NOTICE

THIS DOCUMENT HAS BEEN REPRODUCED FROM MICROFICHE. ALTHOUGH IT IS RECOGNIZED THAT CERTAIN PORTIONS ARE ILLEGIBLE, IT IS BEING RELEASED IN THE INTEREST OF MAKING AVAILABLE AS MUCH INFORMATION AS POSSIBLE
NASA:CR-2002-211762
ICASE Report No. 2002-28

ICASE

P₁ Nonconforming Finite Element Method for the Solution of Radiation Transport Problems

Kab Seok Kang
ICASE, Hampton, Virginia

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited

August 2002

20021023 040
The NASA STI Program Office... in Profile

Since its founding, NASA has been dedicated to the advancement of aeronautics and space science. The NASA Scientific and Technical Information (STI) Program Office plays a key part in helping NASA maintain this important role.

The NASA STI Program Office is operated by Langley Research Center, the lead center for NASA’s scientific and technical information. The NASA STI Program Office provides access to the NASA STI Database, the largest collection of aeronautical and space science STI in the world. The Program Office is also NASA’s institutional mechanism for disseminating the results of its research and development activities. These results are published by NASA in the NASA STI Report Series, which includes the following report types:

- TECHNICAL PUBLICATION: Reports of completed research or a major significant phase of research that present the results of NASA programs and include extensive data or theoretical analysis. Includes compilations of significant scientific and technical data and information deemed to be of continuing reference value. NASA’s counterpart of peer-reviewed formal professional papers but having less stringent limitations on manuscript length and extent of graphics presentations.

- TECHNICAL MEMORANDUM: Scientific and technical findings that are preliminary or of specialized interest, e.g., quick release reports, working papers, and bibliographies that contain minimal annotation. Does not contain extensive analysis.

- CONTRACTOR REPORT: Scientific and technical findings by NASA-sponsored contractors and grantees.

- CONFERENCE PUBLICATIONS: Collected papers from scientific and technical conferences, symposia, seminars, or other meetings sponsored or cosponsored by NASA.

- SPECIAL PUBLICATION: Scientific, technical, or historical information from NASA programs, projects, and missions, often concerned with subjects having substantial public interest.

- TECHNICAL TRANSLATION: English-language translations of foreign scientific and technical material pertinent to NASA’s mission.

Specialized services that complement the STI Program Office’s diverse offerings include creating custom thesauri, building customized databases, organizing and publishing research results... even providing videos.

For more information about the NASA STI Program Office, see the following:

- Access the NASA STI Program Home Page at http://www.sti.nasa.gov

- Email your question via the Internet to helpdesk@sti.nasa.gov

- Fax your question to the NASA STI Help Desk at (301) 621-0134

- Telephone the NASA STI Help Desk at (301) 621-0390

- Write to NASA STI Help Desk, NASA Center for Aeronautics, Information, 7127, Standard Drive, Hanover, MD 21076-1320
P₁ Nonconforming Finite Element Method for the Solution of Radiation Transport Problems

Kab Seok Kang
ICASE, Hampton, Virginia
A NONCONFORMING FINITE ELEMENT METHOD FOR THE SOLUTION OF RADIATION TRANSPORT PROBLEMS

KAJ SEOK KANG

Abstract. The simulation of radiation transport in the optically thick flux-limited diffusion regime has been identified as one of the most time-consuming tasks within large simulation codes. Due to the multiaether complex geometry, the radiation transport system must often be solved on unstructured grids. In this paper, we investigate the behavior and the benefits of the unstructured $P_1$ nonconforming finite element method, which has proven to be flexible and effective on related transport problems, in solving unsteady implicit nonlinear radiation diffusion problems using Newton and Picard linearization methods.

Key words. nonconforming finite elements, radiation transport, inexact Newton linearization, multigrid preconditioning

Subject classification. Applied and Numerical Mathematics

1. Introduction. Radiation transport in astrophysical phenomena and inertial confinement fusion is often modeled using a diffusion approximation [12, 17, 18, 20, 21, 22, 24]. When the radiation field is not in thermodynamic equilibrium, a material-approximated set of nonlinear equations is used to describe energy transport. These equations are highly nonlinear and exhibit multiple time and space scales. Implicit integration methods are desired to overcome time step restrictions.

Nonconforming finite-element methods have been flexible and effective for incompressible fluid flow problems such as incompressible Stokes and Navier–Stokes equations [10, 11]. In the $P_1$ nonconforming method, the degrees of freedom lie on midpoints of edges. Therefore, the number of connections of all degrees of freedom with each other at at least four (four at interior edges and two at boundary edges) is the same number of connections of degrees of freedom in structured finite-difference methods. In contrast, in the $P_1$ conforming method, the number of connections of degrees of freedom is at least four except at boundary points, and depends on the triangulation and position of points. The number of connections of degrees of freedom determines the number of nonzero entries of generated matrices and plays an essential role in performance of parallel implementations of the communication required in kernel operations like matrix-vector multiplication. $P_1$ nonconforming methods generate matrices that have a constant small number of nonzero entries for each row, and therefore have some advantages in parallel implementations and performance.

Because many nonlinear elliptic problems are well solved by conforming finite element methods, nonconforming methods are still rare for such problems. However, nonconforming methods may resolve features of solutions of nonlinear problems not well represented by conforming methods. In this research, a nonconforming method is shown to resolve very sharp changes of energies on heterogeneous domains. The results are very similar to the solutions of the finite volume method with an edge-based flux limiter [19].

