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STRUCTURING DISTRIBUTED RELATION-BASED COMPUTATIONS WITH SCDRC

Nicola Botta, Cezar Ionescu, Ciaron Linstead, Rupert Klein

POTSDAM INSTITUTE
FOR
CLIMATE IMPACT RESEARCH (PIK)

Corresponding author:
Dr. Nicola Botta
Potsdam Institute for Climate Impact Research
P.O. Box 60 12 03, D-14412 Potsdam, Germany
Phone: +49-331-288-2657
Fax: +49-331-288-2695
E-mail: Nicola.Botta@pik-potsdam.de

Herausgeber:
Prof. Dr. F.-W. Gerstengarbe

Technische Ausführung:
U. Werner

POTSDAM-INSTITUT
FÜR KLIMAFOLGENFORSCHUNG
Telegrafenberg
Postfach 60 12 03, 14412 Potsdam
GERMANY
Tel.: +49 (331) 288-2500
Fax: +49 (331) 288-2600
E-mail-Adresse:pik@pik-potsdam.de

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Abstract

In this report we present a set of software components for distributed relation-based computations (SCDRC).We explain how SCDRC can be used to structure parallel computations in a single-program multiple-data computational environment.

First, we introduce relation-based algorithms and relation-based computations as generic patterns in scientific computing. We then discuss the problems that have to be solved to parallelize such patterns and propose a high-level formalism for specifying these problems.

This formalism is then applied to derive parallel distributed relation-based computations. These are implemented in the C++ library SCDRC. We present language independent elements of SCDRC and discuss C++ specific aspects of its design and architecture.

Finally, we discuss how to use SCDRC in a simple application and provide preliminary performance figures.

Contents

1. Introduction

1.1. **What is SCDRC?** SCDRC is a set of software components for structuring distributed relation-based computations.

Relation-based computations are simple but general patterns found in many scientific computing domains. In climate research, they are at the core of grid-based numerical methods for partial differential equations (ocean and atmosphere models), of inference algorithms for Bayesian networks and of viability kernel algorithms (viability studies). They also arise in data interpolation between regular and irregular grids (pre-processing, model coupling).

Relation-based computations are often nested in expensive, iterative programs. These programs could, in principle, take advantage of distributed parallel architectures to speed up computations.

In climate research, faster computations allow simulations on longer time scales, improved resolution and more representative sets of realizations in uncertainty studies.

In practice, however, computational tools for climate research do not take full advantage of parallel computers. Although based on a small set of common computational patterns, climate models are traditionally developed for specific domains in a sequential computational environment. They are neither easy to parallelize nor cheap to adapt to other domains. If those common patterns could be organized in a generic library, which can be used across different domains, substantial development efforts could be saved and the degree of parallelism could be increased.

SCDRC is a prototype of such a generic library.

1.2. **What are relation-based computations?** The notion of relation-based computations is introduced and discussed in detail in the next section. Examples of relation-based computations are: the computation of neighbor elements on a grid; the computation of geometrical properties of grid elements, e.g., element center, area, boundary integrals; sparse matrix-vector multiplications.

Relation-based computations which can be easily implemented in a sequential, single program single data (SPSD) computational environment are often difficult to implement in a parallel, single program multiple data (SPMD) distributed case.

Consider, for instance, the problem of computing the centers of the triangles of a triangulation. Let the triangulation be represented by an integer table vt: the j-th row of vt contains the three indexes of the vertexes of the j-th triangle. Given vt and an array x of vertex coordinates, a sequential computation of the centers could read:

Algorithm 1 : triangle centers

```
for $j$ in $[\,0\dots\mathrm{size}(vt)\,)$ do
    compute $(1/3) * (x(vt(j)(0)) + x(vt(j)(1)) + x(vt(j)(2)))$
end for
```

In algorithm 1, $[a\dots b)$ represents the interval of natural numbers a, $a+1$, $\dots$, $b-1$. It is not obvious how to implement the above rule on a parallel computer with distributed memory. If one requires the implementation to be reasonably *efficient*, one has to answer, among others, the following questions:

(1) How are vt and x distributed among remote partitions[1]?
(2) Which vertex coordinates are needed on the local partition which are stored on remote partitions?
(3) Which vertex coordinates stored on the local partition are needed by which remote partition?
(4) How can these coordinates be exchanged between partitions?

A few remarks are appropriate here: if the *efficiency* requirement can be neglected, a parallel implementation of algorithm 1 can be easily derived by just duplicating the whole x on all partitions. This approach is, for for most practical problems, unaffordable. Moreover, it raises the non-trivial question of how to ensure the consistency of duplicated data.

Message passing libraries, e.g. MPI, provide efficient and portable answers to question 4: how to exchange data between partitions. However, they cannot provide answers to questions 1-3: these questions are concerned with the *structuring* of the

[1]we do not attempt at defining the concept of a *partition* here: in a SPMD (single program multiple data) distributed computational environment, different partition may correspond to remote memory spaces.

parallel computation. In particular, the answers to question 2 and 3 essentially depend on how question 1 is answered.

Of course, structuring rules or guidelines cannot be given in general but only for certain classes of computations or computational patterns. Relation-based computations are a family of such patterns.

1.3. **Who can take advantage from SCDRC?**

As a set of components for structuring distributed relation-based computations, SCDRC is a software layer above message passing libraries but below applications. It is not meant to be directly used by application developers. Instead, SCDRC is designed to be the basis on which application dependent software components are written. In other words, applications are expected to use SCDRC indirectly via application dependent abstractions.

As an example, consider a triangulation class supporting the implementation of finite element discrete differential operators. This is an application dependent abstraction (in the sense that it will implement, among others, methods which are specific to finite element computations) which could be written on top of SCDRC. A finite element program for approximating incompressible flows is an example of an application.

Being a low-level software layer (w.r.t. applications), SCDRC does not attempt at hiding the communication steps which are needed in relation-based computations. Communication steps which are conceptually complementary but distinct are represented by distinct data structures or function calls.

This means that developers have a high degree of control over communication and can take advantage of such control for optimizations. However, communication is structured in a set of primitives which have been specifically designed for relation-based computations. In particular, SCDRC users do not have direct access to standard message passing (MPI) primitives and do not need to care about synchronization, mutual exclusion, deadlock or race condition problems. They can develop application dependent software components on the top of SCDRC which hide communication or leave it visible to the user.

