapting Beale's approach in Beale (2009) for the second part of our argument, a technique from analytic semigroup theory now allows us to obtain maximum resolvent estimates through the Laplace transform representation of the resolvent:

$$D_h^\gamma (z - A_h)^{-1} = \int_0^\infty e^{-zt} D_h^\gamma e^{A_h t}\, dt.$$

For this step, it is critical that our estimates on $D_h^\gamma e^{A_h t}$ be valid on a wedge containing the positive real axis so that we can extend our resolvent estimates to a large enough portion of the complex plane.

With maximum norm estimates on $D_h^\gamma (z - A_h)^{-1}$ in hand, we are finally able to examine the regularity of fully discrete schemes. The simplest time-stepping method for which our regularity result holds for the homogeneous equation is the familiar L-stable implicit Euler method. For the implicit Euler method with time step k, we approximate the solution of the ODE

$$y_t = \lambda y$$

at time nk by

$$\begin{aligned} y^n &= (1 - k\lambda)^{-1} y^{n-1} \\ &= s(k\lambda) y^{n-1}, \end{aligned}$$

where $s(k\lambda) = (1 - k\lambda)^{-1}$ is the time-stepping function. In a similar fashion, we approximate the solution to the exact problem (1.3) by

$$u^n = s(kA_h)^n u^0.$$

More generally, for a multi-step method, we have operators $s_n(kA_h)$ for which

$$u^n = s_n(kA_h) u^0.$$

For L-stable methods we can write the operator $s_n(kA_h)$ or its spatial differences as a contour integral:

$$D_h^\gamma s_n(kA_h) = \int_\Gamma s_n(z) D_h^\gamma (z - kA_h)^{-1} \, dz$$

for Γ a contour originating at $e^{-i\theta_0}\infty$ and ending at $e^{i\theta_0}\infty$, for $\theta_0 \in (\pi/2, \pi)$, enclosing the spectrum of A_h. Using our maximum norm resolvent estimates in this representation of the fully discrete solution gives regularity results for the fully discrete problem.

The maximum norm fully discrete regularity results for the inhomogeneous problem and the resolvent estimates on the elliptic operator can then be used to obtain regularity results for the inhomogeneous problem.

As an application, we derive improved maximum norm resolvent estimates for discrete divergence form elliptic operators on the space of periodic grid functions of mean value zero. The results in this section apply to the popular second-order accurate discretization for mixed derivatives found in Samarskii (2001). By restricting our attention to periodic grid functions of mean value zero, we ensure that the elliptic operators are invertible. For such an elliptic operator A_h, we show that $(A_h)^{-1}$ and $D_h(A_h)^{-1}$ have maximum norm uniformly bounded in h, and second differences of $(A_h)^{-1}$ are uniformly bounded except for logarithmic factors.

The key to discovering these maximum norm estimates is to write

$$\begin{aligned} D_h^\gamma (A_h)^{-1} &= \int_0^\infty D_h^\gamma e^{A_h t}\, dt \\ &= \int_0^1 D_h^\gamma e^{A_h t}\, dt + \int_1^\infty D_h^\gamma e^{A_h t}\, dt \end{aligned}$$

and estimate each term separately. The first integral can be handled by our previous semi-discrete results. The second integral requires more care. We show that the maximum norm of $D_h^\gamma e^{A_h t}$ is controlled by the H^m norm of $A_h^{m/2} e^{A_h t}$, which decays exponentially. This requires adapting the semigroup theory of Renardy and Rogers (2004) and the elliptic regularity of Evans (1998). More sophisticated discrete elliptic regularity results have been shown by Thomée and Westergren (1968), Shreve (1973) and Bondesson (1973) for operators with smooth coefficients on bounded domains. Our assumption of periodic data with mean value zero simplifies the regularity theory here significantly, allowing us to reduce the regularity of the coefficients.

To obtain the elliptic resolvent estimates, we make use of the discrete Poincaré inequality and discrete Sobolev inequality. The discrete Poincaré inequality (also known in the literature as Wirtinger's inequality) first appeared in Schoenberg (1950). The discrete Sobolev inequality was proved originally by Sobolev (1940), and is stated in Shreve (1973).

In Chapter 2, we state preliminaries and present our main results. In Chapter 3 we discuss the semi-discrete problem. It is here that we construct the fundamental solution and prove the maximum norm regularity of the semi-discrete evolution operator. In the first section of Chapter 4, we use the results of Chapter 3 to obtain maximum norm resolvent estimates on discrete elliptic operator. In the second section of Chapter 4, we apply our resolvent estimates to obtain fully discrete maximum norm regularity results. In Chapter 5 we apply the theory to obtain almost sharp maximum norm resolvent estimates for divergence form discrete elliptic operators on periodic grids. In Chapter 6 we present experimental numerical results confirming the main results of Chapter 2, and compare the superior regularity properties of certain L-stable methods with the weaker regularity of the Crank-Nicolson method. Appendix A is the proof of the convergence result. In Appendix B, we explain the decay property of the semi-discrete fundamental solution.

2

Preliminaries and Parabolic Regularity Results

We state maximum norm regularity properties of L-stable implicit finite difference schemes valid for large time steps for second-order parabolic equations with time-independent coefficients posed on $\mathbb{R}^d \times [0, \infty)$. We are interested finite difference methods for the Cauchy problem

$$\begin{gathered} u_t = Au + f \\ A = \sum_{jl} a_{jl}(x)\partial_j\partial_l + \sum_j b_j(x)\partial_j + c_0(x) \\ u(x, 0) = u_0(x). \end{gathered} \tag{2.1}$$

Here the operator A satisfies the uniform ellipticity condition

$$\sum_{jl} a_{jl}(x)\xi_j\xi_l \geq c_0|\xi|^2 \tag{2.2}$$

for all $\xi \in \mathbb{R}^d$, with c_0 independent of x. Furthermore, the coefficients a_{jl}, b_j and c must be uniformly bounded and uniformly Hölder continuous.

2.1 Preliminaries

The discretized problem will be posed on the spatial grids

$$\mathbb{R}_h^d = h\mathbb{Z}^d = \left\{x = jh : j \in \mathbb{Z}^d\right\}, \tag{2.3}$$

where $0 < h \leq 1$ is the grid spacing. We define the Banach space $L^\infty(\mathbb{R}_h^d)$:

$$L^\infty(\mathbb{R}_h^d) = \left\{u(x) : \sup_{x \in \mathbb{R}_h^d} |u(x)| < \infty\right\} \tag{2.4}$$

where $u(x)$ is a complex-valued function defined on $\mathbb{R}_h^d$. The norm for $L^\infty(\mathbb{R}_h^d)$ is given by

$$||u||_{L^\infty(\mathbb{R}_h^d)} = \sup_{x \in \mathbb{R}_h^d} |u(x)|. \tag{2.5}$$

We will suppress the subscript when there is no ambiguity. For an operator L with domain and range $\mathbb{R}_h^d$, we define the norm

$$||L||_\infty = \sup_{\substack{x \in R_h^d \\ x \neq 0}} \frac{||Lx||}{||x||}. \tag{2.6}$$

We need a discrete Fourier transform in order to express the ellipticity requirement for discrete operators. The discrete Fourier transform $\hat{f}$ of the grid function f is defined as

$$\hat{f}(\xi) = \sum_{x \in \mathbb{R}_h^d} f(x) e^{-i<x,\xi>/h}. \tag{2.7}$$

The inverse transform is then given by

$$f(x) = (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{f}(\xi) e^{i<x,\xi>/h}\, d\xi. \tag{2.8}$$

The symbol of a difference operator is obtained by replacing the shift operator $u(x) \to u(x + \beta h)$ by $e^{i<\beta,\xi>}$. For instance, the symbol of D_j^+, the forward difference in the x_j direction, is $(e^{i\xi_j} - 1)/h$. For a multi-index γ, we define the difference operator $D_h^\gamma = (D_1^+)^{\gamma_1} \cdots (D_d^+)^{\gamma_d}$. We denote the symbol of D_h^γ by $\widehat{D_h^\gamma}$.

2.2 Parabolic Regularity Results

We select a consistent discretization A_h of A given by

$$A_h = \sum_{jl,\sigma} a_{jl,\sigma}(x,h) S_h^\sigma D_j^+ D_l^+ + \sum_{j,\sigma} b_{j,\sigma}(x,h) S_h^\sigma D_j^+ + \sum_{\sigma} c_\sigma(x,h) S_h^\sigma \tag{2.9}$$

where $h \in (0,1]$ is the grid spacing, $x \in \mathbb{R}_h^d$ are grid points, σ lies in a finite subset of $\mathbb{Z}^d$, and $a_{jl,\sigma}$, $b_{j,\sigma}$ and c_σ are real-valued functions defined for all x and $0 \leq h \leq 1$. The coefficients $a_{jl,\sigma}, b_{j,\sigma}$ and c_σ must be uniformly bounded and must satisfy a uniform Hölder continuity condition such as

$$|a_{jl,\sigma}(x,h) - a_{jl,\sigma}(y,h)| \leq C|x-y|^\alpha, \tag{2.10}$$

with C independent of h. We define the shift operators $S_h^\sigma = (S_1^+)^{\sigma_1} \cdots (S_d^+)^{\sigma_d}$, where $S_j^+ u = u(x + he_j)$ is the forward shift operator in the x_j coordinate direction, and $(S_j^+)^{-1} u(x) = S_j^- u(x) = u(x - he_j)$ is the backward shift operator in the x_j direction. We note that the coefficients $a_{jl,\sigma}(x,h)$ appearing in the discretization (2.9) do not have to be the same as the coefficients $a_{jl}(x)$ appearing in (2.1).

For each fixed y, we define the principal symbol $p_h(y,\xi)$ to be the symbol associated with the difference operator

$$\sum_{jl,\sigma} a_{jl,\sigma}(y,h) S_h^\sigma D_j^+ D_l^+.$$

We require that $p_h(y,\xi)$ satisfy the uniform ellipticity condition

$$\text{Re}\left\{h^2 p_h(y,\xi)\right\} \leq -c|\xi|^2 \tag{2.11}$$

with constant c independent of y and h. For completeness, we also define the full symbol $P_h(y,\xi)$ to be the symbol associated with $A_h(y)$. Hereafter, A_h operates on the x variable alone of a function of x and y, regarding the y variable as fixed.

The discretizations permitted by (2.9) range from the simple discretization

$$\sum_{jl} a_{jl}(x) D_j^+ D_l^- + \sum_j b_j(x) D_j^0 + c(x)$$

to the divergence form discretization appearing in (5.6), provided the a_{jl} are at least $C^{1+\alpha}$.

We note that the ellipticity condition here is stronger than the uniform ellipticity condition for the exact problem, as not all consistent discretizations satisfy it. For instance, if we were to replace each derivative in the exact problem by a centered difference, the resulting scheme would fail to satisfy (2.11) as the principal symbol would be zero for the non-zero vector πe_j. However, as we will show in Chapter 5, if we replace ∂_j by D_j^+ and ∂_l by D_l^-, the resulting scheme does satisfy (2.11).

The time discretization with time step k and $u^n = u(\cdot, nk)$ is implemented by

$$u^n = s_n(kA_h)u^0 \tag{2.12}$$

where $s_n(k\lambda)$ is the time-stepping function for solving numerically the ordinary differential equation $y_t = \lambda y$. For some constant k_0, when $0 < k \leq k_0$, we have that $s_n(kA_h)$ is well-defined as a bounded operator on $L^\infty(\mathbb{R}_h^d)$. For single step methods, we can write $s_n(kA_h) = s(kA_h)^n$.

We restrict our attention to the class of A-stable and L-stable time-stepping methods, i.e.

$$|s_n(z)| \leq 1, \qquad s_n(\infty) = 0 \tag{2.13}$$

on the left half-plane. We require that there exist a disk B_0 about the origin on which

$$|s_n(z)| \leq C_0(1 + c_0|z|)^n. \tag{2.14}$$

Furthermore, for each $\delta' > 0$, we must have an estimate of the form

$$|s_n(z)| \leq C_1(1 + c_1|z|)^{-\rho n} \tag{2.15}$$

for some positive constants p, C_1 and c_1, with constants depending on δ', for all $z \in \Sigma_{\delta'}$, where

$$\Sigma_{\delta'} = \left\{ z = z_1 + iz_2 : z_1 \leq 0, z_2 \leq \delta'|z_1| \right\}. \tag{2.16}$$

Theorem 1. *Under the assumptions (2.13)-(2.15) on s_n, there exist a constant k_0 and constants C_0, C_1, C_2 and C_3, independent of $0 < h \leq 1$ and $0 < k \leq k_0$, for which*

$$||s_n(kA_h)||_\infty \leq C_1 e^{C_0 nk} \tag{2.17}$$

$$||D_h^\gamma s_n(kA_h)||_\infty \leq C_2 (nk)^{-1/2} e^{C_0 nk}, \qquad |\gamma| = 1 \tag{2.18}$$

$$||D_h^\gamma s_n(kA_h)||_\infty \leq C_3 (nk)^{-1}(1 + |\log h| + |\log nk|) e^{C_0 nk}, \qquad |\gamma| = 2. \tag{2.19}$$

A large portion of this dissertation is the proof of Theorem 1.

From Theorem 1, we can deduce the following result, the proof of which is a simple modification of the proof of Theorem 1.2 in Beale (2009):

Theorem 2. *For the choice of single-step method time-stepping function s satisfying the constraints in (2.13)-(2.15), if the problem*

$$u_t = A_h u + f \tag{2.20}$$

$$u(x, 0) = 0 \tag{2.21}$$

is approximated by

$$u^{n+1} = s(kA_h)u^n + k \sum_{i=1}^{m} q_i(kA_h)(1 - \eta_i k A_h)^{-1} f(\cdot, nk + \tau_i k) \tag{2.22}$$

where $k = ch$ for some $c > 0$, $\eta_i > 0$ and τ_i are fixed numbers and q_i is an analytic function on $\Sigma_{\delta'}$ for which $q_i(kA_h)$ is bounded in norm on $L^\infty(R_h^d)$ independently of h and k for k sufficiently small, then for $0 < nk \leq T$ we have

$$||u^n||_\infty \leq C_0 \sup_{t \leq T} ||f(\cdot, t)||_\infty \tag{2.23}$$

$$||D_h^\gamma u^n||_\infty \leq C_1 \sup_{t \leq T} ||f(\cdot, t)||_\infty, \qquad |\gamma| = 1 \tag{2.24}$$

$$||D_h^\gamma u^n||_\infty \leq C_2 (1 + |\log h|^2) \sup_{t \leq T} ||f(\cdot, t)||_\infty, \qquad |\gamma| = 2. \tag{2.25}$$

for constants C_0, C_1 and C_2 depending on c and T but not on h or n.

This result may also be extended to multi-step methods. See Beale (2009) for the extension to BDF2.

2.3 Parabolic Convergence Result

As an application of Theorem 2, we derive a convergence result for the inhomogeneous problem.

We suppose that U is a classical solution to

$$u_t = Au + f$$

$$A = \sum_{jl} a_{jl}(x)\partial_j\partial_l + \sum_j b_j(x)\partial_j + c(x) \tag{2.26}$$

$$u(x,0) = u_0(x)$$

for continuous u_0.

We examine discrete schemes consistent with (2.26) given by the discretization

$$u^{n+1} = s(kA_h)u^n + k\sum_{i=1}^{m} q_i(kA_h)(1-\eta_i kA_h)^{-1} f(\cdot, nk + \tau_i k) \tag{2.27}$$

$$u^0 = u_0$$

for a rational time-stepping function $s(z) = q(z)/r(z)$ and rational q_i. We require that $q_i(kA_h)$ be bounded independently of h and k for k sufficiently small. We also require that s be L-stable, so that $s(\infty) = 0$ implies that the degree of r must be strictly greater than that of q. The consistency of the scheme enables us to take the polynomials $q(z), r(z) = 1 + O(z)$ as $z \to 0$.

To state our convergence result, we must define the local truncation error of the scheme. To do this, we re-express the scheme in a form that directly approximates the exact equation.

Multiplying the scheme by $r(kA_h)$, we may rewrite it as

$$r(kA_h)u^{n+1} = q(kA_h)u^n + k\sum_{i=1}^{m} q_i'(kA_h) f(\cdot, nk + \tau_i k)$$

for rational functions functions $q_i'(z) = r(z)q_i(z)(1-\eta_i z)^{-1}$. Using the fact that $q(z), r(z) = 1 + O(z)$ as $z \to 0$, we may rewrite the scheme as

$$u^{n+1} - u^n = (1 - r(kA_h))u^{n+1} + (q(kA_h) - 1)u^n + k\sum_{i=1}^{m} q_i'(kA_h)f(\cdot, nk + \tau_i k)$$

for polynomials $1 - r(z)$ and $q(z) - 1$ having no constant term. Dividing by k yields a scheme in the classical formulation

$$\frac{u^{n+1} - u^n}{k} = A_*(u^{n+1}, u^n) + \sum_{i=1}^{m} q_i'(kA_h)f(\cdot, nk + \tau_i k), \tag{2.28}$$

where $A_*(u^{n+1}, u^n) = k^{-1}(1 - r(kA_h))u^{n+1} + k^{-1}(q(kA_h) - 1)u^n$ discretizes A_h and $\sum_{i=1}^{m} q_i'(kA_h)f(\cdot, nk + \tau_i k)$ discretizes f. For conditions on the functions q_i that guarantee consistency and a procedure for generating q_i for practical computation, see Chapter 8 of Thomée (2006).

Having re-expressed the scheme in (2.28), the local truncation error $\mathcal{T}$ is defined in the standard way as the quantity satisfying

$$\frac{U^{n+1} - U^n}{k} = A_*(U^{n+1}, U^n) + \sum_{i=1}^{m} q_i'(kA_h)f(\cdot, nk + \tau_i k) + \mathcal{T}^n. \tag{2.29}$$

The total error $\mathcal{E}$ is defined by

$$\mathcal{E}^n = U^n - u^n. \tag{2.30}$$

Starting from (2.29) and reversing the steps used to obtain (2.28) from (2.27) enables us to write

$$\begin{aligned} U^{n+1} = s(kA_h)U^n &+ k\sum_{i=1}^{m} q_i(kA_h)(1 - \eta_i kA_h)^{-1} f(\cdot, nk + \tau_i k) \\ &+ kQ(kA_h)(1 - \eta kA_h)^{-1}\mathcal{T}^n \end{aligned} \tag{2.31}$$

for $Q(z) = (1 - \eta z)/r(z)$ with η a positive constant. $Q(kA_h)$ is uniformly bounded in h and k for k sufficiently small as the degree of r is at least one and r has no roots in the left half-plane.

We can now state our convergence result, the proof of which appears in Appendix A. Although this result requires the more restrictive hypothesis that s be a rational function, the theorem still applies to implicit Euler, TGA, and SDIRK2.

Theorem 3. *Suppose U is a classical solution to (2.26) and u^n is the numerical solution at time step n given by the L-stable scheme in (2.27) for rational s with $k = ch$. If $\mathcal{E}$ is the total error and $\mathcal{T}$ is the local truncation error, then, on any finite interval $[0, T]$, we have:*

$$||\mathcal{E}||_\infty \leq C_0 \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty \tag{2.32}$$

$$||D_h^\gamma \mathcal{E}||_\infty \leq C_1 \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty, \qquad |\gamma| = 1 \tag{2.33}$$

$$||D_h^\gamma \mathcal{E}||_\infty \leq C_2 \left(1 + |\log h|^2\right) \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty \qquad |\gamma| = 2 \tag{2.34}$$

with constants depending on c and T, but not on h or n for k sufficiently small.

3

The Semi-Discrete Problem

3.1 The Semi-Discrete Problem and its Fundamental Solution

To bound $D_h^\gamma e^{A_h t}$ as an operator on $L^\infty(\mathbb{R}_h^d)$, we introduce the semi-discrete problem. The semi-discrete initial value problem for a grid function u is given by

$$L_h u = \left(A_h - \frac{\partial}{\partial t}\right) u = 0 \qquad (3.1)$$

$$u(x,0) = u_0(x)$$

for A_h in (2.9).

For simplicity of exposition, in this chapter we suppose that

$$A_h = \sum_{jl} a_{jl}(x) D_{jl}^2 + \sum_j b_j(x) D_j^1 + c(x), \qquad (3.2)$$

where D_{jl}^2 is a consistent discretization of $\partial_j \partial_l$ and D_j^1 is a consistent discretization of ∂_j. We may express D_{jl}^2 and D_j^1 as finite sums of shift operators:

$$D_{jl}^2 u = h^{-2} \sum_\sigma w_\sigma u(x + \sigma h) \qquad (3.3)$$

$$D_j^1 u = h^{-1} \sum_\sigma w_\sigma u(x + \sigma h) \qquad (3.4)$$

for σ in a finite subset of $\mathbb{Z}^d$. The proofs for general A_h as defined in (2.9) are straightforward modifications of those presented in this chapter.

For each h, A_h is a bounded operator on $L^\infty(\mathbb{R}^d_h)$ (whose bound depends on h), so that $e^{A_h t}$ is well-defined as a bounded operator for $t \in \mathbb{C}$. We find that $e^{A_h t}$ is more well-behaved and, along with its spatial differences, can be bounded uniformly in h.

Theorem 4. *There exists a constant $M > 0$ and constants C and μ, depending on M but not on h, for which*

$$\left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty(\mathbb{R}^d_h)} \leq C|t|^{-|\gamma|/2} e^{\mu t}, \quad |\gamma| \leq 2 \tag{3.5}$$

for all t in the wedge

$$\mathbb{T}_M = \{t = t_1 + it_2 : |t_2| \leq M\,|t_1|\,,\, t_1 > 0\}. \tag{3.6}$$

Furthermore, if the principal symbol of the difference scheme is real whenever ξ is real, M may be taken to be any positive real number.

To prove Theorem 4, we construct a fundamental solution $\Gamma_h(x, t; y)$ for (3.1) satisfying

$$\Gamma_h(x, 0; y) = \delta_{xy} \tag{3.7}$$

$$L_h \Gamma_h = \left(A_h - \frac{\partial}{\partial t}\right) \Gamma_h = 0 \quad (t \in \mathbb{T}_M)$$

where $x, y \in \mathbb{R}^d_h$ are grid points, and

$$\delta_{xy} = \begin{cases} 1 & x = y \\ 0 & x \neq y \end{cases}. \tag{3.8}$$

For such a fundamental solution, the solution of (3.1) may be written

$$u(x, t) = \sum_{x_*} \Gamma_h(x, t; x_*) u_0(x_*). \tag{3.9}$$

The construction of $\Gamma_h(x,t;y)$ is in the spirit of Levi's parametrix. In the parametrix construction, the fundamental solution is realized as a correction applied to the fundamental solution of the constant-coefficient problem obtained by freezing the coefficients of L_h at the grid point y. The frozen coefficient problem with coefficients held constant at y is

$$u_t = A_h(y)u \tag{3.10}$$
$$u(x,0) = u_0(x).$$

Associated with the frozen coefficient problem is its fundamental solution $G_h(x,t;y)$ satisfying

$$G_h(x,0;y) = \delta_{x,0} \tag{3.11}$$

$$L_h(y)G_h = \left(A_h(y) - \frac{\partial}{\partial t}\right) G_h = 0 \quad (t \in \mathbb{T}_M) \tag{3.12}$$

for which the solution $u(x,t)$ to (3.10) can be expressed by

$$u(x,t) = \sum_{x_*} G_h(x - x_*, t; y)u_0(x_*). \tag{3.13}$$

We now build $\Gamma_h(x,t;y)$ as a perturbation of G_h, writing

$$\Gamma_h(x,t;y) = G_h(x-y,t;y) + \int_0^t \left[\sum_{x_*} G_h(x-x_*, t-s; x_*)\Phi_h(x_*,s;y)\right] ds, \tag{3.14}$$

which expresses Γ as the sum of the solution of the frozen coefficient problem and a corrective term depending on a function $\Phi_h(x,t;y)$, to be determined. From the requirement that $L_h\Gamma_h = 0$ in (3.7) we can derive an integral equation for $\Phi_h(x,t;y)$.

We have that

$$
\begin{aligned}
0 &= L_h\Gamma_h \\
&= L_hG_h(x-y,t;y) + \left(A_h - \frac{\partial}{\partial t}\right)\int_0^t \sum_{x_*} G_h(x-x_*,t-s;x_*)\Phi_h(x_*,s;y)\,ds \\
&= L_hG_h(x-y,t;y) + \int_0^t \sum_{x_*} A_hG_h(x-x_*,t-s;x_*)\Phi_h(x_*,s;y)\,ds \\
&\quad - \sum_{x_*} G_h(x-x_*,0;x_*)\Phi_h(x_*,t;y) \\
&\qquad - \int_0^t \sum_{x_*} \frac{\partial}{\partial t}G_h(x-x_*,t-s;x_*)\Phi_h(x_*,s;y)\,ds \\
&= L_hG_h(x-y,t;y) - \Phi_h(x,t;y) \\
&\quad + \int_0^t \sum_{x_*} L_hG_h(x-x_*,t-s;x_*)\Phi_h(x_*,s;y)\,ds.
\end{aligned}
$$

In the final step of the computation we have used the fact that $G_h(x-x_*,0;x_*) = \delta_{x,x_*}$. This yields the integral equation for Φ_h:

$$
\Phi_h(x,t;y) = L_hG_h(x-y,t;y) + \int_0^t \left[\sum_{x_*} L_hG_h(x-x_*,t-s;x_*)\Phi_h(x_*,s;y)\right] ds. \tag{3.15}
$$

We can solve (3.15) by seeking $\Phi_h(x,t;y)$ in the form

$$
\Phi_h(x,t;y) = \sum_{m=0}^{\infty} \Phi_h^{(m)}(x,t;y), \tag{3.16}
$$

where

$$
\Phi_h^{(0)}(x,t;y) = L_hG_h(x-y,t;y) \tag{3.17}
$$

and

$$
\Phi_h^{(m)}(x,t;y) = \int_0^t \left[\sum_{x_*} \Phi_h^{(0)}(x,t-s;x_*)\Phi_h^{(m-1)}(x_*,s;y)\right] ds. \tag{3.18}
$$

To establish the existence of Φ_h, we require pointwise bounds on $\Phi_h^{(m)}$.

3.2 The Frozen Coefficient Fundamental Solution

As the construction and estimation of Φ_h depends heavily on the frozen coefficient fundamental solution, we turn our attention to G_h next. It is profitable to examine G_h through the Fourier transform, where we can exploit the analyticity properties of the symbol to find spatial decay.

We begin with a bound on the symbol of $A_h(y)$.