To solve nonlinear problems, one usually employs linearization techniques. Many models use Picard and Newton methods to linearize. Picard’s method is easy to understand and implement, but converges...
slowly. Newton's method has a second-order convergence rate but requires the Jacobian of the original nonlinear system. In many nonlinear problems, an inexact Newton method works well, with less storage and operation count expense [9]. In this paper, we study the behavior of these three methods on a model radiation transport problem.

Because the system generated from some linearization of the nonlinear problem is usually nonsymmetric, we use preconditioned GMRES [23]. As a preconditioner, we consider multigrid. Multigrid represents an important advance in algorithmic efficiency for the solution of large problems [2, 3, 4, 14, 19, 25].

To use multigrid, we need to define intergrid transfer operators between nonconforming finite-element spaces. Due to the non-nestedness of nonconforming spaces, there is no natural intergrid transfer operator. In previous studies of the nonconforming multigrid method, the average value of two adjacent elements is used to get the interpolated value at a node. Nonconforming multigrid with this intergrid transfer operator is a good solver for linear systems and some nonlinear systems with smooth nonlinear coefficients [1, 5, 6, 9, 15, 16]. However, this intergrid transfer operator does not preserve positivity of functions, which is an essential part of radiation transport problems because energy and temperature are always positive. Therefore, some nonlinear problems with discontinuous coefficients, bound constraints on solutions, and rapidly changing solutions, like the radiation transport problem, cannot use this intergrid transfer operator because the coarse level approximation obtained from the fine level approximation does not satisfy solution bounds, and one cannot generate the coarse level systems or solve the coarse level problems [18]. To overcome these difficulties, we use a new and simple intergrid transfer operator that preserves positivity and solves the above-mentioned problem. However, multigrid with this intergrid transfer operator is slower than with the previous operator. Therefore, we use the simple intergrid transfer operator to derive coarse level systems and the average value intergrid operator to solve the linear systems.

The rest of the paper is organized as follows. In section 2, we describe a model radiation transport and its P1 nonconforming discretization. In section 3, we consider a discretization in time, derive the linearization by Picard and Newton method, and describe the inexact Newton method. In section 4, we describe preconditioned GMRES and the nonconforming multigrid preconditioner. Numerical experiments are given in section 5.

2. Radiation transport model and P1 nonconforming discretization. Under the assumption of an optically thick medium (short mean free path of photons) a first-principles statement of radiation transport reduces to the radiation diffusion limit. A particular idealized dimensionless form of such a system, known as the "2T" model can be written as

\[
\frac{\partial E}{\partial t} - \nabla \cdot (D_\sigma \nabla E) = \sigma_a T^4 - E, \tag{22.1}
\]

\[
\frac{\partial T}{\partial t} - \nabla \cdot (D_T \nabla T) = - \sigma_a T^4 - E, \tag{22.2}
\]

with

\[
\sigma_a = \frac{I_0}{2T^4}, \quad D_\sigma(T, E) = \frac{1}{\sigma_a + \frac{1}{2} \mu \nabla E}, \quad \text{and} \quad D_T(T) = \sigma T^4 \tag{22.3}
\]

Here, \(E(x, t)\) represents the photon energy, \(T(x, t)\) is the material temperature, \(\sigma_a\) is the opacity and \(\mu\) is the material conductivity. In the non-equilibrium case, the nonlinear source terms on the right-hand side are nonzero and govern the transfer of energy between the radiation field and material temperature. Additional nonlinearities are generated by the particular form of the diffusion coefficients, which are functions of the \(E\) and \(T\) fields. In particular, the energy diffusion coefficient, \(D_\sigma(T, E)\) contains the term \(\nabla E\), which
Figs. 1. Domain of model problem.

Refers to the gradient of E. This limiting term is an artificial means of ensuring physically meaningful energy propagation speeds (i.e., no faster than the speed of light). The atomic number z is a material coefficient, and while it may be highly variable, it is only a function of position (i.e., \( z = f(x, y) \) in two dimensions).

The two model problems considered in this study are taken from [19] and depicted in Figure 1. We consider a unit square domain of similar material with atomic number \( z = 1 \) and a unit square domain of two dissimilar materials, where the outer region contains material with an atomic number of \( z = 1 \) and the inner region \( (1/3 < x < 2/3, 1/3 < y < 2/3) \) contains material with an atomic number of \( z = 10 \). The top and bottom walls are insulated and inlet and outlet boundaries are specified using mixed (Robin) boundary conditions, as shown in the figure. For convenience, we represent the boundary \( x = 0 \), \( 0 \leq y \leq 1 \) and \( x = 1 \), \( 0 \leq y \leq 1 \) by \( \Gamma_0 \), and otherwise by \( \Gamma_1 \). Then the boundary condition of the problem is

\[
\frac{\partial E}{\partial n} = 0, \quad \text{on} \quad \Gamma_0,
\]

\[
\frac{\partial E}{\partial n} = g, \quad \text{on} \quad \Gamma_0 - \Gamma_3,
\]

\[
\frac{\partial T}{\partial n} = 0, \quad \text{on} \quad \Gamma_0.
\]

where \( n \) is the local outward normal vector of the boundary.

Equations (2.2.1) and (2.2.2) form a system of coupled nonlinear partial differential equations which must be discretized in space and time. In this section, we consider a discretization in space and will consider a discretization in time in the next section.

The variational form of (2.2.1) and (2.2.2) can be written as follows. Find \( (E, T) \in (H^1(\Omega))^2 \) such that

\[
\int_{\Omega} \frac{\partial E}{\partial t} w dx + \int_{\Omega} D_{T} \nabla E \cdot \nabla w dx + \int_{\Gamma_1} \mathbb{I} E w ds = 0,
\]

\[
- \int_{\Omega} \sigma_s ((T)^4 - E) w dx - \int_{\Gamma_1} 2g w ds = 0,
\]

\[
\int_{\Omega} \frac{\partial T}{\partial t} w dx + \int_{\Omega} D_{T} \nabla T \cdot \nabla w dx - \int_{\Gamma_1} \sigma_s ((T)^4 - E) w ds = 0,
\]

for all \((w, \sigma) \in (H^1(\Omega))^2 \) and for all \( t \in [0, t_{\text{max}}] \).

