Parallelization Using TH–Collocation

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In recent years, the innovation of Massively Parallel Processor Systems has created the need of a new algorithms for these architectures. The TH-collocation method is very suitable for parallelization. In this paper, the implementation of the TH-Collocation Method on a Massively Parallel System is carried out using the CRAY T3D emulator and a CRAY T3D supercomputer. A distributed memory programming model is used, as it is explained here; furthermore, the analysis points to particular procedures that produce optimal accuracy. The techniques for the optimization of this program, using the CRAY utilities are discussed. Example calculation illustrate the computational procedure and verify the theorical convergence rates.

1. Introduction

Field-scale simulations of fluids in porous media often involve problems that are so large that solution on the full computational domain is either impossible or extremely inefficient. Parallelization techniques [Bramble,1986], [Bramble, 1988], [Ewing, 1990], have been developed to allow these large processes to be split into pieces that can be solved independently and then put back together to give an approximation of the total solution. The independence of the solution processes on the separate parts of the problem gives extreme flexibility in the methods and allows efficient use of parallel architecture supercomputers. The methods can simply separate sub domain solutions to divide the computational effort, or can allow the use of different discretizations or even different model equations on the separate domains. Thus, a simplified description of the physics can be used in regions where the simplification is valid, and more rigorous models can be used locally [Buzbee, 1974].

Many applications of fluid flow in porous media involve both large-scale processes and highly-localized phenomena that are often critical to the physical behavior of the flow. For large-scale problems, it is frequently impossible to use a uniform or quasi-uniform grid that is sufficiently fine to resolve the local phenomena. Since these local processes are often dynamic, efficient numerical simulations require the ability to perform dynamic, self-adaptive local grid refinement. Normal introduction of local grid refinement techniques destroys the vectorization capabilities of supercomputers and hence their efficienc. Parallel techniques possess enormous potential for efficient local accuracy improvements in many large-scale problems.

In this paper we will discuss the collocation discretization and the use Parallel System using a CRAY T3D supercomputer. All of these computations illustrate the enormous potential for new advances in the use of supercomputers in simulation using the local refinement techniques. Finally, example calculations are presented to illustrate the methodology.

2. Preliminary Concepts

In this section, Herrera's algebraic theory of boundary value problems [Herrera, 1977], [Herrera, 1982], [Herrera, 1984], [Herrera, 1985a, 1985b, 1985c], is briefly explained.

Consider a region Ω and the linear spaces D_1 and D_2 of trial and test functions defined in Ω, respectively. Assume further that functions belonging to D_1 and D_2 may have jump dicontinuities across some internal boundaries whose union will be denoted by Σ. For example, in applications or the theory to finite element methods, the set Σ will be the union of all the inter element boundaries. In this setting, the general boundary value problem to be considered is one with prescribed jumps across Σ. The differential equation is

$$\mathcal{L}u = f_\Omega \quad \text{in} \quad \Omega, \tag{2.1}$$

where Ω may be a purely spatial region or, more generally, a space-time region. Certain boundary and jump conditions are specified on the boundary $\partial\Omega$ of Ω and on Σ, respectively. When Ω is a space-time region, such conditions generally include initial conditions. In the literature on mathematical modeling of macroscopic physical systems, there are a variety of examples of initial-boundary value problems with prescribed jumps. To mention just one, problems of elastic wave diffraction can be formulated as such [Herrera, 1985c, 1986]. The jump conditions that the sought solution must satisfy across Σ, in order to define a well posed problem, depend on the specific applications and on the differential operator considered. For example, for elliptic problems of second order, continuity of the sought solution and its normal derivative is usually required, but the problem in which the solution and its normal derivative jump across Σ in a prescribed manner is also well posed [Herrera, 1986].