Theorem 5. *Let $0 < B < 1$. There exists a positive constant M and constants c, κ and ω depending on M and B, but not on h or y, for which*

$$\text{Re}\,\{P_h(y, \xi + i\beta)t\} \leq -c|\xi|^2 \frac{|t|}{h^2} + \kappa|\beta|^2 \frac{|t|}{h^2} + \omega|t| \tag{3.19}$$

for all $(\xi + i\beta) \in S_B$, all $t \in \mathbb{T}_M$ and all grid points y, where

$$S_B = \left\{(\xi + i\beta) \in \mathbb{C}^d : |\xi_j| \leq \pi, |\beta_j| \leq B\right\}. \tag{3.20}$$

Furthermore, if $p_h(y, \xi)$ is real whenever ξ is real, $M > 0$ may be taken arbitrarily large.

Proof. We first consider the principal symbol $p_h(y, \xi + i\beta)$ of $A_h(y)$. Multiplying by h^2, the function $h^2 p_h(y, \xi + i\beta)$ is analytic on S_B and bounded in magnitude independent of $0 < h \leq 1$. The real part of $h^2 p_h(y, \xi + i\beta)t$ is given by

$$\begin{aligned} &\text{Re}\,\left\{h^2 p_h(y, \xi + i\beta)t\right\} = \\ &\quad = \left(\text{Re}\,\left\{h^2 p_h(y, \xi + i\beta)\right\}\right) t_1 - \left(\text{Im}\,\left\{h^2 p_h(y, \xi + i\beta)\right\}\right) t_2. \end{aligned} \tag{3.21}$$

We denote the symbol of D^2_{jl} by $\widehat{D^2_{jl}}$. As $h^2 \widehat{D^2_{jl}}$ is a polynomial in $e^{\pm i\xi_j}, e^{\pm i\xi_l}$, we can extend it to an entire function of $\xi_j + i\beta_j$ and $\xi_l + i\beta_l$. We write the Taylor expansion for $h^2 \widehat{D^2_{jl}}$:

$$h^2 \widehat{D^2_{jl}}(\xi_j + i\beta_j, \xi_l + i\beta_l) = \sum_{\substack{\mu,\nu \in \mathcal{N} \\ \mu+\nu \geq 2}} c_{\mu\nu}(\xi_j + i\beta_j)^\mu (\xi_l + i\beta_l)^\nu. \tag{3.22}$$

As $\widehat{D^2_{jl}}$ is consistent with $\partial_j\partial_l$, the first coefficient, $c_{1,1}$, in the Taylor expansion must be -1. If we expand the products, we may separate the resulting terms into three categories: terms containing only powers of ξ_j and ξ_l, terms containing only powers of β_j and β_l, and the remaining cross terms. As we are restricting our attention to the compact set S_B and each cross term contains at least one component of ξ and one component of β, the cross terms have sum of magnitude at most $O(|\xi||\beta|)$. Likewise, as the terms containing only powers of β have at minimum two factors of β, their sum has magnitude at most $O(|\beta|^2)$ on S_B. Thus, we may write

$$\begin{aligned} h^2\widehat{D^2_{jl}}(\xi_j+i\beta_j,\xi_l+i\beta_l) &= \left(\sum_{\substack{\mu,\nu\in\mathcal{N}\\ \mu+\nu\geq 2}} c_{\mu\nu}(\xi_j)^{\mu}(\xi_l)^{\nu}\right) + O(|\xi||\beta|) + O(|\beta|^2) \\ &= h^2\widehat{D^2_{jl}}(\xi_j,\xi_l) + O(|\xi||\beta|) + O(|\beta|^2). \end{aligned}$$

Substituting this into the formula for $p_h(y,\xi+i\beta)$, we have

$$\begin{aligned} h^2 p_h(y,\xi+i\beta) &= h^2\left(\sum_{jl} a_{jl}(y)\widehat{D^2_{jl}}(\xi_j,\xi_l)\right) + O(|\xi||\beta|) + O(|\beta|^2) \qquad (3.23) \\ &= h^2 p_h(y,\xi) + O(|\xi||\beta|) + O(|\beta|^2). \end{aligned}$$

This bound may be taken independent of y as the a_{jl} are uniformly bounded.

Using the uniform ellipticity hypothesis on the first term, we have

$$\mathrm{Re}\left\{h^2 p_h(y,\xi+i\beta)\right\} \leq -c|\xi|^2 + O(|\xi||\beta|) + O(|\beta|^2).$$

For each $\epsilon > 0$ we may bound the $O(|\xi||\beta|)$ term by $\epsilon|\xi|^2 + C_\epsilon|\beta|^2$. By choosing ϵ sufficiently small we find

$$\mathrm{Re}\left\{h^2 p_h(y,\xi+i\beta)\right\} \leq -c'|\xi|^2 + \kappa|\beta|^2$$

for some positive constants c' and κ.

For the imaginary part of $p_h(y,\xi+i\beta)$, we use the elementary bound

$$\left|\mathrm{Im}\left\{h^2 p_h(y,\xi+i\beta)\right\}\right| \leq C\left(|\xi|^2+|\beta|^2\right).$$

Therefore, for $t \in \mathbb{T}_M$, we have that

$$\begin{aligned}\text{Re }\left\{h^2 p_h(y,\xi+i\beta)t\right\} &= \left(\text{Re }\left\{h^2 p_h(y,\xi+i\beta)\right\}\right)t_1 - \left(\text{Im }\left\{h^2 p_h(y,\xi+i\beta)\right\}\right)|t_2| \\ &\leq \left(-c'|\xi|^2+\kappa|\beta|^2\right)t_1 + C\left(|\xi|^2+|\beta|^2\right)|t_2| \\ &\leq -c'|\xi|^2 t_1 + \kappa|\beta|^2 t_1 + CM|\xi|^2 t_1 + CM|\beta|^2 t_1. \end{aligned} \tag{3.24}$$

If we take M so that $CM < c'$, then we have, for some constants c'' and κ':

$$\text{Re }\left\{h^2 p_h(y,\xi+i\beta)t\right\} \leq -c''|\xi|^2 t_1 + \kappa'|\beta|^2 t_1.$$

Dividing through by h^2 and using the fact that $(1+M^2)^{-1/2}|t| \leq t_1 \leq |t|$ on $\mathbb{T}_M$, we discover

$$\text{Re }\{p_h(y,\xi+i\beta)t\} \leq -c''\frac{|\xi|^2}{h^2}|t| + \kappa'\frac{|\beta|^2}{h^2}|t|. \tag{3.25}$$

We now turn to the full symbol. From the elementary bound

$$\left|\sum_j b_j(y)\widehat{D_j^1} + c(y)\right| \leq C\left(\frac{|\xi|}{h} + \frac{|\beta|}{h} + 1\right),$$

we have for each $\epsilon > 0$:

$$\left|\sum_j b_j(y)\widehat{D_j^1} + c(y)\right| \leq \epsilon\frac{|\xi|^2}{h^2} + \epsilon\frac{|\beta|^2}{h^2} + C_\epsilon.$$

Consequently,

$$\text{Re }\left\{\left(\sum_j b_j(y)\widehat{D_j^1} + c(y)\right)t\right\} \leq \epsilon\frac{|\xi|^2}{h^2}|t| + \epsilon\frac{|\beta|^2}{h^2}|t| + C_\epsilon|t|. \tag{3.26}$$

Adding the bounds in (3.25) and (3.26) gives the result.

In the case where $p_h(y,\xi)$ is real whenever ξ is real, (3.23) yields the improved bound

$$\left|\text{Im }\left\{h^2 p_h(y,\xi+i\beta)\right\}\right| \leq \epsilon|\xi|^2 + C_\epsilon|\beta|^2,$$

as

$$\operatorname{Im}\left\{h^2 p_h(y,\xi)\right\} = 0.$$

This allows us to take M to be as large as we wish in (3.24) provided we first choose ϵ sufficiently small.

□

Theorem 6. *For the box S_B in Theorem 5, there exists a constant C independent of h for which*

$$|P_h(x,\xi+i\beta) - P_h(y,\xi+i\beta)| \leq C|x-y|^\alpha \left(\frac{|\xi|^2}{h^2} + \frac{|\beta|^2}{h^2} + 1\right) \tag{3.27}$$

for all $x, y \in \mathbb{R}^n_h$ and all $(\xi + i\beta) \in S_*$.

Proof. We estimate:

$$\begin{aligned}
&|P_h(x,\xi+i\beta) - P_h(y,\xi+i\beta)| = \\
&\qquad = \left|\sum_{jl}\left[a_{jl}(x) - a_{jl}(y)\right]\widehat{D^2_{jl}} + \sum_j \left[b_j(x) - b_j(y)\right]\widehat{D^1_j} + \left[c(x) - c(y)\right]\right| \\
&\qquad \leq C|x-y|^\alpha\left(\frac{|\xi|^2}{h^2} + \frac{|\beta|^2}{h^2}\right) + C|x-y|^\alpha\left(\frac{|\xi|}{h} + \frac{|\beta|}{h}\right) + C|x-y|^\alpha \\
&\qquad \leq C|x-y|^\alpha\left(\frac{|\xi|^2}{h^2} + \frac{|\beta|^2}{h^2} + 1\right)
\end{aligned}$$

using the uniform Hölder continuity of the coefficients and elementary bounds on $\widehat{D^2_{jl}}$ and $\widehat{D^1_j}$.

□

In order to prove several pointwise bounds on the fundamental solution to the frozen coefficient problem, we will need a short lemma.

Lemma 7. *Suppose*

$$\beta_j = \text{sign}\{x_j - y_j\} \min\left\{\frac{|x_j - y_j|h}{2\kappa|t|}, B\right\} \tag{3.28}$$

for some positive constants B and κ. Then for some constants c and C depending on B and κ, we have

$$e^{-<x-y,\beta>/h+\kappa|\beta|^2\frac{|t|}{h^2}} \leq Ce^{-c|x-y|/h}, \qquad |t| \leq 2h^2 \tag{3.29}$$

$$e^{-<x-y,\beta>/h+\kappa|\beta|^2\frac{|t|}{h^2}} \leq Ce^{-c|x-y|/\sqrt{|t|}}, \qquad |t| \geq h^2. \tag{3.30}$$

Proof. Without loss of generality, suppose that the first k components of β satisfy

$$\beta_j = \frac{|x_j - y_j|h}{2\kappa|t|},\ j = 1, \cdots, k$$

and the last are given by

$$\beta_j = B,\ j = k+1, \cdots, d.$$

Then we have

$$\frac{-<x-y,\beta>}{h} = \sum_{j=1}^{k} \frac{-|x_j - y_j|^2}{2\kappa|t|} + \sum_{j=k+1}^{d} \frac{-B|x_j - y_j|}{h} \tag{3.31}$$

and

$$\frac{\kappa|\beta|^2|t|}{h^2} = \sum_{j=1}^{k} \kappa\left(\frac{|x_j - y_j|^2h^2}{4\kappa^2|t|^2}\right)\frac{|t|}{h^2} + \sum_{j=k+1}^{d} \frac{\kappa B^2|t|}{h^2}$$

$$= \sum_{j=1}^{k} \frac{|x_j - y_j|^2}{4\kappa|t|} + \sum_{j=k+1}^{d} \frac{\kappa B^2|t|}{h^2}. \tag{3.32}$$

However, in the second sum of the last line, we have that $B \leq \dfrac{|x_j - y_j|h}{2\kappa|t|}$ so that $B^2 \leq \dfrac{B|x_j - y_j|h}{2\kappa|t|}$ and thus

$$\frac{\kappa B^2|t|}{h^2} \leq \frac{B|x_j - y_j|}{2h}. \tag{3.33}$$

Using (3.33) in (3.32) gives us

$$\frac{\kappa|\beta|^2|t|}{h^2} \leq \sum_{j=1}^{k} \frac{|x_j - y_j|^2}{4\kappa|t|} + \sum_{j=k+1}^{d} \frac{B|x_j - y_j|}{2h}.$$

Combining (3.31) with (3.32) yields the estimate

$$\frac{-<x-y,\beta>}{h} + \frac{\kappa|\beta|^2|t|}{h^2} \leq -\sum_{j=1}^{k} \frac{|x_j - y_j|^2}{4\kappa|t|} - \sum_{j=k+1}^{d} \frac{B|x_j - y_j|}{2h}.$$

Exponentiating, we find

$$e^{-<x-y,\beta>/h+\kappa|\beta|^2\frac{|t|}{h^2}} \leq e^{-\sum_{j=1}^{k}|x_j-y_j|^2/4\kappa|t|} e^{-\sum_{j=k+1}^{d} B|x_j-y_j|/2h}.$$

Applying the fact that $e^{-r^2} \leq Ce^{-r}$ for $r \geq 0$ to the first factor on the right, we have

$$e^{-<x-y,\beta>/h+\kappa|\beta|^2\frac{|t|}{h^2}} \leq Ce^{-\sum_{j=1}^{k}|x_j-y_j|/(2\sqrt{\kappa}\sqrt{|t|})} e^{-\sum_{j=k+1}^{d} B|x_j-y_j|/2h},$$

and the result follows immediately.

□

We now examine the frozen coefficient fundamental solution $G_h(x,t;y)$. Our primary strategy will be to consider G_h in the Fourier Transform. Analyticity of the transform of G_h enables us to employ contour deformation techniques from complex analysis to exhibit exponential spatial decay in G_h.

Theorem 8. *With M as in Theorem 5, for any multi-index γ, there exist constants C_1, C_2 and ω for which*

$$|D_h^\gamma G_h(x-y,t;y)| \leq C_1 h^{-|\gamma|} e^{-C_2|x-y|/h} e^{\omega|t|}, \qquad |t| \leq 2h^2 \tag{3.34}$$

$$|D_h^\gamma G_h(x-y,t;y)| \leq C_1 h^d\, |t|^{-d/2-|\gamma|/2} e^{-C_2|x-y|/\sqrt{|t|}} e^{\omega|t|}, \qquad |t| \geq h^2 \tag{3.35}$$

for all $x, y \in \mathbb{R}_h^d$, $0 < h \leq 1$ and $t \in \mathbb{T}_M$.

Proof. Writing G_h in the transform, we have

$$|D_h^\gamma G_h(x-y,t;y)| = \left| (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi) e^{P_h(y,\xi)t + i<x-y,\xi>/h} \, d\xi \right|. \tag{3.36}$$

Using Cauchy's integral formula and the periodicity of $P_h(y, \xi + i\beta)$, in each integral we may deform the contour of integration from the real axis to the segment joining $-\pi + i\beta$ and $\pi + i\beta$ where $|\beta| \leq B$ as in (5). This allows us to express

$$|D_h^\gamma G_h(x-y,t;y)| = \left| (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi + i\beta) e^{P_h(y,\xi+i\beta)t + i<x-y,\xi>/h - <x-y,\beta>/h} \, d\xi \right|.$$

We first assume that $|t| \leq 2h^2$. We bound the difference operator by $C/h^{|\gamma|}$ and use (3.19) to obtain

$$|D_h^\gamma G_h(x-y,t;y)| \leq Ch^{-|\gamma|} e^{\kappa|\beta|^2|t|/h^2 - <x-y,\beta>/h + \omega|t|} \int\limits_{[-\pi,\pi]^d} e^{-c|\xi|^2|t|/h^2} \, d\xi.$$

The integral is bounded by a constant, so that we have

$$|D_h^\gamma G_h(x-y,t;y)| \leq Ch^{-|\gamma|} e^{\kappa|\beta|^2|t|/h^2 - <x-y,\beta>/h + \omega|t|}.$$

The result follows by choosing β_j as in Lemma 7.

We proceed to the case $|t| \geq h^2$. From the bound

$$|\hat{D}_h^\gamma(\xi + i\beta)| \leq C \left(\frac{|\xi|^{|\gamma|}}{h^{|\gamma|}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}} \right) \tag{3.37}$$

on the symbol of the difference operator and (3.19) applied in (3.36) we find that

$$|D_h^\gamma G_h(x-y,t;y)| \leq Ce^{\kappa|\beta|^2|t|/h^2 - <x-y,\beta>/h + \omega|t|} \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^{|\gamma|}}{h^{|\gamma|}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}} \right) e^{-c|\xi|^2|t|/h^2} \, d\xi \tag{3.38}$$

on the sector $\mathbb{T}_M$ guaranteed by (3.19). Making the change of variables $\xi_j' = \xi_j\sqrt{|t|}/h$ and extending the integral over all of $\mathbb{R}^d$ we have

$$|D_h^\gamma G_h(x-y,t;y)| \le Ce^{\kappa|\beta|^2|t|/h^2 - <x-y,\beta>/h+\omega|t|}h^d|t|^{-d/2}\times$$

$$\times\int\limits_{\mathbb{R}^d}\left(\frac{|\xi'|^{|\gamma|}}{|t|^{|\gamma|/2}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}}\right)e^{-c|\xi'|^2}\,d\xi'$$

$$\le Ch^d|t|^{-d/2}\left(\frac{1}{|t|^{|\gamma|/2}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}}\right)e^{\kappa|\beta|^2|t|/h^2 - <x-y,\beta>/h+\omega|t|}.$$

With the choice of β_j in Lemma 7, we find

$$|D_h^\gamma G_h(x-y,t;y)| \le Ch^d|t|^{-d/2}\left(\frac{1}{|t|^{|\gamma|/2}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}}\right)e^{-c|x-y|/\sqrt{|t|}+\omega|t|}.$$

As our choice of β has each component bounded by $\dfrac{|x-y|h}{2\kappa|t|}$, we are guaranteed that

$$\frac{|\beta|^{|\gamma|}}{h^{|\gamma|}} \le C\frac{|x-y|^{|\gamma|}}{|t|^{|\gamma|}}.$$

Using this fact, factoring and absorbing constants leads us to find

$$|D_h^\gamma G_h(x-y,t;y)| \le Ch^d|t|^{-d/2}|t|^{-|\gamma|/2}\left(1+\left(\frac{|x-y|}{\sqrt{|t|}}\right)^{|\gamma|}\right)e^{-c|x-y|/\sqrt{|t|}+\omega|t|}.$$

Employing the fact that

$$r^k e^{-cr} \le C_{\epsilon,k}e^{-(c-\epsilon)r}, \qquad r\ge 0 \tag{3.39}$$

for real-valued functions and exploiting the scaling in $|x-y|/\sqrt{|t|}$ in the exponential enables us to conclude

$$|D_h^\gamma G_h(x-y,t;y)| \le Ch^d|t|^{-d/2-|\gamma|/2}e^{-c'|x-y|/\sqrt{|t|}}e^{\omega'|t|}.$$

□

Theorem 9. *Let γ be any multi-index for which $|\gamma| \le 2$. With M as in Theorem 5, there exist constants C_1, C_2 and ω for which*

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| \le C_1 h^{-|\gamma|}|y_1-y_2|^\alpha \times \times e^{-C_2|x-y|/h} e^{\omega|t|}, \qquad |t| \le 2h^2 \tag{3.40}$$

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| \le C_1 h^d |t|^{-d/2-|\gamma|/2}|y_1-y_2|^\alpha \times \times e^{-C_2|x-y|/\sqrt{|t|}} e^{\omega|t|}, \qquad |t| \ge h^2 \tag{3.41}$$

for all $x, y, y_1, y_2 \in \mathbb{R}_h^d$, $0 < h \le 1$ and $t \in \mathbb{T}_M$.

Proof. We again turn to the transform to obtain the estimate. We have that

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| =$$

$$= \left|(2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi+i\beta)\left(e^{P_h(y_1,\xi+i\beta)t} - e^{P_h(y_2,\xi+i\beta)t}\right) e^{i<x-y,\xi>/h-<x-y,\beta>/h}\, d\xi\right|$$

$$= \left|(2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi+i\beta)\left(e^{P_h(y_1,\xi+i\beta)t-P_h(y_2,\xi+i\beta)t} - 1\right) \times \times e^{P_h(y_2,\xi+i\beta)} e^{i<x-y,\xi>/h-<x-y,\beta>/h}\, d\xi\right|.$$

We use (3.19), (3.37) and the fact that

$$|e^z - 1| \le |z|e^{|z|} \tag{3.42}$$

to find

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| \le$$

$$\le Ce^{-<x-y,\beta>/h+\kappa|\beta|^2|t|/h^2+\omega|t|} \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^{|\gamma|}}{h^{|\gamma|}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}}\right) \times$$

$$\times |P_h(y_1,\xi+i\beta) - P_h(y_2,\xi+i\beta)|\,|t|e^{|P_h(y_1,\xi+i\beta)-P_h(y_2,\xi+i\beta)||t|} e^{-c|\xi|^2|t|/h^2}\, d\xi.$$

We use the bound in Theorem 6 to obtain

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| \le$$

$$\le Ce^{-<x-y,\beta>/h+\kappa|\beta|^2|t|/h^2+\omega|t|} \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^{|\gamma|}}{h^{|\gamma|}} + \frac{|\beta|^{|\gamma|}}{h^{|\gamma|}}\right) |y_1-y_2|^\alpha \times$$

$$\times \left(\frac{|\xi|^2}{h^2}|t| + \frac{|\beta|^2}{h^2}|t| + |t|\right) e^{C|y_1-y_2|^\alpha\left(|\xi|^2|t|/h^2+|\beta|^2|t|/h^2+|t|\right)} e^{-c|\xi|^2|t|/h^2}\, d\xi.$$

For small enough δ, with $|y_1 - y_2| \le \delta$, we then find

$$|D_h^\gamma G_h(x-y,t;y_1) - D_h^\gamma G_h(x-y,t;y_2)| \le$$

$$\le C|y_1-y_2|^\alpha e^{-<x-y,\beta>/h+\kappa'|\beta|^2|t|/h^2+\omega|t|} \times$$

$$\times \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^{|\gamma|+2}}{h^{|\gamma|+2}} + \frac{|\beta|^{|\gamma|+2}}{h^{|\gamma|+2}} + 1\right) |t| e^{-c'|\xi|^2|t|/h^2}\, d\xi.$$

The remainder of the proof is similar to the proof of Theorem 8, continuing from (3.38). The factor of $|t|$ is absorbed into the exponential, causing an increase in ω.

For $|y_1 - y_2| > \delta$, the result is a straightforward consequence of Theorem 8.

□

Theorem 10. *Let γ be any multi-index for which $|\gamma| \le 2$. With M as in Theorem 5, there exist constants C_1, C_2 and ω for which*

$$|D_h^\gamma G_h(x_1-y,t;y) - D_h^\gamma G_h(x_2-y,t;y)| \le$$

$$\le C_1 h^{-(|\gamma|+1)}|x_1-x_2| e^{-C_2|x_2-y|/h} e^{\omega|t|}, \qquad |t| \le 2h^2 \tag{3.43}$$

$$|D_h^\gamma G_h(x_1-y,t;y) - D_h^\gamma G_h(x_2-y,t;y)| \le$$

$$\le C_1 h^d |t|^{-d/2-|\gamma|/2-1/2}|x_1-x_2| e^{-C_2|x_2-y|/\sqrt{|t|}} e^{\omega|t|}, \qquad |t| \ge h^2 \tag{3.44}$$

for all $x_1, x_2, y \in \mathbb{R}_h^d$ with $|x_1 - x_2| \le \sqrt{|t|}$, $0 < h \le 1$ and $t \in \mathbb{T}_M$.

Proof. We write the difference in the transform, deform the contour of integration, and factor the integrand to obtain

$$|D_h^\gamma G_h(x_1 - y, t; y) - D_h^\gamma G_h(x_2 - y, t; y)| =$$

$$= \left| (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi + i\beta) \times \right.$$

$$\left. \times \left(e^{P_h(y,\xi+i\beta)t + i<x_1-y,\xi+i\beta>/h} - e^{P_h(y,\xi+i\beta)t+i<x_2-y,\xi+i\beta>/h} \right) d\xi \right|$$

$$= \left| (2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} \hat{D}_h^\gamma(\xi + i\beta) \times \right.$$

$$\left. \times\, e^{P_h(y,\xi+i\beta)t+i<x_2-y,\xi>/h-<x_2-y,\beta>/h} \left(e^{i<x_1-x_2,\xi+i\beta>/h} - 1 \right) d\xi \right|.$$

Using (3.42), we bound the factor

$$\left| e^{i<x_1-x_2,\xi+i\beta>/h} - 1 \right| \le |x_1 - x_2| \frac{|\xi + i\beta|}{h} e^{|x_1-x_2| \frac{|\xi+i\beta|}{h}}$$

$$\le |x_1 - x_2| \left(\frac{|\xi|}{h} + \frac{|\beta|}{h} \right) e^{\epsilon|x_1-x_2|^2|\xi^2|/h^2 + \epsilon|x_1-x_2|^2|\beta^2|/h^2 + 1/\epsilon}$$

$$\le C|x_1 - x_2| \left(\frac{|\xi|}{h} + \frac{|\beta|}{h} \right) e^{\epsilon|x_1-x_2|^2|\xi^2|/h^2 + \epsilon|x_1-x_2|^2|\beta^2|/h^2}.$$

As $|x_1 - x_2| \le \sqrt{|t|}$ by hypothesis,

$$\left| e^{i<x_1-x_2,\xi+i\beta>/h} - 1 \right| \le C|x_1 - x_2| \left(\frac{|\xi|}{h} + \frac{|\beta|}{h} \right) e^{\epsilon|\xi|^2|t|/h^2 + \epsilon|\beta|^2|t|/h^2}.$$

Combining this with (3.19) gives us

$$|D_h^\gamma G_h(x_1 - y, t; y) - D_h^\gamma G_h(x_2 - y, t; y)| \le$$

$$\le C|x_1 - x_2| e^{-<x_2-y,\beta>/h + \kappa'|\beta|^2|t|/h^2 + \omega|t|} \times$$

$$\times \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^{|\gamma|+1}}{h^{|\gamma|+1}} + \frac{|\beta|^{|\gamma|+1}}{h^{|\gamma|+1}} \right) e^{-c'|\xi|^2|t|/h^2}\, d\xi.$$

The remainder of the proof is similar to the proof of Theorem 8, continuing from (3.38).

□

Theorem 11. *With M as in Theorem 5, there exist constants C_1, C_2 and ω for which*

$$|L_h G_h(x-y,t;y)| \leq C_1 h^{-2+\alpha} e^{-C_2|x-y|/h} e^{\omega|t|}, \qquad |t| \leq 2h^2 \tag{3.45}$$

$$|L_h G_h(x-y,t;y)| \leq C_1 h^d |t|^{-d/2-1+\alpha/2} e^{-C_2|x-y|/\sqrt{|t|}} e^{\omega|t|}, \qquad |t| \geq h^2, \tag{3.46}$$

for all $x, y \in \mathbb{R}^d_h$, $0 < h \leq 1$ and $t \in \mathbb{T}_M$.

Proof. Writing $L_h G_h(x-y,t;y)$ in the transform, we have

$$|L_h G_h(x-y,t;y)| = \Bigg|(2\pi)^{-d} \int\limits_{[-\pi,\pi]^d} (P_h(x,\xi+i\beta) - P_h(y,\xi+i\beta)) \times \\ \times e^{P_h(y,\xi+i\beta)t + i<x-y,\xi>/h - <x-y,\beta>/h}\, d\xi\Bigg|.$$

By (3.19) and Theorem 6, we find

$$|L_h G_h(x-y,t;y)| \leq \\ \leq C|x-y|^\alpha e^{-<x-y,\beta>/h + \kappa|\beta|^2 \frac{|t|}{h^2} + \omega|t|} \int\limits_{[-\pi,\pi]^d} \left(\frac{|\xi|^2}{h^2} + \frac{|\beta^2|}{h^2} + 1\right) e^{-c|\xi|^2 \frac{|t|}{h^2}}\, d\xi.$$

The remainder of the proof is similar to the proof of Theorem 8, continuing from (3.38).