We discretize \( \Omega \) by using a triangular grid consisting of triangles, shown in Figure 2. The grid is generated by connecting the midpoints of the edges of the triangles from the coarsest discretization \( T_0 \) which contains
edges and conforms to the material interface boundaries in such a way that no triangle edges cross this boundary. Let \( h_j \) and \( T_j \), \( j = 1, \ldots, J \), be given, where \( T_j \) is a partition of \( \Omega \) into triangles and \( h_j \) is the maximum diameter of the elements of \( T_j \).

Define the \( P_1 \) nonconforming finite element spaces

\[
V_j = \{ v \in L^2(\Omega) : v|_K \text{ is linear for all } K \in T_j, \quad v \text{ is continuous at the midpoints of interior edges} \}.
\]

Then the nonconforming finite element discretization of (2.24) and (2.25) can be written as: Find \( (E, T) \in (V_j \times [0, t_{\text{max}}])^2 \) such that

\[
\int_{0}^{1} \frac{\partial E}{\partial t} \triangledown v \, dx + \int_{\Gamma_0} D(E, T) \triangledown E \cdot \triangledown v \, ds + \int_{T_j} \frac{1}{2} E \, v \, dx
\]

\[= \int_{\Gamma_0} \sigma(T)(T_k)^4 - E_k \, v \, ds - \int_{T_j} 2 \rho u \, dx = 0, \]

\[\int_{0}^{1} \frac{\partial \phi}{\partial t} \triangledown v \, dx + \int_{\Gamma_0} D(v, T) \triangledown \phi \cdot \triangledown v \, ds - \int_{\Gamma_0} \sigma(T)(T_k)^4 - E_k \, v \, ds = 0, \quad (2.27)
\]

for all \( (u, v) \in V_j^2 \) and for all \( t \in [0, t_{\text{max}}] \).

In above equations, to perform the integration in space, we use a three-point quadrature rule on each triangle in \( T_j \). Because the points where the degrees of freedom are defined and the quadrature points of triangle are the same, we can easily compute the integration on each triangle and

\[
\int_{\Omega} D(x; \phi, \psi) \, dx = \frac{D(x)}{3} \delta_{\phi \psi}
\]

for all basis functions \( \phi, \psi \) of \( V \) and \( K \in T_j \). Also, because \( v_k \) is a piecewise constant on each triangle in \( T_j \) for all \( k \in V \), we compute \( v_k \) needed in \( D_k \) exactly.

3. Time integration and nonlinear iteration. In this section, we consider a discretization in time and three nonlinear iterations i.e., Newton, Picard and inexact Newton iteration.
The time derivatives are discretized as first-order backward differences, with lumping of the mass matrix, leading to an implicit scheme which requires the solution of a nonlinear problem at each time step. This approach is first-order accurate in time, and is chosen merely for convenience, since the principal objective is the study of the solution of the nonlinear system. Higher order temporal discretizations are demonstrated to be worthwhile in [18].

To solve the nonlinear problem (2.2.6) and (2.2.7) we consider the Picard linearization method and the Newton linearization method. In both methods, we need to solve linear systems to get corrections at each nonlinear iteration step.

The fully implicit Picard linearization method separates the operators into linear parts and nonlinear parts and all nonlinear parts are evaluated at the previous nonlinear iteration level, \( k - 1 \). This results in the following system of equations:

\[
\begin{align*}
\int_0^{T_k} \frac{E_k^a - F_k^a}{\Delta t} \, u \, dx + \int_0^{T_k} D_k^{a-1} \nabla E_k^a \cdot \nabla u \, dx &= \int_{T_k}^{1} E_k^a \, v \, dx, \\
- \int_0^{T_k} \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, v \, dx &= \int_{T_k}^{1} 2g \, u \, dx = 0, \\
\end{align*}
\]

\[
\int_0^{T_k} \frac{T_k^a - T_k^{a-1}}{\Delta t} \, v \, dx + \int_0^{T_k} D_k^{a-1} \nabla T_k^a \cdot \nabla v \, dx &= \int_{T_k}^{1} \nabla \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, v \, dx = 0.
\]

for all \((u, v) \in V^2\). Because (3.3.1) and (3.3.2) are linear systems in \((E_k^a, T_k^a)\), we can easily calculate their Jacobian.

To get the corrections \((\delta E, \delta T)\) in the Picard Method at level \( k \), we solve the following linear systems:

\[
\begin{align*}
\int_0^{T_k} \frac{\delta E}{\Delta t} \, u \, dx + \int_0^{T_k} D_k^{a-1} \nabla \delta E \cdot \nabla u \, dx &= \int_{T_k}^{1} \frac{1}{2} \delta E \, u \, dx, \\
- \int_0^{T_k} \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, \delta T \, dx &= F_k^{a-1} (u), \\
\int_0^{T_k} \frac{\delta T}{\Delta t} \, v \, dx + \int_0^{T_k} D_k^{a-1} \nabla \delta T \cdot \nabla v \, dx &= \int_{T_k}^{1} \nabla \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, \delta E \, v \, dx = F_k^{a-1} (v),
\end{align*}
\]

for all \((u, v) \in V^2\) where

\[
\begin{align*}
F_k^{a-1} (u) &= - \int_0^{T_k} E_k^a - F_k^a \, u \, dx - \int_0^{T_k} D_k^{a-1} \nabla E_k^a \cdot \nabla u \, dx \\
&\quad - \int_{T_k}^{1} \frac{1}{2} E_k^a \, v \, dx + \int_0^{T_k} \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, v \, dx + \int_{T_k}^{1} 2g \, u \, dx, \\
F_k^{a-1} (v) &= - \int_0^{T_k} T_k^a - T_k^{a-1} \, v \, dx - \int_0^{T_k} D_k^{a-1} \nabla T_k^a \cdot \nabla v \, dx \\
&\quad + \int_{T_k}^{1} \nabla \sigma_k^{a-1} \left( \left( T_k^{a-1} \right)^{1/2} I_k^{a-1} - E_k^a \right) \, v \, dx.
\end{align*}
\]