The definition of a formal disjoint requires that a differential operator $\mathcal{L}$ and its formal adjoint $\mathcal{L}^*$ satisfy the condition that $w\mathcal{L}u - u\mathcal{L}^*w$ be a divergence, i. e.,

$$w\mathcal{L}u - u\mathcal{L}^*w = \nabla \cdot \{\underline{\mathcal{D}}(u,w)\} \tag{2.2}$$

for suitable vector-valued bilinear function $\underline{\mathcal{D}}(u,w)$. Integration of Eq. (2.2) over Ω and multiplication of the generalized divergence theorem [Allen, 1988] yields

$$\int_\Omega \{w\mathcal{L}u - u\mathcal{L}^*w\}\, dx = \int_{\partial\Omega} \mathcal{R}_\partial(w,u)\, dx + \int_\Sigma \mathcal{R}_\Sigma(u,w)\, dx$$

where

$$\mathcal{R}_\partial(u,w) = \underline{\mathcal{D}}(u,w)\cdot\underline{\mathbf{n}} \text{ and } \mathcal{R}_\Sigma(u,w) = -[\underline{\mathcal{D}}(u,w)]\cdot\underline{\mathbf{n}}. \tag{2.4}$$

Here the square brakets stand for the "jumps" across Σ of the function contained inside, i.e., limit on the positive side minus limit on the negative side. Here, as in what follows, the positive side of Σ is chosen arbitrarily and then the unit normal vector $\mathbf{n}$ is taken pointing towards the positive side of Σ. Observe that generally $\mathcal{L}u$ will not be defined on Σ, since u and its derivatives may be discontinuous. Thus, in this article, it is understood that integrals over Ω are carried out excluding Σ. Consequently, differential operators will always be understood in an elementary sense and not in a distributed sense.

In the general theory of partial differential equations, Green's formulas are used extensively. For the construction of such formulas it is standard to introduce a decomposition of the bilinear function $\mathcal{R}_\partial$ (see, for example, Lions and Magenes [Lions, 1972]). Indicating transposes of bilinear forms by means of an asterisk, the general form of such

decomposition is

$$\mathcal{R}_\partial(u,w) = \underline{\mathcal{D}}(u,w)\cdot\underline{\mathbf{n}} = \mathcal{B}(u,w) - \mathcal{C}^*(u,w), \tag{2.5}$$

where $\mathcal{B}(u,w)$ and $\mathcal{C}(w,u) = \mathcal{C}^*(u,w)$ are two bilinear functions. When considering initial-boundary value problems, the definitions of these bilinear forms depend on the type of boundary and initial conditions to be prescribed. A basic property required of $\mathcal{B}(u,w)$ is that for any u that satisfies the prescribed boundary and initial conditions, $\mathcal{B}(u,w)$ is a well-defined linear function of w, independent of the particular choice of u. This linear function will be denoted g_∂ (thus its value for any given function w will be $g_\partial(w)$), and the boundary conditions can be specified by requiring that $\mathcal{B}(u,w) = g_\partial(w)$ for every $w \in D_2$ (or more briefly: $\mathcal{B}(u,\cdot) = g_\partial$). For example, for the Dirichlet problem of the Laplace equation, it will be seen later that $\mathcal{B}(u,w)$ can be taken to be $u\frac{\partial u}{\partial n}$ on $\partial\Omega$. Thus, if u is the prescribed value of u on $\partial\Omega$ one has $\mathcal{B}(u,w) = u_\partial\frac{\partial w}{\partial n}$ for any function u that satisfies the boundary conditions. Thus $g(w) = u_\partial\frac{\partial w}{\partial u}$ in this case.

The linear function $\mathcal{C}^*(u,\cdot)$, on the other hand, cannot be evaluated in terms of the prescribed boundary values, but it also depends exclusively on certain boundary values of u (the "complementary boundary values"). Generally, such boundary values can only be evaluated after the initial-boundary value problem has been solved. Taking the example of the Dirichlet problem for the Laplace equation, as before, $\mathcal{C}^*(u,w) = w\frac{\partial u}{\partial n}$ and the complementary boundary values correspond to the normal derivative on $\partial\Omega$.