□

Theorem 12. *With M as in Theorem 5, there exist constants C_1, C_2 and ω for* *which*

$$|(L_hG_h)(x_1-y,t;y)-(L_hG_h)(x_2-y,t;y)| \leq$$
$$\leq C_1 h^{-2+\alpha/2}|x_1-x_2|^{\alpha/2}\left(e^{-C_2|x_1-y|/h}+e^{-C_2|x_2-y|/h}\right)e^{\omega|t|}, \qquad |t|\leq 2h^2 \quad (3.47)$$
$$|(L_hG_h)(x_1-y,t;y)-(L_hG_h)(x_2-y,t;y)| \leq$$
$$\leq C_1 h^{d}|t|^{-d/2-1+\alpha/4}|x_1-x_2|^{\alpha/2}\left(e^{-C_2|x_1-y|/\sqrt{|t|}}+e^{-C_2|x_2-y|/\sqrt{|t|}}\right)e^{\omega|t|},\ |t|\geq h^2 \quad (3.48)$$

for all $x_1, x_2, y \in \mathbb{R}_h^d$, $0 < h \leq 1$ *and* $t \in \mathbb{T}_M$.

Proof. We treat the case $|t| \geq h^2$ explicitly. The case $|t| \leq 2h^2$ is handled similarly.

We begin by supposing $|x_1 - x_2| \leq \sqrt{|t|}$. We write out

$$L_hG_h(x_1-y,t;y) - L_hG_h(x_2-y,t;y) = B_2 + B_1 + B_0$$

where

$$\begin{aligned} B_2 &= \sum_{jl}\left(a_{jl}(x_1)-a_{jl}(y)\right)D^2_{jl}G_h(x_1-y,t;y) \\ &\qquad - \sum_{jl}\left(a_{jl}(x_2)-a_{jl}(y)\right)D^2_{jl}G_h(x_2-y,t;y) \\ &= \sum_{jl}\left(a_{jl}(x_1)-a_{jl}(x_2)\right)D^2_{jl}G_h(x_1-y,t;y) \\ &\qquad + \sum_{jl}\left(D^2_{jl}G_h(x_1-y,t;y)-D^2_{jl}G_h(x_2-y,t;y)\right)\left(a_{jl}(x_2)-a_{jl}(y)\right) \\ &= F_1 + F_2 \end{aligned}$$

and B_1 and B_0 are defined similarly for the lower-order discretizations. Here we have re-arranged the terms so that our previous estimates are directly applicable. We bound F_1 using the uniform Hölder continuity of the a_{jl} and (3.35), giving us

$$|F_1| \leq C|x_1-x_2|^{\alpha}h^d|t|^{-d/2-1}e^{-C_2|x_1-y|/\sqrt{|t|}}e^{\omega|t|}.$$

As $|x_1 - x_2| \le \sqrt{|t|}$ by hypothesis, we have that $|x_1 - x_2|^\alpha \le |x_1 - x_2|^{\alpha/2}|t|^{\alpha/4}$, which gives us

$$|F_1| \le C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} e^{-C_2|x_1-y|/\sqrt{|t|}} e^{\omega|t|}.$$

We may bound F_2 using the uniform Hölder continuity of the a_{jl} and (3.44), yielding

$$|F_2| \le C|x_2 - y|^\alpha |x_1 - x_2| h^d |t|^{-d/2-3/2} e^{-C_2|x_2-y|/\sqrt{|t|}} e^{\omega|t|}.$$

We can rewrite the above as

$$|F_2| \le C \left(\frac{|x_2 - y|}{\sqrt{|t|}} \right)^\alpha |t|^{\alpha/2} |x_1 - x_2| h^d |t|^{-d/2-3/2} e^{-C_2|x_2-y|/\sqrt{|t|}} e^{\omega|t|}.$$

The scaling in the exponent now gives us

$$|F_2| \le C|x_1 - x_2| h^d |t|^{-d/2-3/2+\alpha/2} e^{-C_3|x_2-y|/\sqrt{|t|}} e^{\omega|t|}.$$

We split up $|x_1 - x_2| = |x_1 - x_2|^{\alpha/2}|x_1 - x_2|^{1-\alpha/2}$ and use the hypothesis $|x_1 - x_2| \le \sqrt{|t|}$ on the second factor to find

$$\begin{aligned} |F_2| &\le C|x_1 - x_2|^{\alpha/2} |t|^{1/2-\alpha/4} h^d |t|^{-d/2-3/2+\alpha/2} e^{-C_3|x_2-y|/\sqrt{|t|}} e^{\omega|t|} \\ &\le C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} e^{-C_3|x_2-y|/\sqrt{|t|}} e^{\omega|t|}. \end{aligned}$$

Summing the bounds for F_1 and F_2 (along with similar bounds for B_1 and B_0) yields the result in the case $|x_1 - x_2| \le \sqrt{|t|}$.

The result for $|x_1 - x_2| \ge \sqrt{|t|}$ is an immediate consequence of Theorem 11.

□

Theorem 13. *Let M be as in Theorem 5. Suppose γ is a multi-index with $|\gamma| = 2$. Then there exists a constant C depending on M but not on h or x for which:*

$$\left| \sum_{x_*} D_h^\gamma G_h(x - x_*, t; x_*) \right| \le C h^{-2+\alpha} e^{\omega|t|}, \qquad |t| \le 2h^2 \tag{3.49}$$

$$\left| \sum_{x_*} D_h^\gamma G_h(x - x_*, t; x_*) \right| \le C|t|^{-1+\alpha/2} e^{\omega|t|}, \qquad |t| \ge h^2, \qquad |t| \ge h^2 \tag{3.50}$$

for $t \in \mathbb{T}_M$.

Proof. We prove the case where $|t| \geq h^2$ explicitly. The case where $|t| \leq 2h^2$ is similar.

Let $\chi : \mathbb{R} \to \mathbb{R}$ be a C_0^∞ function with $\chi(r) \equiv 1$ for $|r| \leq 1$ and $\chi(r) \equiv 0$ for $|r| \geq 2$. For an arbitrary grid point q, we express

$$\sum_{x_*} [D_h^\gamma G_h(x - x_*, t; x_*)] =$$

$$\begin{aligned}
&= \sum_{|x-x_*|\leq 2} [(D_h^\gamma G_h(x - x_*, t; x_*) - D_h^\gamma G_h(x - x_*, t; q))\, \chi(|x - x_*|)] \\
&\quad + \sum_{|x-x_*|\leq 2} [D_h^\gamma G_h(x - x_*, t; q) \chi(|x - x_*|)] \\
&\quad + \sum_{|x-x_*|\geq 2} [D_h^\gamma G_h(x - x_*, t; x_*)(1 - \chi(|x - x_*|))] \\
&= J_1 + J_2 + J_3
\end{aligned}$$

To handle J_1, we use Theorem 9 and the fact that χ is bounded to find that

$$|J_1| \leq C \sum_{|x-x_*|\leq 2} h^d |t|^{-d/2-1} |x_* - q|^\alpha e^{-C_2|x-x_*|/\sqrt{|t|}} e^{\omega|t|}.$$

For the particular choice $q = x$, we have

$$\begin{aligned}
|J_1|\big|_{q=x} &\leq C \sum_{|x-x_*|\leq 2} h^d |t|^{-d/2-1} |x_* - q|^\alpha e^{-C_2|x-x_*|/\sqrt{|t|}} e^{\omega|t|} \\
&\leq C \sum_{|x-x_*|\leq 2} h^d |t|^{-d/2-1} |x_* - x|^\alpha e^{-C_2|x-x_*|/\sqrt{|t|}} e^{\omega|t|} \\
&\leq C \sum_{|x-x_*|\leq 2} h^d |t|^{-d/2-1+\alpha/2} e^{-C_3|x-x_*|/\sqrt{|t|}} e^{\omega'|t|},
\end{aligned}$$

where in the last step we have exploited the scaling in the exponential to trade Hölder regularity for temporal regularity. The final inequality can be rewritten as

$$|J_1|\big|_{q=x} \leq C|t|^{-1+\alpha/2} e^{\omega|t|} \sum_{|x-x_*|\leq 2} h^d |t|^{-d/2} e^{-C_3|x-x_*|/\sqrt{|t|}}.$$

The sum on the right can be regarded as a Riemann sum. If we select $\delta z = h/\sqrt{|t|}$, then $\delta z \le 1$, and the sum is bounded by

$$\sum_{j\in\mathbb{Z}^d} e^{-C_3|j\delta z|}\delta z^d.$$

This is a Riemann sum for the exponentially decaying function $e^{-C_3|x|}$ and is uniformly bounded in $0 < \delta z \le 1$ by a constant. Therefore,

$$|J_1|\big|_{q=x} \le C|t|^{-1+\alpha/2}e^{\omega|t|}.$$

To handle J_2, we interpret the difference as acting on x_* and difference by parts, so that

$$J_2 = -\sum_{|x-x_*|\le 2}[D_h^{\gamma_1}G_h(x-x_*,t;q)D_h^{\gamma_2}\chi(|x-x_*|)]$$

where $|\gamma_1| = |\gamma_2| = 1$ are multi-indices. As χ is C_0^∞, $D_h^{e_2}\chi(|x-x_*|) \le C$ for C independent of h and x. We use this fact and Theorem 8 for $|\gamma| = 1$ to find

$$|J_2| \le C\sum_{|x-x_*|\le 2} h^d|t|^{-d/2-1/2}e^{-C_2|x-x_*|/\sqrt{|t|}}e^{\omega|t|}$$

The sum on the right is $C|t|^{-1/2}e^{\omega|t|}$ multiplied by the discretization of an integral, so that

$$|J_2| \le C|t|^{-1/2}e^{\omega|t|}.$$

For J_3, we use the fact that χ is bounded and apply the estimate in Theorem 8 with $|\gamma| = 2$ to find

$$|J_3| \le C\sum_{|x-x_*|\ge 2} h^d|t|^{-d/2-1}e^{-C_2|x-x_*|/\sqrt{|t|}}e^{\omega|t|}.$$

As $|x-x_*| \ge 2$, we can multiply the sum on the right by $|x-x_*|$, and exploit the scaling in the exponential to find

$$|J_3| \le C\sum_{|x-x_*|\ge 2} h^d|x-x_*||t|^{-d/2-1}e^{-C_2|x-x_*|/\sqrt{|t|}}e^{\omega|t|}$$

$$h^d|t|^{-d/2-1/2}e^{-C_4|x-x_*|/\sqrt{|t|}}e^{\omega|t|}.$$

The final step can be expressed as the rescaling of an integral, enabling us to conclude that

$$|J_3| \leq C|t|^{-1/2}e^{\omega|t|}.$$

Adding the bounds on J_1, J_2 and J_3 (for the choice $q = x$) gives the result.

□

3.3 Two Lemmas

Two lemmas simplify the proof that the series for Φ_h converges. We define

$$\Psi^{(m)}(x,\tau,y) = \exp\left(-(C_2 - m\epsilon)\frac{|x-y|}{\tau}\right) \tag{3.51}$$

where C_2 is given in Theorem 11.

Lemma 14. *Suppose ϵ is a positive constant and m is a positive integer for which $(m+1)\epsilon < C_2$. Let x and y be generic grid points, and $0 < s < t$.*

There exists a constant $d(\epsilon)$ (independent of x, y, C_2 and m) for which:

(i) *With no other restriction on t or s:*

$$\sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x,h,x_*)\Psi^{(m)}(x_*,h,y) \leq d(\epsilon)\Psi^{(m)}(x,h,y). \tag{3.52}$$

(ii) *If $t \geq 2h^2$:*

$$\sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x,h,x_*)\Psi^{(m)}(x_*,\sqrt{s},y) \leq d(\epsilon)\Psi^{(m)}(x,\sqrt{t},y). \tag{3.53}$$

(iii) *If $t \geq 2h^2$:*

$$\sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x,\sqrt{t-s},x_*)\Psi^{(m)}(x_*,h,y) \leq d(\epsilon)\Psi^{(m+1)}(x,\sqrt{t},y) \tag{3.54}$$

(iv) *If* $t \geq 2h^2$ *and* $(t-s) \geq h^2$*:*

$$h^d (t-s)^{-d/2} \sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x, \sqrt{t-s}, x_*) \Psi^{(m)}(x_*, h, y) \leq d(\epsilon) \Psi^{(m)}(x, \sqrt{t}, y). \tag{3.55}$$

(v) *If* $t \geq 2h^2$ *and* $(t-s) \geq h^2$*:*

$$h^d (t-s)^{-d/2} \sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x, \sqrt{t-s}, x_*) \Psi^{(m)}(x_*, \sqrt{s}, y) \leq d(\epsilon) \Psi^{(m)}(x, \sqrt{t}, y). \tag{3.56}$$

(vi) *If* $t \geq 2h^2$ *and* $s \geq h^2$*:*

$$h^d s^{-d/2} \sum_{x_* \in \mathbb{R}_h^n} \Psi^{(0)}(x, \sqrt{t-s}, x_*) \Psi^{(m)}(x_*, \sqrt{s}, y) \leq d(\epsilon) \Psi^{(m+1)}(x, \sqrt{t}, y). \tag{3.57}$$

Furthermore, a similar result holds when m *is replaced by* 0 *on the left hand side and* m *is replaced by* 1 *on the right hand side of (i),(ii), (iv) and (v), and (iii) and (vi) hold for* $m = 0$ *without modification.*

Proof. (i) Applying the triangle inequality to the grid points x, y and x_* and multiplying by the negative constant $-(C_2 - m\epsilon)/h$ results in the relationship:

$$-(C_2 - m\epsilon)|x - x_*|/h - (C_2 - m\epsilon)|x_* - y|/h \leq -(C_2 - m\epsilon)|x - y|/h.$$

From this we subtract $m\epsilon|x - x_*|/h$ from both sides to obtain that

$$-C_2|x - x_*|/h - (C_2 - m\epsilon)|x_* - y|/h \leq -(C_2 - m\epsilon)|x - y|/h - m\epsilon|x - x_*|/h.$$

This inequality and the monotonicity of the exponential allow us to reason

$$\sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x, h, x_*) \Psi^{(m)}(x_*, h, y) = \sum_{x_*} e^{-C_2|x - x_*|/h} e^{-(C_2 - m\epsilon)|x_* - y|/h}$$

$$\leq \sum_{x_*} e^{-(C_2 - m\epsilon)|x-y|/h} e^{-m\epsilon|x - x_*|/h} \leq e^{-(C_2 - m\epsilon)|x-y|/h} \sum_{x_*} e^{-m\epsilon|x - x_*|/h}$$

$$\leq d(\epsilon) e^{-(C_2 - m\epsilon)|x-y|/h} = d(\epsilon) \Psi^{(m)}(x, h, y).$$

The sum is independent of h, and as m is a positive integer, we may take the constant $d(\epsilon)$ to be the sum when $m = 1$, so that $d(\epsilon)$ is independent of m.

(ii) Starting with an easy consequence of the triangle inequality,

$$-(C_2 - m\epsilon)|x - x_*|/\sqrt{t} - (C_2 - m\epsilon)|x_* - y|/\sqrt{t} \le -(C_2 - m\epsilon)|x - y|/\sqrt{t},$$

we replace $\sqrt{t}$ in the denominator by positive real numbers of smaller magnitude, leading to:

$$-(C_2 - m\epsilon)|x - x_*|/h - (C_2 - m\epsilon)|x_* - y|/\sqrt{s} \le -(C_2 - m\epsilon)|x - y|/\sqrt{t}.$$

By subtracting $m\epsilon|x - x_*|/h$ from each side, we have that

$$-C_2|x - x_*|/h - (C_2 - m\epsilon)|x_* - y|/\sqrt{s} \le -(C_2 - m\epsilon)|x - y|/\sqrt{t} - m\epsilon|x - x_*|/h.$$

The remainder of the proof is similar in spirit to the proof of (i).

(iii) We apply the triangle inequality to the grid points x, x_* and y and multiply by $-(C_2 - (m+1)\epsilon)$ to obtain

$$- (C_2 - (m+1)\epsilon)|x - x_*|/\sqrt{t} - (C_2 - (m+1)\epsilon)|x_* - y|/\sqrt{t} \le$$
$$\le -(C_2 - (m+1)\epsilon)|x - y|/\sqrt{t}.$$

We replace $\sqrt{t}$ on the left hand side by smaller constants, so that

$$- (C_2 - (m+1)\epsilon)|x - x_*|/\sqrt{t-s} - (C_2 - (m+1)\epsilon)|x_* - y|/h \le$$
$$\le -(C_2 - (m+1)\epsilon)|x - y|/\sqrt{t}.$$

Subtracting $\epsilon|x_* - y|/h$ from each side and subtracting $(m+1)\epsilon|x - x_*|/\sqrt{t-s}$ from the left gives

$$- C_2|x - x_*|/\sqrt{t-s} - (C_2 - m\epsilon)|x_* - y|/h \le$$
$$\le -(C_2 - (m+1)\epsilon)|x - y|/\sqrt{t} - \epsilon|x_* - y|/h.$$

The remainder of the proof is similar in spirit to the proof of (i).

(iv) The proof is very similar to the proof of (v), presented below.

(v) We begin by applying the triangle inequality to the grid points x, x_* and y, and multiply by the negative constant $-(C_2 - m\epsilon)$ to find

$$-(C_2 - m\epsilon)|x - x_*|/\sqrt{t} - (C_2 - m\epsilon)|x_* - y|/\sqrt{t} \le -(C_2 - m\epsilon)|x - y|/\sqrt{t}.$$

We replace both occurrences of $\sqrt{t}$ in the denominators on the left hand side by smaller constants, so that

$$-(C_2 - m\epsilon)|x - x_*|/\sqrt{t-s} - (C_2 - m\epsilon)|x_* - y|/\sqrt{s} \le -(C_2 - m\epsilon)|x - y|/\sqrt{t}.$$

Subtracting $m\epsilon|x - x_*|\sqrt{t-s}$ from both sides gives

$$\begin{aligned} - C_2|x - x_*|/\sqrt{t-s} - (C_2 - m\epsilon)|x_* - y|/\sqrt{s} \le \\ \le -(C_2 - m\epsilon)|x - y|/\sqrt{t} - m\epsilon|x - x_*|/\sqrt{t-s}. \end{aligned}$$

We can now bound the sum on the left in (3.56) by

$$\begin{aligned} h^d(t-s)^{-d/2} \sum_{x_* \in \mathbb{R}_h^d} \Psi^{(0)}(x, \sqrt{t-s}, x_*)\Psi^{(m)}(x_*, \sqrt{s}, y) = \\ = h^d(t-s)^{-d/2} \sum_{x_*} e^{-C_2|x-x_*|/\sqrt{t-s}} e^{-(C_2-m\epsilon)|x_*-y|/\sqrt{s}} \\ \le h^d(t-s)^{-d/2} \sum_{x_*} e^{-(C_2-m\epsilon)|x-y|/\sqrt{t}} e^{-m\epsilon|x-x_*|/\sqrt{t-s}}. \end{aligned}$$

We define $\eta = h/\sqrt{t-s}$. Then $\eta \le 1$, and

$$\begin{aligned} h^d(t-s)^{-d/2} \sum_{x_* \in \mathbb{R}_h^d} e^{-C_2|x-x_*|/\sqrt{t-s}} e^{-(C-m\epsilon)|x_*-y|/\sqrt{s}} \le \\ \le e^{-(C_2-m\epsilon)|x-y|/\sqrt{t}} \left(\sum_{j \in \mathbb{Z}^d} e^{-m\epsilon j\eta} \eta^d \right) \\ \le d(\epsilon) e^{-(C_2-m\epsilon)|x-y|/\sqrt{t}} \\ = d(\epsilon)\Psi^{(m)}(x, \sqrt{t}, y). \end{aligned}$$

In the second to last step, we have recognized that the expression involving η is the discretization of an integral and is uniformly bounded for $0 < \eta \le 1$.

(vi) The proof is similar in spirit to the proofs of (iii) and (v).

We note that the only bounds among (i)-(vi) that *require* giving up some exponential decay are (iii) and (vi). When $m = 0$, each bound requires giving up some exponential decay, and the proofs begin similarly to that of (iii).

□

Lemma 15. *Let* $0 < \gamma_1 < 1 < \gamma_2$ *and* $t > 0$. *Then*

$$\int_0^t (t-s)^{-1+\gamma_1} s^{-1+\gamma_2}\, ds = \frac{\Gamma(\gamma_1)\Gamma(\gamma_2)}{\Gamma(\gamma_1+\gamma_2)} t^{-1+\gamma_1+\gamma_2}, \tag{3.58}$$

where Γ *with one argument is the standard* Γ *function.*

Proof. We make the change of variables $s' = s/t$, so that the integral becomes

$$\int_0^1 (t-ts')^{-1+\gamma_1}(ts')^{-1+\gamma_2}(t)\, ds' = t^{-1+\gamma_1+\gamma_2}\int_0^1 (1-s')^{-1+\gamma_1}(s')^{-1+\gamma_2}\, ds'. \tag{3.59}$$

We recognize the integral on the right as a standard form of the Beta function, and, by a well-known property of the Beta function, we have

$$\int_0^1 (1-s')^{-1+\gamma_1}(s')^{-1+\gamma_2}\, ds' = B(\gamma_1,\gamma_2) = \frac{\Gamma(\gamma_1)\Gamma(\gamma_2)}{\Gamma(\gamma_1+\gamma_2)},$$

from which the result follows immediately.

□

3.4 Constructing Φ_h

To show that Φ_h converges, we seek pointwise bounds on each term $\Phi_h^{(m)}$. The estimate on the first term, $\Phi_h^{(0)}(x,t;y) = L_h G_h(x-y,t;y)$, was handled specially by way of a contour deformation in Theorem 11. The subsequent terms $\Phi_h^{(m)}$ for $1 \le m \le \hat{m}$ for $\hat{m}$ defined below contain singularities of diminishing order in t, and for these $\hat{m}$ terms, the bound on each successive term in Φ_h requires abandoning some decay in $|x-y|/\sqrt{|t|}$ (or $|x-y|/h$). However, the terms beyond the $(\hat{m}+1)$-*th* contain positive powers of t, have uniform decay in $|x-y|/\sqrt{|t|}$ and possess coefficients that decay like $\Gamma(1+m\alpha/2)^{-1}$, which are essential to the proof of the convergence of the series for Φ_h.

We begin by defining

$$\hat{m} = \lfloor \frac{(d+2)-\alpha}{\alpha} \rfloor. \tag{3.60}$$

Theorem 16. *With M as in Theorem 5 and C_2 as in Theorem 11, there exist constants C_1 and ω (independent of x, y and $0 < h \le 1$) such that for every $0 < \epsilon < C_2/(\hat{m}+2)$, there is a constant $d(\epsilon)$ so that*

(i) *for $0 \le m \le \hat{m}$ we have:*

$$\left|\Phi_h^{(m)}(x,t;y)\right| \le C_1 d(\epsilon)^m h^{-2+(m+1)\alpha} \Psi^{(m)}(x,h,y) e^{\omega|t|}, \qquad |t| \le 2h^2 \tag{3.61}$$

$$\left|\Phi_h^{(m)}(x,t;y)\right| \le C_1 d(\epsilon)^m h^d \, |t|^{-d/2-1+(m+1)\alpha/2} \Psi^{(m)}(x,\sqrt{|t|},y) e^{\omega|t|}, \qquad |t| \ge h^2. \tag{3.62}$$

(ii) *for all $m > 0$, we have:*

$$\left|\Phi_h^{(\hat{m}+m)}(x,t;y)\right| \le \frac{4^m C_1^{m+1} d(\epsilon)^{\hat{m}+m} \Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} \times$$
$$\times\, h^d \, |t|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \Psi^{(\hat{m}+1)}(x,h,y) e^{\omega|t|}, \quad |t| \le 2h^2 \tag{3.63}$$

$$\left|\Phi_h^{(\hat{m}+m)}(x,t;y)\right| \le \frac{4^m C_1^{m+1} d(\epsilon)^{\hat{m}+m} \Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} \times$$
$$\times\, h^d \, |t|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \Psi^{(\hat{m}+1)}(x,\sqrt{|t|},y) e^{\omega|t|}, \quad |t| \ge h^2. \tag{3.64}$$

We remark that $\Psi^{(m)}$ is best thought of as keeping track of the $|x-y|/\sqrt{|t|}$ (or $|x-y|/h$) scaling in the decay of $\Phi_h^{(m)}$.

Proof. We have already addressed $\Phi_h^{(0)}$ in Theorem 11.

To prove (3.61), we restrict our attention to $|t| \leq 2h^2$. Substituting the small $|t|$ estimate in (3.61) into (3.18) inductively, we find

$$|\Phi_h^{(m+1)}(x,t;y)| \leq Cd(\epsilon)^m h^{-4+(m+2)\alpha} e^{\omega|t|} \int_0^t \sum_{x_*} \Psi^{(0)}(x,h,x_*)\Psi^{(m)}(x_*,h,y)\, ds.$$

Here we have multiplied out all the the factors that do not depend on the index of summation and placed them in front of the sum. We note that $e^{\omega|t-s|}e^{\omega|s|} = e^{\omega|t|}$ as t, s and $t-s$ all lie on the same ray from the origin. The sum is in a form amenable to Lemma 14 part (i). We apply the lemma to find that

$$|\Phi_h^{(m+1)}(x,t;y)| \leq Cd(\epsilon)^m h^{-4+(m+2)\alpha} e^{\omega|t|} \int_0^{|t|} d(\epsilon)\Psi^{(m+1)}(x,h,y)\, ds.$$

Here we have given up some spatial decay by replacing $\Psi^{(m)}$ in the conclusion of the lemma by $\Psi^{(m+1)}$, as $\Psi^{(m)}$ is an increasing function of m. The integrand is independent of s, and $|t| \leq 2h^2$, so that the right hand side is bounded by

$$|\Phi_h^{(m+1)}(x,t;y)| \leq Cd(\epsilon)^{m+1} h^{-2+(m+2)\alpha} \Psi^{(m+1)}(x,h,y) e^{\omega|t|},$$

proving (3.61).

We move on to proving (3.62). We note that (3.61) immediately implies (3.62) for $h^2 \leq |t| \leq 2h^2$. To prove (3.62) for $|t| \geq 2h^2$, we split the path of integration defining $\Phi_h^{(m)}$ into four parts. We take the path of integration in the definition of $\Phi_h^{(m)}(x,t;y)$ to be the segment joining the origin and t. We define I_1 to be the integral over the segment from 0 to $h^2 t/|t|$, I_2 over the segment joining $h^2 t/|t|$ to $t/2$, I_3 over the segment joining $t/2$ to $(1-h^2/|t|)t$ and I_4 over the segment joining $(1-h^2/|t|)t$ to t, so that $\Phi_h^{(m)}(x,t;y) = I_1 + I_2 + I_3 + I_4$.

