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N. P. Chrisochoides
C. E. Houstis
Elias N. Houstis
Purdue University, enh@cs.purdue.edu
S. K. Kortesis
John R. Rice
Purdue University, jrr@cs.purdue.edu

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C. E. Houstis
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N.P. Chrisochoides, C.E. Houstis†, E.N. Houstis, S.K. Kortesis†, and J.R. Rice

Computer Sciences Department
Purdue University
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Abstract

In this paper we study the partitioning and allocation of computations associated with the numerical solution of partial differential equations (PDEs). Strategies for the mapping of such computations to parallel MIMD architectures can be applied to different levels of the solution process. We introduce and study heuristic approaches defined on the associated geometric data structures (meshes). Specifically, we study methods for decomposing finite element and finite difference meshes into balanced, nonoverlapping subdomains which guarantee minimum communication and synchronization among the underlying associated subcomputations. Two types of algorithms are considered: clustering techniques based on sequential orderings of the discrete geometric data and optimization based techniques involving geometric or graphical metric criteria. These algorithms support the automatic mode of a geometry decomposition tool developed in the parallel ELLPACK environment which is implemented under X11-window systems. A brief description of this tool is presented.

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FOR PDE COMPUTATIONS

N.P. Chrisochoides, C.E. Houstis, E.N. Houstis,
S.K. Kortesis and J.R. Rice

Department of Computer Science
Purdue University
West Lafayette, IN 47907

Abstract

In this paper we study the partitioning and allocation of computations associated with the numerical solution of partial differential equations (PDEs). Strategies for the mapping of such computations to parallel MIMD architectures can be applied to different levels of the solution process. We introduce and study heuristic approaches defined on the associated geometric data structures (meshes). Specifically, we study methods for decomposing finite element and finite difference meshes into balanced, nonoverlapping subdomains which guarantee minimum communication and synchronization among the underlying associated subcomputations. Two types of algorithms are considered: clustering techniques based on sequential orderings of the discrete geometric data and optimization based techniques involving geometric or graphical metric criteria. These algorithms support the automatic mode of a geometry decomposition tool developed in the parallel ELLPACK environment which is implemented under X11-window systems. A brief description of this tool is presented.

1. INTRODUCTION

In this paper we consider the problem of partition and allocation of computations associated with the numerical solution of Partial Differential Equations (PDEs) into load balanced tasks requiring minimum synchronization and communication. The efficient solution of this problem is essential for the parallel processing of such computations. Its formulation can be based either on the geometric or the algebraic data structures associated with the PDE solution process or on the precedence graph of the PDE solver. In [Hous 88] we present a methodology for partitioning and allocation which is applicable to the computation graph of the PDE solution process. In this paper we formulate and analyze partitioning methodologies for computations defined on geometric data structures. The approach has been implemented as a special software tool in the parallel ELLPACK environment [Hous 89b]. The issue of automatic partitioning has been raised in [Fara 88] in conjunction with finite element computations on local memory machines and in [Fox 86a,b] for certain algebraic computations. Some partitioning strategies for nonuniform problems on multiprocessors are studied in [Berg 85]. In Section 2 we present several partitioning strategies and formulate various criteria that are used to determine them. A new algorithm based on geometric graph partitioning (GCP) ideas is developed and presented in Section 3, together with the description of existing clustering approaches. In Section 4 we present the performance evaluation of four automatic partitioning strategies. The results obtained indicate that the new GGP algorithm produces "optimum" partitions within reasonable time intervals. Finally, Section 5 contains a brief
description of the geometry decomposition software tool implemented under X-windows, which allows the user to specify and manipulate domain decompositions interactively, as well as to display the automatically generated ones. A detailed description of this tool will appear in [Hous 89b].

