Data-parallel support for numerical irregular problems

E.L. Zapata*, O. Plata, R. Asenjo, G.P. Trabado

Department of Computer Architecture, University of Málaga, P.O. Box 4114, E-29080 Málaga, Spain

Abstract

A large class of intensive numerical applications show an irregular structure, exhibiting an unpredictable runtime behavior. Two kinds of irregularity can be distinguished in these applications. First, irregular control structures, derived from the use of conditional statements on data only known at runtime. Second, irregular data structures, derived from computations involving sparse matrices, grids, trees, graphs, etc. Many of these applications exhibit a large amount of parallelism, but the above features usually make that exploiting such parallelism becomes a very difficult task. This paper discusses the effective parallelization of numerical irregular codes, focusing on the definition and use of data-parallel extensions to express the parallelism that they exhibit. We show that the combination of data distributions with storage structures allows to obtain efficient parallel codes. Codes dealing with sparse matrices, finite element methods and molecular dynamics (MD) simulations are taken as working examples. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

Scientific and engineering applications are computational expensive, and so important efforts have been devoted to find efficient implementations on multiprocessors. This general situation, however, deserves to be analyzed in more detail. There is a class of numerical applications that exhibit a regular structure. Computationally,
these problems are typically characterized by the existence of a simple relationship between the indices of two data dependent array accesses (often a linear function analyzable by the compiler).

Regular applications are usually easy to parallelize, making efficient use of the processor cycles and the memory hierarchy of current multiprocessor architectures. These codes make easy to devise a simple mechanism to access remote data, as regular data dependences can often be satisfied, with little or no communication, by distributing data structures across memories using simple mapping strategies (block, cyclic or mixed block–cyclic).

Many important numerical applications, however, show an irregular structure. These problems arise in sparse matrix computations, computational fluid dynamics (CFD), image processing, molecular dynamics (MD) simulations, climate modeling, optimization problems, etc. [32,42]. They exhibit an irregular and unpredictable runtime behavior, that does not fit directly the architectural features of contemporary multiprocessors. This makes that writing an efficient parallel program becomes a very difficult task.

We can distinguish two kinds of irregularity in these applications. First, irregular control structures may appear in the code, that is, conditional statements on data only known at runtime. Second, irregular data structures may also appear in the code, which include sparse matrices, grids, trees, graphs, etc. Usually these data structures are organized as arrays in the code, but in such a way that arise pairs of dependent array elements whose indices appear to be related by a complex function or by an array lookup (indirection access). Both kinds of irregularities cause irregular communication patterns and workload balancing problems. Issues like data layout, data/control dependences, locality, workload balancing, communication optimization, and others, become hard problems to be assessed.

Private memory (message-passing) architectures have been the most used machines to solve large numerical problems. Typically these machines are programmed using a standard sequential language, like FORTRAN or C, augmented with constructs for message-passing, like PVM or MPI. In this programming model, the programmer must explicitly deal with complex aspects, like data distribution, work partitioning, task communications, workload balance, and others. This fact leads to high developing costs and slow software production.

To facilitate the productivity of parallel numerical software, two more options are being available in recent years [13,19,41]. On one hand, a data-parallel programming model has been standardized, the High Performance Fortran (HPF) [14,15,26,27,31]. This paradigm is based on a single thread of control and a globally shared address space. On the other hand, scalable distributed shared memory machines [30] are starting to be used for solving numerical applications. For these systems shared memory is the native programming model. Recently there has been an important effort to develop a new standard for portable, high level, scalable and incremental shared memory parallelization, called OpenMP [34].

In any of the above parallel programming models a good distribution of data across the memories is a key point for obtaining a scalable parallel program [36]. It would be desirable to have a compiler capable of selecting the appropriate data
distribution with no intervention from the programmer. However, this is a very tough task for numerical irregular problems. Currently the problem is open and unsolved, except for some simple classes of irregular codes [2,9,10]. The compilation task can be simplified if the programmer is allowed to be involved through the use of compiler directives. These directives may help the compiler in identifying the class of irregular application, that is the role of the main data structures in the code, as well as express directly data distributions and alignments. Data-parallel and scalable shared memory programming models permit this alternative.

This paper reviews our research experience in parallelizing numerical irregular problems in scalable parallel systems, mainly message-passing machines, in the context of a data-parallel programming model. It shows a sample of the methods we have developed in the case of three example codes, that cover a representative set of irregular applications. In all cases we explain how to use and improve the data-parallel language HPF to inform the compiler about key aspects of the program and hence obtain an efficient and scalable parallel code.

The rest of the paper is organized as follows. Section 2 discusses the difficulties in the parallelization of numerical irregular programs, and how we can obtain efficient parallel codes if the compiler is aware of some problem properties. Sections 3 and 4 explain the method we follow to obtain such parallel codes for various code examples, one in the sparse matrix area (Section 3) and two dealing with unstructured domains (Section 4). In Section 5 some related work is described, and finally, we draw some conclusions in Section 6.