We begin by examining I_1, using the bounds in (3.61) and (3.62) inductively and collecting factors, to obtain

$$|I_1| = \left| \int_0^{h^2 t/|t|} \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*)\Phi_h^{(m)}(x_*, s; y)\, ds \right|$$

$$\leq Cd(\epsilon)^m h^{d-2+(m+1)\alpha} e^{\omega|t|} \times$$

$$\times \int_0^{h^2} |t-s|^{-d/2-1+\alpha/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(m)}(x_*, h, y)\, ds.$$

As $|t-s| \geq |t|/2$ on the segment defining I_1, we use the fact that $|t-s|^{-d/2-1+\alpha/2} \leq (|t|/2)^{-d/2-1+\alpha/2}$ to find

$$|I_1| \leq Cd(\epsilon)^m |t|^{-d/2-1+\alpha/2} h^{d-2+(m+1)\alpha} e^{\omega|t|} \times$$

$$\times \int_0^{h^2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(m)}(x_*, h, y)\, ds$$

$$\leq Cd(\epsilon)^{m+1} |t|^{-d/2-1+\alpha/2} h^{d-2+(m+1)\alpha} e^{\omega|t|} \int_0^{h^2} \Psi^{(m+1)}(x, \sqrt{|t|}, y) ds$$

$$\leq Cd(\epsilon)^{m+1} |t|^{-d/2-1+\alpha/2} h^{d+(m+1)\alpha} e^{\omega|t|} \Psi^{(m+1)}(x, \sqrt{|t|}, y),$$

where we have made use of Lemma 14 part (iii) to handle the sum. Keeping in mind that $h \leq \sqrt{|t|}$, we have

$$|I_1| \leq Cd(\epsilon)^{m+1} h^d |t|^{-d/2-1+(m+2)\alpha/2} \Psi^{(m+1)}(x, \sqrt{|t|}, y) e^{\omega|t|}.$$

Next, we turn our attention to I_2. We begin in a similar fashion to the estimate of I_1, applying the bounds in (3.62) inductively, enabling us to conclude that

$$|I_2| = \left| \int_{h^2 t/|t|}^{t/2} \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*)\Phi_h^{(m)}(x_*, s; y)\, ds \right|$$

$$\leq Cd(\epsilon)^m h^d e^{\omega|t|} \int_{h^2}^{|t|/2} |t-s|^{-d/2-1+\alpha/2} h^d s^{-d/2-1+(m+1)\alpha/2} \times$$

$$\times \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(m)}(x_*, \sqrt{|s|}, y)\, ds.$$

As $|t-s| \geq |t|/2$, we bound $|t-s|^{-d/2-1+\alpha/2} \leq |t/2|^{-d/2-1+\alpha/2}$ and absorb the resulting factors of 2, obtaining

$$|I_2| \leq Cd(\epsilon)^m h^d |t|^{-d/2-1+\alpha/2} e^{\omega|t|} \int_{h^2}^{|t|/2} s^{-1+(m+1)\alpha/2} \times$$
$$\times \left(h^d |s|^{-d/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*) \Psi^{(m)}(x_*, \sqrt{|s|}, y) \right) ds.$$

Applying Lemma 14 part (vi), we find that

$$|I_2| \leq Cd(\epsilon)^{m+1} h^d |t|^{-d/2-1+\alpha/2} e^{\omega|t|} \Psi^{(m+1)}(x, \sqrt{|t|}, y) \int_{h^2}^{|t|/2} |s|^{-1+(m+1)\alpha/2} \, ds.$$

The integral in s can be extended over the interval $[0, |t|/2]$ and evaluated explicitly, giving a multiple of $|t|^{(m+1)\alpha/2}$. After absorbing the resulting constant from the integration, we have

$$|I_2| \leq Cd(\epsilon)^m h^d |t|^{-d/2-1+(m+2)\alpha/2} \Psi^{(m+1)}(x, \sqrt{|t|}, y) e^{\omega|t|}.$$

The integrals I_3 and I_4 are handled similarly to I_2 and I_1, respectively, with the roles of s and $t-s$ interchanged. Summing the estimates of each integral produces the desired bound, establishing (3.62).

We will now prove (3.63) and (3.64) for $m = 1$ as the base case for an inductive argument. This term is the first for which the power of $|t|$ in our desired estimate is positive, and so some care must be taken to account for the signs of the exponents.

We begin by focusing on $\Phi_h^{(\hat{m}+1)}$ for $|t| \leq 2h^2$, multiplying out the estimates in (3.61) to discover that

$$|\Phi_h^{(\hat{m}+1)}(x, t; y)| = \left| \int_0^t \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*) \Phi_h^{(\hat{m})}(x_*, s; y) \, ds \right|$$
$$\leq Cd(\epsilon)^{\hat{m}} h^{-4+(\hat{m}+2)\alpha} e^{\omega|t|} \int_0^{|t|} \sum_{x_*} \Psi^{(0)}(x, h, x_*) \Psi^{(\hat{m})}(x_*, h, y) \, ds.$$

By Lemma 14 part (i), we have

$$|\Phi_h^{(\hat{m}+1)}(x,t;y)| \le Cd(\epsilon)^{\hat{m}+1} h^{-4+(\hat{m}+2)\alpha} e^{\omega|t|} \int_0^{|t|} \Psi^{(\hat{m}+1)}(x,h,y)\,ds.$$

Rewriting the integrand slightly and recognizing the integrand is independent of s gives us

$$|\Phi_h^{(\hat{m}+1)}(x,t;y)| \le Cd(\epsilon)^{\hat{m}+1} h^d h^{-d-4+(\hat{m}+2)\alpha} |t| \Psi^{(\hat{m}+1)}(x,h,y) e^{\omega|t|}.$$

From the definition of $\hat{m}$ in (3.60) we can verify that $-d-4+(\hat{m}+2)\alpha \le 0$, and as $|t| \le 2h^2$, we can bound $h^{-d-4+(\hat{m}+2)\alpha}$ by a multiple of $|t|^{-d/2-2+(\hat{m}+2)\alpha/2}$, to find

$$|\Phi_h^{(\hat{m}+1)}(x,t;y)| \le Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+2)\alpha/2} \Psi^{(\hat{m}+1)}(x,h,y) e^{\omega|t|}.$$

Multiplication by a suitable constant reveals this to be (3.63) for $m=1$ in disguise.

As in the proof of (3.61), we note that (3.64) for $m=1$ follows from (3.63) for $h^2 \le |t| \le 2h^2$, so we concentrate only on the case where $|t| \ge 2h^2$. To prove (3.64) for $m=1$, we again divide the path of integration into the same four segments as in the proof of (3.62); we take J_1 to be the integral over the segment from 0 to $h^2t/|t|$, J_2 over the segment joining $h^2t/|t|$ to $t/2$, J_3 over the segment joining $t/2$ to $(1-h^2/|t|)t$ and J_4 over the segment joining $(1-h^2/|t|)t$ to t, so that $\Phi_h^{(m)}(x,t;y) = J_1+J_2+J_3+J_4$.

We examine J_3 and J_4 in detail. The integrals J_2 and J_1 are handled similarly, with the roles of s and $t-s$ interchanged. For J_3, we have

$$\begin{aligned}
|J_3| &= \left| \int_{t/2}^{(1-h^2/|t|)t} \sum_{x_*} \Phi_h^{(0)}(x,t-s;x_*) \Phi_h^{(\hat{m})}(x_*,s;y)\,ds \right| \\
&\le Cd(\epsilon)^{\hat{m}} h^d e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-d/2-1+\alpha/2} h^d |s|^{-d/2-1+(\hat{m}+1)\alpha/2} \times \\
&\qquad \times \sum_{x_*} \Psi^{(0)}(x,\sqrt{|t-s|},x_*) \Psi^{(\hat{m})}(x_*,\sqrt{|s|},y)\,ds.
\end{aligned}$$

As $|s| \ge |t|/2$ and $-d/2-1+(\hat{m}+1)\alpha/2 < 0$, we can bound $|s|^{-d/2-1+(\hat{m}+1)\alpha/2}$ by a multiple of $|t|^{-d/2-1+(\hat{m}+1)\alpha/2}$ and absorb the resulting power of 2, obtaining

$$|J_3| \leq Cd(\epsilon)^{\hat{m}} h^d |t|^{-d/2-1+(\hat{m}+1)\alpha/2} e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/2} \times$$

$$\times \left(h^d |t-s|^{-d/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*) \Psi^{(\hat{m})}(x_*, \sqrt{|s|}, y) \right) ds.$$

A direct application of Lemma 14 part (v) yields

$$|J_3| \leq Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+1)\alpha/2} e^{\omega|t|} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) \times$$

$$\times \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/2} \, ds.$$

The integral in s can be extended over the interval $[|t|/2, |t|]$ and evaluated explicitly, yielding a multiple of $|t|^{\alpha/2}$. After absorbing the constant resulting from the integration, we have

$$|J_3| \leq Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+2)\alpha/2} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|}.$$

For J_4, we write

$$|J_4| = \left| \int_{(1-h^2/|t|)t}^{t} \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*) \Phi_h^{(\hat{m})}(x_*, s; y) \, ds \right|$$

$$\leq Cd(\epsilon)^{\hat{m}} e^{\omega|t|} \int_{|t|-h^2}^{|t|} h^{-2+\alpha} h^d |s|^{-d/2-1+(\hat{m}+1)\alpha/2} \times$$

$$\times \sum_{x_*} \Psi^{(0)}(x, h, x_*) \Psi^{(\hat{m})}(x_*, \sqrt{|s|}, y) \, ds.$$

As $|s| \geq |t|/2$ on the interval over which J_4 is defined and $-d/2-1+(\hat{m}+1)\alpha/2 \leq 0$, we bound $|s|^{-d/2-1+(\hat{m}+1)\alpha/2} \leq C|t|^{-d/2-1+(\hat{m}+1)\alpha/2}$, so that

$$|J_4| \leq Cd(\epsilon)^{\hat{m}} h^d |t|^{-d/2-1+(\hat{m}+1)\alpha/2} e^{\omega|t|} \times$$

$$\times \int_{|t|-h^2}^{|t|} h^{-2+\alpha} \sum_{x_*} \Psi^{(0)}(x, h, x_*) \Psi^{(\hat{m})}(x_*, \sqrt{|s|}, y) \, ds.$$

We use Lemma 14 part (ii) to bound the sum, so that

$$|J_4| \le Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+1)\alpha/2} e^{\omega|t|} \int_{|t|-h^2}^{|t|} h^{-2+\alpha} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y)\, ds.$$

The integrand is independent of s, which gives us

$$|J_4| \le Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+1)\alpha/2} e^{\omega|t|} h^{\alpha} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y).$$

Bounding $h^\alpha \le |t|^{\alpha/2}$, we conclude

$$|J_4| \le Cd(\epsilon)^{\hat{m}+1} h^d |t|^{-d/2-1+(\hat{m}+2)\alpha/2} e^{\omega|t|} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y).$$

Summing the estimates for J_3 and J_4 with similar estimates for J_1 and J_2 gives (3.64) for $\hat{m}+1$ (in disguise).

We now establish (3.63) by induction. For this portion of the proof, we keep careful track of constants. For $m \ge 1$, in the case $|t| \le 2h^2$ we have that

$$\begin{aligned}
&|\Phi_h^{(\hat{m}+m+1)}(x,t;y)| = \\
&\quad = \left| \int_0^t \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*) \Phi_h^{(\hat{m}+m)}(x_*, s; y)\, ds \right| \\
&\quad \le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m} \Gamma(\alpha/2)^m}{\Gamma(-d/2 + (\hat{m}+m+1)\alpha/2)} e^{\omega|t|} h^d \times \\
&\qquad \times \int_0^{|t|} h^{-2+\alpha} |s|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \sum_{x_*} \Psi^{(0)}(x, h, x_*) \Psi^{(\hat{m}+1)}(x_*, h, y)\, ds.
\end{aligned}$$

The sum is again handled by Lemma 14 part (i), so that

$$\begin{aligned}
|\Phi_h^{(\hat{m}+m+1)}(x,t;y)| &\le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1} \Gamma(\alpha/2)^m}{\Gamma(-d/2 + (\hat{m}+m+1)\alpha/2)} e^{\omega|t|} h^d \Psi^{(\hat{m}+1)}(x, h, y) \times \\
&\qquad \times \int_0^{|t|} h^{-2+\alpha} |s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\, ds.
\end{aligned}$$

As $|t| \le 2h^2$, we have that $h^{-2+\alpha} \le 2^{1-\alpha/2}|t-s|^{-1+\alpha/2} \le 2|t-s|^{-1+\alpha/2}$, so that

$$|\Phi_h^{(\hat{m}+m+1)}(x,t;y)| \le 2\frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} e^{\omega|t|} h^d \Psi^{(\hat{m}+1)}(x,h,y) \times$$
$$\times \int_0^{|t|} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\, ds.$$

Lemma 15 handles the integral explicitly, so that

$$|\Phi_h^{(\hat{m}+m+1)}(x,t;y)| \le 2\frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} e^{\omega|t|} h^d \Psi^{(\hat{m}+1)}(x,h,y) \times$$
$$\times \frac{\Gamma(\alpha/2)\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)}{\Gamma(-d/2+(\hat{m}+m+2)\alpha/2)} |t|^{-d/2-1+(\hat{m}+m+2)\alpha/2}.$$

Multiplying everything out gives us

$$|\Phi_h^{(\hat{m}+m+1)}(x,t;y)| \le 2\frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^{m+1}}{\Gamma(-d/2+(\hat{m}+m+2)\alpha/2)} \times$$
$$\times h^d |t|^{-d/2-1+(\hat{m}+m+2)\alpha/2} e^{\omega|t|} \Psi^{(\hat{m}+1)}(x,h,y).$$

The desired result now follows immediately.

For $h^2 \le |t| \le 2h^2$, (3.64) follows directly from (3.63).

Finally, we establish (3.64) with $|t| \ge 2h^2$ for general $m \ge 1$. We split the path of integration defining $\Phi_h^{(\hat{m}+m)}(x,t;y)$ into three integrals: L_1 over the segment from 0 to $h^2 t/|t|$, L_2 over the segment from $h^2 t/|t|$ to $(1-h^2/|t|)t$ and L_3 over the segment $(1-h^2/|t|)t$ to t.

We begin by examining L_1. Using (3.63) we have that

$$|L_1| = \left| \int_0^{h^2 t/|t|} \sum_{x_*} \Phi_h^{(0)}(x,t-s;x_*)\Phi_h^{(\hat{m}+m)}(x_*,s;y)\, ds \right|$$
$$\le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|} \int_0^{h^2} |t-s|^{-d/2-1+\alpha/2} \times$$
$$h^d |s|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \sum_{x_*} \Psi^{(0)}(x,\sqrt{|t-s|},x_*)\Psi^{(\hat{m}+1)}(x_*,h,y)\, ds.$$

We re-arrange the factors into a form amenable to Lemma 14 part (iv):

$$|L_1| \leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|} \int_0^{h^2} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \times$$
$$\times\, h^d |t-s|^{-d/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(\hat{m}+1)}(x_*, h, y)\, ds.$$

Applying the lemma we deduce

$$|L_1| \leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|} \times$$
$$\times\, \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) \int_0^{h^2} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\, ds.$$

We bound the integral by applying Lemma 15, and multiplying everything out gives us a suitable bound on L_1:

$$|L_1| \leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^{m+1}}{\Gamma(-d/2+(\hat{m}+m+2)\alpha/2)} h^d |t|^{-d/2-1+(\hat{m}+m+2)\alpha/2} e^{\omega|t|} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y).$$

We focus next on the integral L_2. We have

$$|L_2| = \left| \int_{h^2 t/|t|}^{(1-h^2/|t|)t} \sum_{x_*} \Phi_h^{(0)}(x, t-s; x_*)\Phi_h^{(\hat{m}+m)}(x_*, s; y)\, ds \right|$$
$$\leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|} \int_{h^2}^{|t|-h^2} |t-s|^{-d/2-1+\alpha/2} \times$$
$$\times\, h^d |s|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(\hat{m}+1)}(x_*, \sqrt{|s|}, y)\, ds.$$

With some re-arrangement, we have

$$|L_2| \leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|} \int_{h^2}^{|t|-h^2} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2} \times$$
$$\times\, h^d |t-s|^{-d/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*)\Psi^{(\hat{m}+1)}(x_*, \sqrt{|s|}, y)\, ds.$$

The sum is addressed by Lemma 14 part (v), so that we have

$$|L_2| \le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d e^{\omega|t|}\Psi^{(\hat{m}+1)}(x,\sqrt{|t|},y)\times$$

$$\times \int_{h^2}^{|t|-h^2} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\, ds.$$

We may bound the integral by Lemma 15, and multiplying out the resulting factors yields, after some cancellation,

$$|L_2| \le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1}\Gamma(\alpha/2)^{m+1}}{\Gamma(-d/2+(\hat{m}+m+2)\alpha/2)} h^d |t|^{-d/2-1+(\hat{m}+m+2)\alpha/2}\Psi^{(\hat{m}+1)}(x,\sqrt{|t|},y)e^{\omega|t|}.$$

We now bound L_3. We have

$$\begin{aligned}|L_3| &= \left|\int_{(1-h^2/|t|)t}^{t} \sum_{x_*} \Phi_h^{(0)}(x,t-s;x_*)\Phi_h^{(\hat{m}+m)}(x_*,s;y)\, ds\right| \\ &\le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} e^{\omega|t|}\int_{|t|-h^2}^{|t|} h^{-2+\alpha}h^d|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\times \\ &\quad \times \sum_{x_*} \Psi^{(0)}(x,h,x_*)\Psi^{(\hat{m}+1)}(x_*,\sqrt{|s|},y)\, ds.\end{aligned}$$

As $|t-s| \le h^2$, we have that $|t-s|^{-1+\alpha/2} \le h^{-2+\alpha}$, so

$$|L_3| \le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} e^{\omega|t|}\int_{|t|-h^2}^{|t|} h^{-2+\alpha}h^d|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\times$$

$$\times \sum_{x_*} \Psi^{(0)}(x,h,x_*)\Psi^{(\hat{m}+1)}(x_*,\sqrt{|s|},y)\, ds.$$

We bound the sum using Lemma 14 part (ii), finding that

$$|L_3| \le \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m}\Gamma(\alpha/2)^m}{\Gamma(-d/2+(\hat{m}+m+1)\alpha/2)} h^d \Psi^{(\hat{m}+1)}(x,\sqrt{|t|},y)e^{\omega|t|}\times$$

$$\times \int_{|t|-h^2}^{|t|} |t-s|^{-1+\alpha/2}|s|^{-d/2-1+(\hat{m}+m+1)\alpha/2}\, ds.$$

Using Lemma 15 to handle the integral and cancelling out the resulting factors yields the bound

$$|L_3| \leq \frac{4^m C_1^{m+2} d(\epsilon)^{\hat{m}+m+1} \Gamma(\alpha/2)^{m+1}}{\Gamma(-d/2+(\hat{m}+m+2)\alpha/2)} h^d |t|^{-d/2-1+(\hat{m}+m+2)\alpha/2} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|}.$$

Summing the bounds for L_1, L_2 and L_3 proves (3.64).

□

Adding the pointwise bounds on the terms $\Phi^{(m)}$ yields the existence of Φ_h satisfying similar estimates.

Theorem 17. *There exist constants C_1, C_2 and ω for which*

$$|\Phi_h(x,t;y)| \leq C_1 h^{-2+\alpha} \Psi^{(\hat{m}+1)}(x,h,y) e^{\omega|t|}, \qquad |t| \leq 2h^2 \qquad (3.65)$$

$$|\Phi_h(x,t;y)| \leq C_1 h^d\, |t|^{-d/2-1+\alpha/2} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|}, \qquad |t| \geq h^2, \qquad (3.66)$$

on the sector $t \in \mathbb{T}_M$ appearing in Theorem 5.

Proof. We give the proof for the case $|t| \geq h^2$. For the case $|t| \leq 2h^2$, the proof is similar.

We split the series for $\Phi_h(x,t;y)$ into two pieces:

$$\begin{aligned} \Phi_h(x,t;y) &= \sum_{m=0}^{\hat{m}} \Phi_h^{(m)}(x,t;y) + \sum_{m=\hat{m}+1}^{\infty} \Phi_h^{(m)}(x,t;y) \\ &= S_1 + S_2. \end{aligned}$$

The first sum contains the terms which we have estimated by negative powers of $|t|$, and the second sum contains those which are bounded by positive powers of $|t|$ and have rapidly decaying coefficients.

We first examine S_1. From the estimates in (3.62), as $\Psi^{(m)}$ is an increasing function of m, replacing $\Psi^{(m)}(x, \sqrt{|t|}, y)$ by $\Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y)$ yields the bound

$$\Phi_h^{(m)}(x,t;y) \leq h^d |t|^{-d/2-1+(m+1)\alpha/2} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|} y) e^{\omega|t|}.$$

Using this in the summation S_1 gives us

$$|S_1| \le h^d \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|} \sum_{m=0}^{\hat{m}+1} |t|^{-d/2-1+(m+1)\alpha/2}.$$

As $-d/2 - 1 + (m+1)\alpha/2 \le 0$ for $0 \le m \le \hat{m}$, we may bound the sum on the right by $C\left(|t|^{-d/2-1+(m+1)\alpha/2} + 1\right)$. (Each term in the sum is bounded by $|t|^{-d/2-1+\alpha/2}$ if $|t| \le 1$, and each term is bounded by 1 if $|t| \ge 1$.) We may then bound

$$\left(|t|^{-d/2-1+\alpha/2} + 1\right) \le C|t|^{-d/2-1+(m+1)\alpha/2} e^{C'|t|},$$

so that we conclude

$$|S_1| \le Ch^d |t|^{-d/2-1+\alpha/2} e^{\omega'|t|}.$$

We now turn our attention to S_2. From (3.64), we can derive the bounds

$$|\Phi_h^{(m)}(x, t; y)| \le h^d |t|^{-d/2-1+\alpha/2} \frac{(C|t|)^{m\alpha/2}}{\Gamma(-d/2 + (m+1)\alpha/2)} \Psi^{(\hat{m}+1)}(x, t; y) e^{\omega|t|}$$

for $m \ge \hat{m} + 1$ by rewriting the constants. Therefore,

$$|S_2| \le h^d |t|^{-d/2-1+\alpha/2} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|} \sum_{m=\hat{m}+1}^{\infty} \frac{(C|t|)^{m\alpha/2}}{\Gamma(-d/2 + (m+1)\alpha/2)}. \quad (3.67)$$

We first suppose $C|t| > 1$. We have that

$$|S_2| \le Ch^d |t|^{-1} \Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y) e^{\omega|t|} \sum_{m=\hat{m}+1}^{\infty} \frac{(C|t|)^{-d/2+(m+1)\alpha/2}}{\Gamma(-d/2 + (m+1)\alpha/2)}. \quad (3.68)$$

For each integer $n \ge 1$, the sum on the right possesses at most $\lfloor 2/\alpha \rfloor + 1$ terms for which $n \le (-d/2 + (m+1)\alpha/2) < n + 1$. The numerator of each of these terms is bounded above by $(C|t|)^{n+1}$, and the denominator is bounded below by $\Gamma(n)$. Therefore

$$\begin{aligned}\sum_{m=\hat{m}+1}^{\infty} \frac{(C|t|)^{-d/2+(m+1)\alpha/2}}{\Gamma(-d/2 + (m+1)\alpha/2)} &\le (\lfloor 2/\alpha \rfloor + 1) \sum_{n=1}^{\infty} \frac{(C|t|)^{n+1}}{\Gamma(n)} \\ &\le C' e^{C''|t|}.\end{aligned}$$

Using this in (3.68), for $C|t| > 1$ we have that

$$|S_2| \leq Ch^d|t|^{-1}\Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y)e^{\omega'|t|}$$
$$\leq Ch^d|t|^{-d/2-1+\alpha/2}\Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y)e^{\omega''|t|}.$$

If instead $C|t| \leq 1$, then the sum on the right in (3.67) is bounded independent of $|t|$ by a constant, so that we have $|S_2| \leq C'h^d|t|^{-d/2-1+\alpha/2}\Psi^{(\hat{m}+1)}(x, \sqrt{|t|}, y)e^{\omega|t|}$ for $C|t| \leq 1$.

The result follows from adding the bounds on S_1 and S_2.

□

We also require a notion of Hölder continuity in Φ_h.

Theorem 18. *For M as in Theorem 5, there exist constants C, C_2 and ω for which*

$$|\Phi_h(x_1, t; y) - \Phi_h(x_2, t; y)| \leq Ch^{-2+\alpha/2}|x_1 - x_2|^{\alpha/2}\times$$
$$\times \left(e^{-C_2|x_1-y|/h} + e^{-C_2|x_2-y|/h}\right)e^{\omega|t|}, \qquad |t| \leq 2h^2 \tag{3.69}$$

$$|\Phi_h(x_1, t; y) - \Phi_h(x_2, t; y)| \leq Ch^d|t|^{-d/2-1+\alpha/4}|x_1 - x_2|^{\alpha/2}\times$$
$$\times \left(e^{-C_2|x_1-y|/\sqrt{|t|}} + e^{-C_2|x_2-y|/\sqrt{|t|}}\right)e^{\omega|t|}, \quad |t| \geq h^2 \tag{3.70}$$

for $t \in \mathbb{T}_M$.

Proof. We restrict our attention to the case where $|x_1 - x_2| \leq \sqrt{|t|}$ and $|t| \geq 2h^2$. The result is an easy consequence of Theorem 17 for the case $|t| \leq 2h^2$ and the case $|x_1 - x_2| \geq \sqrt{|t|}$ for $|t| \geq h^2$.

Recalling (3.15), the integral equation that Φ_h satisfies, we have

$$\Phi_h(x_1,t;y)-\Phi_h(x_2,t;y)=$$

$$=L_hG_h(x_1-y,t;y)-L_hG_h(x_2-y,t;y)+$$

$$+\int_0^t\sum_{x_*}\left(L_hG_h(x_1-x_*,t-s;x_*)-L_hG_h(x_2-x_*,t-s;x_*)\right)\Phi(x_*,s;y)\,ds$$

$$=S_1+S_2$$

By Theorem 12 we have already seen that

$$|S_1|\leq C|x_1-x_2|^{\alpha/2}h^d|t|^{-d/2-1+\alpha/4}\left(e^{-C_2|x_1-y|/\sqrt{|t|}}+e^{-C_2|x_2-y|/\sqrt{|t|}}\right)e^{\omega|t|}.$$

To estimate S_2, we split the integral into four parts. As with previous estimates, we define I_1 to be the integral over the segment from 0 to $h^2t/|t|$, I_2 over the segment joining $h^2t/|t|$ to $t/2$, I_3 over the segment joining $t/2$ to $(1-h^2/|t|)t$ and I_4 over the segment joining $(1-h^2/|t|)t$ to t.