In a similar fashion, convenient formulations of boundary value problems with prescribed jumps require constructing Green's formulas in discontinuos fields. This can be done by introducing a general decomposition of the bilinear function $\mathcal{R}_\Sigma(u,w)$ whose definition is pointwise. The general theory includes the treatment of differential operators with discontinuous coefficients [Herrera, 1985c]. However, in this article, only continuous coefficients will be considered. In this case, such decomposition is easy to obtain, and it stems from the algebraic identity:

$$[\underline{\mathcal{D}}(u,w)] = \underline{\mathcal{D}}([u],\dot{w}) + \underline{\mathcal{D}}(\dot{u},[w]), \tag{2.6}$$

where

$$[u] = u_+ - u_-, \quad \dot{u} = (u_+ + u_-)/2. \tag{2.7}$$

The desired decomposition is obtained by combining the second of Eqs (2.4) with (2.6):

$$\mathcal{R}_\Sigma(u,w) = \mathcal{J}(u,w) - \mathcal{K}^*(u,w)$$

with

$$\mathcal{J}(u,w) = -\underline{\mathcal{D}}([u],\dot{w})\cdot\underline{\mathbf{n}}, \tag{2.9a}$$

$$\mathcal{K}^*(u,w) = \mathcal{K}(w,u) = \underline{\mathcal{D}}(\dot{u},[w])\cdot\underline{\mathbf{n}}. \tag{2.9b}$$

An important property of the bilinear function $\mathcal{J}(u,w)$ is that, when the jump of u is specified, it defines a unique linear function of w, which is independent of the particular choice of u. When considering initial-boundary value problems with prescribed jumps, the linear function defined by the prescribed jump in this manner will be denoted by J_Σ (thus its value for any given function w will be $J_\Sigma(w)$ and the jump conditions at any point of Σ can be specified by means of the equation $\mathcal{J}(u,\cdot) = J_\Sigma$. In problems with prescribed jumps, the linear functional $\mathcal{K}^*(u,\cdot)$ plays a role similar to that of the complementary boundary values $\mathcal{C}^*(u,\cdot)$. It can only be evaluated after the initial-boundary value problem has been solved and certain information about the average of the solution and its derivatives on Σ is known. Such information will be called the "generalized averages".

Introducing the notation

$$\langle Pu, w\rangle = \int_\Omega w\mathcal{L}u\, dx, \qquad \langle Q^*u, w\rangle = \int_\Omega w\mathcal{L}^*u\, dx, \tag{2.10a}$$

$$\langle Bu, w\rangle = \int_{\partial\Omega} \mathcal{B}(u, w)\, dx, \quad \langle C^*u, w\rangle = \int_{\partial\Omega} \mathcal{C}(w, u)\, dx, \tag{2.10b}$$

$$\langle Ju, w\rangle = \int_\Sigma \mathcal{J}(u, w)\, dx, \quad \langle K^*u, w\rangle = \int_{\partial\Omega} \mathcal{K}(w, u)\, dx \tag{2.10c}$$

Eq (2.3) can be written as

$$\langle Pu, w\rangle - \langle Q^*u, w\rangle = \langle Bu, w\rangle - \langle C^*u, w\rangle + \langle Ju, w\rangle - \langle K^*u, w\rangle. \tag{2.11}$$

This is an identity between bilinear forms and can be written more briefly, after rearranging, as

$$P - B - J = Q^* - C^* - K^*. \tag{2.12}$$

This is the Green-Herrera formula for operators in discontinuous fields [Ewing, 1990], [Herrera, 1985a].

The initial-boundary value problem with prescribed jumps can be formulated pointwise by means of Eq. (2.1) together with

$$\mathcal{B}(u, \cdot) = g_\partial \text{ and } \mathcal{J}(u, \cdot) = j_\Sigma. \tag{2.13}$$

In order to associate a variational formulation with this problem, define the linear functionals $f, g, j \in D_2^*$ by means of

$$\langle f, w\rangle = \int_\Omega w f_\Omega\, dx, \ \langle g, w\rangle = \int_{\partial\Omega} g_\Omega(w)\, dx, \ \langle j, w\rangle = \int_\Sigma j_\Sigma(w)\, dx. \tag{2.14}$$