2. PARTITIONING STRATEGIES FOR PDE COMPUTATIONS

The numerical solution of partial differential equations usually is represented by an approximate function defined over a given mesh of the PDE domain. This function is determined by solving a system of algebraic equations that depends on the discretization method used. For the solution of this set of equations with a parallel MIMD machine consisting of many processors, a partitioning of the underlying computation is required. The strategy of allocating the partitions of the computations to processors affects the performance of the parallel processing. Any optimal partitioning/allocating strategy has the following objectives (a) the workloads of all processors are balanced, and (b) the processor synchronization and communication cost is kept to a minimum. Partitions of PDE computations that satisfy the above goals can be defined either on the geometric data structures (meshes) or algebraic data structures (discrete systems) or on the computation graph of the selected PDE solver. In this paper we consider partitioning strategies applied to fixed PDE meshes $\Omega_k$, which are referred as geometry decomposition approaches. Instances of the other two approaches are formulated and studied in [Fox 86] and [Hous 83]. Throughout this paper we assume that $\Omega_k$ is a finite element mesh consisting of $\{n_i(x,y,z)\}_{i=1}^{N_k}$ nodes with $\{w_{i}\}_{i=1}^{N_k}$ connectivity and, $\{e_j(n_1,\ldots,n_\rho)\}_{j=1}^{M_k}$ elements. The case of finite difference meshes can be handled in a similar way. In the geometry decomposition strategy, we seek a partition of the underlying PDE computation determined by a decomposition of $\Omega_k$ into $P$ (number of processing elements) nonoverlapping subdomains $\{D_j\}_{j=1}^{P}$ such that

(i) each subdomain contains almost the same number of elements,

(ii) they are "circular" or "spherical" and connected, and

(iii) the number of interface nodes or interior boundary elements among subdomains is minimum.

It has been observed that a nearest neighbor allocation of such partitioning computations tends to be close to optimum. For the mathematical formulation of this partitioning problem, we introduce Euclidean and graphical metrics. Throughout we denote by $(x_{k},y_{k})$ the geometric center of a 2-D element $e_i$, $|D_k| = c_k$ the number of elements in this subdomain, $D_k$ the interface interior elements of $D_k$, $C_{e_i}$ the subset of $\Omega_k$ consisting of all adjacent elements to $e_i$, and $\chi(e_i,e_j)$, the characteristic function $\{\chi(e_i,e_j) = 1$ if $e_i \in C_{e_j}$ and $e_i$ and $e_j$ are in different domains or $\chi(e_i,e_j) = 0$ otherwise$. In the case of 2-dimensional meshes we define the mass center of each subdomain $D_k$ to be the point

$$x_{D_k} = \frac{1}{c_k} \sum_{e_i \in D_k} x_i, \quad y_{D_k} = \frac{1}{c_k} \sum_{e_i \in D_k} y_i$$

and the Euclidean distance between two subdomains $(D_k,D_{l})$ to be the distance between mass centers

$$d_{D_k,D_l} = \sqrt{(x_{D_k} - x_{D_l})^2 + (y_{D_k} - y_{D_l})^2}.$$ 

Furthermore, we denote by $r_{k} = \sqrt{|D_k|/\pi}$ the radius of the subdomain $D_k$. The topology of a finite element mesh $\Omega_k$ is represented by a graph $G(\mathcal{V},L)$ whose vertices $\mathcal{V}$ correspond to the elements of $\Omega_k$ and edges $L$ correspond to adjacent pairs of elements. A P-way domain decomposition of $\Omega_k$ is viewed as a P-way graph decomposition of $G$. The problem of partitioning graphs has been studied by many researchers [Barn 82], [Dona 73], [Gold 84], [Chri 76]. In this paper we are particularly interested in the techniques presented in [Kern 70]. For the formulation of P-way graph partitioning techniques, we define the mass center $CR_k$ of a subgraph $G_k(V_k,L_k)$ as follows:

$$CR_k = \{v_i \in V_k : \min \sum_{v_j \in V_k} p(v_i,v_j)\}$$

where $p(v_i,v_j)$ denotes the minimum path that connects the pair $v_i, v_j$ in $V_k$. The distance of vertex $v_i \in V_k$ from $CR_k$ is defined by the quantity

$$d_{v_i,CR_k} = \sqrt{(x_{v_i} - x_{CR_k})^2 + (y_{v_i} - y_{CR_k})^2}.$$
while the distance between subdomains (subgraphs) $D_k(G_k)$ and $D_l(G_l)$ is defined to be

$$d_{D_k,D_l} = \frac{1}{|CR_k| \cdot |CR_l|} \sum_{v_i \in CR_k} (\rho(v_i,v_j))^2.\$$

In the case of graphical metrics, the radius $r_k$ of $D_k$ is defined as the minimum $d_{v_i,C(R_k)}$ for all vertices $v_i \in G_k$ for which the corresponding element belongs to the interface $D_k'$ of the subdomain $D_k$.

3. AUTOMATIC LOAD BALANCED GEOMETRY PARTITIONING STRATEGIES

In this section we formulate and analyze various heuristic domain decomposition techniques for finite element meshes. Specifically, we identify and study two classes of methods. The first class consists of partitioning strategies which are based on some global ordering of elements which minimize the bandwidth or envelope of the discrete PDE system. The other class involves optimization based methods using Euclidean or graphical metrics.

3.1 Clustering techniques

The simplest load balanced decomposition strategy is to group the first $NE/P$ elements of the mesh into subdomains, assuming some a priori global ordering of the mesh elements. Figure 3.1 depicts a domain partitioning based on an ordering of elements along vertical mesh lines. Although this ordering scheme leads to banded systems with minimum bandwidth, it produces partitions whose subdomains are "non-spherical", sometimes disconnected and with lengthy interior interfaces.

A second, more sophisticated clustering approach is based on the Cuthill and McKee ordering scheme. This approach tries to determine subdomains $D_k$ around some specific element $e_i$ such that $\sum \rho(e_i,e_j) > 0$ over all elements $e_j \in C_{e_i}$. If the cardinality of $|D_k| < c_k$, then $D_k$ is enlarged recursively by including the elements $C_{e_k} - (C_{e_k} \cap D_k)$ where $e_k \in D_k$ until $|D_k| = c_k$. This expansion of the Cuthill-McKee ordering ensures to some degree local minimization of sub-domain interfaces while it forces two consecutive subdomains to be adjacent. This ensures the global minimization of the subdomain interface lengths. Our experiments indicate that this scheme leads to partitioning with disconnected subdomains (Figure 3.1b). Different
implementations of the above strategy are presented in [Fahr 88] and [Hous 89b].

3.2 Optimization based techniques

We now consider $P$-way balanced partitions which optimize certain objective functions. Specifically the problem of determining a load balanced $P$-way partition with minimum interface length is reduced to the minimization of the communication or cut cost function

$$\frac{1}{2} \sum_{k,t=1}^{P} \sum_{i \in D_k, j \in D_t} \chi(i,j)$$

provided $|D_k| = c_k > 0$, $\Omega = \bigcup_{k=1}^{P} D_k$ and $D_k \cap D_t = \emptyset$ for all subdomains. The number of feasible solutions of a $P$-way partitioning is prohibitively large [Kern 70] even for a moderate number $P$ of subdomains. A good alternative is to determine semi-optimal solutions using fast heuristics. It appears that the most efficient heuristic strategy for partitioning graphs is the so-called Kernighan-Lin (Ker-Lin) approach [Kern 70]. According to this technique, a given feasible solution is improved with respect to the minimization of the objective function (3.1) by interchanging the pair of elements $(e_i, e_j) \in D_k \times D_t$ such that the so-called profit function

$$f(e_i, e_j) = 2 \sum_{e \in C_i} \chi(e) - |C_i|$$

$$+ 2 \sum_{e \in C_j} \chi(e) - |C_j| - 2\chi(e_i, e_j)$$

is maximum. Although the method is capable of determining a "good" local minimum as Figure 3.2 indicates, its time complexity is significantly large.