We show the estimate for I_1 explicitly. The general procedure for each of the other integrals is similar: we first use the bounds in Theorem 12 and Theorem 17, and then re-organize the resulting sum to estimate it in a way similar to the proof of Lemma 14. The remaining powers of $|s|$ and $|t-s|$ are integrable. We perform the integration, and any remaining powers of h may be bounded by powers of $|t|$.

We estimate:

$$|I_1|=$$

$$\left|\int_0^{h^2t/|t|}\sum_{x_*}\left(L_hG_h(x_1-x_*,t-s;y)-L_hG_h(x_2-x_*,t-s;x_*)\right)\Phi(x_*,s;y)\,ds\right|$$

$$\leq C|x_1-x_2|^{\alpha/2}h^dh^{-2+\alpha}\int_0^{h^2}|t-s|^{-d/2-1+\alpha/4}\times$$

$$\times\left[\sum_{x_*}\left(e^{-c|x_1-x_*|/\sqrt{|t-s|}}+e^{-c|x_2-x_*|/\sqrt{|t-s|}}\right)e^{-c|x_*-y|/h}\right]ds.$$

As $|t-s| \geq |t|/2$ we bound $|t-s|^{-d/2-1+\alpha/4} \leq C|t|^{-d/2-1+\alpha/4}$, giving us

$$|I_1| \leq C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} h^{-2+\alpha} \times$$
$$\times \int_0^{h^2} \left[\sum_{x_*} \left(e^{-c|x_1-x_*|/\sqrt{|t-s|}} + e^{-c|x_2-x_*|/\sqrt{|t-s|}} \right) e^{-c|x_*-y|/h} \right] ds.$$

The sum can be bounded in a way analogous to the proof of Lemma 14 part (iv), so that we have

$$\left[\sum_{x_*} \left(e^{-c|x_1-x_*|/\sqrt{|t-s|}} + e^{-c|x_2-x_*|/\sqrt{|t-s|}} \right) e^{-c|x_*-y|/h} \right] \leq$$
$$\leq C \left(e^{-C_3|x_1-y|/\sqrt{|t|}} + e^{-C_3|x_2-y|/\sqrt{|t|}} \right).$$

This yields

$$|I_1| \leq C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} h^{-2+\alpha} \times$$
$$\times \int_0^{h^2} \left(e^{-C_3|x_1-y|/\sqrt{|t-s|}} + e^{-C_3|x_2-y|/\sqrt{|t-s|}} \right) ds$$
$$\leq C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} h^{\alpha} \left(e^{-C_3|x_1-y|/\sqrt{|t|}} + e^{-C_3|x_2-y|/\sqrt{|t|}} \right)$$
$$\leq C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} \left(e^{-C_3|x_1-y|/\sqrt{|t|}} + e^{-C_3|x_2-y|/\sqrt{|t|}} \right).$$

Summing similar bounds from each of the remaining three integrals with the bound on I_1 gives the estimate for S_2:

$$|S_2| \leq C|x_1 - x_2|^{\alpha/2} h^d |t|^{-d/2-1+\alpha/4} \left(e^{-C_3|x_1-y|/\sqrt{|t|}} + e^{-C_3|x_2-y|/\sqrt{|t|}} \right).$$

Summing the bounds on S_1 and S_2 yields the result.

□

3.5 Bounding the Fundamental Solution

With our pointwise estimates for Φ_h, G_h and differences of G_h in hand, we can establish the needed pointwise bounds on $D_h^{\gamma}\Gamma_h$.

Theorem 19. *For M as in Theorem 5 and for each multi-index γ with $|\gamma| \le 2$ there exist constants C_1, C_2 and ω depending on M but not on h, x or y for which:*

$$|D_h^\gamma \Gamma_h(x,t;y)| \le C_1 h^{-|\gamma|} e^{-C_2|x-y|/h} e^{\omega|t|}, \qquad |t| \le 2h^2 \tag{3.71}$$

$$|D_h^\gamma \Gamma_h(x,t;y)| \le C_1 h^d |t|^{-d/2-|\gamma|/2} e^{-C_2|x-y|/\sqrt{|t|}} e^{\omega|t|}, \qquad |t| \ge h^2 \tag{3.72}$$

for $t \in \mathbb{T}_M$.

Proof. We give the proof for $|t| \ge 2h^2$ explicitly. The proof for $|t| \le 2h^2$ is similar.

For any multi-index γ with $|\gamma| \le 2$, we difference the constructed form of Γ_h in (3.14), noting that because the difference acts on the x variable, it falls only on G_h. We find that

$$D_h^\gamma \Gamma_h(x,t;y) =$$

$$= D_h^\gamma G_h(x-y,t;y) + \int_0^t \left[\sum_{x_*} \left(D_h^\gamma G_h(x-x_*, t-s; x_*) \right) \Phi_h(x_*, s; y) \right] ds.$$

The estimates in Theorem 8 take care of the first term, so we focus our attention on the integral. As in the estimates of similar integrals prior, we split the path of integration into four segments. We define I_1 to be the integral over the segment from 0 to $h^2 t/|t|$, I_2 over the segment joining $h^2 t/|t|$ to $t/2$, I_3 over the segment joining $t/2$ to $(1-h^2/|t|)t$ and I_4 over the segment joining $(1-h^2/|t|)t$ to t, so that $\Phi_h^{(m)}(x,t;y) = I_1 + I_2 + I_3 + I_4$. We begin by examining I_1, the integral taken over the segment joining the origin with $h^2 t/|t|$. Using the bounds in Theorem 8 and Theorem 17, we have

$$|I_1| \le C e^{\omega|t|} h^d h^{-2+\alpha} \int_0^{h^2} |t-s|^{-d/2-|\gamma|/2} \sum_{x_*} \Psi^{(0)}(x, \sqrt{|t-s|}, x_*) \Psi^{(\hat{m}+1)}(x_*, h, y)\, ds$$

$$\le C_\epsilon e^{\omega|t|} h^d |t|^{-d/2-|\gamma|/2} h^{-2+\alpha} \int_0^{h^2} \Psi^{(\hat{m}+2)}(x, \sqrt{|t|}, y)\, ds,$$

where we have again used Lemma 14 to handle the sum. As the integrand is independent of s and $h^\alpha \leq |t|^{\alpha/2}$, we discover

$$\begin{aligned}|I_1| &\leq C_\epsilon h^d |t|^{-d/2-|\gamma|/2} h^\alpha \Psi^{(\hat{m}+2)}(x, \sqrt{|t|}, y) e^{\omega|t|} \\ &\leq C_\epsilon h^d |t|^{-d/2-|\gamma|/2+\alpha/2} \Psi^{(\hat{m}+2)}(x, \sqrt{|t|}, y) e^{\omega|t|}.\end{aligned}$$

The integrals I_2 and I_4 are similar, as is the integral I_3 for $|\gamma| \leq 1$. In each of these cases, the general procedure is the same: we write out the estimates for $D_h^\gamma G_h$ and Φ_h, collecting powers of h, $(t-s)$ and s within the integral so that we may bound the summation in the same manner as in the proof of Lemma 14. We then perform the integration in s; any remaining powers of h are non-negative, and so are bounded by powers of $|t|$, and collecting all powers of $|t|$ yields the result. The only obstruction to this general procedure occurs when estimating I_3 for $|\gamma = 2|$, where attempting to apply the estimates for $D_h^\gamma G_h$ and Φ_h directly results in the appearance of an integral whose integrand contains a singularity like $(t-s)^{-1}$.

For I_3 when $|\gamma| = 2$, we write

$$|I_3| = \int_{t/2}^{(1-h^2/|t|)t} \left[\sum_{x_*} \left(D_h^\gamma G_h(x - x_*, t - s; x_*) \right) \Phi_h(x_*, s; y) \right] ds.$$

We rewrite and split the integral in a form that will allow us to apply the known continuity properties of Φ_h:

$$\begin{aligned}|I_3| &= \int_{t/2}^{(1-h^2/|t|)t} \left[\sum_{x_*} D_h^\gamma G_h(x - x_*, t - s; x_*) \left(\Phi_h(x_*, s; y) - \Phi_h(x, s; y) \right) \right] ds \\ &\quad + \int_{t/2}^{(1-h^2/|t|)t} \left[\sum_{x_*} D_h^\gamma G_h(x - x_*, t - s; x_*) \right] \Phi_h(x, s; y) \, ds \\ &= J_1 + J_2.\end{aligned}$$

We first examine J_1. By Theorem 8 and Theorem 18 we have

$$|J_1| \le Ch^d e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1}|s|^{-d/2-1+\alpha/4} h^d |t-s|^{-d/2} \times$$
$$\times \sum_{x_*} |x-x_*|^{\alpha/2} e^{-C_2|x-x_*|/\sqrt{|t-s|}} \left(e^{-C_2|x-y|/\sqrt{|s|}} + e^{-C_2|x_*-y|/\sqrt{|s|}} \right) ds.$$

We use the fact that $|s| \ge |t|/2$ and trade Hölder continuity for regularity in $(t-s)$ by exploiting the scaling in the exponential to find

$$|J_1| \le Ch^d |t|^{-d/2-1+\alpha/4} e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/4} h^d |t-s|^{-d/2} \times$$
$$\times \sum_{x_*} e^{-C_3|x-x_*|/\sqrt{|t-s|}} \left(e^{-C_2|x-y|/\sqrt{|s|}} + e^{-C_2|x_*-y|/\sqrt{|s|}} \right) ds.$$

The sum can be bounded in a way similar to the sums in Lemma 14. We obtain

$$|J_1| \le Ch^d |t|^{-d/2-1+\alpha/4} e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/4} e^{-C_4|x-y|/\sqrt{|t|}} \, ds.$$

This leads to the estimate

$$|J_1| \le Ch^d |t|^{-d/2-1+\alpha/2} e^{-C_4|x-y|/\sqrt{|t|}} e^{\omega|t|}.$$

To address J_2, we use Theorem 13 and Theorem 17, finding

$$|J_2| \le Ce^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/2} h^d |s|^{-d/2-1+\alpha/2} e^{-c|x-y|/\sqrt{|s|}} \, ds.$$

We use the bounds $|t|/2 \le |s| \le |t|$ to find

$$|J_2| \le Ch^d |t|^{-d/2-1+\alpha/2} e^{-c|x-y|/\sqrt{|t|}} e^{\omega|t|} \int_{|t|/2}^{|t|-h^2} |t-s|^{-1+\alpha/2} \, ds$$
$$\le Ch^d |t|^{-d/2-1+\alpha} e^{-c|x-y|/\sqrt{|t|}} e^{\omega|t|}.$$

The desired result now follows from the bounds on J_1 and J_2. □

The estimates on Γ_h in Theorem 19 enable us to prove Theorem 4.

Proof of Theorem 4. The bounds in Theorem 4 follow almost immediately from using Theorem 19 in (3.9). We suppose $|t| \geq h^2$; the case $|t| \leq h^2$ is similar. We estimate:

$$\begin{aligned} \left|\left|D_h^\gamma e^{A_h t} u_0\right|\right|_\infty &= \left|\left|\sum_{x_*} D_h^\gamma \Gamma_h(x,t;x_*) u_0(x_*)\right|\right|_\infty \\ &\leq \left(\sup_x \sum_{x_*} \left|D_h^\gamma \Gamma_h(x,t;x_*)\right|\right) ||u_0||_\infty \\ &\leq C|t|^{-|\gamma|/2} e^{\omega|t|} \left(\sup_x \sum_{x_*} e^{-C|x-x_*|/\sqrt{|t|}} h^d |t|^{-d/2}\right) ||u_0||_\infty . \end{aligned} \tag{3.73}$$

In the last step the sum

$$\sum_{x_*} e^{-C|x-x_*|/\sqrt{|t|}} h^d |t|^{-d/2}$$

is actually independent of x, as it is taken over all grid points. We may thus set $x = 0$, so that the sum becomes

$$\sum_{x_*} e^{-C|x_*|/\sqrt{|t|}} h^d |t|^{-d/2}.$$

We define $\eta = h/\sqrt{|t|}$. As $|t| \geq h^2$, we have that $0 < \eta \leq 1$. With this substitution, the sum becomes

$$\sum_{j \in \mathbb{Z}^d} e^{-C|j\eta|} \eta^d.$$

This is the discretization of an integral with exponentially decaying integrand, and is bounded independent of $0 < \eta \leq 1$. Noting that the sum is bounded in (3.73) allows us to conclude that

$$\left|\left|D_h^\gamma e^{A_h t} u_0\right|\right|_\infty \leq C|t|^{-|\gamma|/2} e^{\omega|t|} ||u_0||_\infty$$

and Theorem 4 follows, with μ in the statement of the theorem equal to ω. □

4

Resolvent Estimates and Fully Discrete Parabolic Regularity

4.1 Resolvent Estimates for A_h

The bounds on the evolution operator $e^{A_h t}$ and its spatial differences in Theorem 4 enable us to obtain resolvent estimates for A_h and its spatial differences by means of the Laplace transform representation the resolvent.

Theorem 20. *Let $\delta = 2/M$ for M in Theorem 4. There exist constants C_0, C_1, C_2 and ω, depending on δ but not on h, for which*

$$\left|\left|((A_h - \omega) - z)^{-1}\right|\right|_\infty \leq C|z|^{-1} \tag{4.1}$$

$$\left|\left|D_h^\gamma \left((A_h - \omega) - z\right)^{-1}\right|\right|_\infty \leq C|z|^{-1/2}, \qquad |\gamma| = 1 \tag{4.2}$$

$$\left|\left|D_h^\gamma \left((A_h - \omega) - z\right)^{-1}\right|\right|_\infty \leq C(1 + |\log|z|| + |\log h|), \qquad |\gamma| = 2 \tag{4.3}$$

for all z on the sector

$$S_\delta = \mathbb{C} - \left(\{z = z_1 + iz_2 : z_1 < 0, |z_2| < \delta|z_1|\} \cup \{0\}\right). \tag{4.4}$$

Proof. Let $\omega > (1 + M^2)^{1/2}\mu$ for μ in Theorem 4, and consider the operator $A_h - \omega I$.

We have

$$\left|\left|D_h^\gamma e^{(A_h-\omega)t}\right|\right| = \left|\left|D_h^\gamma e^{A_h t} e^{-\omega t}\right|\right|$$
$$= \left|\left|e^{-\omega t} D_h^\gamma e^{A_h t}\right|\right|$$

as A_h and ωI commute and $e^{-\omega t}$ is a multiplication operator. Then, using $\left|\left|D_h^\gamma e^{A_h t}\right|\right|_\infty \leq C_1 |t|^{-|\gamma|/2} e^{\mu |t|}$ on $\mathbb{T}_M$ with constants independent of h (but depending on M) and the fact that $|e^{-\omega t}| \leq e^{-\omega(1+M^2)^{-1/2}|t|}$ on $\mathbb{T}_M$, we find

$$\left|\left|D_h^\gamma e^{(A_h-\omega I)t}\right|\right| \leq C_1 |t|^{-|\gamma|/2} e^{\mu|t|} e^{-\omega(1+M^2)^{-1/2}|t|}$$
$$\leq C_1 |t|^{-|\gamma|/2}. \tag{4.5}$$

For $z \in \mathbb{C}$ with $\operatorname{Re} z > 0$, we can write

$$D_h^\gamma (z - (A_h - \omega))^{-1} = \int_0^\infty e^{-zt} D_h^\gamma e^{(A_h-\omega)t}\, dt. \tag{4.6}$$

On the sector $S_1 = \{z \in \mathbb{C} : z_1 > 0, |z_2| \leq \delta z_1\}$, we bound $|e^{-zt}| = e^{-z_1 t} \leq e^{-c|z|t}$ for $t > 0$ and constant depending on δ. Combining this fact with (4.5) for $|\gamma| = 0$ yields (4.1) for $z \in S_1$. Using (4.5) with $|\gamma| = 1$ instead gives

$$\left|\left|D_h^\gamma (z - (A_h - \omega))^{-1}\right|\right| \leq C \int_0^\infty \frac{e^{-c|z|t}}{\sqrt{t}}\, dt \leq C|z|^{-1/2}, \tag{4.7}$$

establishing (4.2) for $z \in S_1$.

To verify (4.3) for $z \in S_1$, we split the interval of integration. On the interval $[0, h^2]$, we bound the second difference by Ch^{-2}, and apply (4.5) directly on $[h^2, \infty]$. This gives us

$$\left|\left|D_h^\gamma (z - (A_h - \omega))^{-1}\right|\right| = \left|\left|\int_0^{h^2} e^{-zt} D_h^\gamma e^{(A_h-\omega)t}\, dt + \int_{h^2}^\infty e^{-zt} D_h^\gamma e^{(A_h-\omega)t}\, dt\right|\right|$$
$$\leq Ch^2 h^{-2} + C \int_{h^2}^\infty \frac{e^{-c|z|t}}{t}\, dt$$
$$\leq C(1 + |\log |z| h^2|). \tag{4.8}$$

We now extend the estimates from S_1 to the sectors $S_2 = \{z : z_2 > 0, |z_1| \leq z_2/\delta\}$ and the sector $S_3 = \{z : z_2 < 0, |z_1| \leq |z_2|/\delta\}$ conjugate to S_2. We write $z = z_1 + iz_2$ and $t = t_1 + it_2$, so that $\operatorname{Re} tz = t_1z_1 - t_2z_2$. If $z_1 > 0$, $z_2 \geq 0$, $t_1 \geq 0$ and $t_2 \leq 0$, then $\operatorname{Re} tz \geq t_1z_1$ and $|e^{-zt}| = e^{-z_1t_1}$. This permits us to deform the path of integration in (4.6) to the ray $R = \{t = t_1 - iMt_1, t_1 \geq 0\}$. For $z \in S_2$ and $t \in R$ we have $\operatorname{Re} tz = t_1(z_1 + Mz_2) \geq t_1(-1/\delta z_2 + 2/\delta z_2) \geq z_2t_1/\delta \geq C|z||t|$ for some constant C depending on M. We therefore have that $|e^{-zt}| \leq e^{-c|z||t|}$, and we can estimate in a fashion similar to (4.7) and (4.8). The sector S_3 is handled similarly, and as $S_\delta = S_1 \cup S_2 \cup S_3$, the theorem is established.

□

4.2 Fully Discrete Regularity

We restate and prove Theorem 1, beginning with the assumptions on the time-stepping method s_n.

We assume that s_n is A-stable and L-stable, i.e. that s_n is analytic and

$$|s_n(z)| \leq 1, \qquad s_n(\infty) = 0 \tag{4.9}$$

on the left half-plane. We require that there exist a disk B_0 about the origin on which

$$|s_n(z)| \leq C_0(1 + c_0|z|)^n. \tag{4.10}$$

Furthermore, for each $\delta' > 0$, we must have an estimate of the form

$$|s_n(z)| \leq C_1(1 + c_1|z|)^{-\rho n}, \tag{4.11}$$

for all $z \in \Sigma_{\delta'}$, where

$$\Sigma_{\delta'} = \{z = z_1 + iz_2 : z_1 \leq 0, z_2 \leq \delta'|z_1|\} \tag{4.12}$$

and p, C_1 and c_1 are positive constants depending on δ'.

Theorem 21. *Under the assumptions (4.9)-(4.11) on s_n, there exists a constant k_0 and constants C_0, C_1, C_2 and C_3 independent of $0 < h \le 1$, $0 < k \le k_0$ for which*

$$||s_n(kA_h)||_\infty \le C_0 e^{C_3 nk} \tag{4.13}$$

$$||D_h^\gamma s_n(kA_h)||_\infty \le C_1 (nk)^{-1/2} e^{C_3 nk}, \qquad |\gamma| = 1 \tag{4.14}$$

$$||D_h^\gamma s_n(kA_h)||_\infty \le C_2 (nk)^{-1}(1 + |\log h| + |\log nk|) e^{C_3 nk}, \qquad |\gamma| = 2. \tag{4.15}$$

Proof. For δ in Theorem 20, we rewrite the resolvent estimates in Theorem 20 for kA_h on $S_\delta + \omega k$, the horizontal translation of S_δ by ωk:

$$S_\delta + \omega k = \{z : z = z' + \omega k,\ z' \in S_\delta\}. \tag{4.16}$$

For z outside $\Sigma_\delta + \omega k$ we have

$$\left|\left|(z - kA_h)^{-1}\right|\right|_\infty \le C|z - \omega k|^{-1} \tag{4.17}$$

$$\left|\left|D_h^\gamma (z - kA_h)^{-1}\right|\right|_\infty \le Ck^{-1/2}|z - \omega k|^{-1/2}, \qquad |\gamma| = 1 \tag{4.18}$$

$$\left|\left|D_h^\gamma (z - kA_h)^{-1}\right|\right|_\infty \le Ck^{-1}(1 + |\log(|z - \omega k|/k)| + |\log h|), \qquad |\gamma| = 2. \tag{4.19}$$

For any positively oriented piecewise smooth simple closed curve Γ (depending on h) in $\mathbb{C}$ enclosing the spectrum of kA_h we can write

$$s_n(kA_h) = \frac{1}{2\pi i}\int_\Gamma s_n(z)(z - kA_h)^{-1} dz.$$

We first restrict our attention to the case $n > n_0$ for some fixed $n_0 > 2/p$. For $\delta' > \delta$, using (4.11) and (4.17), we can deform the contour of integration to the contour $\Gamma_{n,k}$ that includes the arc

$$R_0 = \left\{z = (\epsilon/n)e^{i\theta} + \omega k,\ |\theta| \le \theta_0\right\} \tag{4.20}$$

and the rays

$$R_\pm = \left\{z = re^{\pm i\theta_0} + \omega k,\ r \ge \epsilon/n\right\}, \tag{4.21}$$

where θ_0 is the angle between $z_2 = -\delta' z_1$ and the real axis. We must take ϵ and k_0 sufficiently small so that R_0 lies within the disk B_0 guaranteed by (4.10) for $0 < k \leq k_0$ and $R_\pm$ each lie in $B_0 \cup \Sigma_{\delta'}$.

A short segment of each ray may extend past the region $\Sigma_{\delta'}$ where (4.11) is valid (depending on the relative size of ϵ/n and ωk), so we further divide each of the rays $R_\pm$ into two parts. We label the segment $(R_\pm \cap S_{\delta'}) \subset B_0$ by $R_{1,\pm}$ and label the portion $(R_\pm \cap \Sigma_{\delta'})$ by $R_{2,\pm}$. Elementary algebra can be used to show that the segment $R_{1,\pm}$ has length bounded above by Ck for some constant C.

We first work to establish (4.13). On R_0, we bound $|s_n(z)| \leq C(1+c\epsilon/n+c\omega k)^n \leq Ce^{Cnk}$ using (4.10). By (4.17), we bound

$$\left|\left|(z - kA_h)^{-1}\right|\right| \leq |((\epsilon/n)e^{i\theta} + \omega k) - \omega k|^{-1} \leq n/\epsilon. \tag{4.22}$$

The arc has length less than $2\pi\epsilon/n$. This gives us the bound

$$\left|\left|\int_{R_0} s_n(z)(z - kA_h)^{-1} dz\right|\right| \leq Ce^{Cnk}(n/\epsilon)(2\pi\epsilon/n) \leq Ce^{Cnk}.$$

We next consider the portion of the integral over $R_{1,\pm}$. This segment has length of order k, so that $|z| \leq C(k+\epsilon/n)$ for $z \in R_{1,\pm}$. As $R_{1,\pm}$ is contained within the disk B_0 on which (4.10) is applicable, we have that $|s_n(z)| \leq Ce^{Cnk}$ on $R_{1,\pm}$. Furthermore, on $R_{1,\pm}$ we have $|z - \omega k| \geq \epsilon/n$, so that $||(z - kA_h)^{-1}|| \leq n/\epsilon$. Therefore

$$\left|\left|\int_{R_{1,\pm}} s_n(z)(z - kA_h)^{-1} dz\right|\right| \leq Ce^{Cnk}(n/\epsilon)k \leq Ce^{Cnk}.$$

Finally, we bound the contribution from the ray $R_{2,\pm}$. By (4.11), for $z \in R_{2,\pm}$, we have

$$\begin{aligned} |s_n(z)| &= |s_n(re^{i\theta_0} + \omega k)| \\ &\leq C(1 + C|re^{i\theta_0} + \omega k|)^{-\rho n}. \end{aligned}$$

As $|re^{i\theta} + \omega k| \geq Cr$ we have that

$$|s_n(z)| \leq C(1 + Cr)^{-\rho n}$$

on the ray $R_{2,\pm}$.

Therefore, as $r \geq \epsilon/n$ on $R_{2,\pm}$, we have

$$\left|\left|\int_{R_{2,\pm}} s_n(z)(z - kA_h)^{-1} dz\right|\right| \leq \int_{\epsilon/n}^{\infty} C(1 + Cr)^{-\rho n} r^{-1}\, dr$$

$$\leq C(n/\epsilon) \int_0^{\infty} (1 + Cr)^{-\rho n}\, dr \leq C(n/\epsilon)(\rho n - 1)^{-1} \leq C.$$

The argument for $|\gamma| = 1$ is a straightforward modification of the above, using (4.18) in place of (4.17). On R_0 and $R_{1,\pm}$, this results in the factor n/ϵ being replaced by $(n/(\epsilon k))^{1/2}$, changing the bound by a factor of $(nk)^{-1/2}$. On $R_{2,\pm}$, the factor r^{-1} is replaced by $r^{-1/2}$, producing a similar change in the bound.

We proceed to verifying (4.15). On R_0, we bound $|s_n(z)| \leq Ce^{Cnk}$, and, for $|\gamma| = 2$,

$$\begin{aligned} \left|\left|D_h^{\gamma}(z - kA_h)^{-1}\right|\right| &\leq Ck^{-1}(1 + |\log|(z - \omega k)/k|| + |\log h|) \\ &\leq Ck^{-1}(1 + |\log(\epsilon/(nk))| + |\log h|) \\ &\leq Ck^{-1}(1 + |\log nk| + |\log h|). \end{aligned}$$

The arc has length less than $2\pi\epsilon/n$, so

$$\begin{aligned} \left|\left|\int_{R_0} s_n(z) D_h^{\gamma}(z - kA_h)^{-1} dz\right|\right| &\leq Ce^{Cnk}k^{-1}(1 + |\log nk| + |\log h|)(2\pi\epsilon/n) \\ &\leq C(nk)^{-1}(1 + |\log nk| + |\log h|)e^{Cnk}. \end{aligned}$$

We move on to the portion of the integral over the segment $R_{1,\pm}$. We bound the length of the segment by a multiple of k, use the estimate that $|s_n(z)| \leq Ce^{Cnk}$ on the segment and apply the resolvent estimate (4.19) to find

$$\left\| \int_{R_{1,\pm}} s_n(z) D_h^\gamma (z - kA_h)^{-1} dz \right\| \leq$$

$$\leq (Ck)(Ce^{Cnk}) \left(Ck^{-1}(1 + |\log(|z - \omega k|/k)| + |\log h|) \right)$$

$$\leq C(1 + |\log \epsilon/(nk)| + |\log(\epsilon/(nk) + C) + |\log h|)e^{Cnk}$$

$$\leq C(1 + |\log nk| + |\log h|)e^{Cnk}.$$

In the second step in the above calculation, we have used the fact that $\epsilon/(nk) \leq |z - \omega k|/k \leq \epsilon/(nk) + C$.

