A PARALLEL PRECONDITIONED CONJUGATE GRADIENT FOR THE SCHUR COMPLEMENT IN NON-LINEAR HEAT CONDUCTION PROBLEMS

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ABSTRACT

A computational strategy for nonlinear finite element computations on local-memory multiprocessor is presented. The proposed strategy exploits all the parallelism inherent in the finite element methodology. The method is based on a fine domain decomposition that is mapped onto the set of local memory processors. The finite element equations are constructed using a form of one-way dissection. Within each processor a direct method is applied for the solution of its linearized subsystem while the preconditioned conjugate gradient is applied to the Schur complement. A numerical test experiment is given and the results are discussed.

INTRODUCTION

In view of the size and structure of the problem, finite element analysis is a promising candidate for parallel and distributed computations. Until recently, most increases in the speed of finite element computations come via the speed of vector processors. Now, the true potential for execution time improvement lies in concurrent multiprocessors. "A multiprocessor is a computer with two or more central processing units, each of which executes instructions independently of the others except when a processor needs to communicate or synchronize with one or more of the others" [1].

In this work we consider the local-memory multiprocessors where each processor has its independent attached memory. communication with other processors is done by sending or receiving messages through an interconnect scheme.

Farhat et al. [2] have proposed a computational algorithm based on a direct method for solving structural mechanics linear problems on local-memory multiprocessors. Recently, Farhat and Crivelli [3] have designed a computational strategy for nonlinear finite element computations that can be applied on shared-memory or local-memory multiprocessors. In this strategy, explicit computations are carried out at the element level and implicit computations at the subdomain level. Also Wait and El Attar [4], have proposed an element - by - element parallel technique on local-memory transputer architecture.

In this paper, a parallel computation strategy for nonlinear finite element analysis is presented. The domain over which the finite element solution is required is decomposed into a number of subdomains, then the equations are constructed in parallel using a form of one-way nested dissection [5, 6]. The aim of nested dissection is the partitioning of the main linearized system into two subsystems. The first subsystem is solved concurrently using direct schemes (each processor factorizes and solves its own part of the subsystem). The solution of the entire problem is completed by taking the interaction between the subdomains into account. This yields what is called the "Schur Complement". This reduced subsystem is solved using the preconditioned conjugate gradient (PCG) iterative method. The use of an iterative scheme (within each nonlinear iteration) permits no explicit computation nor storage of the Schur complement.

NON-LINEAR FINITE ELEMENT EQUATIONS

In this section, the finite element equations arising from the solution of problems in non-linear heat conduction are formulated. First, the weighted residual or weak form is defined. Next, the Galerkin approximation is introduced

which, along with an assumed spatial discretization, leads to the finite element matrix form of the problem. The solution of the resulting nonlinear matrix equations motivates the development of an iterative algorithm. Finally, the linear problem generated by the iterative algorithm is discussed.

The problem is posed for a body occupying a spatial domain Ω, a finite region R^{ND}, where R is the set of real numbers and ND is the number of space dimensions. The boundary of Ω, denoted Γ, is assumed to be piecewise smooth. Γ can be subdivided into two disjoint subsets, Γ_g and Γ_h. In order to model a wide variety of nonlinear heat conduction problems, very few restrictions will be placed on the material composing the body. The material is considered inhomogeneous, therefore the conductivity K and the internal heat generation Q may vary through the body. Nonlinear temperature dependence is allowed in K and Q.

The strong form of the boundary value problem, based on a generalization of the Fourier law of heat conduction [7, 8], is stated as

$$\nabla . (K \nabla T) + Q = 0 \quad \text{on } \Omega \tag{1}$$

where T(x) is the temperature and x represents a general point in Ω, $x = \{x_i\}$; i = 1, 2, ..., ND.

Different types of boundary conditions are defined on the subsets Γ_g and Γ_h of Γ. On Γ_g, the temperature is prescribed g that may depend on position. On Γ_h, a natural boundary condition is applied. This type of boundary condition applies a heat flux h which may depend on temperature as well as position, hence

$$T = g \quad \text{on } \Gamma_g \tag{2}$$

$$n . (K \nabla T) = h \quad \text{on } \Gamma_h \tag{3}$$

where n is the outward normal unit vector on Γ_h.