For the fully implicit Newton linearization method it is somewhat more complicated to compute the Jacobian at approximate solution points. To get the Jacobian we have to calculate the derivatives of the system with respect to \((\phi, \psi)\) for all basis functions in \(V^2 \times V^2\).
As the result of differentiation with respect to \((\phi, \theta)\), to get the corrections \((\delta E, \delta T)\) in Newton's Method at level \(k\), we solve the following linear systems.

\[
\begin{align*}
\int_D \delta E \, \text{d}x + \int_D D_{\phi}^a \delta E \cdot \nabla \text{d}x + \int_D D_{\phi}^b \delta E \cdot \nabla \text{d}x + \int_D D_{\phi}^c \delta E \cdot \nabla \text{d}x = \\
+ \int_D D_{\phi}^d \delta E \cdot \nabla \text{d}x + \int_D \frac{1}{2} \delta E \text{d}x \int_D \frac{1}{2} \delta E \text{d}x = F_{\phi}^{a-1}(u),
\end{align*}
\]

(3.3.7)

\[
\begin{align*}
\int_D \delta E \, \text{d}x + \int_D D_{\theta}^a \delta E \cdot \nabla \text{d}x + \int_D D_{\theta}^b \delta E \cdot \nabla \text{d}x + \int_D D_{\theta}^c \delta E \cdot \nabla \text{d}x = \\
+ \int_D D_{\theta}^d \delta E \cdot \nabla \text{d}x + \int_D \frac{1}{2} \delta E \text{d}x \int_D \frac{1}{2} \delta E \text{d}x = F_{\theta}^{a-1}(v),
\end{align*}
\]

(3.3.8)

for all \((u, v) \in V^2\) where

\[
\begin{align*}
D_{\phi}^a &= \left( \frac{\partial^2 E_{\phi}^a}{\partial \phi^2} \right) \nabla \nabla E_{\phi}^a \nabla \left( \frac{\partial^2 E_{\phi}^a}{\partial \phi^2} \right) \nabla E_{\phi}^a, \\
D_{\phi}^b &= \left( \frac{\partial^2 E_{\phi}^a}{\partial \phi \partial \theta} \right) \nabla \nabla E_{\phi}^a \nabla E_{\phi}^a, \\
D_{\phi}^c &= \left( \frac{\partial^2 E_{\phi}^a}{\partial \theta \partial \phi} \right) \nabla \nabla E_{\phi}^a \nabla E_{\phi}^a, \\
D_{\phi}^d &= \left( \frac{\partial^2 E_{\phi}^a}{\partial \theta^2} \right) \nabla \nabla E_{\phi}^a \nabla E_{\phi}^a,
\end{align*}
\]

\[
\begin{align*}
D_{\theta}^a &= \left( \frac{\partial^2 E_{\theta}^a}{\partial \theta^2} \right) \nabla \nabla E_{\theta}^a \nabla E_{\theta}^a, \\
D_{\theta}^b &= \left( \frac{\partial^2 E_{\theta}^a}{\partial \theta \partial \phi} \right) \nabla \nabla E_{\theta}^a \nabla E_{\theta}^a, \\
D_{\theta}^c &= \left( \frac{\partial^2 E_{\theta}^a}{\partial \phi \partial \theta} \right) \nabla \nabla E_{\theta}^a \nabla E_{\theta}^a, \\
D_{\theta}^d &= \left( \frac{\partial^2 E_{\theta}^a}{\partial \phi^2} \right) \nabla \nabla E_{\theta}^a \nabla E_{\theta}^a.
\end{align*}
\]

where \(\frac{\partial^2 E_{\phi}^a}{\partial \phi^2} \nabla \nabla E_{\phi}^a \nabla E_{\phi}^a\) can be easily evaluated on each triangle in \(T_j\).

After linearization, we have to solve the linear systems

\[
J^{a-1} \begin{pmatrix} \delta E \\ \delta T \end{pmatrix} = \begin{pmatrix} F_{\phi}^{a-1} \\ F_{\theta}^{a-1} \end{pmatrix}
\]

(3.3.9)

for each step where \(J^{a-1}\) is a Jacobian, which is computed by Picard's method or Newton's method.

In either method, we need for robustness to control the step length \(\alpha\) where

\[
\begin{align*}
E_{\phi}^{a-1} &= E_{\phi}^{a-1} - \alpha \frac{\delta E}{\delta T}.
\end{align*}
\]

In this study, we control the step length by simply halving \(\alpha\) until the residual of the updated solution is less than the previous residual. In this control, we sometimes fail to get a proper step length, so we stop at a fixed step length and perform the next nonlinear iteration. If the number of failures exceeds a fixed number, then we go to next time steps by using the best approximation, which has the smallest nonlinear residual.

**Remark 3.1** The Newton method has, asymptotically, a second order convergence for nonlinear problems and the Picard method has only a first order convergence. However, the resulting linear problem of the Picard method is easier solved than that of the Newton method because the Picard method lacks the correction term as described in ref. [7].