Then the variational formulation of the initial-boundary value problem with prescribed jumps is

$$Pu = f, \quad Bu = g, \quad Ju = j. \tag{2.15}$$

The bilinear functional J just constructed, as well as B, are boundary operators for P, which are fully disjoint. (For the definitions of the concepts that appear in italics here, the reader is referred to Herrera's original papers [Herrera, 1977, 1982, 1984, 1985a, 1985b, 1985c, 1986]). When this is the case, the system of equations (2.15) is equivalent to the single variational equation

$$\langle (P - B - J)u, w\rangle = \langle f - g - j, w\rangle \quad \forall w \in D_2. \tag{2.16}$$

This is said to be "the variational formulation in terms of the data of the problem", because Pu, Bu and Ju are prescribed. Making use of formula (2.12), the variational formulation (2.16) is transformed into

$$\langle (Q^* - C^* - K^*)u, w\rangle = \langle f - g - j, w\rangle \quad \forall w \in D_2. \tag{2.17}$$

This is said to be "the variational formulation in terms of the sought information" because Q^*u, C^*u and K^* are not prescribed. The variational formulation (2.16) and (2.17) are equivalent by virtue of the identity (2.12). The linear functionals Q^*u, C^*u and K^*u

supply information about the sought solution at points in the interior of the region Ω, the complementary boundary values at $\partial\Omega$, and the generalized averages of the solution at Σ, respectively, as can be verified by inspection of Eqs. (2.10), and are illustrated in the examples that follow.

Localized adjoint methods are based on the following observations. When the method of weighted residuals is applied, an approximate solution $\hat{u} \in D_1$ satisfies

$$\langle (P - B - J)\hat{u}, w^\alpha \rangle = \langle f - g - j, w^\alpha \rangle, \quad \alpha = 1, \ldots, N, \tag{2.18}$$

where $\{w^1, \ldots, w^N\} \subset D_2$ is a given system of weighting functions. However, these equations, when they are expressed in terms of the sought information, become

$$\langle (Q^* - C^* - K^*)\hat{u}, w^\alpha \rangle = \langle f - g - j, w^\alpha \rangle, \quad \alpha = 1, \ldots, N. \tag{2.19}$$

Since the exact solution satisfies (2.17), it must be that

$$\langle (Q^* - C^* - K^*)\hat{u}, w^\alpha \rangle = \langle (Q^* - C^* - K^*)u, w^\alpha \rangle = \langle f - g - j, w^\alpha \rangle, \quad \alpha = 1, \quad , N. \tag{2.20}$$

Either in this form or in the form

$$\langle (Q^* - C^* - K^*)(\hat{u} - u), w^\alpha \rangle = 0, \quad \alpha = 1, ..., N \tag{2.21}$$

Eqs (2.20) can be used to analyze the information about the exact solution that is contained in an approximate one. In localized adjoint methods, these observations have been used as a framework for selecting more convenient test functions.

In section 3, attention will be restricted to functions which are continnous across Σ, with a possibly discontinous first derivative. Then, for the most general elliptic operator of second order, to be considered there, we have

$$\mathcal{B}(u, w) = (\mathbf{a}_n \frac{\partial w}{\partial n} + b \cdot n)u, \qquad \mathcal{C}(w, u) = \mathbf{a}_n w \frac{\partial u}{\partial n}; \tag{2.22}$$

while

$$\mathcal{J}(u, w) = \mathbf{a}_n w[\frac{\partial u}{\partial n}], \qquad \mathcal{K}(w, u) = \mathbf{a}_n u[\frac{\partial w}{\partial n}] \tag{2.23}$$

with $\mathbf{a}_n = \underline{\mathbf{n}} \cdot \underline{\underline{\mathbf{a}}} \cdot \underline{\mathbf{n}}$.

3. TH—Collocation.

To illustrate Trefftz-Herrera Domain Decompositions, let us discuss the general elliptic differential equation of second order defined by

$$\pounds u \equiv -\nabla \cdot (\underline{\underline{\mathbf{a}}} \cdot \nabla u) + \nabla \cdot (\underline{\mathbf{b}}\, u) + c\, u \tag{3.1a}$$

whose formal adjoint is:

$$\pounds^* w \equiv -\nabla \cdot (\underline{\underline{\mathbf{a}}} \cdot \nabla w) - \underline{\mathbf{b}} \cdot \nabla w + c\, w, \tag{3.1b}$$

in two dimensions. Referring to Fig. 1 of *Herrera et. al*, 1996, in these proceedings, $C^0(\Omega)$ weighting functions which are bi-cubic —i.e., cubic in x and in y, separately— on the elemental rectangles, will be used. When standard collocation is applied, it is usual to represent such polynomials by means of Hermites; however, that will not be done here since it is not convenient for our purposes.

