A FAST MULTILEVEL ALGORITHM FOR THE SOLUTION OF NONLINEAR SYSTEMS OF CONDUCTIVE-RADIATIVE HEAT TRANSFER EQUATIONS IN TWO SPACE DIMENSIONS *

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Abstract. In this paper we describe a fast multilevel algorithm for the solution of a system of nonlinear integro-differential equations that model steady-state combined conductive-radiative heat transfer in two space dimensions. This extends our previous work in one space dimension. We formulate the equations as a compact fixed point problem with the temperature as the unknown. The fixed point map requires both a Poisson solve and a transport solve for its evaluation. As a solver for both the transport problem and the full system we apply the Atkinson-Brakhage algorithm, using Newton-GMRES as the solver on the coarse mesh. We compare our solver choices with Newton-GMRES. Under modest stability and convergence assumptions on the transport solver, we prove convergence of the multilevel method for the complete system.

Key words. conductive-radiative heat transfer, multilevel algorithm, compact fixed point problems

AMS subject classifications. 45G10, 45L10, 65H10, 65J15, 82A70,

1. Introduction. In this paper we describe a fast multilevel algorithm for the solution of a system of nonlinear integro-differential equations that model steady-state combined conductive-radiative heat transfer in two space dimensions. This extends our previous work in one dimension from [6] and [21]. Such models arise in the study of the temperature distribution within molten glass in a furnace and during heat treatment of glass plates [1], [11], [13], [19], the study of the thermal properties of coating materials such as glassy materials, ceramics, and cryodeposits [17], [7], [27], and in the study of porous materials such as fibers, powders, and foams used in insulation at either very high or very low temperatures [26], [37].

In much of the literature [10], [15], [22], [30], [32], [34], [35], [40], methods for finding approximate solutions to these models rely on fixed point iteration, also known as the method of successive substitution, Picard iteration, or nonlinear Richardson iteration. Convergence is linear at best and the iteration may fail to converge if the fixed point map is not a contraction, and such failure has been observed [35]. The multilevel methods in this paper do not suffer from these convergence problems.

We describe the system of equations in § 1.1 and then in § 1.2 show how the system can be reduced to a single equation, a nonlinear completely continuous fixed point problem, in temperature alone. We derive a fixed point formulation that is commonly used in § 1.2 and use results from [28] to show that the fixed point map is completely continuous on the space of continuous functions if the boundary data are continuous. In § 2 we describe a fast algorithm for the solution of this compact fixed point problem. We present numerical results in § 3.

1.1. The equations. We begin with the equations for the dimensionless radiative intensity ψ and temperature Θ in a convex bounded domain $\mathcal{D} \subset R^2$, [30], [34], [39].

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The isotropic, monoenergetic, radiative transport equation is [10], [25], [34],

$$\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}\left(\psi(\mathbf{r},\mathbf{\Omega})\right)+\psi(\mathbf{r},\mathbf{\Omega})=(1-c(\mathbf{r}))\Theta^4(\mathbf{r})+c(\mathbf{r})\int_S\psi(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}'\qquad\text{for }\mathbf{r}\in\mathcal{D}. \tag{1.1}$$

In (1.1) the integration for the collision term

$$\int_S\psi(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}',$$

where S is the unit circle and $d\mathbf{\Omega}'$ is Lebesgue measure normalized so that S has measure one. Hence, in terms of the direction cosines

$$\mu=\cos\theta,\eta=\sqrt{1-\mu^2}\cos\phi$$

the integral of a function g defined on S is

$$\int_S g(\mathbf{\Omega}')d\mathbf{\Omega}'=\frac{1}{2\pi}\int\int_{\mu^2+\eta^2\le1}\frac{g(\mu,\eta)}{\sqrt{1-\mu^2-\eta^2}}\,d\mu\,d\eta.$$

The intensity ψ is a function of a position variable $\mathbf{r}=(x,y)$ and $\mathbf{\Omega}=(\theta,\phi)$ is a direction vector on the unit sphere. The spectral albedo $0\le c(\mathbf{r})\le1$ is a property of the physical domain and is known. We will consider Dirichlet boundary conditions on the incoming radiation of the form

$$\psi(\mathbf{r},\Omega)=\Theta_0^4(\mathbf{r})\text{ for }\mathbf{r}\in\partial\mathcal{D}\text{ and }\mathbf{n}^T\mathbf{\Omega}<0, \tag{1.2}$$

where $\Theta_0\ge0$ is a given function on $\partial\mathcal{D}$ and $\mathbf{n}$ is the outward normal to $\partial\mathcal{D}$ at r. We assume that $\mathcal{D}$ is piecewise smooth and hence $\mathbf{n}$ is defined almost everywhere on $\partial\mathcal{D}$. If $0<c(\mathbf{r})<1$ then (1.1) has a unique solution for any given $\Theta\in C(\overline{\mathcal{D}})$ [28].