2. Revealing problem structure

Numerical applications that operate on regular data structures can often be efficiently implemented by using data-parallel language constructs. The regular nature of the problem to be solved can be easily comprised at the language and compiler levels. The same cannot be said about irregular numerical applications, that use irregular data structures. It is usual that in the process of expressing an irregular application using language constructs some problem properties are lost. For instance, codes may not exhibit key properties such as spatial or temporal localities associated to the nature of the problem. It is crucial, however, to exploit this kind of properties in order to obtain efficient parallel codes.

There is, therefore, usually a mismatch between the problem-level representation of the application (data and operations needed to process the data, as well as the problem properties of such data and operations) and its language-level representation (code using some conventional data-parallel language). In order to obtain an efficient parallel program the compiler needs to know the role of some key data structures in the code as well as some general properties that the data stored on such structures fulfill. Let us explain this using two small code examples, as shown in Fig. 1. In Fig. 1(a), a sparse matrix–vector multiplication code (SpMxV) is sketched. The source and resulting vectors are dense, and are represented by arrays X and Y. The matrix, however, is sparse and it is represented using a compressed row storage (CRS) format.
This format uses three arrays, Data, Col and Row to represent the matrix. Data stores the non-zero entries of the matrix, as they were traversed in a rowwise fashion. Col stores the column indices of the entries in Data, and Row stores the locations in Data that start a row (by convenience, Row(n+1) stores the number of non-zero entries of the matrix plus one, where n is the number of rows of the matrix).

The SpMxV code shown in Fig. 1(a) is efficient, as only non-zero matrix entries are considered for the multiplication, avoiding a large amount (depending on the matrix fill-in) of null operations. However, the nature of the problem has been lost. A simple analysis of the code only sees a two-level nested loop that operates on five dense one-dimensional arrays. A naive parallelization of the nested loop probably produces an inefficient parallel code, as the length of the inner loop cannot be predicted at compile-time and the array X is accessed through an indirection. Simple block/cyclic distributions of the arrays may imply an unbalanced workload distribution and a high communication overhead.

A much better parallel code can be obtained if the knowledge that the three arrays Data, Col and Row actually represents a sparse matrix (problem property) is considered. If the compiler knows that the arrays Row and Col only contains index information about the location of the values stored in Data on a matrix space, then a uniform distribution of Data is enough to assure a well-balanced code workload distribution. In addition, a careful assignment of the particular elements in Data to the processors allows us to optimize the communication requirements. The definition of this mapping may also be facilitated if the sparse matrix nature of the problem is known. When using a data-parallel language, such data distribution and assignment must be done at the language level. Hence, the sparse matrix problem property should also be at that level.

A different situation is represented in Fig. 1(b). The code shown is a section of a simple MD simulation [5]. A neighbour list (NeighbourList) was previously built by storing pairs of interacting particles. The inner loop k sweeps over those pairs and, if the separation between the interacting particles is less than some cut-off distance,
pairwise force contributions on them are computed. Afterwards, velocities and positions of all the particles in the system are updated. These computations are repeated during a small number of consecutive timesteps (outermost loop ts).

The force calculation stage is usually the most time-consuming part of the simulation. Through the use of a neighbour list, only non-null force contributions are computed, speeding up this stage. However, this fact increases the algorithmic complexity of the code, as indirections appear at both sides (LHS and RHS) of the statements computing the forces. A naive distribution of the particles across the processors (block distribution of the arrays, for instance) probably produces a parallel code with high communication requirements at the most computational part of the MD simulation.

However, if only short-range interactions are considered in the simulation (problem property), then the neighbour list exhibits a high degree of spatial locality. This knowledge does not appear in the code, but only in the input data. Exhibiting this knowledge at the language/compiler level, the communication overhead can be minimized. For instance, a spatial decomposition of the domain can be accomplished. Communication requirements are very low, as only particles near the frontier of the sub-domains interact with non-local particles (belonging to other sub-domains).

There are many parallel implementations of the above two codes, and of many other numerical irregular applications. Most of these implementations, in the case of large applications at least, has been done on massively parallel computers, resorting to message-passing libraries to deal with communication. All these parallel codes take advantage, in same way, of problem properties, such as the ones discussed above, in order to get efficiency. However, data-parallel language constructs are less flexible than message-passing routines. The execution model is single-threaded with a globally shared address space. With these languages we have similar difficulties to expose problem properties than with a sequential language. While there are many efficient message-passing irregular numerical codes, for many problems, however similar implementations using a data-parallel language is currently an open question.

The approach we follow consists in defining new data-parallel language constructs in the context of HPF that permit to identify the role of the important data structures in the code, to express exploitable key properties of the problem nature (data properties) and to manipulate irregular data structures. The compiler is in turn instructed to recognize the new constructs to use them when producing the parallel code. For large applications, the complexity of the compiler may be lightened by leaving most of the work associated with data distribution, communication and synchronization to an external runtime library. The rest of the paper is dedicated to show the proposed solutions for a number of representative numerical irregular codes.

3. Sparse matrix algebra

Sparse matrices arise naturally when discretizing continuous operators. They appear in a large number of important scientific and engineering codes, which are
classified as irregular applications [17,29,50]. This is because sparse matrices are represented using compact data formats, which necessitates heavy use of indirect addressing through pointers stored in index arrays. Such compact formats are used in order to not store zero elements, saving memory and avoiding arithmetic with zero elements to save floating-point operations.