1.4. **How does SCDRC compare to other approaches?**

A discussion of the many and different approaches towards introducing abstraction layers between message passing libraries and scientific computing applications goes beyond the scope of this report.

For an overview of the role of *subroutine libraries* and of *frameworks* in generic software components for scientific computing we refer the reader to [4]. A comprehensive discussion of *domain specific languages*, frameworks and *toolkits* from the point of view of *domain engineering* can be found in [9]. The concepts of *grid* and of *algorithm oriented design* of software components for grids and geometries are discussed in [1], [3] and [5].

SCDRC has been designed around patterns which are found in numerical methods for partial differential equations (PDE) *and* in other applications domain: adaptive stochastic sequential decision processes and Bayesian network inference are two prominent examples. Up to now, the most significant efforts towards developing frameworks of generic, reusable software components have been done in the PDE application domain. In the following, we point out differences and similarities between SCDRC and well established frameworks for solving PDEs.

A very elementary difference between SCDRC and frameworks like POOMA[2], Overture[3], Amatos[4] and OpenFoam[5] is in terms of size. SCDRC is a very small, *thin* software layer: at the present stage, `sloccount`[6] counts about 12000 source lines of code in the main directory tree of SCDRC. As a comparison, OpenFoam version 1.2 consists of about one million lines of code!

Another important difference between SCDRC and computational frameworks for PDE lies in the level of abstraction. The central concepts in SCDRC are relations and relation-based computations. The main problems addressed by SCDRC are how to represent distributed relations and how to implement parallel relation-based computations.

In numerical frameworks for PDEs, *grid* concepts play an outstanding role. Grids are much more complex concepts than relations. One can think of relations in a couple of different ways – as sets of pairs, as characteristic functions or as functions – and one can distinguish between different *kinds* of relations: regular relations, irregular relations, etc. This complexity, however, is very little when compared to the complexity of grid concepts. The grids needed in computational frameworks for PDEs have *geometrical* and *topological* aspects. The latter are described by a whole set of grid relations. Grid representations depend on the choice of a *coordinate system*, on the number of *dimensions* of the geometrical space in which they are embedded, on a number of *grid coordinates*. One can distinguish between *structured* and *unstructured* grids, between *regular* and *irregular* grids, between *rectangular*, *skew* and *curvilinear* grids. *Adaptive* grids, *hierarchical* grids, *overlapping* and *non-overlapping* grids are other aspects of different grid taxonomies.

The development of SCDRC is an attempt at tackling the problem of structuring algorithm-oriented parallel computations on the basis of the smallest common concept and of the simplest computational patterns found in a wide class of scientific computing problems: relations and relation-based computations.

Since it tackles the parallelization problem at an elementary level, the SCDRC approach is more similar to the *algorithmic skeletons* or to POOMA's *stencil*-based approach than to grid-based domain decomposition approache. As it will become clear in the following sections, relation-based algorithms and relation-based computations are, in fact, non-trivially parallelizable data parallel algorithmic skeletons in the sense of [14].

Special kind of relations – symmetric, anti-reflexive graphs – play a fundamental role in graph partitioning algorithms such as those implemented in the Metis [12] and ParMetis [8] library. As we will see in the next section, SCDRC provide an interface to these libraries. The interface allows one to apply partitioning algorithms to SCDRC relations. The application domains of Metis and ParMetis – graph and grid partitioning – on the one side and of SCDRC on the other side are complementary but clearly separated.

As a set of software components for structuring distributed relation-based computations, SCDRC provides a subset of the functionalities provided by the Janus framework, see [10]. In fact, the initial phase of the SCDRC development has been done in collaboration with Dr. J. Gerlach, the main developer of Janus. As we will show

[2]`http://acts.nersc.gov/pooma`
[3]`http://acts.nersc.gov/overture`
[4]`http://www.amatos.info`
[5]`http://www.opencfd.co.uk/openfoam`
[6]By David A. Wheeler, `http://www.dwheeler.com/sloccount`

in section 3, SCDRC shares with Janus (and with ParMetis) the conceptual model of representing distributed functions and relations. There are, however, important differences between SCDRC and Janus. These differences are both in implementation independent aspects and in the implementation design.

A major implementation independent difference is architectural. In contrast to Janus, the architecture of SCDRC is based on the formal specification of a small set of problems. These problems are informally introduced at the end of the next section and problem specifications are discussed in detail in section 3.

Another difference between SCDRC and Janus is in how solution algorithms for the problem specifications of section 3 have been derived. In SCDRC, this has been done on the basis of a single communication primitive in the spirit of the BSP (bulk synchronous parallel processing) model, see [7], [6]. This communication primitive is discussed in detail in 3 and 4. In contrast to SCDRC, Janus algorithms are not explicitly designed around a single communication primitive, and attempt to hide the distinction between parallel and sequential execution.

A third major difference between Janus and SCDRC is in the approach towards constructing relations. Janus supports incremental construction with a very flexible (albeit non trivial) two-phase model. SCDRC takes a more straightforward approach and does not support incremental construction.

1.5. **What is the state of development of SCDRC?** SCDRC is in a prototypical stage. Its sources are available under the GPL licence but have not been released (please contact botta@pik-potsdam.de). SCDRC has been compiled with gcc version 3.3.6 and 4.0.2 and tested on a linux-cluster under lam-mpi and mpich and on a 240 CPU IBM p655 cluster. At the present, no application dependent software components have been built on the top of SCDRC but a few simple examples are provided.

1.6. **Outline.** The rest of this report is organized as follows. In section 2 we introduce and discuss relation-based algorithms and relation-based computations following the triangle center example outlined above. Section 3 describes implementation independent design elements of SCDRC. In this section we discuss, among others, how distributed functions and distributed relations are conceptually represented – remember question 1) above – and which aspects of this representation are visible to SCDRC users. In section 4 we discuss implementation dependent aspects and architecture of SCDRC. In the last section we comment a simple application and discuss preliminary results.

2. Relation-based algorithms and relation-based computations

2.1. **Relation-based algorithms.** Let's go back to algorithm 1 introduced in section 1 to represent a triangle center computation. In this rule we have used $x(i)$ (for i equal to $vt(j)(0)$, $vt(j)(1)$ and $vt(j)(0)$) to represent the i-th element of the array x.