Let H_o and H_1 be the trial and test spaces respectively, such that

$$H_o = \{u: u = g \text{ on } \Gamma_g\} \tag{4}$$

$$H_1 = \{v : v = 0 \text{ on } \Gamma_g\} \tag{5}$$

where u and v denote temperature like fields.

The weak form is obtained by multiplying (1) by $v \in H_1$, integrating over Ω, applying the divergence theorem and making use of the boundary conditions (2) and (3). This yield the following weak form:

Find $u \in H_o$ such that for every $v \in H_1$

$$a(w;u,v) = b(w;Q,v) + d(w;h,v). \tag{6}$$

The operators a, b, d and (.,.) are defined as

$$a(w;u,v) = \int \nabla u(x).K[w(x),x]\nabla v(x) \; d\Omega \tag{7}$$

$$b(w;Q,v) = \int Q\,[w\,(x)]\;\; v(x)\;\; d\Omega \tag{8}$$

$$d(w;\, h,\, v) = \int h\,[w\,(x),\, x]\;\; v(x)\;\; d\Gamma \tag{9}$$

$$(u,\, v) = \int u(x)\; v(x)\; d\Omega \tag{10}$$

where w (x) is a temperature-like field.

The Galerkin form is derived from the weak form by approximating the trial and test spaces with finite-dimensional subspaces. Let H^h_1 be a subspace of H_1 spanned by the functions v^h such that

$$H^h_1 = \{v^h : v^h = \sum_{A=1}^{n} N_A(x)\, d_A \;;\; v^h = 0 \quad \text{on } \Gamma_g\} \subset$$

where N_A, A = 1, 2, 3, ..., n are n linearly independent functions in H_1 and d_A are constants.

Similarly, the approximation of the trial space is defined as:

$$H^h_o = \{u^h;\, u^h = v^h + g^h \;;\; v^h \in H_1{}^h \;;\; g^h \in H_o\} \subset H_o$$

The Galerkin approximation is stated as:

Find $u^h = v^h + g^h$ such that

$$a\,(u^h;\, v^h,\, w^h) = b\,(u^h;\, Q,\, w^h) + d(u^h;\, h,\, w^h) - a(u^h;\, g^h,\, w^h) \tag{11}$$

Now the finite element matrix equations are derived from the Galerkin form by defining the approximation of the test and trial spaces based on a given spatial discretization. The domain Ω is discretized into disjoint elements Ω^e, e = 1, 2, ..., N_e, where N_e is the number of elements. Each element is defined by an ordered set of nodal points. In the finite element approximation N_A (x) are called the shape functions such that

$$N_A(x) = \begin{cases} 1\, x = x_A \\ 0x = x_B \\ 0x \text{ is 'no-local} \end{cases} \quad (12)$$

where x_A and x_B are the coordinates of nodes A and B respectively, and "local" is taken to mean in elements connected to the node under consideration. Thus, the finite element matrix form of the boundary value problem is:

Find q such that

$$\mathbf{N(q)} = \mathbf{F(q)} \quad (13)$$

where

$$N(q) = \sum_{e=1}^{N_e} n^e(q) \quad (14)$$

where $\sum_{e=1}^{N_e}$ is a combination of summation and a Boolean map which expands the element contribution $\mathbf{n}^e(q)$ to global size. The element contribution is given by

$$\mathbf{n}^e(\mathbf{q}^e) = \{n^e_a(q^e)\} \quad (15)$$

with components

$$n^e_a(q^e) = \int_{\Omega^e} B^T_a(x)\ K(u^h, x)\ B_b(x)\ q^e_b\ d\Omega \quad (16)$$

The vector $\mathbf{B}_a$ contains the spatial derivatives of the shape functions as

$$B_a(x) = \frac{\partial N_a(x)}{\partial x} \quad (17)$$

The right-hand-side vector $\mathbf{F(q)}$ is

$$F(q) = \sum_{e=1}^{N_e} f^e(q^e) \quad (18)$$

where the element contribution is given by

$$\mathbf{f}^e(q) = \{f^e_a(q^e)\} \quad (19)$$

with components

$$f^e_a(q^e) = \int_{\Omega^e} N_a(x)\, Q(u^h,x)\, d\Omega + \int_{\Gamma^e \cap \Gamma_h} N_a(x)\, h(u^h,x)\, d\Gamma \quad (20)$$