The temperature satisfies the normalized diffusion equation

$$\nabla_{\mathbf{r}}\cdot(\nabla_{\mathbf{r}}\Theta(\mathbf{r}))=\frac{1-c(\mathbf{r})}{N_c}\left(\Theta^4(\mathbf{r})-f(\mathbf{r})\right)\qquad\text{for }\mathbf{r}\in\mathcal{D} \tag{1.3}$$

where the flux f is defined by

$$f(\mathbf{r})=\int_S\psi(\mathbf{r},\mathbf{\Omega}')d\mathbf{\Omega}', \tag{1.4}$$

and N_c is the conduction-to-radiation parameter, [35], [34]. The boundary conditions for (1.3) are

$$\Theta(\mathbf{r})=\Theta_0(\mathbf{r})\text{ on }\partial\mathcal{D}. \tag{1.5}$$

1.2. Fixed point formulation. As with the one-dimensional case considered in [21] and [6] the system of equations (1.1) and (1.3) can be formulated as a fixed point problem in Θ alone.

$$\Theta=\mathcal{H}(\Theta). \tag{1.6}$$

The map $\Theta\to\mathcal{H}(\Theta)$ is computed by

1. solving (1.1) with boundary data (1.2) to obtain f,
2. using Θ and f to form the right side of (1.3), and
3. solving (1.3) subject to (1.5).

Our assumptions on c imply that the boundary value problem (1.1) – (1.2) has a unique solution, [28]. We define the solution operator for the transport equation by considering the boundary value problem

$$\mathbf{\Omega} \cdot \nabla_{\mathbf{r}} (\psi(\mathbf{r}, \mathbf{\Omega})) + \psi(\mathbf{r}, \mathbf{\Omega}) = (1 - c(\mathbf{r}))q(\mathbf{r}) + c(\mathbf{r}) \int_S \psi(\mathbf{r}, \mathbf{\Omega}') d\mathbf{\Omega}' \qquad \text{for } \mathbf{r} \in \mathcal{D} \tag{1.7}$$

subject to (1.2) and let $\mathcal{S}$ be the affine map that takes the data q to the flux f defined by (1.4). It is known that if Θ_0 is continuous, then $\mathcal{S}$ is a compact map on $C(\overline{\mathcal{D}})$, [28], where $\overline{\mathcal{D}}$ denotes the closure of $\mathcal{D}$.

Similarly, we let $\mathcal{G}$ be the solution operator for the diffusion equation. This means that $u = \mathcal{G}(p)$ is the solution of

$$\nabla^2 u = p$$

subject to (1.5). $\mathcal{G}$ is an affine compact map on $C(\overline{\mathcal{D}})$ [14]. With this notation,

$$\mathcal{H}(\Theta) = \mathcal{G}\left(\alpha \left[\Theta^4 - \mathcal{S}(\Theta^4)\right]\right), \tag{1.8}$$

where

$$\alpha(\mathbf{r}) = \frac{1 - c(\mathbf{r})}{N_c}.$$

Since $\mathcal{S}$ is bounded on $C(\overline{\mathcal{D}})$ and $\mathcal{G}$ is compact, $\mathcal{H}$ is a completely continuous map on $C(\overline{\mathcal{D}})$ if the boundary function Θ_0 is continuous on $\partial\mathcal{D}$.

Our numerical methods are Newton-like methods for the nonlinear equation

$$\mathcal{R}(\Theta) = \Theta - \mathcal{H}(\Theta) = 0. \tag{1.9}$$

We assume that the standard assumptions for local convergence of Newton's method hold.

ASSUMPTION 1.1.

1. *$\mathcal{R}$ is a Lipschitz continuously Fréchet differentiable map on $C(\overline{\mathcal{D}})$.*
2. *There is a solution $\Theta^* \in C(\overline{\mathcal{D}})$ of* (1.9) *and $\mathcal{R}'(\Theta^*)$ is nonsingular.*

2. Compactness and Multilevel Algorithms. The algorithms we discuss here are local in the sense that the initial iterate must be near the solution for the convergence analysis to be valid. We assume that initial iterates far from the solution are refined via a globalized nonlinear solve, such as a line search [20], on the coarse mesh.