To improve the efficiency of the Newton method, we can use an inexact Newton method [6]. When the Newton iteration is "far" from convergence (i.e., the residual is large) there is no reason to solve the linear system accurately. However, when the Newton iteration is "close" (i.e., the residual is "small") the convergence rate of Newton's method is tightly coupled to the accuracy of the linear solution. To adjust the amount of work done in the linear solve (via a convergence tolerance) we employ an inexact Newton method.
In the inexact Newton approach, the convergence criteria for the linear solver is proportional to the residual in the nonlinear iteration. In equation form this is

$$\left\| F^{s+1} \left( \frac{\delta F}{\delta T} \right) - \left( \frac{F^s}{F^s} \frac{\delta F}{\delta T} \right) \right\| \leq \gamma_1 \left\| \left( \frac{F^s}{F^s} \frac{\delta F}{\delta T} \right) \right\|,$$  

(3.3.10)

where $\gamma_1 = 1.0 \times 10^{-2}$ is the value used in this study unless otherwise noted. We note that [13] shows how to adaptively select $\gamma_1$ to recover asymptotically full second order convergence.

4. PGMRES and multigrid preconditioning. In this section, we explain PGMRES, which is a combination of a Krylov-based linear iterative method, and multigrid, which is well known as a successful preconditioner, as well as a scalable solver even in unaccelerated form, for many problems.

GMRES [23] is a well known solver for non-Hermitian problems. In practice, GMRES can be restarted after $m$ steps, where $m$ is some fixed integer parameter, to save storage by accepting a generally less rapid convergence.

We describe the restarted PGMRES for solving

$$Ax = b$$  

(4.4.1)

with preconditioning matrix $B_j$.

PGMRES(m) Algorithm 4.1.
(1) Start: Choose $x_0$ and compute $r_0 = B_j(b - A_jx_0)$. $\alpha = \|r_0\|$ and $\beta = \alpha / 3$.
(2) Iterate: For $j = 1, \ldots, m$ do:
   Compute $w = B_jA_jx_j$.
   For $i = 1, \ldots, j$ do:
   $$h_{j,i} = (w, v_i)$$
   $$w = w - h_{j,i}v_i$$
   Enddo.
   Compute $h_{j+1,i} = \|w\|$ and $v_{j+1} = w / h_{j+1,i}$.
Enddo.
(3) Form the approximation solution:
   Define $V_m = \{v_1, \ldots, v_m\}$.
   $$\hat{N}_m = \{h_{j,i} \mid j, i : 1 \leq j \leq m\}$$
and set $x_m = x_0 + V_m y_m$ where $y_m$ minimizes $\beta e_1 - \hat{N}_m y$, $y \in R^n$.
(4) Restart:
   Compute $r_m = B_j(b - A_jx_m)$, if satisfied then stop
   else compute $x_0 := x_m$, $\beta = \|r_m\|$ and $\alpha = \alpha / 3$ and go to (2).
Arnoldi iteration constructs an orthogonal basis of the left preconditioned Krylov subspace

$$\text{Span}(\beta_1, B_jA_jr_0, \ldots, (B_jA_j)^{n-1}r_n)$$

It uses a modified Gram-Schmidt process, in which the new vector to be orthogonalized is obtained from the previous vector in the process. All residual vectors and their norms that are computed by the algorithm.
correspond to the preconditioned residuals, namely, \( z_m = B_j(b - A_jx_m) \), instead of the original (unpreconditioned) residual \( b - A_jx_m \). In addition, there is no easy access to these unpreconditioned residuals, unless they are computed explicitly. So we monitor these preconditioned residuals to stop PGMRES iteration to solve linear problem.

Next, we consider Multigrid Preconditioner \( B_j \).

To define a multigrid method, we need to define intergrid transfer operators - between nonconforming finite element spaces. Due to the non-nestedness of nonconforming spaces, there is not a natural intergrid transfer operator. In previous studies of nonconforming multigrid methods[1, 5, 6, 9], average value of two adjacent elements are used to set the value of a node. A nonconforming multigrid method with this intergrid transfer operator is a good solver for linear systems and some nonlinear systems that have smooth nonlinear coefficients.

To get the coarse level approximate linear system for (3.3.7), we need coarse level approximations of \((E_h^{(k+1)}, T_h^{(k+1)})\) and \((E_h^{(k)}, T_h^{(k)})\). If the approximate solution \((E_h^{(k+1)}, T_h^{(k+1)})\) varies rapidly in space, then some coarse level approximations of \((E_h^{(k+1)}, T_h^{(k+1)})\) may have negative values. However \((E_h^{(k+1)}, T_h^{(k+1)})\) are required to be positive for the computation of \(D_h^{(k+1)}\). Either we cannot generate the coarse level systems or they may become nearly singular, making it hard to solve the coarse level problems.

To overcome these difficulties, we use a new and simple intergrid transfer operator called the covolume-based intergrid transfer operator, which preserves only piecewise constant functions [15]. It is well known that, to get a good convergence factor in multigrid algorithms, intergrid transfer operators should preserve higher order functions [16]. Therefore the multigrid method with this intergrid transfer operator converges slowly compared to average value intergrid operator to solve linear systems. However preservation of positivity of nodal values of the fields is critical. So, we use the covolume-based intergrid transfer operator to obtain the coarse level systems and the average value intergrid operator to interpolate the solution between levels (coarse-to-fine and fine-to-coarse) when solving the linear systems in Picard method or Newton's method.