THE NON-LINEAR ITERATIVE ALGORITHM

In the preceding section we reduced the solution of the nonlinear partial differential equation to the solution of a set of nonlinear algebraic equations. The discrete equilibrium equations arising from finite element nonlinear formulation may be written in the general compact form

$$r(q) = 0 \quad (21)$$

where

$$r(q) = N(q) - F(q)$$

The Newton-Raphson method and its numerous variants, collectively known as Newton-like methods are the most popular class of methods for the solution of (21). The Newton-like methods are usually related to the following iteration scheme

$$\text{solve} \quad r'(q_k)\ p_k = -\, r(q_k)$$

$$\text{set } q_{k+1} = q_k + p_k$$

then at each iteration step, a linearized system of equations

$$\mathbf{A}\, x = b \quad (22)$$

is to be solved. The matrix $\mathbf{A}$ is a sparse, symmetric and positive definite.

PARALLEL CONSTRUCTION OF THE FINITE ELEMENT MATRICES

The spatial domain Ω is decomposed into a set of subdomains Ω_i (i = 1, 2, ..., N_p), where N_p is the number of the local-memory processors in the machine. On each processor, there is a subset containing the interior nodes and a subset containing the separators. The separators are the nodes on the interface between the subdomains. If the global ordering of the nodes is such that all the interior

nodes come before any of the separators, then it is possible to partition the system (22) as

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix} \qquad (23)$$

where x_o, x_1 correspond to the unknowns at the interior nodes and separators respectively. A_{oo} is block diagonal with one block on each processor. The partitioning of the system (23) is analogous to one-way dissection [7], as there is only one level of subdivision of the matrix. It is possible to eliminate the interior unknowns x_o in terms of the separators x_1 to give the reduced system

$$S\, x_1 = b^*_1 \qquad (24)$$

where S is called the "Schur Complement" and is given by

$$S = A_{11} - A_{10}\, A^{-1}_{00}\, A_{01} \qquad (25)$$

and

$$b_1^* = b_1 - A_{10}\, A^{-1}_{00}\, b_0 \qquad (26)$$

It follows that the solution of (23) can be performed in stages as

Stage 1:

$$A_{00}\, y_0 = b_0 \qquad (27)$$

This stage is completely parallizable since each processor will factorize its submatrix $A^{(i)}_{00}$ $i = 1, 2, ..., N_p$. A direct algorithm based on Cholesky factorization is applied within each processor.

Stage 2:

$$S\, x_1 = b^*_1 \qquad (28)$$

Since S is symmetric and positive definite, the solution of (28) can be performed using the (PCG) iterative method. Theorem (1) proves that S is a positive definite matrix.

Theorem (1)

If $W = \begin{bmatrix} W_{00} & W_{01} \\ W_{10} & W_{11} \end{bmatrix}$ is symmetric and positive definite and W_{00} is nonsingular, then the matrix $W_{11} - W_{10}\, W^{-1}_{00}\, W_{01}$ is also positive definite.

Proof

We first introduce the congruent transformation as

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$$A = F^t\, \bar{A}\, F \qquad (29)$$

$\bar{A}$ is said to be congruent to A. The congruent transformation preserves the signs of the eigenvalues. From the decomposition

$$\begin{bmatrix} W_{00} & W_{01} \\ W_{10} & W_{11} \end{bmatrix} = \begin{bmatrix} I & 0 \\ W_{10}W_{00}^{-1} & I \end{bmatrix} \begin{bmatrix} W_{00} & 0 \\ 0 & W_{11} - W_{10}W_{00}^{-1}W_{01} \end{bmatrix} \cdot \begin{bmatrix} I & W_{00}^{-1}W_{01} \\ 0 & I \end{bmatrix}$$

it is apparent that

$$\begin{bmatrix} W_{00} & W_{01} \\ W_{10} & W_{11} \end{bmatrix} \text{ is congruent to } \begin{bmatrix} W_{00} & 0 \\ 0 & W_{11} - W_{10}W_{00}^{-1}W_{01} \end{bmatrix}$$

and hence the eigenvalues of $W_{11} - W_{10}\, W_{00}^{-1}\, W_{01}$ are positive, proving that it is a positive definite matrix.