Normally, it can be distinguished two broad categories of sparse matrix representations [50]. *Structured representations*, that exploit some regular structure of the fill (set of locations of the non-zero elements), and *unstructured representations*, that do not impose any requirements to the fill. However, in this sections and the next one, we will consider an operative classification of sparse matrix applications [17]. We will use the term *static* to comprise those applications that only read the sparse matrix fill. That is, the fill of the matrix does not change during computation. The other class is called *dynamic*, including those applications that read and write the sparse matrix structure. In this case, the fill of the matrix may change during computation.

An efficient parallelization of a sparse matrix application requires exploitation of data locality and a simple and fast method to locate non-local data. Most parallel implementations are tuned according to the fill pattern of the sparse matrix, in order to attain maximum efficiency [29]. According to this, some sparse compact representation is more appropriate than others to get the best efficiency.

In a data-parallel environment, such as HPF, we are constrained to the language constructs of a sequential language, such as FORTRAN90/95, and some directives used to express parallelism and to instruct the compiler on how to produce the parallel code. Currently HPF does not include any directive to link the arrays of the sparse matrix representation to the sparse matrix itself [27]. However, having such directive permit to define sparse data distributions with the property of, on the one hand, exploiting data locality and, on the other hand, simplifying the location of non-local data. We have proposed the directive SPARSE to fill this gap [4,49]. For instance, for the example shown in Fig. 1(a), we would write

```
!HPF$ SPARSE(CRS(Data, Col, Row)) :: A(N, N)
```
to express that Data, Col and Row are the arrays associated with the CRS representation of a sparse matrix. In addition, the sparse matrix is giving a name, A in the example shown. This name is actually a template, because it does not exist in the original sequential code. We can use it only inside other HPF directives. The sparse name can be referenced in a distribute directive. For example,

```
!HPF$ DISTRIBUTE(CYCLIC, CYCLIC) :: A
```
specifies that the sparse matrix A should have its rows and columns distributed cyclically over some two-dimensional arrangement of processors. Observe that A names a *complete* (uncompressed) sparse matrix. Therefore, both non-zero and zero elements are considered for distribution. As a consequence of this specification, the arrays Data, Col and Row will be mapped to the processors in such a way that the above distribute directive is obeyed. This kind of sparse distribution was called block row scatter (BRS) in [4,40].
For mapping purposes, the sparse matrix is dealt as a dense matrix. Hence, the workload is balanced using similar techniques than if the code were dense. Besides the compiler can derive simple formulas to determine the location of each sparse data entry. Communication schedules are easy to compute and optimize, with low overhead.

The above BRS pseudo-regular sparse data distribution can be used to obtain efficient parallel codes using static sparse matrices in an efficient way. For instance, [6] shows a simple parallel implementation of the conjugate gradient iterative method for solving large sparse systems of linear equations. A complete discussion of static sparse computations on the framework of the Vienna Fortran compilation system can be found in [49]. BRS (and multiple recursive decomposition, MRD, discussed in the next section) distributions are described in detail and compilation and runtime issues related to their implementation are analyzed.

For dynamic sparse matrix applications, the situation is much more complex. The explained approach must be extended to take into account that the fill of the matrix may change while computing. Our solution is to define a dynamic compact format to represent the sparse matrix, keeping charge of the possible fill-in. The rest of the section is dedicated to discuss in detail a dynamic case study.

3.1. Dynamic case study: Direct sparse solvers

A wide range of numerical applications include the solution of large sparse systems of linear equations. There are two different approaches to solve such systems, direct and iterative methods. In direct methods [17, 22], the system is converted into an equivalent one whose solution is easier to determine by applying a number of elementary row and/or column operations to the coefficient matrix. A different approach is taken in iterative methods [7, 51], where successive approximations to obtain more accurate solutions are carried out.

Direct methods for solving sparse systems exhibit different problems to those of iterative methods. The coefficient sparse matrix is transformed, or factorized, operation that may change the fill of the matrix. The compact representation of the matrix must take into consideration this fact. Also, row and/or column permutations of the coefficient matrix (pivoting) are usually accomplished in order to assure numerical stability and reduce fill-in. All these features make direct methods much harder to parallelize than iterative solvers.

Let us take the sparse LU factorization as a working example [17]. Fig. 2 shows an in-place code for the direct right-looking LU algorithm, where a n-by-n matrix A is factorized. The code includes a row and column pivoting operation (full pivoting) to provide numerical stability and preserve the sparsity rate.

Apart from linking the compact representation arrays to the sparse nature of the problem, as was seen previously with the SPARSE directive, an additional effort is needed to select the appropriate compact format. Standard compressed formats are not the most suitable schemes to support efficiently the fill-in problem and pivoting operations. Dynamic formats, such as linked lists, are more flexible that standard static formats, such as CRS. Pivoting operations are accomplished by just inter-
changing pointer values. Fill-in is easily managed, as entry insertion/deletion operations are simple when using linked lists.