Let $\{\mathcal{S}_h\}$ and $\{\mathcal{G}_h\}$ denote families of approximations to the transport solution operator $\mathcal{S}$ and diffusion solution operator $\mathcal{G}$. Typically the index h is a level of mesh refinement and $h_m = h_{m-1}/2$ and our goal is to solve the approximate equation

$$\mathcal{R}_{h_{min}}(\Theta) = \Theta - \mathcal{H}_{h_{min}}(\Theta) = 0 \tag{2.1}$$

for some small h_{min}. The two algorithms we describe in this section, Newton-GMRES and the Atkinson-Brakhage method solve (2.1) by an approximation of Newton's method. Moreover, both methods exploit the compactness properties of the infinite dimensional problem so that their performance does not depend on h_{min}.

If the transport equation (1.1) and the diffusion equation (1.3) can be simultaneously discretized in such a way that the resulting discrete approximation to $\mathcal{H}$

$$\mathcal{H}_h(\Theta) = \mathcal{G}_h\left(\alpha\left[\Theta^4 - \mathcal{S}_h(\Theta^4)\right]\right), \tag{2.2}$$

satisfies certain strong convergence and collective compactness properties, [2], then either the Atkinson-Brakhage, [5], [8], or a simple multilevel scheme based on applying a Newton-GMRES, [20], iteration on each level, [9], will give fast convergence.

In this section we give a formal description of these algorithms, describe the conditions on $\{\mathcal{S}_h\}$ and $\{\mathcal{G}_h\}$ that are needed for fast convergence, and give modest assumptions on the discretizations of the transport and diffusion equations that make these conditions hold.

2.1. Assumptions on the Discretizations. Our approach is to view all discrete maps as acting on the infinite dimensional space $C(\mathcal{D})$. We begin this subsection by giving a brief indication as to how this can be done. In § 3 we present more detail for a specific example.

If our maps $\{\mathcal{S}_h\}$ and $\{\mathcal{G}_h\}$ require nodal values of their input, it is simple to evaluate a continuous function Θ at the nodes of a discretization to provide the necessary data to $\{\mathcal{S}_h\}$ and $\{\mathcal{G}_h\}$. Similarly, if the output of $\mathcal{S}$, the flux, is given as a cell-average quantity, as it is in many transport codes, a simple averaging procedure (see § 3) can transform the cell-average quantity into the nodal values that $\mathcal{G}_h$ might require. Finally, $\mathcal{G}_h$, as realized by a finite-difference or finite-element approximation would give nodal values as output, which we will convert to a continuous function by linear or bilinear interpolation.

Recall that a family of linear operators $\{B_h\}_{h>0}$ on a Banach space X is *collectively compact* if

$$\cup_{h>0} B_h(\mathcal{B})$$

is precompact in X. Here $\mathcal{B}$ is the unit ball in X. $\{B_j\}_h$ is *strongly convergent* to an operator B if

$$\lim_{h\to 0} B_h u \to Bu$$

for all $u \in X$.

We make the following assumptions on the sequences $\{\mathcal{G}_h\}$ and $\{\mathcal{S}_h\}$.

ASSUMPTION 2.1. *There is $M_O > 0$ and a Banach spaces Y such that $C(\overline{\mathcal{D}}) \subset Y$ and for all $u \in C(\overline{\mathcal{D}})$*

1.

$$\|\mathcal{S}_h'(u)\|_{\mathcal{L}(C(\overline{\mathcal{D}}))} \le M_O \text{ and}$$

and $\mathcal{S}_h(u) \to \mathcal{S}(u)$ in the topology of Y.

2.

$$\|\mathcal{G}_h'(u)\|_{\mathcal{L}(Y,C(\overline{\mathcal{D}}))}, \|\mathcal{G}_h'(u)\|_{\mathcal{COM}(C(\overline{\mathcal{D}}))} \le M_O$$

$\mathcal{G}_h(u) \to \mathcal{G}(u)$ in the topology of $C(\overline{\mathcal{D}})$.

In Assumption 2.1 $\mathcal{L}$ and $\mathcal{COM}$ denote spaces of bounded and compact operators.

In the statement of Assumption 2.1 we refer to the Fréchet derivatives of the affine maps $\mathcal{S}_h$ and $\mathcal{G}_h$. $\mathcal{S}_h'$ and $\mathcal{G}_h'$ are simply solvers for problems with homogeneous boundary conditions. The choice

of space Y and the convergence properties of the transport solver depend on the discretization and we wish to treat the transport solver as a black box.

For example, using $Y = L^2(\mathcal{D})$ asks very little beyond stability of the transport solvers in part 1 of Assumption 2.1 and then part 2 can be verified for simple geometries [16]. For many discretizations, such as the one in § 3, $Y = C(\overline{\mathcal{D}})$ can be used [28], [38].

The Assumptions we make on the discretizations depend on both the transport and diffusion discretizations and solvers. These are sufficient to get the collective compactness conditions on $\mathcal{H}_h'$ needed for the fast solvers we discuss in § 2.2 and 2.3 to converge. We make this precise in Theorem 2.1.