THE PRECONDITIONED CONJUGATE GRADIENT (PCG)

The (PCG) method is an iterative technique for the solution of a symmetric positive definite system of equations [8 - 9]. If the system to be solved is

$$S\, x = b$$

then a preconditioner matrix B is chosen such that $B^{-1}S$ has a small spectral radius. The PCG algorithm is therefore

$$x_0 = B^{-1}b, \quad r_0 = b - Sx_0, \quad p_0 = B^{-1} r_o$$

then for i = 0, 1, 2, ... until convergence

$$\alpha_i = \frac{r_i \cdot B^{-1} r_i}{p_i \cdot S p_i}$$

$$x_{i+1} = x_i + \alpha_i p_i$$

$$r_{i+1} = r_i - \alpha_i S p_i$$

$$\beta_i = \frac{r_{i+1} \cdot B^{-1} r_{i+1}}{r_i \cdot B^{-1} r_i}$$

$$p_{i+1} = B^{-1} r_{i+1} + \beta_i p_i$$

The matrix S in (28) can be expensive to compute and store. However, we notice that Sy (for any vector y) can be computed at the expense of solving a subproblem with the sparse right-hand-side $A_{01}y$ and certain sparse matrix and vector operations. Whenever Sy is to be computed, the following algorithm is applied

-compute $x = A_{11}y$
-compute $y_1 = A_{01}y$
-solve $A_{00}y_2 = y_1$
-compute $y_3 = A_{10}y_2$
-compute $Sy = x - y_3$

The choice of the preconditioner B is based on the subdomain decomposition such that

$$B = \sum_i A_{11}^{(i)} - A_{10}^{(i,i)} A_{00}^{(i)^{-1}} A_{01}^{(i,i)} \qquad (30)$$

$$i = 1, 2, \ldots\ldots, N_p$$

and hence complete parallism is secured during the solution of the set of linear equations to compute $B^{-1}r_i$.

NUMERICAL EXAMPLE

The method is tested for a thermal radiation problem [10]. A square plate with a nonlinear radiation boundary condition and a significantly nonlinear thermal conductivity is to be considered. The problem spatial domain is a square region defined by

$$0 \le x, y \le 1 \text{ m} \qquad (31)$$

The material conductivity is strongly nonlinear

$$K = 2(1 + 5\frac{T}{1000}) \qquad \frac{W}{m.^{\circ}K} \qquad (32)$$

the heat generation per unit volume is constant

$$Q = 2500 \text{ W/m}^3 \qquad (33)$$

The problem has several different types of boundary conditions. There is a prescribed temperature on the lower edge

$$T = 0^{\circ}K \text{ on } y = 0 \text{ m},$$

insulation on the upper edge

$$n.(K \nabla T) = 0 \text{ W/m} \quad \text{on } y = 1 \text{ m}$$

a prescribed constant heat flux on the right edge

$$n.(K \nabla T) = 1000 \text{ W/m on } x = 1 \text{ m},$$

and a radiation boundary condition on the left edge

$$n.(K \nabla T) = h_r (T^4 - T_r^4) \text{ on } x = 0 \text{ m},$$

where

$$h_r = 1.0 \times 10^{-9} \qquad \frac{W}{m(^{\circ}K)^4}$$

$$T_r = 1500^{\circ}K$$

The results were obtained on an IBM 80386 personal computer equipped with 12 Inmos T800 Transputers in the center of mathematical software research in Liverpool University. Table (1) summarizes the results in case of a finite element network of 1200 linear quadrilaterals.

Table (1). Nonlinear radiation Problem.

N_p	N_e	iters outer	iters inner	run time (sec)	speed up	efficiency
1	1200	3	14.2	7426		
8		3	15.6	1141	6.51	81.37 %
12		3	18.3	753	9.86	82.16 %

CONCLUSION

This paper has focused on the development of a parallel computational strategy for nonlinear heat conduction problems. The strategy is based on partitioning the domain of interest into a set of subdomains. The interior unknowns are eliminated in favor of the separators leading to a reduced system (Schur Complement). A Newton-like method is used to solve the nonlinear system of equations. Within each nonlinear iteration a direct and iterative techniques were used. The test example validated the proposed computational strategy. The technique could be extended for large number of local-memory processors, also it can be simply modified to be used with shared-memory machines.

ACKNOWLEDGEMENTS

The author wishes to acknowledge the valuable contributions of Dr. R. Wait at Liverpool University in preparing and testing this work. The author also wishes to express his thanks to the British Council in Alexandria for its support in visiting Liverpool University twice in 1990.

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