In order to guarantee that a $P$-way partition satisfies the criteria (i) to (iii), we introduce the following profit function for elements $e_i, e_j$ in $D_k$ and $D_t$ respectively

$$F(e_i, e_j) = \left\{ \begin{array}{l}
\left[ \frac{d_iCR_k}{r_k} - 1 \right] - \left[ \frac{d_jCR_k}{r_k} - 1 \right], \\
+ \left[ \frac{d_iCR_t}{r_t} - 1 \right] - \left[ \frac{d_jCR_t}{r_t} - 1 \right] \\
+ f(e_i, e_j) \end{array} \right\}$$

Figure 3.2 2-way partitions of a discrete rectangular domain. (a) Cuthill-McKee partition, (b) Ker-Lin partition, (c) GGP solution (optimal solution).
It is easy to see that the maximization of $F$ forces the interchanging of elements outside the "radius" of $D_k, D_l$ which are closer to the current interface of the two selected subdomains. Next, we describe a 2-way optimization based algorithm. Its generalization to a P-way optimization is called GGP-recursion and is obtained by applying the same algorithm recursively. The Cuthill-McKee algorithm and the 2-way GGP have been combined to produce a P-way partition algorithm called CM-GGP. A global non-recursive P-way partitioning geometry graph algorithm is under development and it will appear elsewhere.

/* An automatic 2-way domain decomposition algorithm */

Assume an initial decomposition

$$\Omega = D_1 \cup D_2 \text{ with } |D_1| = c_1, |D_2| = c_2$$

and interfaces $D_i, D_j$.

Step 1: Compute the characteristics of the initial decomposition (center of mass, distance, communication-cost or cut-cost).

Step 2: Determine a pair $(e_i, e_j) \in D_1 \times D_2$ such that the profit function $F(e_i, e_j)$ is positive or maximum and $e_i$ or $e_j$ has not been considered in the previous interchanges with $f(e_i, e_j) > 0$.

Step 3: If the value of the profit function $F$ is positive and the number of interchanges with nonpositive $F$ values is less than the given limit (max-int), then update $D_1, D_2$ and repeat the algorithm with the updated decomposition as the initial decomposition.

If the value of the profit function $F$ is non-positive, the number of unsuccessful interchanges is greater than the given limit (max-int) and the distance $d_{D_i, D_j}$, increases or cut-cost has been reduced then set the number of unsuccessful interchanges equal to 0, update $D_1$ and $D_2$ and repeat the algorithm. OTHERWISE terminate.

The data in Figure 3.3 imply that the new profit function forces interchanges of elements among subdomains $D_1$ and $D_2$ that increase their distance while reducing the objective function (3.1).

![Figure 3.3 The values of the cut-cost function and the distance $d_{D_i, D_j}$ during the execution of the GGP-algorithm for an L-shape domain. A mesh with 406 elements was used.](attachment:figure.png)

4. PERFORMANCE OF GEOMETRY PARTITIONING STRATEGIES

In this section we present the results of some preliminary experiments to measure the degree of satisfiability of the partitioning criteria (i) to (iii) and the time complexity of various geometry decomposition approaches. We have implemented five load balancing algorithms. The two are clustering algorithms based on the natural and Cuthill-McKee orderings which are called Nat-clust and CM-clust, respectively. The other three are graph partitioning type algorithms which try to optimize certain cut-cost functions guided...
by certain profit functions involving Euclidean 
metrics. Their implementation using graphical 
metrics is under way. These are the Kernighan 
Lin (Ker-Lin), the recursive algorithm based on 
the 2-way algorithm described in Section 3 
(GGP-recur) and the GGP-alg algorithm. Figure 
4.1 presents the communication requirements or 
interface lengths for the semi-annulus discrete 
domain of Figure 3.1 obtained using the four 
algorithms. In the case of Ker-Lin and GGP-
recur algorithms the initial feasible partition used 
is the P-way solution of CM-clust. The data indi-
cate clearly that the GGP-recur solution is quan-
titative and qualitative “closer” to the optimum.