We examine the contribution from $R_{2,\pm}$. Applying (4.11) and (4.19), we have

$$\left\| \int_{R_{2,\pm}} s_n(z) D_h^\gamma (z - A_h)^{-1}\, dz \right\| \leq \int_{\epsilon/n}^{\infty} C(1 + Cr)^{-\rho n} k^{-1} (1 + |\log(r/k)| + |\log h|)\, dr.$$

We rewrite $r/k = (rn)/(nk)$ and expand.

$$\left\| \int_{R_{2,\pm}} s_n(z) D_h^\gamma (z - A_h)^{-1}\, dz \right\| \leq$$

$$\leq Ck^{-1} \int_{\epsilon/n}^{\infty} (1 + Cr)^{-\rho n} \left(1 + |\log nk| + |\log h| + |\log nr|\right)\, dr.$$

The integral can be split, estimating the terms with $(1 + |\log h| + |\log nk|)$ and those with $\log nr$ separately. As

$$\left| \int_{\epsilon/n}^{\infty} (1 + Cr)^{-\rho n}\, dr \right| \leq C/n,$$

we have

$$Ck^{-1} \int_{\epsilon/n}^{\infty} (1 + Cr)^{-\rho n} \left(1 + |\log nk| + |\log h|\right)\, dr \leq C(nk)^{-1} \left(1 + |\log nk| + |\log h|\right).$$

The term containing $|\log nr|$ requires more subtlety. As we have restricted our attention to the case $\rho n > 2$, we have $(1 + Cr)^{\rho n/2} \geq 1 + C\rho nr/2$. Using elementary calculus, we find that for $r \geq \epsilon/n$, the ratio $|\log nr|/(1 + C\rho nr/2)$ is bounded by a constant depending on ϵ, so that

$$k^{-1} \int_{\epsilon/n}^{\infty} (1 + Cr)^{-\rho n} |\log nr| \, dr \leq Ck^{-1} \int_{\epsilon/n}^{\infty} (1 + Cr)^{-\rho n/2} \, dr \leq C(nk)^{-1}. \quad (4.23)$$

Summing the bounds on each of the integrals yields (4.15).

We now return to consider the case $1 \leq n \leq n_0$. For such n, the decay in (4.11) is insufficient for convergence of the integrals in the preceding argument. To compensate for this, we modify the function $s_n(z)$ and estimate the modified function. As $s_n(\infty) = 0$, we can express $s_n(z) = c_n z^{-1} + O(|z|^{-2})$. We define $\tilde{s}_n(z) = s_n(z) + c_n(1 - z)^{-1}$ so that $\tilde{s}_n(z) = O(|z|^{-2})$ as $z \to \infty$ on $\Sigma_{\delta'}$. Therefore, we can bound

$$|\tilde{s}_n(z)| \leq C(1 + c|z|)^{-2}, \qquad z \in \Sigma_{\delta'} \quad (4.24)$$

for some constants C and c independent of $1 \leq n \leq n_0$. We can then bound $\tilde{s}_n(kA_h)$ using the Cauchy integral representation as before, so that (4.13)-(4.15) hold for $\tilde{s}_n(kA_h)$ replacing $s_n(kA_h)$. We also recognize that $(1 - kA_h)^{-1}$ satisfies the bounds (4.13)-(4.15) by using $z = 1$ in (4.17)-(4.19) and the fact that $k^{-1} \leq n_0(nk)^{-1} \leq C(nk)^{-1}$. Theorem 21 follows from these bounds and the expression $s_n(kA_h) = \tilde{s}_n(kA_h) - c_n(1 - kA_h)^{-1}$.

□

5

Divergence Form Elliptic Operators on Spatially Periodic Grid Functions

We now restrict our attention to divergence form operators on the space of spatially periodic grid functions of mean value zero. This class of discrete operators is invertible. In Theorem 27, the final theorem of this section, we prove sharp maximum norm estimates for the inverse and its first spatial differences, uniform in the grid spacing, and almost sharp maximum norm estimates for second spatial differences.

For convenience we assume that the interval of interest is $[-\pi, \pi]^d$, that the grid spacing is $h = 2\pi/N$ and that our grid functions are 2π-periodic.

We discretize $[-\pi, \pi]^d$ by I_h^d where $I_h = \{x \in \mathbb{R}_h^1 : -\pi < x \leq \pi\}$. On I_h^d, we can define the space X_h of periodic grid functions of mean value zero by

$$X_h = \left\{ u(x) : \sum_{x_0 \in I_h^d} u(x_0) = 0 \right\} \tag{5.1}$$

and regard X_h as a subset of R_h^d by extending each $u \in X_h$ periodically.

For each non-negative integer m, we define the Sobolev space $H^m(I_h^d)$ with the norm

$$||u||^2_{H^m(I_h^d)} = \sum_{0\le|\gamma|\le k} ||D_h^\gamma u||^2_{L^2(I_h^d)} \,. \tag{5.2}$$

The $L^2(I_h^d)$ norm is induced by the inner product

$$\langle u, v\rangle = \sum_{x_0\in I_h^d} u(x_0)\overline{v(x_0)}h^d, \tag{5.3}$$

so that $L^2(I_h^d)$ can be regarded as a complex Hilbert space.

For simplicity, we introduce the problem

$$\begin{aligned} u_t &= A_h u \\ A_h u &= \sum_{jl} D_j^+\left(a_{jl}(x)D_l^- u\right) \\ u(x,0) &= u_0(x) \in X_h \end{aligned} \tag{5.4}$$

where the $a_{jl} = a_{lj}$ are required to be 2π-periodic $C^{\lfloor d/2\rfloor+3}(\mathbb{R}^d)$ functions for which we have the ellipticity condition

$$\sum_{jl} a_{jl}(x)\xi_i\xi_j \ge c|\xi|^2, \tag{5.5}$$

with c independent of x for all vectors $\xi \in \mathbb{R}^d$. The choice of A_h in (5.4) is only first-order accurate. However, all of the results in this chapter also hold with the commonly used second-order accurate operator

$$\widetilde{A_h} = \sum_{jl}\left[\frac{1}{2}D_j^+\left(a_{jl}(x)D_l^- u\right) + \frac{1}{2}D_j^-\left(a_{jl}D_l^+ u\right)\right] \tag{5.6}$$

replacing A_h. The proofs require only minor modification.

We find that the principal symbol of the difference scheme is real and satisfies an appropriate uniform ellipticity condition.

Theorem 22. *The principal symbol $p(y,\xi)$ of A_h satisfies the uniform ellipticity condition*

$$h^2 p(y,\xi) \leq -c|\xi|^2, \qquad \xi \in [-\pi,\pi]^d, \tag{5.7}$$

for some constant c independent of h and y.

The principal part of A_h is

$$\sum_{jl} a_{jl}(y) D_j^+ D_l^-,$$

with principal symbol

$$p(y,\xi) = h^{-2} \sum_{jl} a_{jl}(y) \left(e^{i\xi_j} - 1\right)\left(1 - e^{i\xi_l}\right).$$

We can factor to obtain

$$h^2 p(y,\xi) = \sum_{jl} a_{jl}(y) e^{i\xi_j/2} e^{-i\xi_l/2} \left(e^{i\xi_j/2} - e^{-i\xi_j/2}\right)\left(e^{i\xi_l/2} - e^{-i\xi_l/2}\right).$$

Using the symmetry of the a_{jl}, we have

$$h^2 p(y,\xi) = \sum_{jl} a_{jl}(y) \frac{1}{2}\left(e^{i\xi_j/2} e^{-i\xi_l/2} + e^{-i\xi_j/2} e^{i\xi_l/2}\right)\left(e^{i\xi_j/2} - e^{-i\xi_j/2}\right)\left(e^{i\xi_l/2} - e^{-i\xi_l/2}\right).$$

With the definitions of sine and cosine, we can rewrite this as

$$h^2 p(y,\xi) = -4 \sum_{jl} a_{jl}(y) \cos\left(\frac{\xi_j}{2} - \frac{\xi_l}{2}\right) \sin\frac{\xi_j}{2} \sin\frac{\xi_l}{2}.$$

The identity for the cosine of a difference allows this to be rewritten as

$$\begin{aligned} h^2 p(y,\xi) &= -4\left[\sum_{jl} a_{jl}(y) \cos\frac{\xi_j}{2} \sin\frac{\xi_j}{2} \cos\frac{\xi_l}{2} \sin\frac{\xi_l}{2}\right] - 4\left[\sum_{jl} a_{jl}(y) \sin^2\frac{\xi_j}{2} \sin^2\frac{\xi_l}{2}\right] \\ &= -\left[\sum_{jl} a_{jl}(y) \sin\xi_j \sin\xi_l\right] - 4\left[\sum_{jl} a_{jl}(y) \sin^2\frac{\xi_j}{2} \sin^2\frac{\xi_l}{2}\right]. \end{aligned}$$

By the uniform positivity of the matrix of $a_{jl}(y)$, we have

$$h^2 p(y,\xi) \leq -c|\sin\xi|^2 - 4c|\sin^2\frac{\xi}{2}|^2$$

for some c independent of y. The function on the right of the preceding inequality is non-positive and non-zero for $\xi \in [-\pi,\pi]^d$, $\xi \neq 0$. Furthermore, on the neighborhood $[-\pi/2,\pi/2]^d$ of the origin, $c|\xi|^2 \leq |\sin\xi|^2 \leq C|\xi|^2$, so that we may conclude

$$h^2 p(y,\xi) \leq -c'|\xi|^2$$

for some constant c' independent of y.

For any grid function $v \in X_h$, it is readily verified that $A_h v \in X_h$ using summation by parts. (The first difference of any periodic grid function is in X_h, and $A_h v$ is the sum of first differences of periodic grid functions.)

This ensures that the solution $u(x,t)$ to (5.4) satisfies $u(x,\cdot) \in X_h$, as

$$\frac{d}{dt}\left(\sum_{x_0} u(x_0,t)\right) = \sum_{x_0} u_t(x_0,t) = \sum_{x_0} A_h u(x_0,t) = 0.$$

For u the solution to (5.4), we calculate for $t > 0$:

$$\begin{aligned}\langle A_h u, u\rangle &= h^d \sum_{x_0}\sum_{jl} D_j^+\left(a_{jl}(x_0) D_l^- u(x_0)\right) u(x_0)\\ &= -h^d \sum_{x_0}\sum_{jl} a_{jl}(x_0)(D_l^- u(x_0))(D_j^- u(x_0)),\end{aligned}$$

after summing by parts. By the uniform ellipticity condition on the matrix $a_{jl}(x)$, we find

$$\langle A_h u, u\rangle \leq -Ch^d \sum_{x_0}\sum_{j}(D_j^- u(x_0))^2$$

for some constant C independent of h. We recognize the right hand side is a sum of norms, so that

$$\langle A_h u, u\rangle \leq -C\sum_j \left|\left|D_j^- u\right|\right|_{L^2}^2.$$

By the translation invariance of the L^2 norm, we have

$$\langle A_h u, u\rangle \leq -C' \sum_j \left|\left|D_j^+ u\right|\right|_2^2. \tag{5.8}$$

The discrete Poincaré inequality then gives us that

$$\langle A_h u, u\rangle \leq -C \left|\left|u\right|\right|_2^2. \tag{5.9}$$

However,

$$\langle A_h u, u\rangle = \langle u_t, u\rangle = \frac{1}{2}\frac{d}{dt}\langle u, u\rangle = \frac{1}{2}\frac{d}{dt}\left|\left|u\right|\right|_{L^2}^2.$$

Using this in (5.9), we find that there exists a positive constant c, independent of h, for which

$$\left|\left|u\right|\right|_{L^2}^2 \leq e^{-ct}.$$

Thus, the solution operator $e^{A_h t}$ satisfies

$$\left|\left|e^{A_h t}\right|\right|_{L^2} \leq e^{-ct}, \qquad t > 0$$

for $c > 0$ independent of h.

As A_h is a bounded operator (with bound depending on h), for each $t \in \mathbb{C}$, $e^{A_h t}$ is a bounded operator (with bound also depending on h). Then for any $M > 0$, and for all t in the wedge $\mathbb{T}_M$ defined in (3.6), we have

$$\left|\left|e^{A_h t}\right|\right|_{L^2} = \left|\left|e^{A_h t_1 + iA_h t_2}\right|\right|_{L^2} = \left|\left|e^{iA_h t_2} e^{A_h t_1}\right|\right|_{L^2}.$$

However, as A_h is self-adjoint, $e^{iA_h s}$ is a unitary group for s real, so $\left|\left|e^{iA_h t_2}\right|\right|_{L^2} = 1$. This leads us to conclude that

$$\left|\left|e^{A_h t}\right|\right|_{L^2} \leq \left|\left|e^{A_h t_1}\right|\right|_{L^2} \leq e^{-ct_1} \leq e^{-c'|t|}, \qquad t \in \mathbb{T}_M \tag{5.10}$$

for some c' depending on M but not on h.

We now modify a theorem from analytic semigroup theory found in Renardy and Rogers (2004).

Theorem 23. *For n a positive integer or half-integer, there exist positive constants ω and C_n, independent of h, for which*

$$\left|\left|A_h^n e^{A_h t}\right|\right|_{L^2} \leq C_n t^{-n} e^{-\omega t}, \qquad t > 0, \tag{5.11}$$

Proof. By (5.10), we have

$$\left|\left|e^{A_h t}\right|\right|_{L^2} \leq e^{-c|t|}, \qquad t \in \mathbb{T}_M$$

for some $c > 0$ independent of h.

If $c_* = c - \epsilon$, then the modified operator $A_h + c_*$ obeys

$$\left|\left|e^{(A_h + c_*)t}\right|\right|_{L^2} \leq e^{-\epsilon|t|}, \qquad t \in \mathbb{T}_M.$$

We define $\delta = 2/M$. Then for $z \in S_1' = \{z = z_1 + iz_2 : z_1 \geq 0, |z_2| \leq \delta z_1\}$, we have

$$\begin{aligned}\left|\left|((A_h + c_*) - z)^{-1}\right|\right|_{L^2} &= \left|\left|\int_0^\infty e^{-zt} e^{(A_h + c_*)t}\, dt\right|\right|_{L^2} \\ &\leq \int_0^\infty e^{-c'|z|t} e^{-\epsilon t}\, dt\end{aligned}$$

for some c' depending on δ. Thus,

$$\left|\left|((A_h + c_*) - z)^{-1}\right|\right|_{L^2} \leq \frac{C}{1 + |z|} \tag{5.12}$$

for all $z \in S_1'$.

We next suppose that $z \in S_2' = \{z = z_1 + iz_2 : z_2 \geq 0, |z_1| \leq z_2/\delta\}$. We deform the contour of integration to the ray $R_2 = t_1 - iMt_1$. On R_2, we have that $\operatorname{Re} zt = t_1(z_1 + Mz_2) = t_1(z_1 + 2/\delta z_2) \geq t_1 z_2/\delta$. This implies $|e^{-zt}| \leq e^{-c''|z||t|}$ for $z \in S_2'$ and $t \in R_2$ with c'' depending on δ. We therefore obtain an estimate of the same form as (5.12), and a similar argument extends the estimate to $S_3' = \{z = z_1 + iz_2 : z_2 \leq 0, |z_1| \leq |z_2|/\delta\}$ and hence $S_\delta' = S_1' \cup S_2' \cup S_3'$.

We now consider $z' + c_* \in S'_\delta$. (i.e. $z' \in S'_\delta - c_*$), so that we can write $z' = z - c_*$ for $z \in S'_\delta$. Then we have:

$$\begin{aligned} \left|\left|(A_h - z')^{-1}\right|\right|_{L^2} &= \left|\left|(A_h - (z - c_*))^{-1}\right|\right|_{L^2} \\ &= \left|\left|(A_h + c_* - z)^{-1}\right|\right|_{L^2}. \end{aligned}$$

We use the resolvent estimate for $z \in S'_\delta$ in (5.12), so that

$$\left|\left|(A_h - z')^{-1}\right|\right|_{L^2} \leq \frac{C}{1+|z|} \leq \frac{C}{1+|z'+c_*|},$$

from which we conclude

$$\left|\left|(A_h - z')^{-1}\right|\right|_{L^2} \leq \frac{C}{1+|z'|}, \qquad z' \in S'_\delta - c_*.$$

This improved resolvent estimate on $S'_\delta - c_*$ now allows us to write, for $t > 0$,

$$A_h^n e^{A_h t} = \int_\Gamma z^n e^{zt}(z - A_h)^{-1}\, dz$$

for the contour $\Gamma = R_+ \cup R_- \subset S'_\delta - c_*$, where

$$R_\pm = \{-\omega + (-1 \pm i\delta)s, s \geq 0\}$$

for $0 < \omega < c_*$. We note that for negative definite A_h, $(-A_h)^{1/2}$ is well-defined, and we take $A_h^{1/2} = i(-A_h)^{1/2}$. As $-A_h$ is positive, it has a well-defined unique self-adjoint square root. Bounding the contour integral, we have that

$$\begin{aligned} \left|\left|A_h^n e^{A_t}\right|\right|_{L^2} &\leq C \int_0^\infty (1 + r^n) e^{-\omega t - rt} \frac{1}{1+r}\, dr \\ &\leq C_n t^{-n} e^{-\omega' t} \end{aligned}$$

for $t > 0$.

□

We require some elliptic regularity results. The theory here is adapted from Evans (1998).

Theorem 24. *Suppose $a_{jl} \in C^m$. If $u \in X_h$ solves $A_h u = f$, then there exists a constant C_m, independent of h, for which*

$$||u||_{H^{m+1}} \leq C_m \, ||f||_{H^{m-1}} \, . \tag{5.13}$$

Proof. As $A_h u = f$, for an arbitrary grid function $v \in X_h$ we have

$$\langle A_h u, v \rangle = \langle f, v \rangle \, . \tag{5.14}$$

Let $v = (-1)^{m+1} D_h^{\gamma -} D_h^{\gamma} u$ for γ a multi-index with $|\gamma| = m$, where $D_h^{\gamma -} = (D_1^-)^{\gamma_1} \cdots (D_d^-)^{\gamma_d}$. Then we have

$$\sum_{jl} \left\langle D_j^+ (a_{jl} (D_l^- u)), (-1)^{m+1} D_h^{\gamma -} D_h^{\gamma} u \right\rangle = \left\langle f, (-1)^{m+1} D_h^{\gamma -} D_h^{\gamma} u \right\rangle . \tag{5.15}$$

We denote the left side of (5.15) by B and the right side by E.

We first examine B. Summing by parts $m+1$ times, we have

$$B = \sum_{jl} \left\langle D_h^{\gamma} (a_{jl} (D_l^- u)), D_j^- D_h^{\gamma} u \right\rangle .$$

This can be expressed as

$$\begin{aligned} B &= \sum_{jl} \left\langle \sum_{\beta \leq \gamma} \binom{\gamma}{\beta} (S_h^{\beta} D_h^{\gamma - \beta} a_{jl}) D_h^{\beta} D_l^- u, D_h^{\gamma} D_j^- u \right\rangle \\ &= \sum_{jl} \left\langle (S_h^{\gamma} a_{jl}) D_l^- D_h^{\gamma} u, D_j^- D_h^{\gamma} u \right\rangle \\ &\quad + \sum_{jl} \left\langle \sum_{\beta < \gamma} \binom{\gamma}{\beta} (S_h^{\beta} D_h^{\gamma - \beta} a_{jl}) D_h^{\beta} D_l^- u, D_j^- D_h^{\gamma} u \right\rangle \\ &= B_1 + B_2. \end{aligned}$$

By the ellipticity hypothesis and translation invariance of the L^2 norm,

$$B_1 \geq C \sum_j \left|\left| D_j^- D_h^{\gamma} u \right|\right|_{L^2}^2 = C \sum_j \left|\left| D_j^+ D_h^{\gamma} u \right|\right|_{L^2}^2 . \tag{5.16}$$

Turning our attention to B_2, by the Cauchy-Schwarz inequality we have

$$|B_2| \leq \sum_{jl} \sum_{\beta<\gamma} \binom{\gamma}{\beta} \left|\left|(S_h^\beta D_h^{\gamma-\beta} a_{jl}) D_h^\beta D_l^- u\right|\right|_{L^2} \left|\left|D_j^- D_h^\gamma\right|\right|_{L^2}.$$

As the $a_{jl} \in C^m$, the differences $D_h^{\gamma-\beta} a_{jl}$ are uniformly bounded, and so

$$|B_2| \leq C_m \sum_{jl} \sum_{\beta<\gamma} \left|\left|D_h^\beta D_l^- u\right|\right|_{L^2} \left|\left|D_j^- D_h^\gamma\right|\right|_{L^2}.$$

Using the Cauchy-Schwarz inequality with ϵ then gives us

$$\begin{aligned} |B_2| &\leq C_m \sum_{jl} \sum_{\beta<\gamma} \left(C_\epsilon \left|\left|D_h^\beta D_l^- u\right|\right|_{L^2}^2 + \epsilon \left|\left|D_j^- D_h^\gamma u\right|\right|_{L^2}^2 \right) \\ &\leq C_{\epsilon'} \left|\left|u\right|\right|_{H^m}^2 + \epsilon' \sum_j \left|\left|D_j^- D_h^\gamma u\right|\right|_{L^2}^2. \end{aligned} \tag{5.17}$$

Combining (5.16) and (5.17), we find

$$-C_1 \left|\left|u\right|\right|_{H^m}^2 + C_2 \sum_j \left|\left|D_j^+ D_h^\gamma u\right|\right|_{L^2}^2 \leq B,$$

with constants depending on m but not on h.

We now bound E. Summing by parts $m-1$ times and using the Cauchy-Schwarz inequality with ϵ gives us

$$|E| \leq C_\epsilon \left|\left|f\right|\right|_{H^{m-1}}^2 + \epsilon \left|\left|u\right|\right|_{H^{m+1}}^2.$$

As $B = E$, we have

$$-C_1 \left|\left|u\right|\right|_{H^m}^2 + C_2 \sum_j \left|\left|D_j^+ D_h^\gamma u\right|\right|_{L^2}^2 \leq C_3 \left|\left|f\right|\right|_{H^{m-1}} + \epsilon \left|\left|u\right|\right|_{H^{m+1}}.$$

Summing over all $|\gamma| = m$, we find that

$$\left|\left|u\right|\right|_{H^{m+1}}^2 \leq C_m \left(\left|\left|f\right|\right|_{H^{m-1}}^2 + \left|\left|u\right|\right|_{H^m}^2 \right). \tag{5.18}$$

Applying this estimate repeatedly, we see that

$$\left|\left|u\right|\right|_{H^{m+1}}^2 \leq C_m' \left(\left|\left|f\right|\right|_{H^{m-1}}^2 + \left|\left|u\right|\right|_{H^1}^2) \right). \tag{5.19}$$

To remove the $||u||_{H^1}$ term on the right, we take $v = -u$ in (5.14), so that

$$\langle A_h u, -u\rangle = \langle f, -u\rangle .$$

We again label the left side B and the right side E.

We have that

$$\begin{aligned} B &= \left\langle \sum_{jl} D_j^+(a_{jl} D_l^- u), -u \right\rangle \\ &= \left\langle \sum_{jl} a_{jl} D_l^- u, D_j^- u \right\rangle \\ &\geq C \sum_j \left|\left|D_j^- u\right|\right|_{L^2}^2 . \end{aligned}$$

By the discrete Poincaré inequality, this gives us that

$$B \geq c' ||u||_{H^1}^2 .$$

For E, we find

$$\begin{aligned} |E| &\leq \epsilon ||u||_{L^2}^2 + C_\epsilon ||f||_{L^2}^2 \\ &\leq \epsilon ||u||_{H^1}^2 + C_\epsilon ||f||_{L^2}^2 . \end{aligned}$$

As $B = E$, we have

$$c' ||u||_{H^1}^2 \leq \epsilon ||u||_{H^1}^2 + C_\epsilon ||f||_{L^2}^2 ,$$

and thus

$$||u||_{H^1}^2 \leq C' ||f||_{L^2}^2 \leq C' ||f||_{H^m}^2 . \tag{5.20}$$

Substituting (5.20) into (5.19) and taking square roots yields the result.

□

By a simple inductive argument, as a consequence of Theorem 24, we can bound differences by powers of A_h. For m odd, we use that $||u||_{H^1} \leq C \left|\left|A_h^{1/2} u\right|\right|_{L^2}$, which is an immediate consequence of (5.8).

Corollary 25. *Suppose $a_{jl} \in C^m$. Then there exists a constant C_m, independent of h, for which*

$$||u||_{H^m} \leq C_m \left|\left|A_h^{m/2} u\right|\right|_{L^2} \tag{5.21}$$

for all $u \in X_h$.

With the aid of Sobolev space theory, we can obtain L^∞ estimates for large time exhibiting exponential decay.

Theorem 26. *There exist constants C and c, independent of h, for which*

$$\left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty} \leq C e^{-ct}, \qquad t \geq 1. \tag{5.22}$$

Proof. Suppose v is an arbitrary vector in X_h. For $m = \lfloor d/2 \rfloor + 1$, the discrete Sobolev lemma gives us

$$\begin{aligned} \left|\left|D_h^\gamma e^{A_h t} v\right|\right|_{L^\infty} &\leq C_m \left|\left|D_h^\gamma e^{A_h t} v\right|\right|_{H^m} \\ &\leq C \left|\left|e^{A_h t} v\right|\right|_{H^{m+2}}. \end{aligned}$$

As the $a_{jl} \in C^{m+2}$, using Corollary 25 we find that

$$\left|\left|D_h^\gamma e^{A_h t} v\right|\right|_{L^\infty} \leq C \left|\left|A_h^{m/2+1} e^{A_h t} v\right|\right|_{L^2}.$$

For $t \geq 1$, Theorem 23 gives us

$$\left|\left|D_h^\gamma e^{A_h t} v\right|\right|_{L^\infty} \leq C e^{-ct} ||v||_{L^2}.$$

Because we are on a bounded domain, for all $u \in X_h$ we have $||u||_{L^2} \leq C ||u||_{L^\infty}$ for some C independent of h. Therefore, we conclude

$$\left|\left|D_h^\gamma e^{A_h t} v\right|\right|_{L^\infty} \leq C e^{-ct} ||v||_{L^\infty}$$

for $t \geq 1$, which establishes the theorem.