We use the notation $x(i)$ — in contrast to the more usual $x[i]$ — to underline the fact that, for the purpose of expressing the triangle center computation, the way the vertex coordinates are obtained is immaterial. In concrete implementations, x does not need to be an array and one can easily think of triangulations in which the vertex coordinates are given by analytical expressions.

Let's take a critical view at algorithm 1: what if the triangulation covers a sphere and the triangles themselves are spherical? In this case, algorithm 1 yields triangle centers that do not lie on the surface of the sphere. This is probably not what a triangle centers algorithm is meant to compute. Algorithm 1 can be easily modified to avoid triangle shape over-specification:

Algorithm 2 : triangle centers

```
for $j$ in $[\,0 \ldots \mathrm{size}(vt)\,)$ do
    compute $\mathrm{center}(x(vt(j)(0)), x(vt(j)(1)), x(vt(j)(2)))$
end for
```

The new rule delegates the computation of the centers to the center function. This function is now assumed to know whether plane of spherical triangles are at stake in any particular case. In fact, algorithm 2 can be easily generalized to compute whatever function of the coordinates of the triangle vertexes, for instance the triangle areas. This is, in contrast to center, a non-linear function. We can go one step further and think of algorithm 2 as a particular instance of a computational pattern in which j is drawn from some array js of positive natural numbers and a function h is applied to the array of values some function f takes at those indexes i which are in relation with j:

Algorithm 3 : relation-based algorithm

```
for $j$ in $js$ do
    compute $h([\,f(i) \mid i \textbf{ in } R(j)\,])$
end for
```

Here $R(j)$ is an array of indexes which are in relation R with j, in the triangle center example $R(j) = [vt(j)(0), vt(j)(1), vt(j)(2)]$. The notation $[\,f(i) \mid i \textbf{ in } R(j)\,]$ is an instance of an array comprehension, which generalises in the natural way the familiar set comprehension, and which is found in many programming languages, among which are Python, Haskell, Perl6.

We call the above computational pattern a relation-based algorithm (RBA). Relation-based algorithms are defined in terms of two functions h and f and of a relation R.

In relation-based algorithms and, in general, in SCDRC, we will only consider relations between zero-based intervals of natural numbers. This restriction is discussed in detail in section 3. For the moment, let's accept this restriction and think of a relation R as a subset of $[0, m) \times [0, n)$ where m and n are the sizes of the *target* and of the *source* of R, respectively. In this report we will always use a left-from-right notation when giving the signature of relations and functions:

$$R :: [\,0 \ldots m\,) \longleftarrow [\,0 \ldots n\,)$$
$$R(\cdot) :: \mathrm{subarrays}([\,0 \ldots m\,)) \longleftarrow [\,0 \ldots n\,)$$

If we allow f to take as argument pairs in $[0, m) \times [0, n)$:

Algorithm 4 : relation-based algorithm

```
for $j$ in $js$ do
    compute $h([\,f(i, j) \mid i \textbf{ in } R(j)\,])$,
end for
```

relation-based algorithms can be easily specialized to represent matrix-vector multiplications. Let A be a sparse matrix and c, e and p be a CRS (compact row storage, see [8]) representation of A that is, c, e and p satisfy the following equivalence:

$$A(j,i) \neq 0 \;\equiv\; \exists!\; k \;\textbf{in}\; [\,p(j) \ldots p(j+1)\,) : \; i == c(k) \;\wedge\; A(j,i) == e(k) \tag{1}$$

An efficient representation of the computation of the product between A and a suitably sized vector b reads:

Algorithm 5 : sparse matrix vector multiplication

```
**for** $j$ **in** $[\,0 \ldots n\,)$ **do**
    **compute** $\text{sum}([\,e(k) * b[c(k)] \mid k$ **in** $[\,p(j) \ldots p(j+1)\,)\,])$,
**end for**
```

Using 1, this rule can be written as a relation-based algorithm with

$$h = \text{sum}$$
$$f(i,j) = e(k(i,j)) * b[i]$$
$$\quad \textbf{where}\; k(i,j) = p(j) + \text{index\_of}(i, R(j))$$
$$R(j) = [\,c(k) \mid k \;\textbf{in}\; [\,p(j) \ldots p(j+1)\,)\,]$$

In the above expression we have used the function index_of which computes the index of a given element in an array:

$$k == \text{index\_of}(s, ls) \;\equiv\; s == ls[k]$$

Of course, index_of is a function only for array arguments which are *nubbed* that is, contain no duplicates. We impose this requirement on any relation representation $R(\cdot)$.

Implementations of sparse matrix-vector multiplications as relation-based algorithms are useful only if the data structures that implement relations provide efficient ways of computing $R(j)$ and $\text{index\_of}(i, R(j))$. We will address this problem in section 4. For the moment let us summarize the results of the above analysis in the following observations:

- Relation-based algorithms are computational patterns (algorithmic skeletons) commonly found in many application domains; we have seen two examples: grid computations and linear algebra. Examples in numerical methods for PDEs and other application domains can be easily made.
- Relation-based algorithms are not, in general, trivially parallelizable; in particular, they are not trivially parallelizable whenever the following conditions occur:
  - the function f is represented by storing f values in memory. In scientific computing it is often the case that f-values are stored in arrays.
  - The relation R is such that any disjoint splitting of its source in np partial relations $R_1 \ldots R_{np-1}$ yields non-disjoint ranges $\text{ran}(R_p)$, $\text{ran}(R_q)$ for distinct $p, q < np$.

  Unfortunately, many interesting computations, among others the examples discussed above, are not trivially parallelizable.

In section 4 we show how *distributed* relation-based algorithms can be defined in SCDRC by specializing a generic *RBA* rule with concrete types for the functions h, f and for the relation R. In SCDRC, concrete *RBA* objects can be constructed by passing concrete distributed objects representing h, f and R to RBA constructors. Distributed f objects can be, in turn, distributed relation-based algorithms. This provides a natural scheme for composing distributed relation-based algorithms to define complex parallel computations.

2.2. **Relation-based computations.** While being powerful patterns, RBAs are certainly not enough for structuring even simple distributed computations like the triangle centers example introduced in section 1. Let's go back to this example and assume, for concreteness, that the table vt and the vertex coordinates array x are initially stored in a file (vt and x can be seen as a minimal representation of a triangulation).