THEOREM 2.1. *Assume that Assumption 1.1 and 2.1 hold. Then*

1. $\mathcal{H}_h(\Theta) \to \mathcal{H}(\Theta)$ *as* $h \to 0$ *for all* $\Theta \in C(\overline{\mathcal{D}})$
2. $\mathcal{H}_h$ *is a Lipschitz continuously Fréchet differentiable map on* $C(\overline{\mathcal{D}})$.
3. *For all* $u \in X$, $\mathcal{H}_h'(u)$ *converges strongly to* $\mathcal{H}'(u)$.
4. *For all* $M > 0$, *there is* γ *such that the*

$$\|\mathcal{H}_h'(\Theta_1) - \mathcal{H}_h'(\Theta_2)\| \leq \gamma \|\Theta_1 - \Theta_2\|$$

   for all $\|\Theta_1\|, \|\Theta_2\| \leq M$.
5. *For all* $h_0 > 0$ *and* $M > 0$, *the family of operators*

$$\{\mathcal{H}_h'(u)\}_{0<h<h_0, \|u\| \leq M}$$

   is collectively compact.

Proof. The convergence and differentiability assertions in parts 1, 2, and 3 follow trivialy from the assumptions of the theorem.

To verify part 4 we note that

$$\mathcal{H}_h'(\Theta)u = 4\mathcal{G}_h' \left(\alpha \left[\Theta^3 u - \mathcal{S}_h'(\Theta^3 u)\right]\right)$$

for all $\Theta \in C(\overline{\mathcal{D}})$. So if $\|\Theta_1\|, \|\Theta_2\| \leq M$ we have, since $\|\cdot\|_Y \geq \|\cdot\|$,

$$\|\mathcal{H}_h'(\Theta_1) - \mathcal{H}_h'(\Theta_2)\| \leq 4\alpha(M_0 + M_0^2)M^3$$

proving the assertion with $\gamma = 4\alpha(M_0 + M_0^2)M^3$.

Finally, if $\|\Theta\| \leq M$ and $q \in C(\overline{\mathcal{D}})$ then, by assumption,

$$\|\mathcal{S}_h'(\Theta^3 u)\|_{H^1} \leq M_0 M^3 \|u\|$$

Hence,

$$\|\mathcal{G}_h'\mathcal{S}_h'(\Theta^3 u)\|_Y \leq M^3 M_0^2 \|u\|$$

Hence

$$\|\mathcal{H}_h'(\Theta)u\|_Y \leq 4\alpha M^3(M_0 + M_0^2)$$

independently of h. This completes the proof. □

A consequence of Theorem 2.1, the Kantorovich theorem, [18], [20], and Assumptions 1.1 and 2.1 is

COROLLARY 2.2. *There is $h_0 > 0$ such that for all $0 < h < h_0$ there is a solution Θ_h to*

$$\Theta_h = \mathcal{H}_h(\Theta_h)$$

and

$$\lim_{h\to 0} \Theta_h = \Theta^*,$$

where Θ^* is a solution to (1.9) *that satisfies Assumption 1.1. Moreover there is $\delta_0 > 0$ such that*

$$\sup_{0<h<h_0, \|\Theta-\Theta^*\|<\delta_0} \|(I - \mathcal{H}_h'(\Theta))^{-1}\| < \infty.$$

2.2. Newton-GMRES. Newton-GMRES is the simplest of the two algorithms considered in this paper. Our formulation in this paper follows that in [6]. Since we will use this algorithm and the Atkinson-Brakhage algorithm in § 2.3 for solving the transport equation as well as solving (1.6) we will describe the algorithms in terms of a general nonlinear completely continuous fixed point problem

$$u = K(u). \tag{2.3}$$

Newton-GMRES is an implementation of Newton's method in which the linear equation for the step

$$s - K'(u)s = -(u - K(u))$$

is solved inexactly [12] by applying the GMRES [33] iteration to the linearized problem until the relative linear residual is small. This means that the linear iteration will terminate when

$$\|s - K'(u)s + F(u)\| \le \eta\|F(u)\|,$$

where F is the nonlinear residual

$$F(u) = u - K(u).$$

For fixed and sufficiently small values of the *forcing term* η, it is known [12], [20], [29], that the nonlinear iteration will converge q-linearly to the solution.

In practice the operator-vector product $K'(u)s$ is approximated by a forward difference at a cost of one additional evaluation of F (and hence of K), [20]. We do this in § 3 and can, therefore, compare algorithms by counting evaluations of K.