Full-pivoting sparse LU decomposition can be represented by two-dimensional doubly linked lists, in order to make data accesses both by rows and by columns. Each item in such a dynamic structure stores not only the non-zero value and the local row and column indices, but also pointers to the previous and next non-zero element in its row and column (four pointers in total). The complexity of the lists can be simplified if the full pivoting is replaced by a partial pivoting, where only columns (or rows) are swapped. This fact may imply large memory and computation savings because we can use a one-dimensional doubly linked list structure as the compact representation. In such structure, each linked list represents one column (row) of the sparse matrix, where its non-zero elements are arranged in growing order of the row (column) index. Each item of the list stores the row (column) index, the matrix non-zero entry and two pointers. These compact representations were called linked list row–column storage (LLRCS) and linked list column storage (LLCS) (or LLRS for rows).

Fig. 3 depicts an HPF declarative section for the parallel sparse LU code (only the HPF directives are shown). Matrix $A$ is defined as sparse and represented by the LLCS format. The arrays of pointers first and last indicate the first and the last non-zero entry, respectively, of each column of $A$. The array vsize stores the number of non-zero entries on each column of $A$. We have also defined a sparse array $VCOL$,}

```fortran
DO k = 1, n
   Find pivot: $A_{ij}$
   IF (i .NE. k)
      swap $A(k,1:n)$ and $A(i,1:n)$
   END IF
   IF (j .NE. k)
      swap $A(1:n,k)$ and $A(1:n,j)$
   END IF
   $A(k+1:n,k) = A(k+1:n,k) / A(k,k)$
   DO j = k+1, n
      DO i = k+1, n
         $A(i,j) = A(i,j) - A(i,k)A(k,j)$
      END DO
   END DO
END DO
```

Fig. 2. Direct right-looking LU algorithm.

Fig. 3. HPF declarative section for the sparse LU code.
which is represented as a compressed (packed) vector (CVS format). This array will contain the normalized pivot column of A, calculated in each outer iteration of the algorithm.

The last sentence in the declaration section distributes cyclically the columns of the sparse matrix A over a one-dimensional arrangement of abstract processors (linear). Previously, three dense arrays, iq, vpiv and vmaxval, were aligned with the columns of A. Therefore, after the distribution of A, these three arrays also appear distributed in a cyclic fashion over the processors. Finally, the sparse array VCOL is aligned with the rows of A. Hence, after distributing A, VCOL is completely replicated over all the processors. The reason of this replication is to make normalized pivot column visible to all processors, enabling the subsequent parallel sub-matrix update.

As sparse data is accessed through pointers, the default owner compute rule is not the most appropriate work distribution scheme for some phases of the computation. For instance, during the update sub-matrix phase (loops j and i in Fig. 2), we want that processor that owns entry j of the pivot row (vpiv()) be in charge of updating row i of the sub-matrix. The approved HPF-2 extension ON permits such computation assignment. The approved extension RESIDENT is also used to assert that column j of A is stored in the same processor that owns vpiv(j), hence no interprocessor data movement is required (see Fig. 4).

```hpf
!HPF$ INDEPENDENT, NEW (aux,i,amul,product)
loopj: DO j = k+1, n
!HPF$ ON HOME (vpiv(j)), RESIDENT (A(*,j)) BEGIN
  aux => vpiv(j)Xp
  IF (.NOT. ASSOCIATED(aux)) CYCLE
  IF (aux%index /= k) CYCLE
  amul = aux%value
  vsize(i) = vsize(j)-1
  vpiv(j)Xp => aux%next
  aux => aux%next
loopi: DO i = 1, size
  product = -amul*vcolv(i)
  DO IF (.NOT. ASSOCIATED(aux)) EXIT
  IF (aux%index >= vcoli(i)) EXIT
  aux => aux%next
END DO
outer_if: IF (ASSOCIATED(aux)) THEN
  IF (aux%index == vcoli(i)) THEN
    aux%value = aux%value + product
    ELSE
      CALL insert(aux,vcoli(i),product,first(j)Xp,vsize(j))
      IF (vpiv(j)Xp%index => aux%prev%index) vpiv(j)Xp => aux%prev
    END IF
    ELSE outer_if
      CALL append(vcoli(i),product,first(j)Xp,last(j)Xp,vsize(j))
      IF (.NOT. ASSOCIATED(vpiv(j)Xp)) vpiv(j)Xp => last(j)Xp
    END IF
  END IF
END IF
END DO loopi
!HPF$ END ON END DO loopj END DO main
```

Fig. 4. Outline for an extended HPF-2 specification of the sub-matrix update phase of the right-looking partial pivoting LU algorithm.
An implementation of the above code was done on a Cray T3E platform. Due to the lack of a complete HPF-2 compiler, all directives were manually translated into calls to the Data Distribution LaYer (DDLY) runtime library [47]. The code was written in FORTRAN90, and the Cray SHMEM library was used for communications. Parallel execution times and speed-up of this implementation is shown in Fig. 5, taking the sparse matrices from the Harwell–Boeing suite [18] and the University of Florida Sparse Matrix Collection [16]. The efficiency of the parallel code is high when the size of the input matrix is significantly large. Due to fill-in, some load imbalances may appear during factorization, but they were not significant in any of our experiments. An in-depth description of the sparse LU factorization can be found in [1,3,45].