If we think of vt as of the relation R and of x as of the function f of a relation-based algorithm, then the following steps have to be done before a parallel computations of the triangle centers can take place:

(1) read vt and x from the file.
(2) compute a partitioning of the source of vt.
(3) compute a partitioning of the source of x.
(4) distribute vt and x according to these partitioning.

We will discuss in detail what it means to distribute a relation and an array according to a given partitioning in the next sections. For the moment, let's consider steps 2 and 3. Computing a partitioning of the source of vt simply means associating a unique partition number to each triangle of vt.

Of course, one would like to partition the triangles of vt is such a way that the subsequent parallel computation of the centers is done efficiently. This boils down to requiring that all partitions contain approximately the same number of triangles (or a number of triangles proportional to the computational capacity associated with the partitions) and that the total number of *edge-cuts* is minimal and equally distributed among partitions. Notice that the number of edge-cuts – pairs (v, t) in vt such that v and t belong to different partitions – can only be computed if a partitioning of the vertexes is already known (or computed together with the partitioning of the triangles). Minimizing the number of edge-cuts means minimizing the number of vertex coordinates that have to be exchanged between partitions in the triangle centers computation.

Grid and relation (graph) partitioning is a well-established research area and SCDRC does not attempt at providing new solutions in this field. Instead, SCDRC provides an interface to Metis [12] and ParMetis [8]. These are very efficient graph partitioning libraries. The SCDRC interface could be easily extended to other partitioning algorithms.

Of course, different partitioning algorithms put different requirements on their argument relations. Metis and ParMetis, for instance, require such relations to be *symmetric* and *anti-reflexive*. This means that

$$(iRj \equiv jRi) \ \wedge \ (iRj \Rightarrow i \neq j)$$

The vertex-triangle relation of our example is certainly non symmetric. This means that, in order to take advantage of Metis and ParMetis for computing a partitioning of vt, one has to construct a symmetric, anti-reflexive auxiliary relation, say avt, that represents vt "well".

Since avt is to be used to compute a partitioning of the source of vt, its source has to coincide with the source of vt. Moreover, partitionings of (the source of) avt

which satisfy minimal edge-cut constraints should lead to minimal or almost minimal edge-cuts for vt as well.

Grid-relations like vt are commonly found in many application domains. They often describe coverings of 1- 2- or 3-dimensional manifolds or neighborhood relationships on such coverings. A common way of computing an auxiliary relation for grid relations like vt is the following:

(1) compute the *converse* of vt, vt°.
(2) compute $tvt = vt^\circ \cdot vt$.
(3) compute $avt = tvt - \mathrm{id}_{[\,0 \ldots \mathrm{source\_size(vt)}\,)}$

We use R° to denote the converse of a relation (or of a function) R. If $R:\ [\,0 \ldots m\,) \longleftarrow [\,0 \ldots n\,)$, then $R^\circ:\ [\,0 \ldots n\,) \longleftarrow [\,0 \ldots m\,)$ and $jR^\circ i\ \equiv\ iRj$.

Notice that tvt is symmetric and represents a *neighborhood* relationship: $tvt(j)$ provides, for the j-th triangle, the indexes of those triangles that share at least one vertex with the j-th triangle. Neighborhood relationships naturally arise, among others, as *stencils* of discrete differential operators in finite volumes, finite elements and finite differences methods for the numerical approximation of partial differential equations.

The relation avt is symmetric and anti-reflexive and its source coincides with the source of vt. Thus avt can be used to compute a partitioning of (the source of) vt with the Metis library. Given such partitioning, say sp, a “suitable” partitioning tp of the target of vt – the source of x in our example – can be easily computed by considering the relation $sp \cdot vt^\circ$. This relation associates to each vertex the partition numbers of those triangles that share the given vertex. A suitable way of partitioning the target of vt (the source of vt°) is then to pick-up, for each vertex i in the source of $sp \cdot vt^\circ$, the partition number that appears most frequently in the array $(sp \cdot vt^\circ)(i)$. This choice, the fact that tvt is a neighborhood relation and the edge-cut properties of the partitioning of avt computed by Metis, guarantee that the partition number of most vertexes will coincide with the partition number of the triangles it belongs to. This, in turn, means that the number of edge-cuts is almost minimal.

Notice also that the computation of tp described above is itself a relation-based algorithm with $R = vt^\circ$, $f = sp$ and $h = \mathrm{most\_frequent}$. Here most_frequent is a function that takes an array of natural numbers and returns a natural number such that no other array element appears more frequently.

2.3. **Core problems.** In this section we have introduced relation-based algorithms as computational patterns. We have seen that, in order to a apply such patterns in a distributed parallel computational environment, other relation-based computations – among others composition and conversion – are needed. Of course, one would like these computations too to run in parallel and on distributed data.

In developing SCDRC, we have focused our attention on a few core problems. In order to implement distributed relation-based algorithms, these problems have to be solved no matter which programming languages and data structures are used for the implementation. Of course, concrete implementations will require the solution of more additional problems.

We close this section by listing the core problems informally, as they have been formulated at the beginning our analysis. In the next two sections we will introduce a more formal specification, discuss the most important elements of the SCDRC architecture and show how SCDRC components can be combined to implement distributed relation-based computations.

(1) Given a *distributed representation* of a function f and of a *partitioning* of its source, compute a new distributed representation of f *consistent* with the given partitioning.
(2) Given a distributed representation of a relation R and of a partitioning of its source, compute a new distributed representation of R consistent with the given partitioning.
(3) Given a distributed representation of a function f and given, on each *partition*, a subset of $\mathrm{dom}(f)$, compute, on each partition, the correspondent values of f.
(4) Given a distributed representation of a relation R and of a partitioning of its target, compute a distributed representation of R° consistent with the given partitioning.
(5) Given consistent, distributed representations of relations S and T, compute a consistent, distributed representation of $S \cdot T$.