Local coordinates will be introduced; more specifically, linear mappings will be used for transforming some subregions of Ω into the unit square $\Omega_I = [0, 1] \times [0, 1]$. Then the formal adjoint, Eq. (4.1b), is transformed into

$$\pounds^* w \equiv -\nabla(\underline{\underline{\mathbf{A}}} \cdot \nabla w) - \underline{\mathbf{B}} \cdot \nabla w + \mathbf{C} w \tag{3.2}$$

where $\underline{\underline{\mathbf{A}}}$,$\underline{\underline{\mathbf{B}}}$ and C are related to $\underline{\mathbf{a}}$, $\underline{\mathbf{b}}$ and c by means of the mapping. Bi-cubic polynomials defined on Ω_1, constitute a linear space, denoted by Π , of dimension $4 \times 4 = 16$. Define ξ and η by $\xi = x - 1$ and $\eta = y - 1$, then the subspace whose members contain the factor $\xi\eta$, denoted by $\Pi_{\xi\eta}$ has dimension 9 and that whose members vanish on the whole boundary $\partial\Omega_I$ of the unit square, denoted by Π_0, has dimension 4. Observe that $\Pi_0 \subset \Pi_{\xi\eta}$ and that the dimension of algebraic complements of Π_0 with respect to $\Pi_{\xi\eta}$, is 5. In Table 1, the functions $N^\nu(x,y)$, $\nu = 1,\ldots,4$ and $B^\nu(x,y)$, $\nu = 0,\ldots,4$, have been defined. The system $\{N^\nu\}$ constitutes a basis of Π_0, while $\{B^\nu\}$ generates an algebraic complement of Π_0 with respect to $\Pi_{\xi\eta}$.

For constructing the weighting functions, Gaussian collocation is applied to the polynomial representation:

$$W_I^\nu(X \quad X_2) = B^\nu(X \quad X_2) + \sum_{j=1}^{4} C_{Ij}^\nu N^j(X_1 \; X_2)$$

and the four coefficients C_j^ν are determined by the condition $\mathcal{L}^* W^\nu = 0$ which is imposed at four Gaussian points of the unit square Ω_I. In principle, five approximate solutions of the adjoint differential equation can be constructed in this manner, corresponding to $\nu = 0,\ldots,4$. However, only the solutions associated with $\nu = 0,1,2$ will be used in the sequel, because otherwise the resulting system of test functions would not be linearly independent since some repetition would occur when developing the test functions associated with neighboring nodes. This yields three approximate solutions and similar sets of solutions can be constructed in the remaining subregions Ω_{II} , Ω_{III} and Ω_{IV} (Fig. 2 of *Herrera et al.*, 1996, in these proceedings), of the square $[-1,1] \times [-1,1]$.

When putting together such solutions in a continuous manner, five approximate solutions, that will be denoted by $W^\nu(X_1,X_2)$, $\nu = 0,\ldots,4$, are obtained. They will be characterized as shown in Fig. 1.

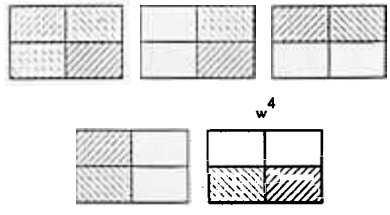


FIGURE 1. The supports of the weighting functions.