4. Unstructured domains

Many scientific and engineering applications work with unstructured domains to provide a general solver being able to handle any problem input to the application. In other case scientists should write specific solvers for the structure of each problem. However, while providing a useful tool for scientists, general solvers represent a challenge for high performance implementation. Some representative examples include finite elements or differences for solving partial differential equation systems, CFD, or MD simulations.

Finite element and difference methods are computational tools for deriving approximate solutions to a system of partial differential equations, that governs the behaviour of some physical system. In order to solve numerically the system, the physical domain is discretizing imposing a grid. In case of finite differences, the grid is usually regular. In general, at each grid point a linear equation that relates the value of some physical magnitude at such point to its value at neighbouring grid points has to be solved. The resulting sparse coefficient matrix of the full equation
system has block diagonal fill structure, and can be solved using some iterative or
direct solver, as was discussed in the previous section. However, new difficulties arise
if the grid is dynamic, as in MD simulations.

In case of finite elements, the grid divides the domain into a large number of small
areas called elements, that comprise sets of interacting grid points. In addition, for
most applications, the grid is not a regular structure, deriving a large, sparse and fill
unstructured coefficient matrix.

These applications contain irregular data access patterns related to unstructured
problem domains. Such common feature poses hard difficulties for automatic par-
allelization or data-parallel implementation. Many types of unstructured problems
have been successfully parallelized [21,29,32]. However, in most cases the software
has been difficult to write. In addition, expressing the irregularities and efficient
mapping onto particular multiprocessors has implied the development of tedious
non-portable code.

In terms of high performance implementation, these applications can be dealt as a
sparse matrix problem, but with the additional difficulty that the sparse coefficient
matrix is often unstructured. A different and more usual approach consists in directly
handling the finite element grid. The grid is irregular but the computations fulfill
locality properties.

As was discussed in Section 2, obtaining an efficient data-parallel implementation
of unstructured application needs to express some problem properties at the lan-
guage and/or compiler level. Codes rely blindly on some simple language constructs
that describes data access patterns, but not the high level structure of the problem
(computations). Data access patterns are irregular, however problem structure tends
to be regular, exhibiting spatial and/or temporal localities. Compilers simply do not
take advantage of such inherent regular properties.

We will explain how to extend the SPARSE HPF directive described in the pre-
vious section to not only relate language data structures to problem data structures,
but also to express regularities inherent to the nature of the problem. Such discussion
will be done for two example cases, a static unstructured domain application (data is
only read), finite element codes, and a dynamic unstructured domain application
(data is read and written), MD simulations.

4.1. Static case study: Finite element codes

In most programs handling unstructured meshes we can find pieces of code similar
in structure to the sample code in Fig. 6. This loop actually represents a matrix–
vector product $\text{PROP2} = \text{WEIGHT} \times \text{PROP1}$. Arrays $L$, $R$, $U$ and $D$ represent the
non-zero weights in matrix $\text{WEIGHT}$. The use of such arrays and the indexing array
$\text{NEIGHBOR}$ is due to the fact that this is an sparse problem and the programmer is
optimizing the representation of the problem by using indirections instead of using
one two-dimensional array for the sparse matrix $\text{WEIGHT}$. Each element in arrays
$\text{PROP1}$ and $\text{PROP2}$ is an associated value corresponding to one mesh element in the
physical model. So, only physically neighboring mesh elements are considered in the
matrix–vector product.
From this code we can extract two observations that will become important while parallelizing unstructured meshes applications. First, the code performs a regular computation stencil which includes a limited number of array elements. Those elements correspond only to physically neighboring mesh elements which are statically defined in the input data of the program. Specifically in the contents of the array NEIGHBOR which is related with the structure of the problem mesh. Second, the term physically neighboring is not related with storage neighboring. Mesh elements adjacent in the space may not be stored contiguously in a memory array representing such mesh. Although the computation stencil is regular, speaking in terms of code analysis, the presented sample code is highly irregular because of the use of an array for indexing another one. Compilation analysis finds that accesses to array PROP1 are unpredictable because they depend on the run time contents of array NEIGHBOR.

The example solver shown in Fig. 6 uses only the array NEIGHBOR to direct computations through the problem domain. Nevertheless, this solver does not use all existing information describing the unstructured mesh. Some other structures (arrays) are often used in external partitioners to compute data distributions. Fig. 7 shows in which way an unstructured mesh is described by X, GRID and NEIGHBOR arrays.