3. Implementation independent elements

3.1. **Set, function and relation representations.** As mentioned in the previous section, SCDRC relations are defined between zero-based intervals of natural numbers. Very often, such relations represent relations between finite sets. In our triangulation example, for instance, vt is understood to be a representation of a vertex-triangle relation $\mathbf{vt}$ into a vertex set $\mathbf{V}$ from a triangle set $\mathbf{T}$:

$$\begin{tikzcd}
\mathbf{V} \arrow[d, "\boldsymbol{\rho_V}"'] & \mathbf{T} \arrow[l, "\mathbf{vt}"'] \arrow[d, "\boldsymbol{\rho_T}"] \\
{[\,0 \ldots m\,)} & {[\,0 \ldots n\,)} \arrow[l, "vt"]
\end{tikzcd}$$

Most applications only deal with representations of finite functions and relations: neither the sets $\mathbf{V}$ and $\mathbf{T}$, nor the relation $\mathbf{vt}$ or the representation functions $\boldsymbol{\rho_V}$ and $\boldsymbol{\rho_T}$ do appear in algorithm 1. One can think of any table vt' obtained via a permutation of the rows of vt as another representation of $\mathbf{vt}$ having the same legitimacy as vt.

For applications that only deal with representations of finite functions and relations, natural numbers (Nat) and zero-based Nat intervals are very convenient abstractions for set elements and finite sets. They are computationally cheap (a zero-based Nat interval is described by a single Nat) and naturally lead to representations of finite functions in terms of arrays. For instance, the vertex coordinates of our example are represented by a simple one-dimensional array x of size m (nd here is the number of dimensions of the space in which the triangulation is embedded, typically 2 or 3, and $V(\mathrm{Real}, nd)$ is the set of nd-dimensional real-valued vectors):

$$\begin{tikzcd}
\mathbb{R}^{nd} \arrow[d, "\boldsymbol{\rho}_{\mathbb{R}^{nd}}"'] & \mathbf{V} \arrow[l, "\mathbf{x}"'] \arrow[d, "\boldsymbol{\rho_V}"] \\
\mathrm{V}(\mathrm{Real}, nd) & {[\,0 \ldots m\,)} \arrow[l, "x"]
\end{tikzcd}$$

In turn, arrays of some generic type X, A(X), are, for many computational purposes, very efficient representations of finite functions.

An alternative approach for representing finite sets of a generic type X is by means of a parameterized data structure: Set(X). Representations of finite sets-based on parameterized types are, of course, more powerful than representations-based on zero-based Nat interval abstractions. They can distinguish between sets of different types but same cardinality. On the other hand, parameterized relation and function representations based on parameterized set representations – data structures of the kind $\mathrm{Rel}(\mathrm{Set}(X), \mathrm{Set}(Y))$ or $\mathrm{Fct}(\mathrm{V}(\mathrm{Real}, nd), \mathrm{Set}(Y))$ in place of $\mathrm{A}(\mathrm{V}(\mathrm{Real}, \mathrm{nd}))$ for functions – make functions and relations dependent on application-specific, possibly inefficient representations of set element types.

Notice that frameworks like Janus support parameterized representations of finite sets but rely on relations between zero-based Nat intervals. In SCDRC we only consider sets, functions and relations which are finite. We adopt the Janus approach for relations but we do not support parameterized representations of finite sets. Of course, there are situations in SCDRC in which sets (most probably of Nats) have to be explicitly represented. In these cases we use suitable containers like lists or arrays.

The analysis presented in this section is based on a simple conceptual representation of finite functions and relations as arrays of some type X and as arrays of arrays of Nats, respectively. We stress the fact that this is a conceptual model. As we will see in section 4, SCDRC relations are implemented by means of specific data structures like CRS_Rel and Reg_Rel(n). While being isomorph to arrays of arrays of natural numbers (both CRS_Rel and Reg_Rel(n) can be constructed in terms of such an array), SCDRC implementation of relations are defined in terms of an iterator-based interface which is very different from the array interface.

3.2. **Distributed functions and distributed relations.** In the list of problems presented at the end of the previous section, we have used the term *distributed representation* for functions and relations. In this paragraph we discuss such representations. We follow the approach outlined above and think of functions and relations as arrays of some type X and of type A(Nat), respectively. Let a be an array. A straightforward way of distributing a on np partitions is:

(1) Cut a into np chunks.
(2) Assign the first chunk to the first partition, the second chunk to the second partition and so on.

For this partitioning scheme, the function $pa :: [\,0 \ldots np\,) \longleftarrow [\,0 \ldots \mathrm{size}(a)\,)$ that associates a partition number in $[\,0 \ldots np\,)$ to each element of a is non-decreasing. As usual, we represent pa with an array of Nats. Therefore, if $\mathrm{size}(a) == \mathrm{size}(pa) >> np$, pa can be more economically represented by an array of *offsets* (again of Nats) of size $np + 1$. In fact, any non-decreasing array ofs satisfying:

$$\begin{aligned} \mathrm{size}(ofs) &== np + 1 \\ ofs(0) &== 0 \\ ofs(np) &== \mathrm{size}(a) \end{aligned} \tag{2}$$

represents the non-decreasing partition function $pa : [\,0 \ldots np\,) \longleftarrow [\,0 \ldots ofs(np)\,)$:

$$ofs(p) <= k < ofs(p+1) \;\equiv\; pa(k) == p \tag{3}$$

Conversely, given pa non-decreasing, the corresponding ofs can be easily computed:

Algorithm 6 : offsets

```
Require: $\text{is\_not\_decreasing}(pa) \wedge \max(pa) < np$
1: $ofs = \text{make\_array}(np+1, 0)$
2: for $k$ in $[\,0 \dots \text{size}(pa)\,)$ do
3:     $p = pa(k)$
4:     $ofs(p+1) = 1 + ofs(p+1)$
5: end for
6: for $p$ in $[\,0 \dots np\,)$ do
7:     $ofs(p+1) = ofs(p) + ofs(p+1)$
8: end for
Ensure: $\text{size}(ofs) == np+1 \wedge ofs(0) == 0 \wedge ofs(np) == \text{size}(pa)$
```

At line 1, ofs is initialized as an array of size $np + 1$ with elements equal to zero. At the end of the first loop $ofs(p + 1)$ contains the number of indexes of pa whose partition number is p. The pre-condition $\max(pa) < np$ guarantees that, inside loop 1, $p + 1 < np + 1$ always holds. Thus, no array bound violation can occur at line 4 and each entry of pa is counted exactly one time in exactly one ofs entry. Therefore, at the end of the first loop, the sum of the entries of ofs is equal to the size of pa. In the second loop this sum is stored in $ofs(np)$.