$W^0(0,0) = 1$ and its support is the whole square $[-1,1]\times[-1,1]$; $W^1(X_1,X_2)$ vanishes identically on $\Omega_{II} \cup \Omega_{III}$; thus, its support is $\Omega_I \cup \Omega_{IV}$; $W^2(X_1,X_2)$ vanishes identically on $\Omega_{III} \cup \Omega_{IV}$; thus, its support is $\Omega_I \cup \Omega_{II}$; $W^3(X_1,X_2)$ vanishes identically on $\Omega_I \cup \Omega_{IV}$; thus, its support is $\Omega_{II} \cup \Omega_{III}$; $W^4(X_1,X_2)$ vanishes identically on $\Omega_I \cup \Omega_{II}$ thus, its support is $\Omega_{III} \cup \Omega_{IV}$.

Let $\partial_\nu\Omega$ ($\nu = 1,\ldots,4$) be the left, lower, right and upper boundary of Ω, respectively, and observe that when a node belongs to $\partial_\nu\Omega$, only W^ν vanishes on the boundary. In conclusion, with every interior node (x_i,y_j) of the partition there are associated five test functions, satisfying approximately

$$(Q - \qquad = 0$$

they will be denoted by w_{ij}^ν ($\nu = 0,\ldots$ at boundary nodes there is only one: and at corner nodes none. If the number of nents in the x and y directions is I and J,

ν		1	2	3	4
$N^\nu(x,y)$		$\xi\eta xy$	$\xi\eta x^2y$	$\xi\eta xy^2$	$\xi\eta x^2y^2$
$B^\nu(x,y)$	$\xi\eta$	$\xi\eta x^2$	$\xi\eta y^2$	$\xi\eta x$	$\xi\eta y$

TABLE 1.

respectively, then this yields a system of $(I+1)(J+1)-4$ linearly independent test functions.

4. The trial functions

The test functions that have been developed have the property that concentrate all the information on the internal boundaries Σ and correspondingly, the trial functions will supply information on Σ, exclusively. In particular, a function $\hat{u}_H \in \hat{D}_{1H}$ will be constructed by collocation which satisfies, approximately, the first of Eqs. (2.3). The following notation is adopted: when p and q are functions defined in Ω, the relation $p \cong q$, means that $p = q$ at each one of the Gaussian points of the elemental rectangles. The basic trial functions will be denoted by Φ^ν_{ij}, where the ranges of i,j and ν, are the same as for the test functions; they satisfy $(P-B-J)u = 0$. More precisely, they satisfy $\pounds\Phi^\nu_{ij} \cong 0$, are continuous and vanish on the external boundary $\partial\Omega$. The construction of such functions is the same as that of weighting functions, except that $\pounds^*$ is replaced by $\pounds$. The approximate solution has the expression

$$\hat{u}_H = \sum U^\nu_{ij}\Phi^\nu_{ij} \tag{4.1}$$

where the coefficients U^ν_{ij} are determined by the system of Eqs.(5.3). This is

$$M^{\mu\nu}_{klij}U^\nu_{ij} = F^\mu_{kl} \tag{4.2}$$

where summation convention is understood —repeated indexes are summed over their ranges— and

$$M^{\mu\nu}_{klij} = -\int_\Sigma \kappa^0(w^\mu_{kl},\Phi^\nu_{ij})dx = -\int_\Sigma \mathbf{a}_n\Phi^\nu_{ij}[\partial w/\partial n]dx \tag{4.3a}$$

while

$$F^\nu_{kl} =< f-g, w^\mu_{kl} >= \int_\Omega w^\mu_{kl}f_\Omega dx - \int_{\partial\Omega} u_\partial(\underline{\underline{\mathbf{a}}}\cdot\nabla w^\mu_{kl} + \underline{\mathbf{b}}\, w^\mu_{kl})\cdot\underline{n}dx. \tag{4.3b}$$