The objective is, inside a data-parallel environment, to distribute this representation of the unstructured mesh preserving spatial locality in all the levels of the representation. The vertices of the mesh are stored in X and hence this array is the key data structure to express at the language level the spatial locality that exhibits the problem. As all data accesses in Fig. 6 are local at the mesh domain, we should distribute array X over the processors in such a way that a spatial decomposition of the mesh is accomplished. This mapping can be expressed by extending the SPARSE directive as follows:

```
!HPFS REAL, DYNAMIC, SPARSE(COORDINATES(X(NV, 2))) :: A(:, :)
!HPFS DISTRIBUTE(BLOCK, BLOCK) :: A
```

Instead of specifying a number of arrays and a compact representation, as with sparse problems, the directive instructs the compiler to consider the indicated array (X) as a set of coordinates of spatial locations. The defined template A represents
such spatial domain, and hence is a construct directly related to the mesh. The BLOCK distribution directive applied to the assigned placeholder A results in a spatial decomposition of the array X into sub-domains, and the mapping of such sub-domains over the processors. This type of decomposition was called MRD in [4,40]. Observe that the distribution operation is executed at runtime, when the contents of X is known.

The next step is distributing other data structures representing higher levels in the mesh (like edges, polygons, cubes or other kind of mesh elements). Such mesh elements contain no geometric information but each one is related to some lower level structures (like vertices) already distributed in the former phase. These distributions can be written as follows:

```
Fig. 7. Up: actual structure of the problem domain. Down: X stores coordinates for mesh vertices, GRID stores the definition of the mesh itself (each element is a set of four vertices), NB stores the list of neighbors for each element of the mesh.
```

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The first alignment is an extension of the standard HPF directive, and was called pointer alignment in [43,48]. This directive distributes an indirection array in such a way that each row of the array is stored in the processor owning the row in some other array referenced by the pointer. Specifically, each \( i \)th row of array \( \text{GRID} \) has been aligned with the row of array \( X \) pointed by \( \text{GRID}(i,1) \). The resulting distribution groups in each partition the elements of the array corresponding to closely located mesh elements. The next two alignment directives places several arrays in such a way that spatial locality is exploited. These are standard directives. The last directive is also a new extension of the standard, that we call target alignment. It is possible that, as consequence of the previous distributions, some partitioned arrays point to non-local array elements. Accesses using such indices can not be translated to local coordinates neither executed without fetching remote data before. But we cannot fetch data before knowing which arrays are going to be accessed through those indirections. The target alignment specifies that array \( \text{PROP1} \) is going to be accessed through the indirections stored in array \( \text{NEIGHBOR} \). This way, the compiler is instructed on how to grab needed non-local data at runtime.

Some evaluation tests have been carried out using a real code of 3-D CFD. The code was parallelized rewriting the HPF directives inserted in it by calls to the DDLY library. The executions presented in Fig. 8 were conducted in a IBM SP2 multicomputer. A PVM implementation of the DDLY library was used. The test data consisted in a mesh with approximately 276 000 cells. The solver computed 340 iterations until convergence was reached.

I/O and distribution time are the initialization phase of the program. The test yields excellent results for the execution of the solver loop, which indicate that the exploitation of the spatial locality through the use of the \textit{SPARSE} directive and \textit{indirection alignments} is nearly optimal. Also, the time spent in communications during the computation remains very low. A more detailed analysis of parallel finite element codes can be found in [43,48].

4.2. Dynamic case study: Molecular dynamics

MD simulations consider a set of particles (atoms or molecules) subject to Newton’s classical equations of motion, which are integrated to compute and understand the movement of each particle. With this technique a number of microscopic and macroscopic values can be estimated, such as transport and diffusion coefficients, phase diagrams, and so on, many of them difficult to obtain experimentally.
To simplify the exposition we will consider the simulation of a two-dimensional ensemble of particles subject to a Lennard-Jones potential, 
\[ v_{\text{LJ}}(r) = \sigma^{12}/r^{13} - (\sigma/r)^{6}, \]
where the cut-off distance is \( r_c = 2.5\sigma \). To integrate the equations of motion of the particles, a finite-difference leapfrog algorithm on a Nosé–Hoover thermostat dynamics is used.

Fig. 9 shows the algorithmic structure of such simple short-range MD simulation. The first action is reading particle positions and velocities (read data). Some other quantities are also read, such as the size of the simulation box, the cut-off distance of the potential, the number of timesteps, etc. After some normalizations and simulation box adjustments (initialization), a loop running over the timesteps is started. This loop is strip-mined into two (not perfectly) nested loops. The outer loop steps between strips of the same size (T Hop), and the inner loop steps between single timesteps within a strip.

The outer loop is used to determine at which timestep the link-cell and the neighbor list are built. These data structures are used as book-keeping methods, that avoid to waste CPU cycles in calculating null force contributions on each particle. For each iteration of that loop particles are sorted into the link-cell lattice, and all the pairs of neighboring particles (separated by a distance somewhat larger than the
potential cut-off) are computed and stored in a list. To avoid border effects periodic boundary conditions are implemented at the link-cell level.

The inner loop reuses the neighbor list during a strip of iterations (THop). Force on each particle is calculated by integrating the discretized equations system, taking the interacting particles from the neighbor list. These computations are halved by resorting to Newton’s third law. Afterwards velocities and positions are updated for each particle and some macroscopic parameters are calculated also. A more detailed description of this phase was shown in Fig. 1(b). Finally, after exhausting all time-steps, positions and velocities of all particles are written in a file, in addition to some macroscopic parameters.