Since SCDRC functions and relations are conceptually represented in terms of arrays, it is natural to conceptually represent functions and relations which are *distributed* on np partitions as np-tuples of arrays, as described above. The cutting up of the array in np pieces induces an array of offsets. Alternatively, we can view the np-tuple as resulting from the non-distributed array according to the array of offsets. In either case, we can assume that both the tuple $(f_0 \dots f_{np-1})$ and the offsets ofs are present: they constitute a valid representation of f if

$$f_0 {+\!\!+} f_1 {+\!\!+} \cdots {+\!\!+} f_{np-1} == f$$
$$ofs(k+1) - ofs(k) == \text{size}(f_k) \ \wedge\ ofs(0) == 0$$

The ++ operator "glues" the chunks together. The two conditions are equivalent to the following ones, which are more useful in practice since they provide an explicit "point-wise" characterization of the elements involved.

$$\begin{aligned}
&ofs(np) == \text{size}(f)\\
&f(j) == f_p(j')\\
&\qquad \textbf{where}\\
&\qquad j' = j - ofs(p)\\
&\qquad p:\ ofs(p)\ <=\ j\ <\ ofs(p+1)\\
&\qquad ofs:\ ofs(0) == 0 \ \wedge\ ofs(q+1) == \sum_{k=0}^{k<q+1} \text{size}(f_k),\ q \textbf{ in } [\,0 \dots np\,)
\end{aligned} \tag{4}$$

Notice that $ofs(np) == \sum_{k=0}^{k<np} \text{size}(f_k)$. Therefore the first equation in 4 can be written as

$$\text{size}(f) == \sum_{k=0}^{k<np} \text{size}(f_k)$$

which states an obvious size-consistency condition between f and $(f_0 \ldots f_{np-1})$. Similarly, $(R_0 \ldots R_{np-1})$ is a distributed representations of R if:

$$
\begin{aligned}
&ofs(np) == \text{source\_size}(R) \\
&iRj == iR_p j' \\
&\quad \textbf{where} \\
&\quad j' = j - ofs(p) \\
&\quad p: \; ofs(p) \; <= \; j \; < \; ofs(p+1) \\
&\quad ofs: \; ofs(0) == 0 \\
&\quad \wedge \\
&\quad ofs(q+1) == \sum_{k=0}^{k<q+1} \text{source\_size}(R_k), \; q \; \textbf{in} \; [\,0 \ldots np\,)
\end{aligned}
$$

A caveat: just like the model for non-distributed functions and relations discussed in the previous paragraph, the model discussed here for *distributed* functions and relations is a conceptual one. It is essential for understanding the formal specification of the problems introduced in the next section. This model, however, does not mean that there are data structures, in SCDRC, representing a function or a relation together with its corresponding offset or partitioning function. In much the same way, you will not find, in SCDRC, functions that formally take tuple arguments that represent distributed functions or relations.

The scheme described above for distributing a one-dimensional array a on np partitions and the corresponding conceptual representation of distributed functions and relations is not new. This scheme is used in ParMetis where it is referred to as distributed CRS format. In Janus, distributed relations are equipped with “descriptors” which contain, among others, informations about sizes and offsets of tuple representations.

One can argue that there are many other ways of distributing an array a on np partitions and some of them might be better than the scheme presented here. For instance, if some “communication” relation is defined between the chunks of a and between the partitions (these could be arranged, for a certain computational architecture, according to some hardware “topology” that makes communication between some partitions faster that between others), one might want to “fit” the structure of a to that of the computing architecture. Beside simplicity and minimality, another consideration supports the conceptual model presented here: the problem of partitioning the source and the target of a relation for efficient distributed computations of relation-based algorithms is not trivial. As mentioned in the previous section, SCDRC delegates the solution of this problem to external libraries like Metis and ParMetis. It is in the solution of the partitioning problem that additional, architecture specific partitioning constraints can and should be naturally accounted for.

3.3. **Problem specification.**

In this paragraph we give a formal specification of the problems informally introduced at the end of section 2. This specification rests on the conceptual representation of function and relations discussed in 3.1 and 3.2.

3.3.1. *Problem 1.* Given a distributed representation of a function f and of a partitioning of its source, compute a new distributed representation of f consistent with the given partitioning.

Given:
$(f_0 \ldots f_{np-1}),\ f_p ::\ \text{A(X)}$
$(pf_0 \ldots pf_{np-1}),\ pf_p ::\ \text{A(Nat)}$
such that:
i) $\text{size}(f_p)\ ==\ \text{size}(pf_p)$
ii) $\text{size}(pf_p)\ ==\ 0\ \vee\ \text{max\_elem}(pf_p)\ <\ np$
find:
$\big(f'_0 \ldots f'_{np-1}\big),\ f'_p ::\ \text{A(X)}$
such that:
iii) $f'_p \cdot perm_p == [\, f(i) \mid i \in [\, 0 \ldots \text{size}(f)\,)\,, pf(i) == p\,]$
where
$perm_p :: [\, 0 \ldots m_p\,) \longleftarrow [\, 0 \ldots m_p\,)$ is bijective
$m_p == \text{size}([\, f(i) \mid i \in [\, 0 \ldots \text{size}(f)\,)\,, pf(i) == p\,])$.

Let us comment on this specification: as discussed in 3.2, f is represented by a tuple of arrays, one array for each partition. On each partition, a partition function pf_p specifies how the elements of f_p have to be redistributed among np partitions. As usual, pf_p is represented with an array. This has to have the same size as f_p and has to take values in $[\, 0 \ldots np\,)$. The solution of problem 1 is a *new* distributed function f'. Condition iii) requires f'_p to contain exactly those values $f(i)$ of f such that $pf(i) == p$. Because of the permutation $perm_p$, these values can appear in any order in f'_p.

In the above specification, we have assumed that non-empty arrays of Nats are equipped with a function max_elem :: Nat $\longleftarrow$ A(Nat) that computes the maximal element. max_elem and size are examples of functions whose implementation depends on the computational environment. The implementation of such functions in SCDRC's SPSD and SPMD-distributed environments is discussed at the beginning of section 4. Let's turn the attention to the second problem introduced at the end of section 2. The specification of problem 2 is completely analogous to that of problem 1:

3.3.2. *Problem 2.* Given a distributed representation of a relation R and of a partitioning of its source, compute a new distributed representation of R consistent with the given partitioning.