Our algorithms assume a sequence of approximations $\{K_h\}$ to K having collectively compact Fréchet derivatives $\{K_h'(u)\}_{h>h_0, u\in\mathcal{N}}$ where $h_0 > 0$ and $\mathcal{N}$ is a neighborhood of a solution u^* which satisfies the standard assumptions for quadratic convergence of Newton's method. For an approximate problem $u - K_h(u) = 0$ the Newton-GMRES algorithm is.

ALGORITHM 2.1. `ngmres`(K_h, u, ϵ, η)

1. *While* $\|F_h(u)\| > \epsilon$
   (a) *Solve* $s - K_h'(u)s = -F_h(u)$ *with GMRES*
   Terminate the GMRES iteration when $\|s - K_h'(u)s + F_h(u)\| \le \eta\|F_h(u)\|$
   (b) $u = u + s$

The forcing term η and the parameter ϵ in the termination criterion for the nonlinear residual could well depend on the initial iterate, [20], or the level h. In the numerical results in § 3, ϵ depends on the initial iterate and η is held constant.

Corollary 2.2 implies that the performance of the linear iteration in Algorithm `ngmres` is independent of h, and, therefore, the number of nonlinear iterations needed to reduce the residual by a fixed amount is also independent of h. This fact implies that a nested iteration scheme, in which the problem at level h is solved to convergence and the converged result used as the initial iteration at level $h/2$, will solve the problem to truncation error at $h = h_{min}$ at a total cost of a few fine-mesh function evaluations [5], [6].

The nested iteration form of Newton-GMRES, asking that the incoming residual be reduced by a factor of 10 at each level is

ALGORITHM 2.2. `nestgmb`$(\{K_h\}, h_{min})$

1. *Solve* $u = K_{h_0}(u)$*;* $h = h_0$
2. *While* $h > h_{min}$
   $h = h/2$*;* $\epsilon_h = \|F_h(u)\|/10$
   `ngmres`$(K_h, u, \epsilon_h, \eta)$

The first step in Algorithm `nestgmb`, the coarse mesh solve, is usually done to very high accuracy to extract as much information from the first mesh as possible. For example, if the discretizations are second order accurate, as they are for the problems considered here, and the coarse mesh solve is accurate to truncation error, then $\eta = 1/10$ and ϵ_h as specified in Algorithm `nestgmb` are conservative choices that should maintain accuracy to truncation error at all levels. The assumptions made in § 2.1 imply [9] that the number of GMRES iterations needed within `ngmres` and that the number of nonlinear iterations needed in step 2 of `nestgmb` will be independent of h. These expectations are supported by the numerical results in § 3.

2.3. Atkinson-Brakhage Iteration. The Atkinson-Brakhage algorithm for solution of linear compact fixed point problems of the form $u - Bu = f$ is a multilevel algorithm based on a sequence of solves at a sequence of levels $\{h_m\}_{m=0}^{\infty}$ using a collectively compact and strongly sequence $\{B_h\}$ of approximations to B. The collective compactness and strong convergence assumptions imply, [2], [5], that

$$I + (I - B_h)^{-1}B_h \to (I - B)^{-1}$$

in the operator norm. Hence, for sufficiently small h_0, the Richardson iteration

$$u_{n+1} = u_n - (I + (I - B_{h_0})^{-1}B_h)(u_n - B_h u_n - f)$$

will converge to the solution $u_h = (I - B_h)^{-1}f$ at level h for all $h \leq h_0$. This linear iteration requires only a coarse-mesh solve and a matrix-vector product.

For nonlinear problems the linear iteration is used to approximate a Newton step. We give the nested iteration form below.

ALGORITHM 2.3. `nestab`$(\{K_h\}, h_{min})$

1. *Solve* $u = K_{h_0}(u)$*;* $h = h_0$
2. *While* $h > h_{min}$
   (a) $h = h/2$*;* $\epsilon_h = \|F_h(u)\|/10$

(b) While $\|F_h(u)\| \geq \epsilon_h$

$$u = u = [I + (F'_{h_0})^{-1} K'_h(u)] F_h(\Theta)$$

A consequence of the assumptions in § 2.1 is that if the coarse mesh is sufficiently fine (*i. e.* h_0 sufficiently small) then only one pass through step 2(b) will be needed. Hence, we would expect the cost of a solution to truncation error to be two evaluations of K_h (one for $F_h(u)$ and the other for the difference approximation of $K'_h(u)$. The cost of evaluating F'_{h_0} is a few coarse-mesh function evaluations and can be neglected.