It is interesting to observe that

$$-\int_\Sigma \kappa^0(w^\mu_{kl},\Phi^\nu_{i,j})dx = \int_\Omega \underline{\underline{\mathbf{a}}}\cdot\nabla w^\mu_{kl}\cdot\Phi^\nu_{i,j} - (\underline{\mathbf{b}}\cdot\nabla w^\mu_{kl} + c\, w^\mu_{kl})\Phi^\nu_{ij}dx, \tag{4.4}$$

which allows replacing the surface integral over Σ by a volume integral, which needs to be carried out over the intersection of the supports of w^μ_{kl} and Φ^ν_{ij}, only. If Gaussian integration is applied, the fact that collocation points and the pivotal points for the quadrature coincide, makes the process very economical. As has already been mentioned, the function $\hat{u}_H$ gives an approximate solution on Σ. If we wish extending this information to the interior of the subregions, it is necessary to construct $\hat{u}_p$ such that $\pounds u_p \cong f_\Omega$ and vanishes on Σ. This involves local problems only and can also be done by collocation, and constitutes postprocessing of the solution. Then $\hat{u}_p + \hat{u}_H$ is an approximation to u everywhere. Finally, it must be mentioned that when $\pounds$ is positive definite, so is the system of equations (5.2).

5. Results

A wide variey of computations have been performed on supercomputers using the techniques described in the previous sections. Many of these computational experiments were of such size and complexity as to test the computational limits of the computers used.

Of course, the implementation of any algorithm in a parallel processing enviroment is extremely sensitive to the data structure and its use. The memory characteristics of the computer govern the algorithms and their efficiencies. The relative success of the compilers for shared memory machines are indicative of the greater difficulty in developing efficient parallel algorithms on distributed memory machines for the complex problems arising in reservoir simulation applications.

The CRAY supercomputer offer multi-tasking for implementation of parallel processing, thus allowing the user to provide separate routines for tasks to be run in parallel. In addition, CRAY also allows "microtasking" for parallelism with each separate routine. However, the data structure determines the efficiency of each of these types of parallel algorithms.

To demonstrate the applicability of the computational algorithm, and to verify the theoretical results of the sections, several numerical examples are solved. A completely general computing program was developed and implemented on a CRAY T3D supercomputer.

The procedure is very easy to program and turns out to be quite versatile. Optimizing a program begins by finding where the main work load is located, that is to say, locating which parts of the code are the most time-consuming. This was done using the CRAY utilities Flowview and Perfview. Compiler options and directives were used to refine the optimization. A very useful one was the AtExpert tool. With this utility one can visualize the parts of the program that run in parallel and estimate its speed-up. Fig. 2, based on an actual ATexpert window, illustrates this.

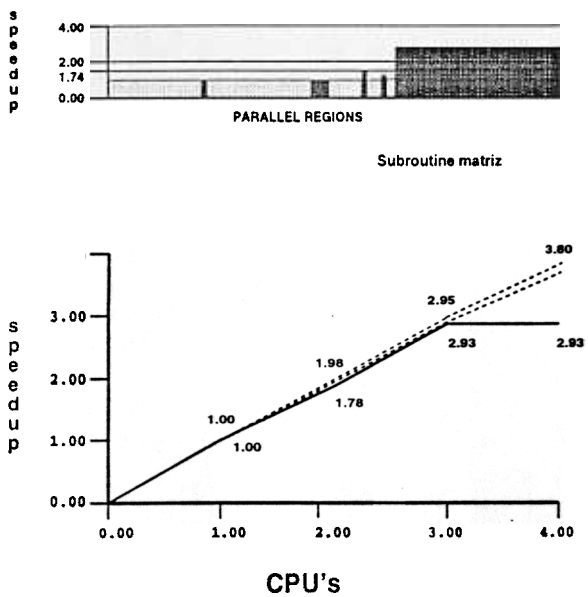
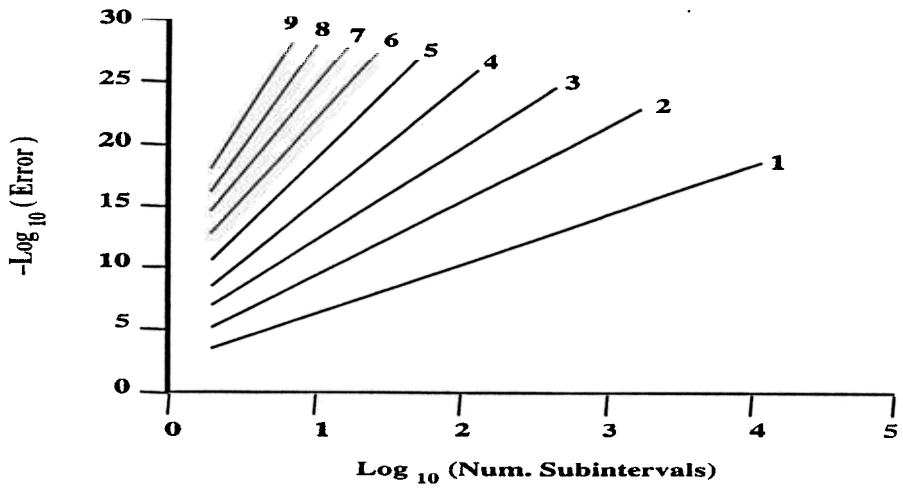