MD codes exhibit a natural parallelism that comes from the fact that the force calculations, and the velocity/position updates, can be done simultaneously for all particles. To exploit this parallelism, a number of partitioning and mapping strategies has been developed. The approach we followed is termed domain decomposition [12,35], as shown in Fig. 10.

An initial blockwise partitioning for the input data to be read is assumed. Each processor reads the input data (particle positions/velocities and input parameters) for its assigned initial partition. At the first timestep, link-cell lattices are built in parallel. A processor will have non-null data only in those cells belonging to its partition. Afterwards a hierarchical partitioning strategy is executed, similar to MRD. The simulation box is first partitioned at the link-cell level along the first dimension. Each strip is then sub-partitioned independently along the second dimension. In general, the number of partition levels equals the number of dimensions of the box. The divisions are accomplished in such a way that some performance parameter is optimized. The imbalance in the number of particles is the most common parameter, but some other can be chosen, such as the imbalance in the number of interactions (density). The partitioner is internal, general enough to cover most cases with average efficiency sufficiently high. Besides, the partitioner generates a compact representation of the decomposition, that permits to optimize subsequent computation stages (mapping arrays are avoided).

After cell-decomposition of the simulation box, a shuffle redistribution of all data arrays (in particular, position and velocity arrays for the particles) is carried out.

Fig. 9. Algorithmic structure of a simple short-range MD simulation.
Each processor will store locally positions/velocities for the particles belonging to its cell-domain. The processors will also store a copy of the particle positions/velocities arranged at nearest neighbor link-cells. This communication interchange between neighbor processors is accomplished by the guest particle update (GPU) stage in Fig. 10. Previously, a GPU particle schedule is built, an array that indicates what processors will receive particles from a particular set of border cells. GPU stage guarantees that all accessed data by a processor is locally available, either as owned data or guest data. As a consequence, all computations can be carried out using only local indices, without any type of control over memory references.

Each cell-domain has the same structure as the original program. A processor can operate on its domain, with no interaction with other processor, until the next synchronization point. A runtime library carries out all synchronization work, in a transparent way for the user. At each synchronization point, the library updates the guest particles across domains (GPU), reusing the first schedule computed (if the cell-domain is not repartitioned, the schedule array does not change). Newton’s third law allow us to replicate force calculations instead of propagating non-local writes, saving communication overhead.

Due to the dynamic nature of the simulation, some particles may change of cell-domain. Instead of carrying out global redistributions, we have implemented a particle migration stage, called particle ownership adjustment (POA), that communicate to the new owner (always a neighboring processor) those particles that have

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Fig. 10. Algorithmic structure of a simple parallel short-range MD simulation.
abandoned its cell-domain. During this stage, the communication schedule for the GPU is also updated.

To exploit the problem spatial locality exhibited by the MD code, the extended SPARSE directive as defined in Section 4.1 is used. For example,

```fortran
!HPF$ REAL, DYNAMIC,
!HPF$ + SPARSE(
!HPF$ + COORDINATES(X(N), Y(N)),
!HPF$ + THRESHOLD = R
!HPF$ + LINKCELL(IX, IY)(LCPNT, LCCNT)
!HPF$+) :: B(0 : LX, 0 : LY)
```

describes a set of N particles with two-dimensional coordinates. Problem domain borders are defined by the intervals [0, LX] and [0, LY]. Note that the dimensions of the placeholder specify real instead of integer bounds because it is not defining an integer index space. The keyword COORDINATES specifies a list with the tables containing geometric information about the elements during program execution. In the particular example, arrays X and Y store the two-dimensional coordinates of the spatial domain.

THRESHOLD controls the behavior of data replication for selected data distributions. It is used to provide an expression for the length of the overlapping area between any neighboring domains of data distribution. Replication guarantees that all particles of neighbor partitions that can be involved in a local computation will be available in local memory as a guest element.

The LINKCELL keyword describes the implementation of the link-cell used in the program. The first argument is the number of cells considered during execution. The second is a list with the arrays which contain link-cell data. We support both linked-lists and dense pointer-arrays implementations as they are the most popular.

The representations of particle sets in FORTRAN programs use to be very heterogeneous. The set of data arrays related to particles depends on what is done in each simulation, though the arrays containing geometric data are always present. For sake of simplicity in directives, the COORDINATES keyword specifies only those arrays, while the other related arrays are specified using standard HPF ALIGN directive with perfect alignment, as for example,

```fortran
!HPF$ ALIGN WITH X :: VX, VY, FX, FY
!HPF$ REDISTRIBUTE(BLOCK, BLOCK) :: B
```

Finally, the placeholder of the problem domain, B must be distributed, using the standard directive. The BLOCK distribution method used in each dimension of the placeholder indicates geometric partitioning (i.e., a value-based distribution) of the set of arrays bound to the placeholder via SPARSE and ALIGN directives.

A DDLY-based implementation of the described MD code was executed on a Cray T3E, with different number of particles (domain size). Fig. 11 shows the speedups and efficiencies obtained on the Cray T3E for each problem size. The
neighbour list was updated every 10 timesteps. The cut-off distance was fixed to $2.5\sigma$
and the size of each link-cell was $2.9\sigma$. The size of the simulation box was $250\sigma \times 250\sigma$. Each test has simulated 1000 timesteps using different number of
processors ranging from 1 to 64. In the case of the 640 000 particle data set, we have
considered speedup 1.0 for 8 processors, as this was the minimum number of pro-
cessors required to execute the simulation.