3. Numerical Examples. Our examples are in two space dimensions in the rectangular domain

$$0 \leq x \leq 1,\ 0 \leq y \leq 1.$$

The diffusion equation is

$$\frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} = \frac{1-c}{N_c}(\Theta^4 - f) \tag{3.1}$$

where

$$\Theta = \Theta(x, y), \quad f = f(x, y).$$

On the boundary we will consider the Dirichlet conditions

$$\begin{aligned} \psi(x, 0, \Omega_{in}) &= \Theta_0(x, 0),\ \psi(x, 1, \Omega_{in}) = \Theta_0(x, 1), \\ \psi(0, y, \Omega_{in}) &= \Theta_0(0, y),\ \psi(1, y, \Omega_{in}) = \Theta_0(y, 1). \end{aligned} \tag{3.2}$$

The radiative transport equation is

$$\mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \psi = cf + q \tag{3.3}$$

where

$$\begin{gathered} \psi = \psi(x, y, \mu, \eta), \\ q(x, y) = (1 - c(x, y))\Theta^4(x, y), \\ c = c(x, y) \end{gathered}$$

is the spectral albedo, and the flux in terms of the direction cosines

$$\mu = \cos\theta, \eta = \sqrt{1 - \mu^2}\cos\phi$$

is given by [24]

$$f = f(x, y) = \frac{1}{2\pi} \int\int_{\mu^2+\eta^2 \leq 1} \frac{\psi(x, y, \mu, \eta)}{\sqrt{1 - \mu^2 - \eta^2}}\, d\mu\, d\eta.$$

On the boundary the incoming intensities of radiation are given by

$$\begin{aligned} \psi(x, 0, \Omega_{in}) &= \Theta_0^4(x, 0),\ \psi(x, 1, \Omega_{in}) = \Theta_0^4(x, 1), \\ \psi(0, y, \Omega_{in}) &= \Theta_0^4(0, y),\ \psi(1, y, \Omega_{in}) = \Theta_0^4(y, 1). \end{aligned} \tag{3.4}$$

We will consider continuous boundary functions Θ_0 to show how the algorithm of the previous sections performs. We will also show how the algorithm can be modified to handle discontinuous boundary conditions.

3.1. Discretizations. Our discretizations use a uniform spatial mesh with meshsize h. We discretize the diffusion equation using finite differences in space. Since $\mathcal{G}_h$ must map C to itself, we must also specify our interpolation method. If we let D_h be the discretization of the Laplacian with boundary conditions (3.2), E_h the evaluation map that takes a continuous function to the vector of evaluations at the mesh points, and P_h the piecewise bilinear interpolation map onto C, we can define

$$\mathcal{G}_h = P_h D_h^{-1} E_h$$

and, if Θ_0 is continuous, satisfy the assumptions on $\mathcal{G}_h$ from § 2. In our computations D_h^{-1} was computed with a fast Poisson solver, [36].

Our assumptions on the transport discretization and solver are more modest, only that $\mathcal{S}_h$ is uniformly bounded in h as a map on C and that the approximation is convergent in some reasonable space Y. We point to [38] for an analysis of several discretizations that do this as well as a description of collective compactness properties of these discretizations. We selected our transport discretization for ease of implementation.

We discretize the transport equation (1.7) in a standard way, [25], using multi-dimensional discrete ordinates. The integrals with respect to $\mathbf{\Omega}'$ in equation (1.7) are discretized using level symmetric quadrature, [25], with the S_{16} ($N_a = 144$ total angular directions) for the angular discretization for all spatial meshes.

The resulting system of equations can be expressed as an affine fixed point problem for the flux alone

$$f = T_h(f) + g_h$$

[25], where g_h depends on the source term q and the boundary conditions. The solution operators for the discrete transport equation, S_h, are given by

$$S_h(q) = (I - T_h)^{-1} g_h$$

and are bounded independently of h, [3], [4], [28], [38]. The operators $\{T_h\}$ are not collectively compact, but are nearly so [28] and we can use both the Atkinson-Brakhage and Newton-GMRES algorithms as solvers with a modest modification.

The issue we must confront is that the nested iteration forms of the Atkinson-Brakhage and Newton-GMRES algorithms need to be modified because the interpolation P_h results in a loss of accuracy (from second order to first order in the transfer from $h \to h/2$). This may well be a result of the ray effects that motivated, in part, the work in [28], or of the lack of collective compactness. To remedy this we add a Nyström interpolation as a smoother at each level.