Let \( A_j : (V_j)^2 \to (V_j)^2 \), \( j = 1, \ldots, J \) be the discretization operator on level \( j \) and \( I_j : (V_{j-1})^2 \to (V_j)^2 \), \( j = 2, \ldots, J \) be the coarse-to-fine intergrid transfer operator. Also, we define the fine-to-coarse intergrid transfer operator \( F_{j-1} : (V_j)^2 \to (V_{j-1})^2 \) by

\[
(I_j,v,w) = (v, F_j^{(g)} w) \quad \forall v \in (V_j)^2 \quad \forall w \in (V_j)^2
\]

Finally, let \( R_j : (V_j)^2 \to (V_j)^2 \) for \( j = 1, \ldots, J \) be the linear smoothing operators, let \( R_j^{(i)} \) denote the adjoint of \( R_j \) with respect to the \( (\cdot , \cdot ) \) inner product, and define

\[
R_j^{(i)} = \begin{cases} R_j & \text{if } i \text{ is odd} \\ R_j^T & \text{if } i \text{ is even} \end{cases}
\]

Following [2], the multigrid operator \( B_j : (V_j)^2 \to (V_j)^2 \) is defined recursively as follows.

**Multigrid Algorithm 4.2** Let \( 1 \leq j \leq J \) and \( p \) be a positive integer. Set \( B_1 = A_1^{-1} \). Assume that \( B_j \) has been defined and define \( B_{j+1} \) for \( p \in (V_j)^p \) by

1. Set \( x^0 = 0 \) and \( q^0 = 0 \).
2. Define \( x^l \) for \( l = 1, \ldots, ml(j) \) by
   
   \[
x^l = x^{l-1} + R_j^{(l-1)} (g - A_j x^{l-1})
   \]
(3) Define $y^{m(j)} = y^{m(j)} + I_2 y^p$, where $y^p$ for $j = 1, \ldots, p$ is defined by

$$y^p = y^{p-1} - B_{p-1} [F_{p-1}(y - A_{p-1} y^{m(j)})]$$

(4) Define $y^l$ for $l = m(j) + 1, \ldots, 2m(j)$ by

$$y^l = y^{l-1} - B_l [F_l(w - A_l y^{m(j)})]$$

(5) Set $B_{m(j)} y = y^{2m(j)}$.

In Multigrid algorithm 4.2, $m(j)$ gives the number of pre- and post-smoothing iterations and can vary as a function of $j$. If $p = 1$, we have a V-cycle multigrid algorithm. If $p = 2$, we have a W-cycle multigrid algorithm. Other versions of multigrid algorithms without pre- or post-smoothing iterative can be analyzed similarly. A variable V-cycle multigrid algorithm is that for which the number of smoothing $m(j)$ increases exponentially as $j$ decreases (i.e., $p = 1$ and $m(j) = 2^j$).

**Remark 4.1.** One can use the multigrid algorithm to solve the systems as a free-standing iterative method. Usually, one uses V-cycle and W-cycle multigrid algorithms to this end and uses V-cycle and variable V-cycle multigrid methods as preconditioners of Krylov-type methods such as PCG, because, when $A_j$ is symmetric positive definite, the V-cycle multigrid operator $B_j$ is a symmetric positive definite operator on $(V_j)^p$, but the W-cycle multigrid operator is not in general [3]. Many researchers have shown convergence of W-cycle multigrid for the nonconforming and conforming cases and of V-cycle multigrid for the conforming case are good preconditioners [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. In this problem, we use V-cycle multigrid method as a preconditioner of GMRES.

5. Algorithm performance and results. In this section, we study the performance of the Newton–Picard and Inexact Newton methods on $P_1$ nonconforming finite element method on two model problems with the only difference between the problems being homogeneity. In the two examples, we use the same triangulations, namely 12800 triangles, 19296 edges, and 6497 vertices. Because nodes are on midpoints of edges in a $P_1$ nonconforming method, the number of degrees of freedom of this problem is 38992.

For problem 1, we consider a homogeneous material with atomic number $z = 1$ and $\kappa = 0.01$ on the whole domain. The initial conditions are $E^o = 1.0 \times 10^{-3}$ and $T^o = (E^o)^{0.3}$. The problem is run to time $t = 3.0$ with nonlinear convergence tolerance within a time step is defined as $|F(w)|_1 \leq 1.0 \times 10^{-6}$ for problem 1. We run with several time steps of 0.001, 0.002, 0.003, and 0.01.

In Figure 3, we plot the contours of temperature $T$ at $t = 1.0, 2.0, 3.0$. Table 1 compares linear solve requirements and nonlinear iterations. Figure 4 depicts the nonlinear convergence behavior of Newton method, Picard method, and Inexact Newton method at time $t = 1.0$.

Figure 3 shows that contours of temperature propagate parallel to the inlet boundary and reproduce on an unstructured grid. The propagation of the one-dimensional case. Table 1 and Figure 4 show that Newton's Method is very efficient compared to Picard's method, and slightly more efficient compared to the Inexact Newton method, in terms of nonlinear iterations per time step.

Inexact Newton needs more nonlinear iterations in comparison to Newton's method, but the best performance overall because this method needs the smallest number of linear iterations. Also, Table 1 shows that the number of linear iterations in each nonlinear iteration of the Picard method is smaller than that of the Newton Method. This means that the linear systems from Picard's method are more easily solved than the linear systems from Newton method.

In Table 2, we report the accuracy as a function of time step by the $L^2$ error of the solution which is defined as $\|u - u_{\text{ref}}\|_2$, where $u_{\text{ref}}$ is obtained by using a time step 0.0001. This result shows that the $L^2$ error in time is first order.
For problem 2, we consider an inhomogeneous material with atomic number $z = 10$ inside the box and $z = 16$ outside, as shown in Figure 5. We changed the nonlinear convergence tolerance within a time step to be $||P(u^*)||_2 \leq 1.0 \times 10^{-4}$ to reduce the simulation time.