FIGURE 2. Serial and parallel portions (upper panel) and overall speedup (lower panel) as determined by ATexpert.

Numerical results computed using this methodology are shown in the convergence plots of Fig. 3. The figure shows the solution error as a function of grid spacing for cases using different choices of interpolation knots. All convergence rates correspond to the theoretical predictions of the previous section.



1:	G=3	m=3.9	4:	G=6	m=9.7	7:	G=9	m=14.5
2:	G=4	m=5.9	5:	G=7	m=11.4	8:	G=10	m=16.1
3:	G=5	m=7.9	6:	G=8	m=13.1	9:	G=11	m=18.4

FIGURE 3. Solution errors for $u'' + (2x^2 + 4x)/[(x+1)(x^2+2x+2)]u' + [1 - 2/(x^2+2x+2)]u = 1/(x^2 + 2x + 2)$ with Dirichlet's conditions $u(0) = 0.5$, $u(1) = 0.2$. The solution is $u(x) = 1/(x^2 + 2x + 2)$; the experimental slope is m.

The computer program was tested by applying it to three equations, but in this article just the results for the first equation are presented; the boundary conditions were Dirichlet conditions. For every one of the examples, one can choose arbitrarily the number E of subintervals and the number n of collocations points. When n is fixed, this defines a straight line of slope $2n$ - 1.

Fig. 3 displays the negative value of the error decimal logarithm, at the nodes, versus the decimal logarithm of the number of subintervals considered in a certain position. As expected, when the weight function degree is imposed, straight lines are obtained as the number of subintervals varies. The experimental slopes of these straight lines also appear for G = 3, 4, 5, 6, 7, 8, 9, 10 and 11.

6. Conclusion

The algebraic theory for numerical methods, as developed by Herrera [Ewing, 1990], [Herrera, 1977, 1982, 1984, 1985a], provides a broad theoretical framework for the development and analysis of numerical approximations. Analysis of the method provides error estimates. Furthermore, the analysis points to particular procedures that produce optimal accuracy. Examples developed in this article illustrate the computational procedure and verify the theoretical convergence rates. Actually, the method presented here has considerable generality and its applicability is not restricted, by any means, to cases where the discretization procedure used is collocation.

From a more general perspective, the results of this article illustrate some of the advan-

tages of an approach for developing algorithms to numerically treat Ordinary Differential Equations that the authors are advocating, and whose basic ingredients consist of (a) identifying the information about the sought solution contained in the approximate one, and (b) using this insight to choose the interpolation procedure.

Finally, we want to emphasize that parallelization using optimal collocation forms a general and powerful framework for investigating and comparing a wide variety of numerical methods for problems for Ordinary Differential Equations. The framework motivates different choices of test functions to approximate different properties of the unknowns, such as fluxes. The general theory is expanding to provide more insight. These techniques appear to have enormous flexibility and potential for treating many applications of fluid flow in porous media.

Acknowledgments. This work was supported by a grant from Universidad Nacional Autónoma de México and Cray Research, Inc. We would also like to thank Dirección General de Servicios de Cómputo Académico for its support and the use of the CRAY Y-MP under its charge and to Consejo Nacional deCiencia y Tecnología for its Conacyt-NSF 1994 grant. Also, Ismael Herrera holds a chair of excellence (Cátedra Patrimonial de Excelencia Nivel I) from CONACYT.

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