Note that $u = T_h(u)$ is a linear problem so the Atkinson-Brakhage is simply a preconditioned Richardson iteration and Newton-GMRES is simply GMRES. We express the algorithms in the nonlinear form because we will refer to them again later in this section. The smoothed formulations of `nestgmb` and `nestab` as applied to a sequence of maps $\{K_h\}$ are

ALGORITHM 3.1. `nestgmb_sm`(K, h_{min})

1. *Solve* $u = K_{h_0}(u)$*;* $h = h_0$
2. *While* $h > h_{min}$
   $h = h/2$*;* $u = K_h(u)$*;* $\epsilon_h = \|u - K_h(u)\|/10$
   `ngmres`$(K_h, u, \epsilon_h, \eta)$

and

ALGORITHM 3.2. `nestab_sm`(K, h_{min})

1. *Solve* $u = K_{h_0}(u)$*;* $h = h_0$
2. *While* $h > h_{min}$
   (a) $h = h/2$*;* $u = K_h(u)$*;* $\epsilon_h = \|u - K_h(u)\|/10$

   (b) While $\|u - K_h(u)\| \geq \epsilon_h$

$$u_h = u_h - [I + (I - K'_{h_0})^{-1} K'_h(u)](u - K_h(u))$$

To convert S_h to a map $\mathcal{S}_h$ on C we must convert the input from a continuous quantity to the cell average quantity used in the transport solve and convert the output back from a cell average to a continuous function. If we let $\hat{E}_h$ map continuous functions to average values on the cell with corners at

$$(ih, jh), ((i+1)h, jh), (ih, (j+1)h), ((i+1)h, (j+1)h)$$

by averaging the values at the corners and $\hat{P}_h$ take cell average quantities to continuous functions by computing interior nodal values by averaging the adjacent cell averages and using the boundary data for exterior nodes, then

$$\mathcal{S}_h = \hat{P}_h S_h \hat{E}_h$$

satisfies the assumptions in § 2 if Θ_0 is continuous.

The number of spatial mesh points was chosen to be $N_s + 1$ in the x direction and $N_s + 1$ in the y direction where $N_s = 2^n$. This way we can easily define nested levels, $h_n = 2^{-n}$, so that as we move from one level to the next the uniform mesh width is reduced by $1/2$. The coarsest mesh m_l was selected so that one iteration per level was needed in the Atkinson-Brakhage iteration and hence varies with the problem to be solved. On the finest mesh m_L, $N_s = 256$. Since we have $N_a = 144$ angular mesh points, this makes a total of approximately 9.4 million unknowns in solving the transport equation on the fine mesh and approximately 65000 unknowns in the diffusion equation. The cost of evaluating $\mathcal{G}_h$ is $O(N_s^2 \ln(N_s))$.

We evaluate the map S_h by solving the transport equation with the Atkinson-Brakhage method applied to the underlying affine fixed point problem for the flux. GMRES was used as the coarse mesh solver. While the collective compactness properties needed to apply the algorithm have not been theoretically verified in more than one space dimension, our numerical experiments indicate that the Atkinson-Brakhage algorithm performed very well. The cost of the transport solve to evaluate S_h is was $O(N_a N_s^2)$ floating point operations. The transport solve is the dominant cost of the entire computation.

The coarse mesh solves were done using Newton-GMRES with the initial iterate that is zero on the interior and satisfies the boundary conditions. The coarse mesh iteration was terminated when the residual was reduced by a factor of 10^{-6} from that of the initial iterate. Based on theory from one dimension [23], [31] we expect our discretizations $\mathcal{H}_h$ to be second-order accurate, for fixed N_a. Hence, as we refine the mesh by a factor of 2, we expect a reduction of 4 in the error. Therefore at the finer meshes we terminate iterations when the residual has been reduced by a factor of 10 with the view that this will safely ensure a reduction by a factor of 4 in the error. For all problems with continuous boundary conditions, we in fact obtain second order accuracy with these choices of stopping criteria. Test problem one is typical of the problems with continuous

boundary conditions. Table 3.1 shows the norm of the incoming residual, r_l, at each level as well as the ratio of this norm with the norm at the previous level. We clearly see the factor of 4 reduction.

TABLE 3.1
L_2-Norm of Incoming Residuals for Problem 1.

Level l	N_s	$R_l = \|r_l\|_2$	R_l/R_{l-1}
2	8	3.75D-03	
3	16	7.74D-04	0.21
4	32	2.20D-04	0.28
5	64	5.47D-05	0.25
6	128	1.38D-05	0.25
7	256	3.46D-06	0.25

We report on numerical work for ten problems in the following subsections. For these problems $N_c = .1$ and $c = .9$ is constant. Experiments with different values of N_c and c produced similar results. The six in § 3.2 have continuous boundary data and are solved with Newton-GMRES and the Atkinson-Brakhage algorithm as discussed in § 2. The four problems in § 3.3 have discontinuous boundary data and the Atkinson-Brakhage algorithm requires modification in order to perform properly.

All computations reported were done on a SUN SPARCstation 4 workstation running SunOS 5.4 version Generic_101945-41 with the SUN f77 compiler version 3.0.1.