□

We can now improve the L^∞ resolvent estimates for A_h.

Theorem 27. *For the operator A_h in (5.4) (or for the operator $\widetilde{A_h}$ in (5.6) replacing A_h) with coefficients $a_{jl} \in C^{\lfloor d/2 \rfloor + 3}(\mathbb{R}^d)$ on the space X_h of periodic grid functions of mean value zero, for multi-indices γ with $|\gamma| \le 2$, there exist constants C_1 and C_2 for which*

$$\left|\left|D_h^\gamma (A_h)^{-1}\right|\right|_{L^\infty(I_h^d)} \le C_1, \qquad |\gamma| = 0, 1 \tag{5.23}$$

$$\left|\left|D_h^\gamma (A_h)^{-1}\right|\right|_{L^\infty(I_d^d)} \le C_2(1 + |\log h|), \qquad |\gamma| = 2. \tag{5.24}$$

Proof. For each multi-index γ with $|\gamma| \le 2$, we can write

$$D_h^\gamma (A_h)^{-1} = \int_0^\infty D_h^\gamma e^{A_h t}\, dt,$$

provided the integral converges.

We estimate in L^∞:

$$\left|\left|D_h^\gamma (A_h)^{-1}\right|\right|_{L^\infty} \le \int_0^\infty \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt.$$

We split the interval of integration, so that

$$\left|\left|D_h^\gamma (A_h)^{-1}\right|\right|_{L^\infty} \le \int_0^1 \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt + \int_1^\infty \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt. \tag{5.25}$$

We first examine the integral on the left. For $|\gamma| = 0, 1$, we use the bound in (4) to find that

$$\int_0^1 \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt \le C \int_0^1 |t|^{-|\gamma|/2}\, dt \le C. \tag{5.26}$$

For $|\gamma| = 2$, we further divide the interval of integration:

$$\int_0^1 \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt = \int_0^{h^2} \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt + \int_{h^2}^1 \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt.$$

We again use (4) for the interval $[h^2, 1]$. However, on the interval $[0, h^2]$, we bound the second difference by C/h^2, so that

$$\begin{aligned}\int_0^1 \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty}\, dt &\le \int_0^{h^2} C h^{-2}\, dt + \int_{h^2}^1 C t^{-1}\, dt \\ &\le C\left(1 + |\log h|\right).\end{aligned} \tag{5.27}$$

For the integral on the right in (5.25), by Theorem 26 we have

$$\int_1^\infty \left|\left|D_h^\gamma e^{A_h t}\right|\right|_{L^\infty} dt \leq C \int_1^\infty e^{-ct}\, dt \leq C'.$$

Combining this with (5.26) for $|\gamma| = 0, 1$ or (5.27) for $|\gamma| = 2$ yields the result.

□

6

Numerical Results

In this chapter we present numerical results for three implicit difference methods applied to a test problem. We compare and contrast the observed superior regularity of the L-stable and A-stable implicit Euler and TGA methods with the lesser regularity of the A-stable (though not L-stable) Crank-Nicolson method when taking large time steps. For the homogeneous problem, we find experimental confirmation of Theorem 1 for implicit Euler and TGA. For these L-stable methods, the first and second differences of the numerical solution exhibit the predicted regularity. In contrast, we find that the conclusion of Theorem 1 does not hold for Crank-Nicolson for first and second differences, as differences of the Crank-Nicolson solution exhibit blow up as the grid spacing tends to zero. For the inhomogeneous problem, we confirm Theorem 2 for implicit Euler and TGA, showing that differences of the inhomogeneous solution are controlled in maximum norm by the maximum norm of the inhomogeneous term. We also observe that Crank-Nicolson possesses the same regularity property for first differences, but may not for second differences.

We discuss and provide graphical representations for each of the regularity properties of first and second differences for all three methods. Although all three methods satisfy the stability properties (2.17) and (2.23) for the solution without differences, we do not discuss these in detail as the regularity properties for first and second differences are more interesting both theoretically and graphically.

We solve numerically the test problem

$$\begin{aligned} u_t &= Au + f \\ A &= a(x)\frac{d^2}{dx^2} \\ a(x) &= 1 + \sin^2(2\pi x) \end{aligned} \tag{6.1}$$

for x on the interval $[0, 1]$ with periodic boundary conditions. We discretize the operator $a(x)d^2/dx^2$ by

$$A_h = a(x)D^+D^-.$$

We compare implicit Euler, TGA and Crank-Nicolson for the time-stepping method. Formulas for these methods appear in the appendix to Beale (2009).

6.1 Homogeneous Results

We first examine the homogeneous problem. We take large time steps of length equal to the grid spacing, i.e. $k = h$. Because the problem is posed on a periodic interval, $D_h^\gamma s^n(kA_h)$ may be regarded as a matrix operator, and its L^∞ norm may be computed as the largest sum of the absolute values in each row. We examine the regularity properties for first and second differences of each method.

We plot the quantities $(nk)^{|\gamma|/2} \left|\left|D_h^\gamma s^n(kA_h)\right|\right|_{L^\infty}$ for $|\gamma| = 1, 2$ and $h = k = 2^{-N}$ at the end of this chapter (note that the computed data is indicated by point markers and the lines are interpolated for ease of viewing). In Figure 6.1 and Figure 6.2 we see the regularity property of first differences of the implicit Euler and TGA solutions, respectively. As the maximum of $(nk)^{1/2} \left|\left|D_h s^n(kA_h)\right|\right|_{L^\infty}$ seems to occur after the first time step for implicit Euler and TGA (as is expected in analogy with the exact problem), we plot the $(k)^{1/2}\,||D_h s(kA_h)||_{L^\infty}$ (the temporally scaled maximum norm after one time step) in Figure 6.7 and Figure 6.8. The maximum value of $(k)^{1/2}\,||D_h s(kA_h)||_{L^\infty}$ levels off quickly as the number of grid points increases, and seems to support the bound $||D_h s^n(kA_h)||_{L^\infty} \leq 3(nk)^{-1/2}$ for $nk \leq 1$. In contrast with the L-stable methods, in Figure 6.3 we see that first differences of the Crank-Nicolson solution blow up as the grid spacing tends to zero.

The regularity property for second differences of the implicit Euler and TGA solutions is depicted in Figure 6.4 and Figure 6.5. It is difficult to determine if the logarithmic factors of $|\log h|$ or $|\log nk|$ are actually required in Theorem 1. In Figure 6.9 and Figure 6.10 we plot the value of $k\,||D_h^2 s(kA_h)||_{L^\infty}$, the maximum norm of the second difference after one time step. While the maximum norms of second differences after one time step do not level off dramatically as they do for first differences, we are still uncertain as to whether the logarithmic factors are required. As in the case of first differences, we see that Crank-Nicolson does not possess the same regularity property as the L-stable methods for large time steps because second differences of its solution blow up as the grid spacing tends to zero.

As Crank-Nicolson fails to have the regularity properties for large time steps of implicit Euler and TGA, we suspect that the assumption of L-stability is critical to obtaining large time step regularity results.

6.2 Inhomogeneous Results

For the inhomogeneous problem, we again take the length of time step to be the same as the spatial grid spacing, i.e. $k = h$. We examine $||D_h^\gamma u||_\infty$ where $|\gamma| = 1, 2$ for u evolved by noisy functions f. The values of various f at (x, t) are taken randomly from $(0, 1)$ and renormalized so that $||f(\cdot, t)||_\infty = 1$. We calculate the numerical solution u for many such f, and at each time step we take the largest value of $||D_h^\gamma u||_\infty$ among all the choices of f (with those depicted being the result of

2000 choices of f). We can then compare to see if $||D_h^\gamma u||$ remains bounded as the grid spacing tends to zero. (Considering particular choices for f, such as having f alternate between -1 and 1 at consecutive grid points, does not seem to affect the results qualitatively.)

The regularity result in (2.24) holds for all three methods, as seen in Figure 6.11, Figure 6.2 and Figure 6.13. In fact, the maximum norm of first differences seem to be decreasing as the grid spacing tends to zero. For Crank-Nicolson, this regularity should not be surprising in light of Corollary 7.2 of Beale (2009), which shows that first differences of the Crank-Nicolson solution for the constant-coefficient heat equation are bounded by the maximum norm of the inhomogeneous term.

For second differences, we observe at least the expected regularity for implicit Euler and TGA. Figure 6.14 and Figure 6.15 indicate that the maximum norm of second differences may be bounded independent of h, so that the logarithmic factor in (2.25) might not be required. In fact, for TGA the maximum norm of the second difference appears to diminish as the grid spacing tends to zero. For Crank-Nicolson, we see in Figure 6.16 that the maximum norm of the second difference increases far more rapidly than it does for implicit Euler as the grid spacing tends to zero, and appears to be unbounded.

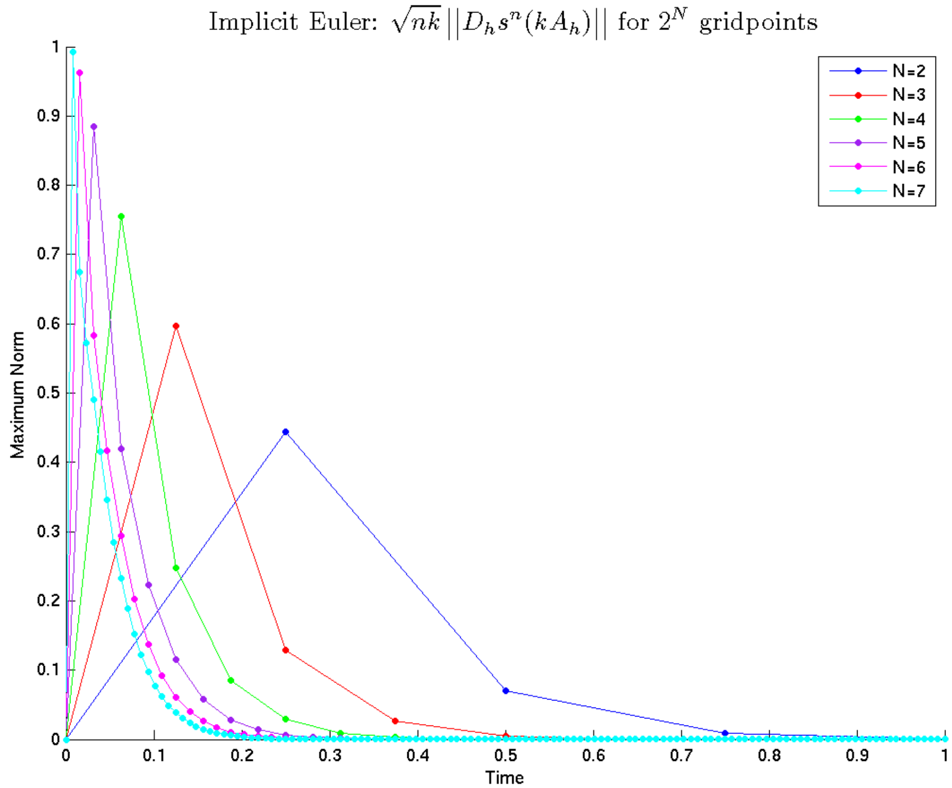

FIGURE 6.1: Temporal control of first difference of implicit Euler solution to homogeneous problem

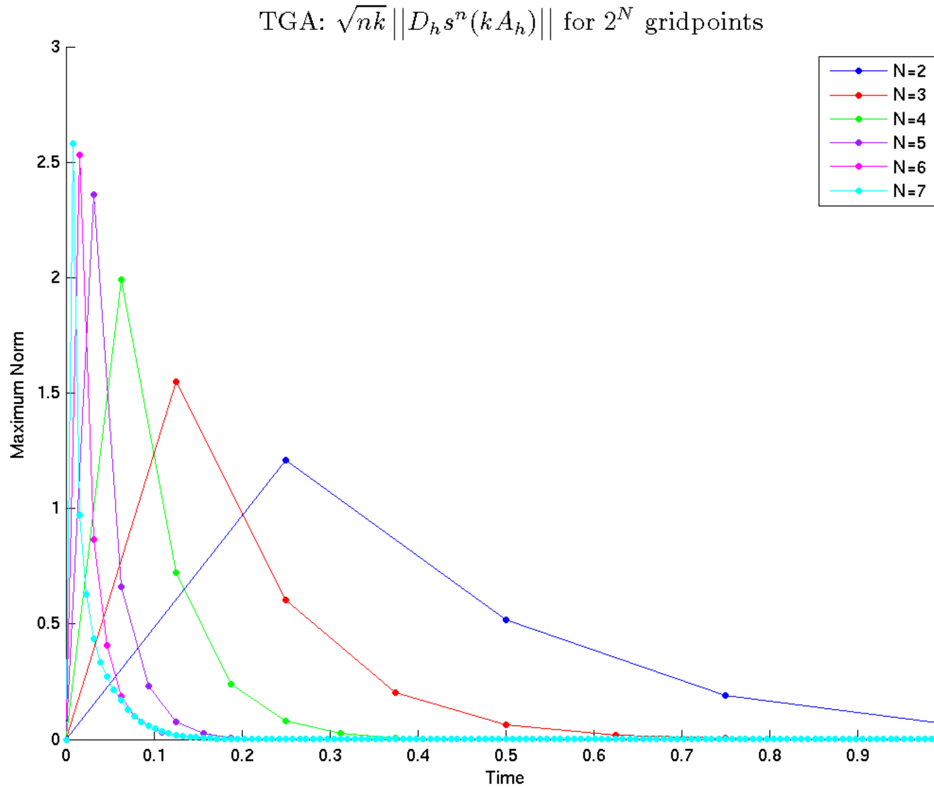

FIGURE 6.2: Temporal control of first difference of TGA solution to homogeneous problem

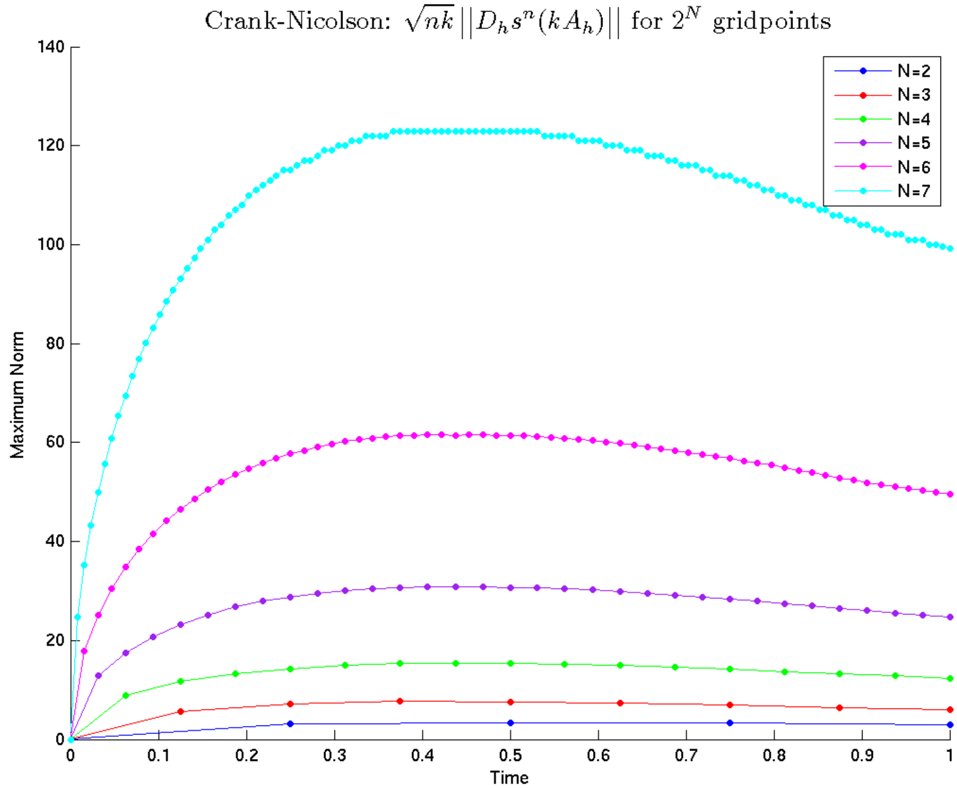

FIGURE 6.3: Lack of temporal control of first difference of Crank-Nicolson solution to homogeneous problem

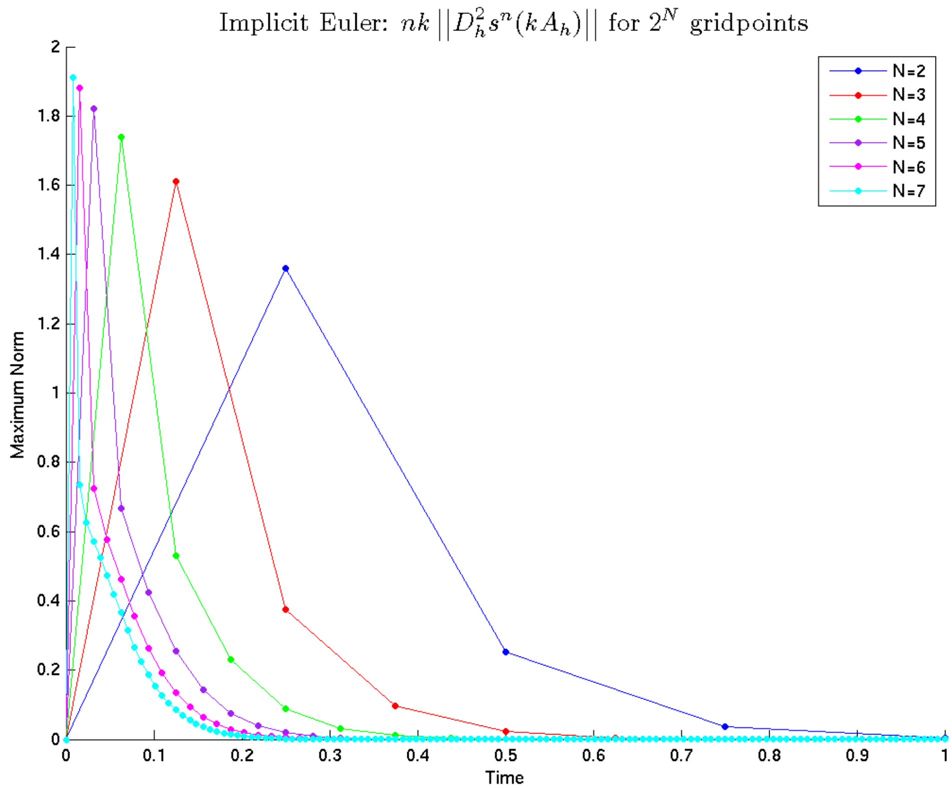

FIGURE 6.4: Temporal control of second difference of implicit Euler solution to homogeneous problem

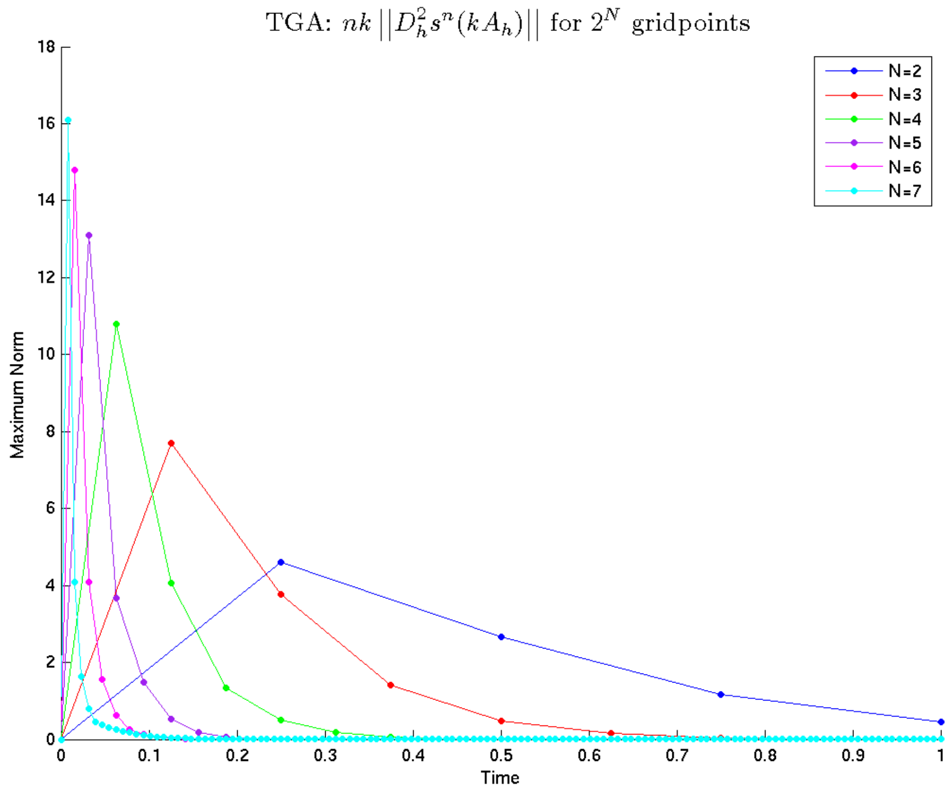

FIGURE 6.5: Temporal control of second difference of TGA solution to homogeneous problem

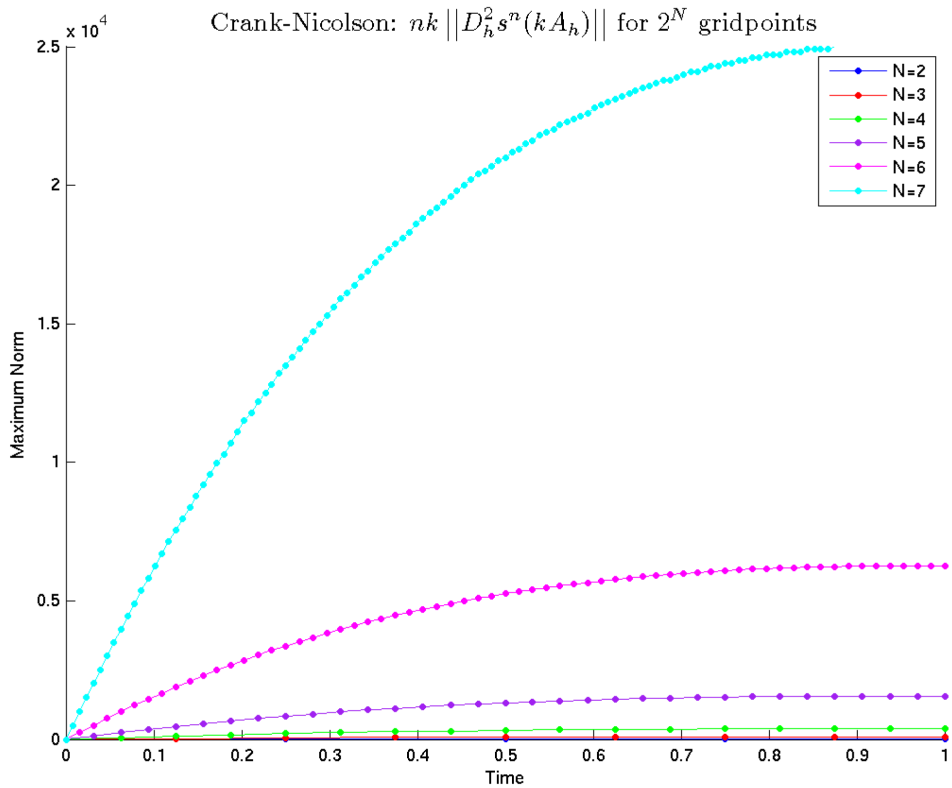

FIGURE 6.6: Lack of temporal control of second difference of Crank-Nicolson solution to homogeneous problem

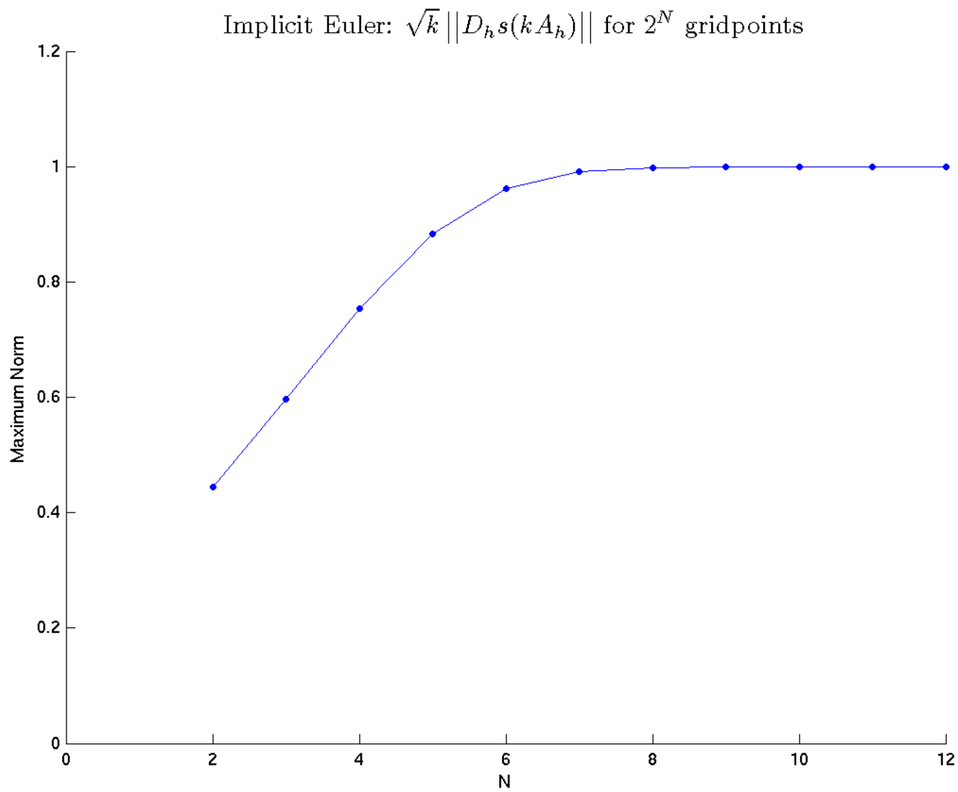

FIGURE 6.7: Temporally rescaled maximum norm of first difference after one time step of implicit Euler