Figure 4.1 The interface lengths of five P-way 
partitions of a 2500 element mesh in 
the semi-annulus domain obtained 
with the one clustering and the three 
graph partitioning algorithms.

In Figure 4.2 we present the number of 
interface nodes as a function of the mesh size, for 
2-way partitions obtained by two optimization 
based algorithms (Ker-lin, GGP-alg). Figure 4.3 
shows the time complexity of these algorithms 
measured in terms of the number of interchange 
elements required for different meshes. The 
results in Figure 4.2 and 4.3 are the average 
values over a population of five domains assum-
ing random initial partition. These results indi-
cate that the GGP solution is closer to the 
optimum partition as defined by criteria (i) to 
(ii). Furthermore, the time complexity measured 
implies that the “better” algorithm (GGP) is the 
faster one.

Figure 4.2 The average number of interface 
nodes for two 2-way optimization 
based partitions for different meshes 
over five different domains.

Figure 4.3 Average time complexity of 2-way 
optimization based methods for 
different size meshes over five 
different domains.

Finally the data in Figures 4.4 and 4.5 sup-
port the conclusion that the proposed GGP algo-
rithm produces “better” partitions among the 
clustering and optimization based algorithms.
5. GEOMETRY DECOMPOSITION

We have built an interactive environment called DecTool to help with domain decomposition. An example display is shown in Figure 5.1. The environment provides facilities for both automatic (using a predefined algorithm), and manual decomposition of a domain. This interactive environment is written using the Toolkit from the third release of X11 windows. Its detailed description is given in [Hous 89b]. DecTool consists of three different windows. The first one is the basic DecTool window which initially appears on the screen (left center in Figure 5.1). It is used to control DecTool using the following three buttons.

DONE: Signals to exit from the tool. After exiting, an output file is produced which contains the description of the last decomposition of the domain in a predefined format.

AUTOMATIC: Invokes the automatically decomposed algorithm.

MANUAL: Allows the user to specify the decomposition explicitly using the mouse.

In this basic window, there are three additional widgets (X Toolkit jargon), for input of editable parameters of the tool. The first, NUMBER OF SUBDOMAINS, specifies the number of subdomains for the decomposition. The user specifies the number of subdomains before using the AUTOMATIC button. When the MANUAL button is used, an estimate of the number of subdomains is entered, which should not be less than the final number of the subdomains. The second widget, MODE, provides two options, SUBDOMAIN and INTERFACE. Every click inside the rectangle changes the mode of the tool. Mode refers to what the user is planning to accomplish, i.e., specify subdomains or specify the assignment of the interface grid points. The last widget is one that shows the currently selected subdomain. If there is none, NONE is displayed, otherwise the color of the selected subdomain and its number are displayed.

The second window displayed is a color palette. A color can be assigned to each subdomain and this assignment is displayed on the palette window. This window is also used to interactively select (change) the currently selected subdomain by clicking inside the color rectangle that corresponds to the subdomain selected.

The third window displays the domain, which is defined in terms of a set of mesh lines and a boundary line. In case there is a decomposition, it is displayed using the color assignment specified by the palette window. This window can also be used to edit interactively, (by using the mouse), the current decomposition. It is also possible to specify a decomposition from scratch by selecting the MANUAL option.
Figure 5.1 Example of the geometry decomposition tool DecTool for an annular region and 16 subdomains. The two DecTool windows are on the left side, the bottom left is for parallel ELLPACK and the right one is the display of the decomposed finite element mesh.

6. REFERENCES