3.2. Results with Continuous Data. For test problems 1, 2, and 3, $\Theta_0(x, y)$ is defined on the boundary of $(0, 1) \times (0, 1)$ by

$$\Theta_0(x, 0) = g(x), \quad \Theta_0(x, 1) = g(1 - x),$$
$$\Theta_0(0, y) = g(y), \quad \Theta_0(1, y) = g(1 - y)$$

where $g(z) = z$ for problem 1, $g(z) = (\cos(2\pi z) + 1)/2$ for problem 2, and $g(z) = -(z - 1)^2 + 1$ for problem 3.

For test problems 4, 5, and 6, $\Theta_0(x, y)$ is defined as the boundary part of the continuous function $g(x, y)$. $g(x, y) = (2 - x - y)/2$ for problem 4, $g(x, y) = (2 - x^2 - y^2)/2$ for problem 5, and $g(x, y) = (\sin(x) + y + 1)/3$ for problem 6.

In Table 3.2 we compare, both in terms of function evaluations and timings the performance of the Atkinson-Brakhage iteration and Newton-GMRES. The Atkinson-Brakhage method outperforms Newton-GMRES by a factor of 2–2.5. The timings nicely correspond to the function evaluation costs, as one would expect in view of the high cost of function evaluations for this problem.

3.3. Results with Discontinuous Data. For discontinuous boundary conditions we must adjust the interpolation maps. In the computations reported in this section, the discontinuities are at the corners. We modified the averaging in the interpolations from vertices to cell averages to only average vertices that do not correspond to discontinuities. With this in mind, we had to use the smoothed algorithms `ngmres_sm` and `nestab_sm` not only in the transport solve but also for the full problem.

TABLE 3.2
Timings (in minutes) and Function Evaluations

	Newton-GMRES		Atkinson-Brakhage		Ratios	
Problem	Time	FMF	Time	FMF	Time	FMF
1	22.8	4	11.8	2	1.9	2.00
2	24.3	4	15.5	2	1.6	2.00
3	28.1	5	13.1	2	2.2	2.50
4	22.4	4	12.7	2	1.8	2.00
5	28.1	5	13.4	2	2.1	2.50
6	23.9	4	13.4	2	1.8	2.00

With the smoothing, we indeed see second order accuracy. Without this smoother we see only first order accuracy. Thus, this smoother is needed in order to maintain the second order accuracy of the discretized maps $\mathcal{H}_h$. For test problem six, which has discontinuous boundary conditions and is defined in below, this smoothing affect can be seen in Tables 3.3 and 3.4. These tables show the norm of the incoming residual, r_l, at each level as well as the ratio of this norm with the norm at the previous level. We clearly see a factor of 4 reduction when using the smoother and a factor of 2 reduction when not using the smoother.

TABLE 3.3
L_2-Norm of Incoming Residuals for Problem 6 without Smoother.

Level l	N_s	$R_l = \|r_l\|_2$	R_l/R_{l-1}
2	8	1.68D-02	
3	16	7.93D-03	0.47
4	32	3.93D-03	0.50
5	64	1.98D-03	0.50
6	128	9.94D-04	0.50
7	256	4.99D-04	0.50

TABLE 3.4
L_2-Norm of Incoming Residuals for Problem 6 with Smoother.

Level l	N_s	$R_l = \|r_l\|_2$	R_l/R_{l-1}
2	8	7.76D-04	
3	16	2.00D-04	0.26
4	32	8.17D-05	0.41
5	64	2.57D-05	0.31
6	128	6.96D-06	0.27
7	256	1.78D-06	0.26

Test problems 7, 8, 9, and 10 are the discontinuous problems. For these problems, $\Theta_0(x, y)$ has the form

$$\Theta_0(x, 0) = \Theta_b, \quad \Theta_0(x, 1) = \Theta_t,$$
$$\Theta_0(0, y) = \Theta_l, \quad \Theta_0(1, y) = \Theta_r$$

where Θ_b, Θ_t, Θ_l, and Θ_r are constants equal to 0 or 1. The values of these constants for the discontinuous test problems are given in Table 3.5.

TABLE 3.5
2D Discontinuous Test Problems.

Problem	Θ_l	Θ_r	Θ_b	Θ_t
7	1.0	0.0	0.0	0.0
8	1.0	1.0	0.0	0.0
9	1.0	0.0	1.0	0.0
10	1.0	1.0	1.0	0.0

The evaluation counts and timings in Table 3.6 conform to the cost analysis above.

TABLE 3.6
Timings (in minutes) and Function Evaluations

	Newton-GMRES		Atkinson-Brakhage		Ratios	
Problem	Time	FMF	Time	FMF	Time	FMF
7	29.6	5	17.8	3	1.7	1.67
8	29.5	5	17.7	3	1.7	1.67
9	29.6	5	17.8	3	1.7	1.67
10	29.6	5	17.8	3	1.7	1.67

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