Given:
$(R_0 \ldots R_{np-1}),\ R_p ::\ \text{A(A(Nat))}$
$(pR_0 \ldots pR_{np-1}),\ pR_p ::\ \text{A(Nat)}$
such that:
i) $\text{source\_size}(R_p)\ ==\ \text{size}(pR_p)$
ii) $\text{size}(pR_p)\ ==\ 0\ \vee\ \text{max\_elem}(pR_p)\ <\ np$
find:
$\big(R'_0 \ldots R'_{np-1}\big),\ R'_p ::\ \text{A(A(Nat))}$
such that:
iii) $R'_p \cdot perm_p == [\, R(i) \mid i \in [\, 0 \ldots \text{source\_size}(R)\,)\,, pR(i) == p\,]$
where
$perm_p :: [\, 0 \ldots m_p\,) \longleftarrow [\, 0 \ldots m_p\,)$ is bijective

$$m_p == \text{size}([\, R(i) \mid i \in [\, 0 \ldots \text{source\_size}(R)\,)\,, pR(i) == p\,]).$$

Notice that, even in the case in which $perm_p$ is taken to be the identity permutation on all partitions both in problem 1 and in problem 2, f', R' are not, in general, equal to f and R. This is because of the fact that pf and pR have not been required to be non-decreasing. In other words, the repartitioning is not required to be a re-cutting.

In section 3.2, we have motivated a conceptual representation of distributed functions and relations that rests on non-decreasing partition functions. From this point of view, the specifications given above seem to be far too general: a (generic) program `redistribute` implementing these specifications, allows one to write a SPMD distributed parallel program to:

(1) on all partitions p in $[\, 0 \ldots np\,)$, do: initialize an empty vertex coordinates array x_p and an empty vertex-triangles relation vt_p.
(2) on partition 0, do: read a vertex coordinates array x and a vertex-triangle relation vt from some file into x_0, vt_0.
(3) on partition 0, do: compute suitable[7] partition functions px_0, pvt_0 of the sources of x_0, vt_0; on all partitions $p \neq 0$ initialize empty px_p, pvt_p.
(4) on all partitions, do: redistribute $(x_0 \ldots x_{np-1})$, $(vt_0 \ldots vt_{np-1})$ according to $(px_0 \ldots px_{np-1})$, $(pvt_0 \ldots pvt_{np-1})$.

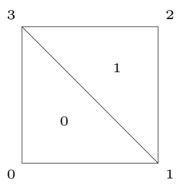
These steps rephrase steps 1-4 of section 2.2 in terms of the notation introduced in this section for distributed representations of functions and relations. Steps 1-4 of section 2.2 have been introduced to set up a SPMD parallel computation of the centers of the triangles of the triangulation represented by the vertex coordinates array x and by the vertex-triangle relation vt. In this section we are going to use this computation as an example of a SPMD parallel relation-based algorithm. We will come back to this example over and over again to motivate and refine formal specifications for the problems introduced at the end of section 2.

Consider steps 1 and 2 above. These yield distributed representations $(x_0 \ldots x_{np-1})$, $(vt_0 \ldots vt_{np-1})$ of x, vt with $x_0 == x$, $vt_0 == vt$ and $x_p == vt_p == [\,]$, p in $[\, 1 \ldots np\,)$. Similarly, step 3 provides distributed representations $(px_0 \ldots px_{np-1})$, $(pvt_0 \ldots pvt_{np-1})$ of px, pvt with $px_0 == px$, $pvt_0 == pvt$ and $px_p == pvt_p == [\,]$, p in $[\, 1 \ldots np\,)$. If px and pvt are *not* non-decreasing, step 4 yields distributed representation $\left(x'_0 \ldots x'_{np-1}\right)$, $\left(vt'_0 \ldots vt'_{np-1}\right)$ of arrays x', vt' such that, in general (i.e. for arbitrary x, vt), $x' \neq x$ and $vt' \neq vt$. The analysis raises two questions:

(Q1) Why do we put forward specifications of redistribution problems that seem to imply more general conceptual representations of distributed functions and relations than the one introduced in section 3.2?
(Q2) If we stick to the conceptual representation of distributed arrays of section 3.2 (and restrict ourselves to partition functions that can be represented by arrays of offsets), isn't it very inefficient to represent px, pvt with tuples of arrays $(px_0 \ldots px_{np-1})$, $(pvt_0 \ldots pvt_{np-1})$ (of total size size(x), source_size(vt)) instead of offsets-based representations of size $np + 1$ independent of the size of the represented function?

To answer these questions and refine the problem specifications presented above, let us discuss steps 1)-4) in a concrete case. Consider a very simple triangulation in

[7]in the sense explained in section 2.2, e.g. using the SCDRC interface to Metis.



which x and vt are:

$$\begin{aligned} x &= [\,[\,0.0, 0.0\,]\,, [\,1.0, 0.0\,]\,, [\,1.0, 1.0\,]\,, [\,0.0, 1.0\,]\,] \\ vt &= [\,[\,0, 1, 3\,]\,, [\,1, 2, 3\,]\,] \end{aligned} \tag{5}$$

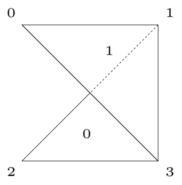
and represent the triangulation of the unit square sketched above. Assume $np == 2$. Then, at the end of step 2, our distributed representation of the triangulation is:

$$\begin{aligned} (\,x_0, x_1\,) &== ([\,[\,0.0, 0.0\,]\,, [\,1.0, 0.0\,]\,, [\,1.0, 1.0\,]\,, [\,0.0, 1.0\,]\,]\,, [\,]) \\ (\,vt_0, vt_1\,) &== ([\,[\,0, 1, 3\,]\,, [\,1, 2, 3\,]\,]\,, [\,]) \end{aligned}$$

where $x_0 == x$, $vt_0 == vt$ and x_1, vt_1 are still empty (remember step 1). Assume that, in step 3, the following partitionings have been computed:

$$\begin{aligned} (\,px_0, px_1\,) &= ([\,1, 1, 0, 0\,]\,, [\,]) \\ (\,pvt_0, pvt_1\,) &= ([\,1, 0\,]\,, [\,]) \end{aligned} \tag{6}$$