We have to remark the good scalability of the parallel code. Efficiency gets closer
to the ideal full parallel program as problem size increases because of the small time
spent in communications (almost constant for different problem sizes and numbers
of processors). The behaviour remains stable as dynamic problems evolve. In [43,46]
a detailed discussion of parallel molecular dynamics codes can be found.

5. Related work

We have distinguished two different approaches to handle irregular computations.
One possibility is based on extending the data-parallel language with new constructs
suitable to express non-structured parallelism. With this information, the compiler
can perform a number of optimizations, usually embedding the rest of them into a
runtime library. In FORTRAN D [20], for instance, the programmer can specify a
mapping of array elements to processors using another array. Vienna-Fortran [52],
on the other hand, lets programmers define functions to specify irregular distributions.
HPF-2 [27] provides a generalized block distribution (GEN-BLOCK), where the
contiguous array partitions may be of different sizes, and an indirect distribution
(INDIRECT), where a mapping array is defined to specify an arbitrary assignment of
array elements to processors.

All these language constructs usually lead to low efficiencies when they are applied
to a wide set of irregular codes. The main drawback is that locating non-local data is
in general an expensive task. Our SPARSE directive, however, allows to specify
pseudo-regular distributions, that do not suffer from this problem.
The second approach is based on runtime techniques, that is, the non-structured parallelism is captured and managed fully at runtime. These techniques automatically manage programmer-defined data distributions, partition loop iterations, remap data and generate optimized communication schedules. Most of these solutions are based on the inspector–executor paradigm [11,33,36].

This technique consists in the insertion of runtime support in the final parallel code to analyze each access and decide if the access is local or remote. In the case of a remote access, remote data is sought and stored locally by the runtime support before the data access is allowed to proceed. The authors produced a runtime library known as PARTI/CHAOS [38,39] that was used in manual parallelization of irregular programs. The introduction of this paradigm in parallel compilation was carried out, for instance, at Rice University in the FORTRAN D compilation system [24,25,44].

The FORTRAN D compiler base domain partitioning on an user-provided function that map array elements to processors depending on their values. Usually, value-based decompositions [23,37] cannot be represented in a compact form, thus a mapping array must be returned by the partitioner. This solution is expensive and inviable for large systems. Also, this distribution method does not guarantee that all accessed data is locally available during all computation stages. As a consequence, inspector code is required to collect references to non-local data. Work distribution for the generated parallel code is derived directly from the computed data decomposition. Although parallel code uses local indices when accessing arrays, indirection data structures keep containing indices pointing to the original global arrays. The presence of indirections through these data structures implies the use of a translation scheme to find out the current location of the requested data (processor + offset). Such translation scheme has a high overhead in memory or communications, as usually involves a problem-size translation table. Communication schedule for gathering non-local data is generated from the above operations.

Our parallelization method, however, is based on a privatization model included on the data-parallel framework. Data that represent the domain of the problem is partitioned using value-based decompositions (domain decompositions) trying to minimize the interactions among the sub-domains. Those interactions (references to non-local data) are dealt transparently to the code by using overlapping areas, where the referenced non-local data elements are stored locally.

Opposite to the inspector–executor strategy, the computation of the overlapping areas is not based on the analysis at runtime of the data references in the code. Overlapping areas are precalculated at compile-time from the information about problem properties introduced in the code through the directive SPARSE, as well as the data distribution specified through the standard DISTRIBUTE directive. Overlapping areas are finally computed in completion during the data distribution phase, when all needed runtime data is known. All irregular computations are executed using the owner compute rule. However, if the data distribution implies non-local writes, these operations are replicated. All processors but the owner of the data element writes on the copy in their overlapping areas. These writes will be simply
discarded. This way there is no need to propagate the non-local write operations and the semantics of the original application is maintained.

Finally, for sparse matrix computations there is a different approach proposed in the literature [8,28], based on the automatic transformation of a dense program, annotated with sparse directives, into a semantically equivalent sparse code. They show this approach on simple and static sparse codes. However, it is not clear its feasibility for more complex programs, like dynamic sparse computations (as in the LU) or simply the transposition of a sparse matrix. The design of such sparse compiler is very complex, in such a way that no implementation of it is available for general and real problems.

6. Conclusions

Numerical irregular applications show subscripted subscripts in their code, usually introduced by the programmer in order to reduce computation overhead and optimize the use of the memory hierarchy. These complexities in the code often hide to the compiler spatial and temporal localities inherent to the application.

Exposing the key data structures in the application as well as some problem properties that the data fulfill, the compiler can analyze the code, exploit data locality and generate efficient parallel code.

This paper describes a number of different applications that show the generality of the method discussed, and that HPF can be used to program efficiently these applications with only a small number of extensions.

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References

[42] Irregular problems in supercomputing applications (special issue), Journal of Parallel and Distributed Computing 50 (1/2) (January 1998).