In Figure 6, we plot the contour of temperature $T$ at $t = 10, 20, 30, 40, 50$. Table 3 compares linear time requirements, linear and nonlinear iterations, and number of failures to meet the convergence tolerance. Figures 8, 9, 10 demonstrate the nonlinear convergence behavior of the Newton and Picard and mixture Newton methods at times $t = 10, t = 25$, and $t = 40$.

As energy propagates, temperatures rapidly change near the front and near the layer where the two different materials meet. As more time passes, the temperature smoothly propagates. Figures 8, 9, 10 show that there are many step length controls to get the solution of the nonlinear problem when the solution changes rapidly ($t = 10, t = 25$) but there is no need for step length control when the solution is smooth ($t = 40$) in any of the three methods.
Table 1: Algorithm performance as a function of time step for problem 1 and time period of 3.0

<table>
<thead>
<tr>
<th>Method</th>
<th>dt</th>
<th># of dt</th>
<th>tot #</th>
<th>ave #</th>
<th>ave lin</th>
<th>hnn dt</th>
<th>ave #</th>
<th>ave # lin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Newton method</td>
<td>0.001</td>
<td>3600</td>
<td>4225</td>
<td>2.1</td>
<td>40981</td>
<td>16.6</td>
<td>8.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.002</td>
<td>1500</td>
<td>4116</td>
<td>2.7</td>
<td>38970</td>
<td>26.0</td>
<td>9.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.005</td>
<td>600</td>
<td>2120</td>
<td>3.5</td>
<td>28167</td>
<td>46.8</td>
<td>13.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>360</td>
<td>1334</td>
<td>4.4</td>
<td>21986</td>
<td>73.7</td>
<td>16.5</td>
<td></td>
</tr>
<tr>
<td>Picard Method</td>
<td>0.001</td>
<td>3600</td>
<td>24235</td>
<td>5.3</td>
<td>181227</td>
<td>60.4</td>
<td>7.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.002</td>
<td>1500</td>
<td>15389</td>
<td>10.3</td>
<td>126132</td>
<td>84.1</td>
<td>8.2</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.005</td>
<td>600</td>
<td>7764</td>
<td>13.0</td>
<td>70165</td>
<td>116.9</td>
<td>9.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>360</td>
<td>5320</td>
<td>17.7</td>
<td>46194</td>
<td>154.0</td>
<td>8.7</td>
<td></td>
</tr>
<tr>
<td>Inexact Newton Method</td>
<td>0.001</td>
<td>3600</td>
<td>8648</td>
<td>2.9</td>
<td>28468</td>
<td>9.5</td>
<td>3.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.002</td>
<td>1500</td>
<td>4534</td>
<td>3.0</td>
<td>15928</td>
<td>10.6</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.005</td>
<td>600</td>
<td>2254</td>
<td>3.8</td>
<td>9878</td>
<td>16.6</td>
<td>4.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.01</td>
<td>360</td>
<td>1450</td>
<td>4.8</td>
<td>7761</td>
<td>25.9</td>
<td>5.4</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: $L_1$-error at $t = 3.0$

<table>
<thead>
<tr>
<th>time steps</th>
<th>$L_1$-error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.00084</td>
</tr>
<tr>
<td>0.002</td>
<td>0.00756</td>
</tr>
<tr>
<td>0.005</td>
<td>0.04060</td>
</tr>
<tr>
<td>0.01</td>
<td>0.06776</td>
</tr>
</tbody>
</table>

Figure 6 shows that the solution of the nonconforming finite element method is very similar to the solution of finite volume method with edge-based flux limiters [26].

In the aspect of performance, the behavior of problem 2 is similar to problem 1 with the exception that problem 1 does not require step length control.

To estimate the accuracy as a function of time step size, we report the $L_1$-error of the solution in Table 4 (based on an accurate solution with $dt = 0.001$). The relative $L_1$-error of simulations with $dt = 0.002$, 0.005, 0.01 compared to the $L_1$-error of $dt = 0.001$ is plotted as a function of time in Figure 7. These results show that the $L_1$-error in time is first order at the beginning of simulation until $t = 3.0$ but gradually deteriorates. This deterioration may be introduced by the nonlinear convergence error within a time step because the accumulation of the nonlinear convergence error will dominate other errors (space and time discretization error) as time steps grow. If we use a finer nonlinear convergence tolerance, then we can delay this deterioration to longer time.

6. Conclusions. We solved unsteady implicit nonlinear radiation diffusion problems by an unstructured $P_1$ nonconforming finite element method. $P_1$ nonconforming finite element methods resolve very sharp changes of energies in the heterogeneous domain similarly to results of the finite volume method with an edge-based flux limiter. The Inexact Newton method has the best performance overall and Preconditioned GMRES with nonconforming multigrid preconditioners to solve linear problems works well. In $P_1$ nonconforming multigrid, the volume-based intergrid transfer operators are useful to solve radiation transport.
problems because the positivity preserving property is needed.