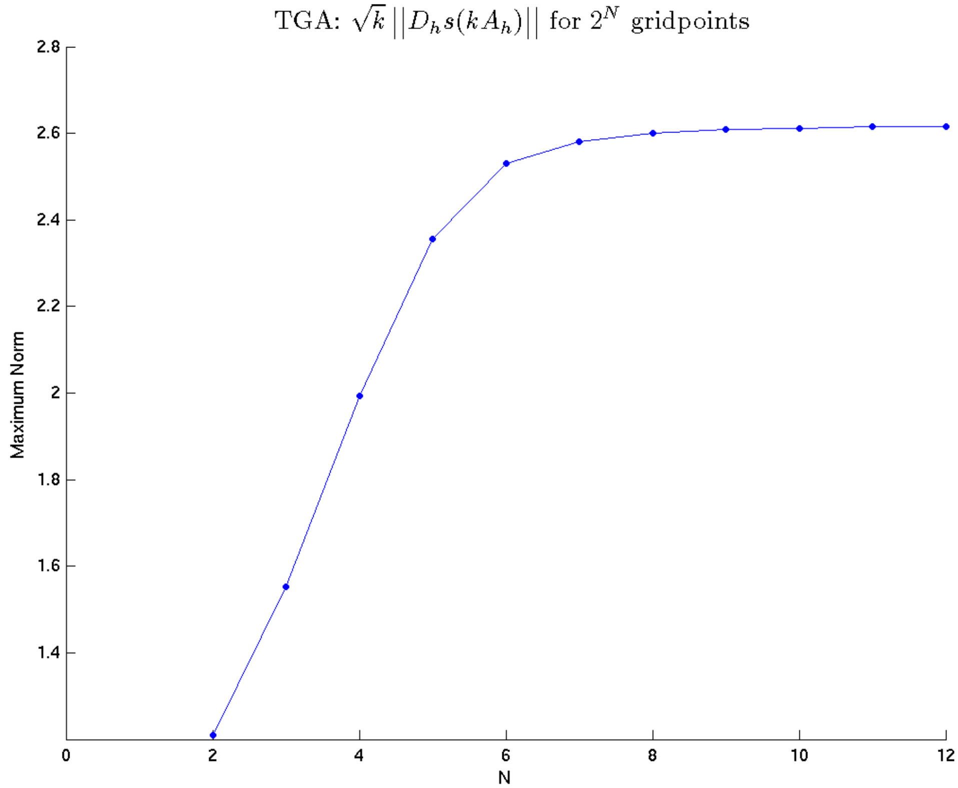

FIGURE 6.8: Temporally rescaled maximum norm of first difference after one time step of TGA

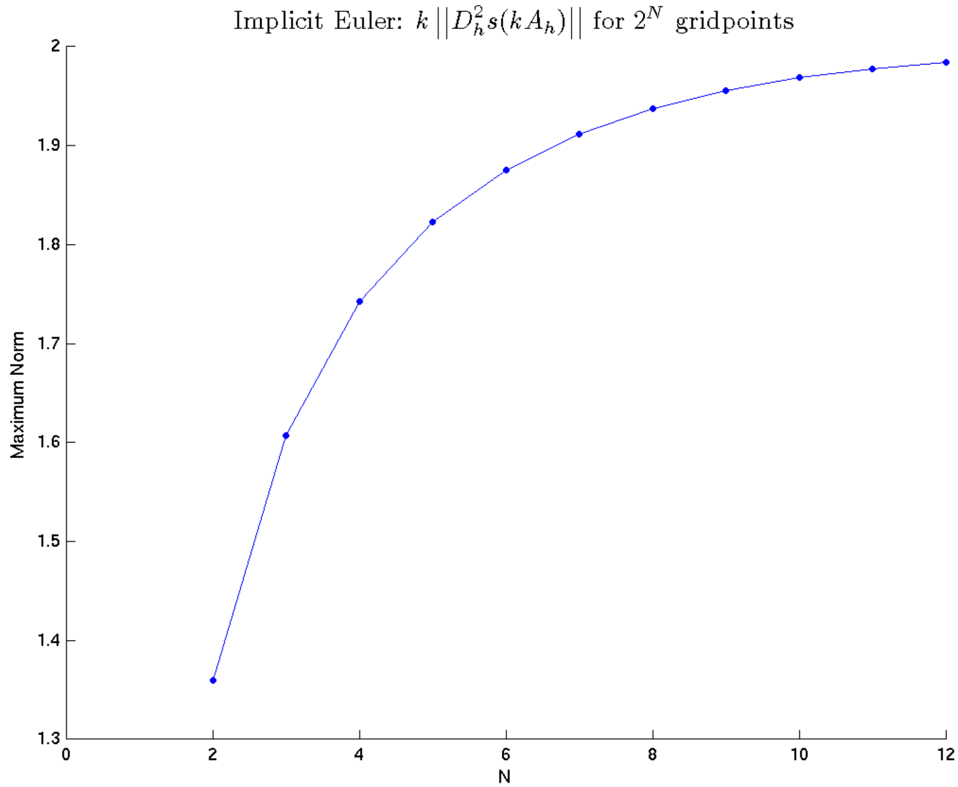

FIGURE 6.9: Temporally rescaled maximum norm of second difference after one time step of implicit Euler

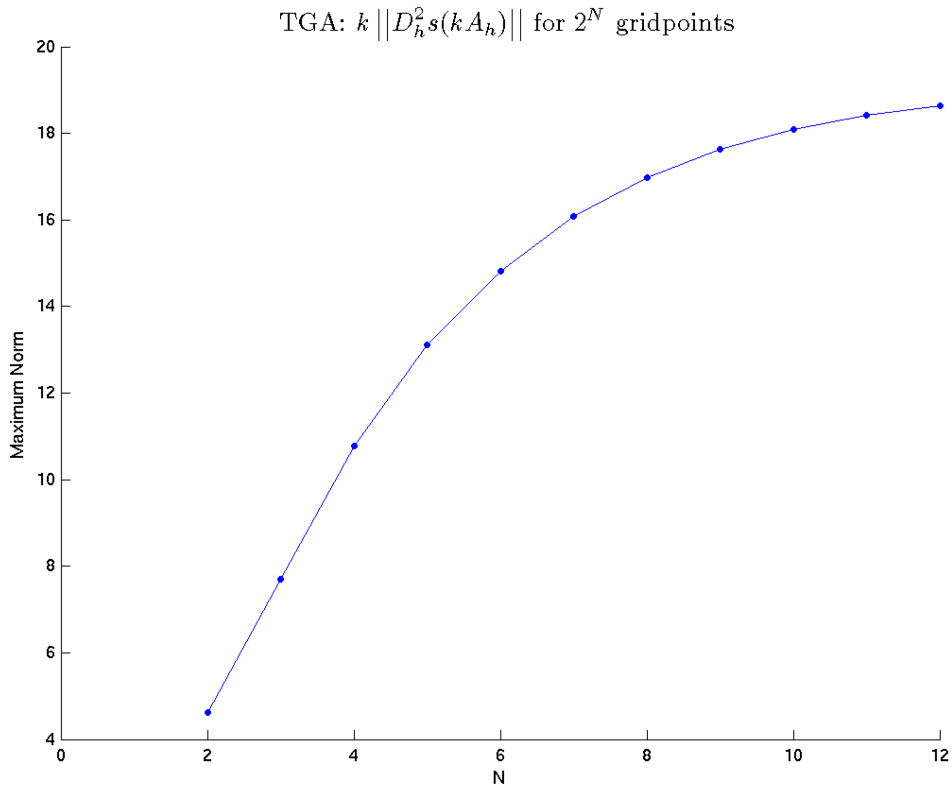

FIGURE 6.10: Temporally rescaled maximum norm of second difference after one time step of TGA

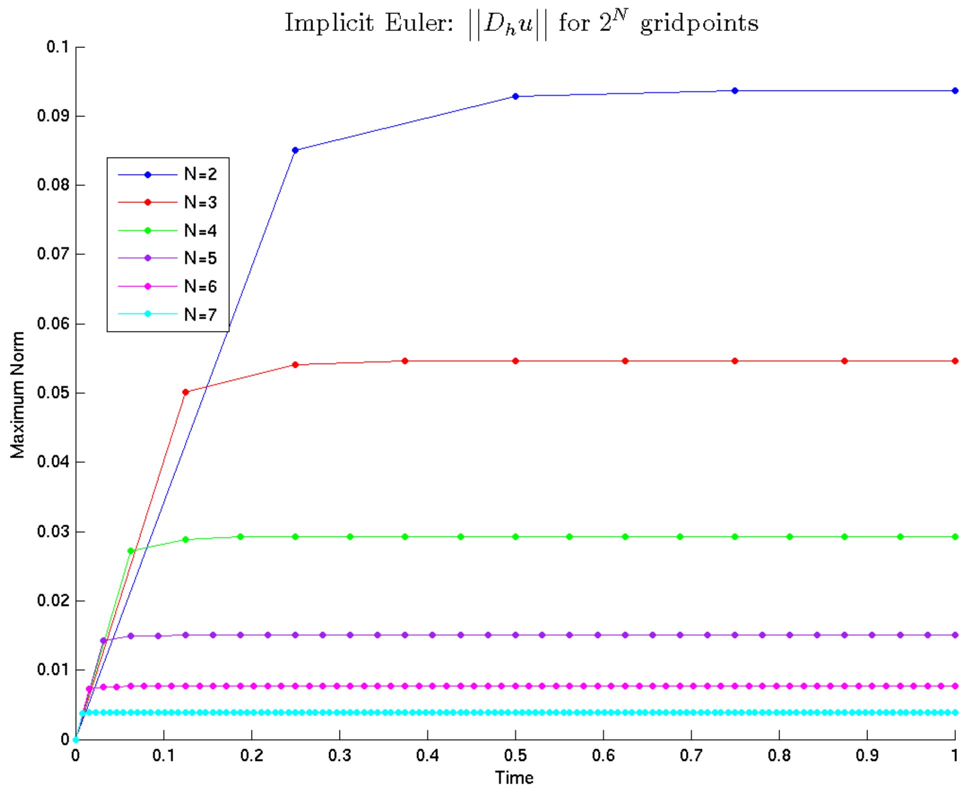

FIGURE 6.11: First difference of implicit Euler solution to inhomogeneous problem

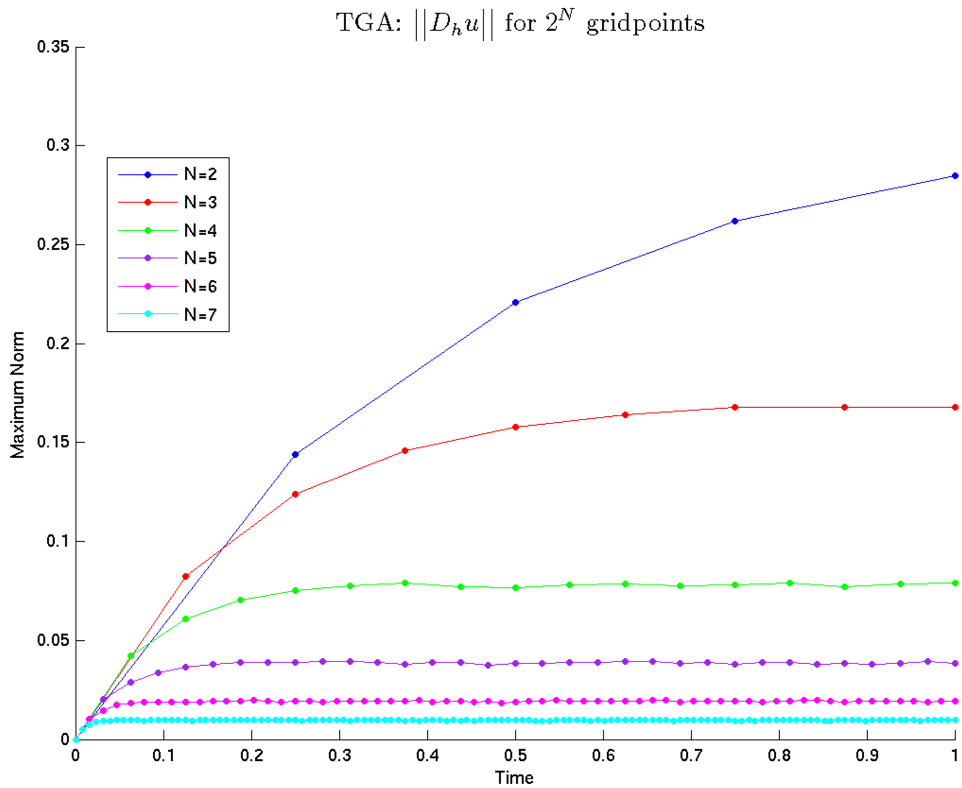

FIGURE 6.12: First difference of TGA solution to inhomogeneous problem

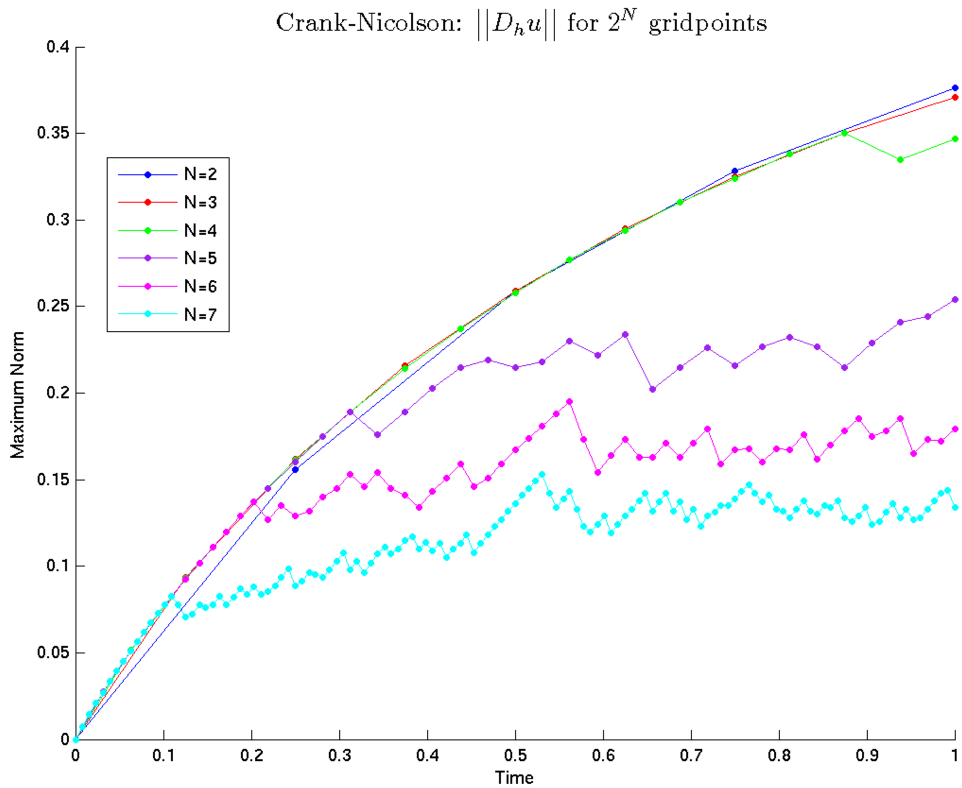

FIGURE 6.13: First difference of Crank-Nicolson solution to inhomogeneous problem

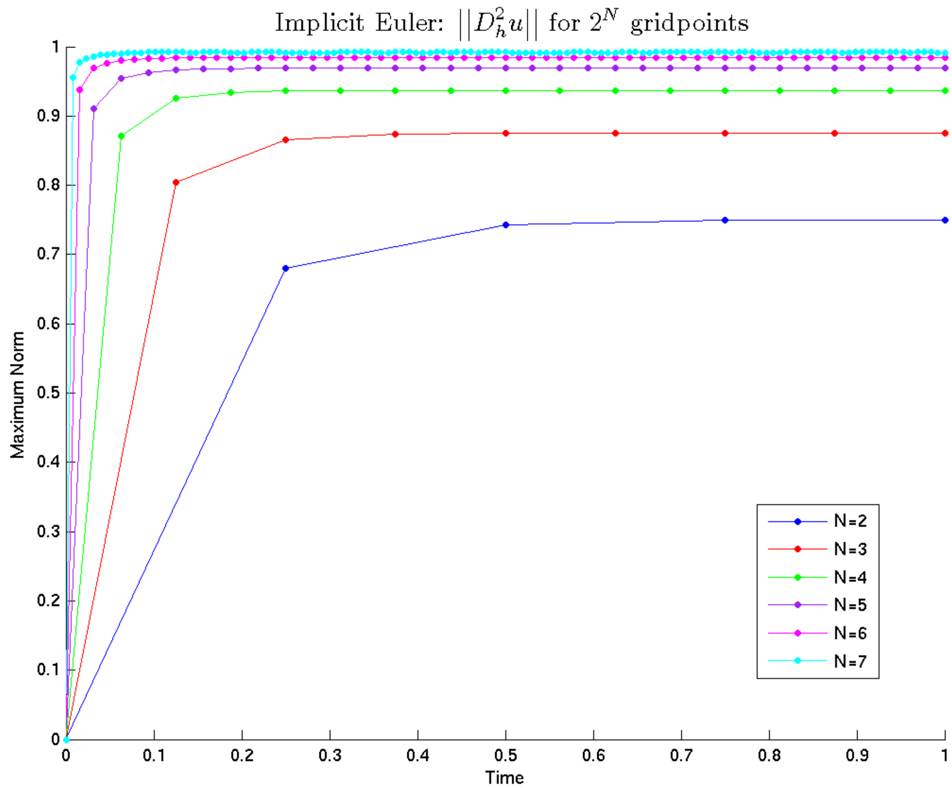

FIGURE 6.14: Second difference of implicit Euler solution to inhomogeneous problem

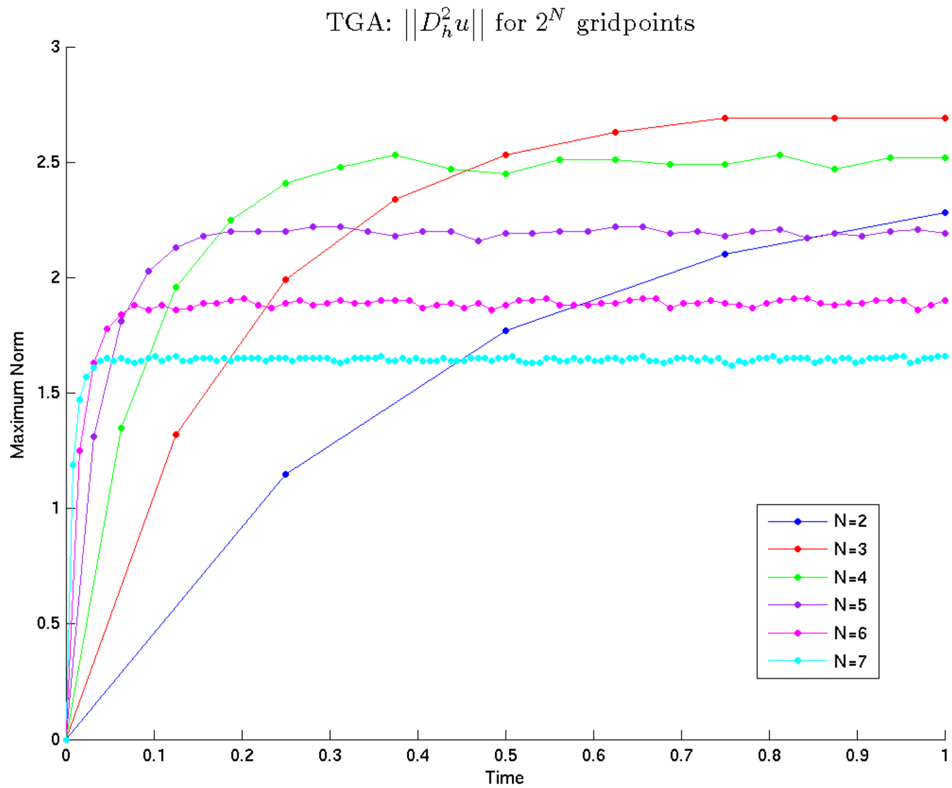

FIGURE 6.15: Second difference of TGA solution to inhomogeneous problem

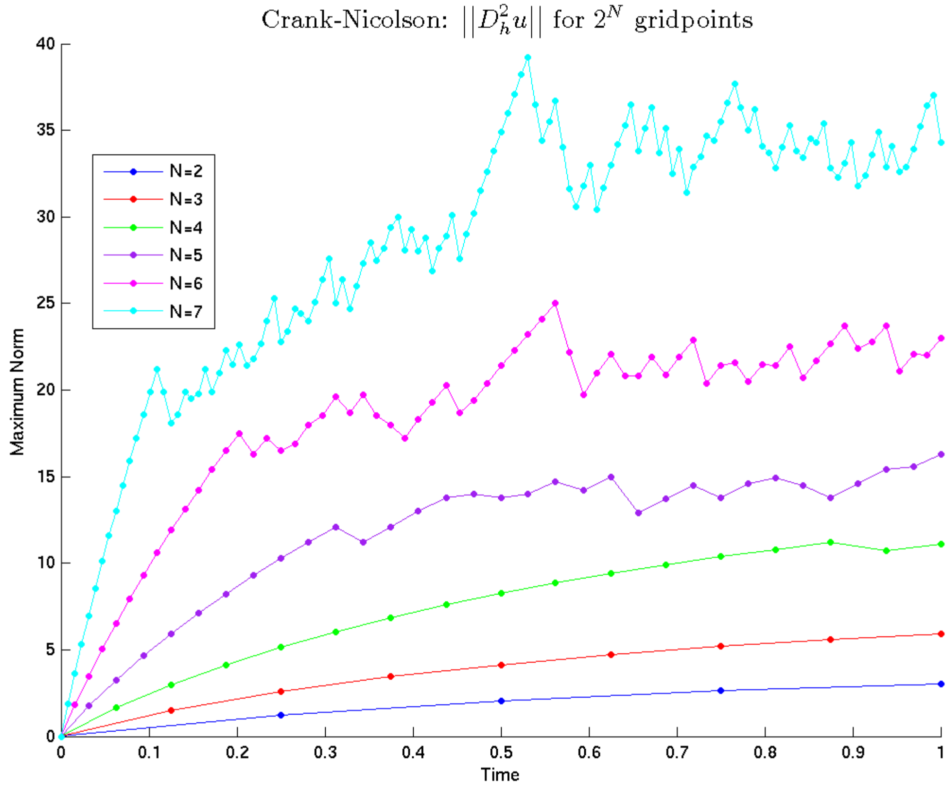

FIGURE 6.16: Second difference of Crank-Nicolson solution to inhomogeneous problem

Appendix A

Proof of Theorem 3

Theorem 3. *Suppose U is a classical solution to (2.26) and u^n is the numerical solution at time step n given by the L-stable scheme in (2.27) for rational s with $k = ch$. If $\mathcal{E}$ is the total error and $\mathcal{T}$ is the local truncation error, then, on any finite interval $[0, T]$, we have:*

$$||\mathcal{E}||_\infty \leq C_0 \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty \tag{A.1}$$

$$||D_h^\gamma \mathcal{E}||_\infty \leq C_1 \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty \,, \qquad |\gamma| = 1 \tag{A.2}$$

$$||D_h^\gamma \mathcal{E}||_\infty \leq C_2 \left(1 + |\log h|^2\right) \sup_{t \leq T} ||\mathcal{T}(\cdot, t)||_\infty \qquad |\gamma| = 2 \tag{A.3}$$

with constants depending on c and T, but not on h or n for k sufficiently small.

Proof. We begin by recalling the definition

$$\mathcal{E}^{n+1} = U^{n+1} - u^{n+1}.$$

In the definition for $\mathcal{E}^{n+1}$, we replace U^{n+1} by the expression in (2.31) relating it to

U^n and $\mathcal{T}^n$, and we replace u^{n+1} by its definition in terms of u^n, so that

$$\mathcal{E}^{n+1} =$$

$$= s(kA_h)U^n + k\sum_{i=1}^{m} q_i(kA_h)(1-\eta_i kA_h)^{-1} f(\cdot, nk+\tau k) + Q(kA_h)(1-\eta kA_h)^{-1}\mathcal{T}^n$$

$$- \left[s(kA_h)u^n + k\sum_{i=1}^{m} q_i(kA_h)(1-\eta_i kA_h)^{-1} f(\cdot, nk+\tau k) \right].$$

The terms involving f cancel, and the linearity of $s(kA_h)$ allows us to write

$$\begin{aligned} \mathcal{E}^{n+1} &= s(kA_h)(U^n - u^n) + Q(kA_h)(1-\eta kA_h)^{-1}\mathcal{T}^n \\ &= s(kA_h)\mathcal{E}^n + Q(kA_h)(1-\eta kA_h)^{-1}\mathcal{T}^n. \end{aligned} \tag{A.4}$$

Because $\mathcal{E}^0 = U^0 - u^0 = u_0 - u_0 = 0$, we can apply Theorem 2 directly to (A.4), establishing the result. $\square$

Appendix B

Decay in the Semidiscrete Fundamental Solution

Our estimates for the decay of the frozen coefficient fundamental solution contain the decay factor $e^{-C|x-y|/\sqrt{|t|}}$ for $|t| \geq h^2$. In analogy with the continuous problem, one might expect that we actually have the decay factor of $e^{-C|x-y|^2/|t|}$. However, this is not the case, even in the simplest possible example.

Consider the one-dimensional constant coefficient semi-discrete problem

$$u_t = A_h u = D^+ D^- u$$

$$u(x, 0) = u_0$$

with fundamental solution $G_h(x, t)$ satisfying

$$G_h(x, 0) = \delta_{x0}$$

$$\left(\frac{\partial}{\partial t} - A_h \right) u = 0.$$

The solution can be expressed in the transform as

$$G_h(x, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-4\sin^2(\xi/2)t/h^2} e^{ix\xi/h} \, d\xi.$$

Using the identity

$$\sin^2 \xi/2 = \frac{1 - \cos \xi}{2}$$

we can rewrite $G_h(x,t)$ as

$$G_h(x,t) = \frac{1}{2\pi} e^{-2t/h^2} \int_{-\pi}^{\pi} e^{-2t/h^2 \cos \xi} e^{ix\xi/h} \, d\xi.$$

Remembering that x/h is an integer and using the fact that sine is odd and cosine even, we have

$$G_h(x,t) = \frac{1}{\pi} e^{-2t/h^2} \int_{0}^{\pi} e^{-2t/h^2 \cos \xi} \cos(x\xi/h) \, d\xi.$$

However, this can be rewritten as

$$G_h(x,t) = \frac{1}{\pi} e^{-2t/h^2} I_{x/h}(2t/h^2)$$

by the integral representation of $I_\nu(z)$, the modified Bessel function of the first kind.

We take $t = 1$ and for simplicity $h = 1$ and $x = \nu \in \mathcal{N}$. Then we are concerned with the behavior in ν of $I_\nu(2)$ as $\nu \to \infty$.

However, the bounds given by Nåsell (1978) imply that for fixed c, $I_{\nu+1}(c)/I_\nu(c) \geq C/(n+1)$, so that the decay in ν cannot be as strong as $e^{-c\nu^2} = e^{-c|x|^2/t}$ for this choice of t. The same argument works for any other fixed values of h with $t = 1$ (or any fixed value of t), and so we cannot hope to obtain decay like $e^{-C|x|^2/t}$ uniform in h and t.

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Biography

Michael Dennis Pruitt was born on August 5, 1985 in Baltimore, MD. He received a B.S. in Mathematics from UMBC in 2005, and a Ph.D. in Mathematics from Duke University in 2011.