Acknowledgments. The author would like to thank D. E. Keyes of Old Dominion University for his valuable advice in the preparation of this paper.
REFERENCES


Fig. 5. Domain of inhomogeneous material

(a) $t = 10$

(b) $t = 20$

(c) $t = 30$

(d) $t = 40$

(e) $t = 50$

Fig. 6. Contour of Temperature of Problem 2.
Table 3. Algorithm performance as a function of time step for problem 2 and time period of 5.0

| Method   | dt   | # of dt | tot # nonlin hits | ave # nonlin hits | tot # linear | ave # linear | ave # lin/| |
|----------|------|---------|-------------------|-------------------|--------------|--------------|------------|
|          |      |         |                   |                   |              |              |           |
| Newton   | 0.001| 5000    | 11980             | 2.4               | 117186       | 23.6         | 9.9        |
| method   |      |         |                   |                   |              |              |           |
|          | 0.002| 2500    | 6745              | 2.7               | 83439        | 33.5         | 12.4       |
|          | 0.006| 1000    | 4314              | 4.3               | 76436        | 76.4         | 17.7       |
|          | 0.01 | 500     | 2973              | 6.0               | 68770        | 137.5        | 23.1       |
| Picard   | 0.001| 5000    | 34074             | 6.8               | 274452       | 54.9         | 8.1        |
| Method   |      |         |                   |                   |              |              |           |
|          | 0.002| 2500    | 21391             | 8.6               | 264772       | 81.9         | 9.6        |
|          | 0.006| 1000    | 12083             | 12.1              | 145675       | 145.9        | 12.1       |
|          | 0.01 | 500     | 7891              | 15.8              | 105284       | 210.5        | 13.3       |
| Implicit | 0.001| 5000    | 11701             | 2.3               | 42069        | 8.5          | 3.6        |
| Newton   |      |         |                   |                   |              |              |           |
|          | 0.002| 2500    | 7045              | 2.8               | 32703        | 13.1         | 4.6        |
| Method   | 0.006| 1000    | 4559              | 4.6               | 30183        | 30.2         | 6.6        |
|          | 0.01 | 500     | 3259              | 6.5               | 27516        | 55.0         | 8.4        |

Table 4. $L^1$-error at $t = 5.0$

<table>
<thead>
<tr>
<th>time steps</th>
<th>$L^1$-error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.00617</td>
</tr>
<tr>
<td>0.002</td>
<td>0.00619</td>
</tr>
<tr>
<td>0.005</td>
<td>0.00648</td>
</tr>
<tr>
<td>0.01</td>
<td>0.00638</td>
</tr>
</tbody>
</table>

Fig. 7. The relative $L^1$-error compared with $L^1$-error of $dt = 0.001$ ($L^1$-error $dt = 0.001$) vs $dt$. First order, $dt = 0.002$, $dt = 0.005$, $dt = 0.01$. $dt = 0.001$. $L^1$-error $dt = 0.001$ $x$ $0.001/dt$. 

10
Fig. 4: Convergence plot at time $t = 1.0$.
FIG 9. Convergence plot at time $t = 2.5$. 

- Newton Method
- Picard Method
- Inexact Newton Method
Fig. 10. Convergence plot at time $t = 4.0$. 

- Newton Method
- Picard Method
- Inexact Newton Method
**REPORT DOCUMENTATION PAGE**

1. **REPORT TYPE**
   - Contractor Report

2. **REPORT DATE**
   - August 2002

3. **REPORT NUMBER**
   - ICASE Report No. 2002-26

4. **AUTHOR(S)**
   - Kuh Seok Kang

5. **PUBLICATION DATE**
   - August 2002

6. **SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**
   - National Aeronautics and Space Administration
   - Langley Research Center
   - Hampton, VA 23681-2199

7. **ABSTRACT**
   - The simulation of radiation transport in the optically thick, diffusion-limited regime has been identified as one of the most time-consuming tasks within large-scale simulation codes. Due to the complexity of nearly geometrical transport systems, the radiation transport operators must often be solved on unstructured grids. The paper investigates the behavior and robustness of the unstructured P1 nonconforming finite element method with a novel transport method, which has proved to be flexible and effective for related transport problems, in solving this system. The paper presents the transcription of radiation diffusion problems using Newton and Picard methods.

8. **FUNDING NUMBERS**
   - ICASE Report No. 1997-15
   - NASA CR 2002-211762

9. **DISTRIBUTION/AVAILABILITY STATEMENT**
   - Uncontrolled, Unlimited
   - Distribution: Nonstandard
   - Availability: NASA-CASI (01/04/97-01/03/98)

10. **DISTRIBUTION CODE**
    - ICASE Report No. 2002-26

11. **SUBJECT TERMS**
    - Nonconforming finite element method, radiation transport, reactor analysis, optimization, parallel preconditioning

**REMARKS**

The simulation of radiation transport in the optically thick, diffusion-limited regime has been identified as one of the most time-consuming tasks within large-scale simulation codes. Due to the complexity of nearly geometrical transport systems, the radiation transport operators must often be solved on unstructured grids. In this paper, we investigate the behavior and robustness of the unstructured P1 nonconforming finite element method, which has proved to be flexible and effective for related transport problems, in solving this system. The paper presents the transcription of radiation diffusion problems using Newton and Picard methods.
REPRODUCTION QUALITY NOTICE

We use state-of-the-art high speed document scanning and reproduction equipment. In addition, we employ stringent quality control techniques at each stage of the scanning and reproduction process to ensure that our document reproduction is as true to the original as current scanning and reproduction technology allows. However, the following original document conditions may adversely affect Computer Output Microfiche (COM) and/or print reproduction:

- Pages smaller or larger than 8.5 inches x 11 inches.
- Pages with background color or light colored printing.
- Pages with smaller than 8 point type or poor printing.
- Pages with continuous tone material or color photographs.
- Very old material printed on poor quality or deteriorating paper.

If you are dissatisfied with the reproduction quality of any document that we provide, particularly those not exhibiting any of the above conditions, please feel free to contact our Directorate of User Services at (703) 767-9066/9068 or DSN 427-9066/9068 for refund or replacement.

END SCANNED DOCUMENT