The tuples $(\,x_0, x_1\,)$, $(\,px_0, px_1\,)$ and $(\,vt_0, vt_1\,)$, $(\,pvt_0, pvt_1\,)$ fulfill the preconditions i) and ii) of the specifications for problems 1 and 2, respectively. Therefore we can apply step 4 using any program that implements these specifications. The distributed representation



$$\begin{aligned} (\,x'_0, x'_1\,) &== ([\,[\,0.0, 1.0\,]\,, [\,1.0, 1.0\,]\,]\,, [\,[\,0.0, 0.0\,]\,, [\,1.0, 0.0\,]\,]) \\ (\,vt'_0, vt'_1\,) &== ([\,[\,1, 2, 3\,]\,]\,, [\,[\,0, 1, 3\,]\,]) \end{aligned} \tag{7}$$

is a legitimate outcome of step 4: with $perm_0 = [\,1, 0\,]$, $x'_0 \cdot perm_0$ is indeed equal to $[\,x(i) \mid i \in [\,0 \ldots \text{size}(x)\,)\,, px(i) == 0\,]$. The remaining requirements are all satisfied with identity permutations.

In the framework of the conceptual representation of distributed arrays introduced in section 3.2, $(\,x'_0, x'_1\,)$, $(\,vt'_0, vt'_1\,)$ is obviously not a distributed representation of *the* triangulation represented by $(\,x_0, x_1\,)$, $(\,vt_0, vt_1\,)$. As sketched in the figure, the triangles of x', vt' are now overlapping ! The *inconsistency* between $(\,x_0, x_1\,)$, $(\,vt_0, vt_1\,)$ on one side and $(\,x'_0, x'_1\,)$, $(\,vt'_0, vt'_1\,)$ on the other side comes into place because, in our example

(1) px is not non-decreasing.
(2) $perm_p$ is not the identity.

The effect of non non-decreasing partitioning functions px and non identical permutations $perm_p$ is obviously that of modifying the order in which the elements of x appear in x': for arbitrary px and $perm_p$ steps 1)-4) yield vertex coordinates x' which are permutations of x:

$$x' == x \cdot perm^{\circ} \tag{8}$$

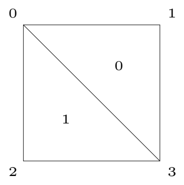
In our example, $perm^{\circ} = [\,3, 2, 0, 1\,]$. The reason why we denote the permutation with the converse symbol will become clear in the following analysis. Notice that, if px were non-decreasing and $perm_p$ were the identity, $perm^{\circ}$ would be the identity permutation and we had $x' == x$.

Of course, we can always choose $perm_p$ to be the identity. However, px is obtained, in SCDRC, from Metis or from other graph partitioning algorithms: it is not possible to require px to be non-decreasing.

We can keep our conceptual representation of distributed functions and relations *and* allow for arbitrary partition functions px if we modify steps 1)-4). To understand how this has to be done, consider equation (8). This can be interpreted in two different ways. On one hand, one can think of $x'(i)$ as of the "new" position of the i-th vertex under the (musical chairs like) motion described by $perm$. On the other hand, one can think of $perm$ as of a renumbering of the vertex set. Under such renumbering, the i-th vertex stays at its own position but gets a "new" index $perm(i)$. Conversely, $perm^\circ$ takes a new index argument of x' into an old index argument of x. This motivates the converse symbol used with equation (8).

The second interpretation of equation (8) suggests how to allow for arbitrary partition functions while keeping our simple conceptual representation of distributed arrays. If equation (8) represents a renumbering of the source of x, then we have to account for this renumbering in vt as well because the target of vt coincides with the source of x. This means that we have to replace the "old" indexes of vt' with the "new" indexes:

$$vt'(j)(i) \leftarrow perm(vt'(j)(i))$$



If we do this replacement in equation (7) we obtain (with $perm == [\,2,3,1,0\,]\,, perm \cdot perm^\circ == \mathrm{id}_{[\,0\ldots 4\,)}$):

$$(9)\qquad \begin{aligned} (\,x'_0, x'_1\,) &== ([\,[\,0.0, 1.0\,]\,, [\,1.0, 1.0\,]\,]\,, [\,[\,0.0, 0.0\,]\,, [\,1.0, 0.0\,]\,]) \\ (\,vt'_0, vt'_1\,) &== ([\,[\,3, 1, 0\,]\,]\,, [\,[\,2, 3, 0\,]\,]) \end{aligned}$$

The new triangulation is now, up to a renumbering of the vertexes and of the triangles, identical to the original one. Notice that the triangle set has been renumbered as well (pvt is not, in our example, non-decreasing).

It is now easy to see how steps 1)-4) have to be modified to allow for arbitrary partition functions px, pvt while keeping the conceptual representation of distributed functions and relations introduced in section 3.2. What we have to do is compute permutations $permx_0^\circ$, $permvt_0^\circ$ of the sources of x_0, vt_0 such that $px_0 \cdot permx_0^\circ$ and $pvt_0 \cdot permvt_0^\circ$ are non-decreasing and modify x_0 and vt_0 accordingly. Then, we redistribute the modified representations with implementations that fulfill our problem 1 and problem 2 specifications and with $perm_d$ equal to the identity. The modified procedure can be described as follows:

(1) on all partitions, do: initialize an empty vertex coordinates array x_p and an empty vertex-triangles relation vt_p.
(2) on partition 0, do: read a vertex coordinates array x and a vertex-triangles relation vt from some file into x_0, vt_0.
(3) on partition 0, do: compute suitable partition functions px_0, pvt_0 of the sources of x_0, vt_0.
(4) on partition 0, do: compute $permx_0^\circ$, $permvt_0^\circ$ such that $px_0 \cdot permx_0^\circ$, $pvt_0 \cdot permvt_0^\circ$ are non-decreasing.
(5) on partition 0, do: replace x_0, px_0, vt_0, pvt_0 with $x_0 \cdot permx_0^\circ$, $px_0 \cdot permx_0^\circ$, $vt_0 \cdot permvt_0^\circ$ and $pvt_0 \cdot permvt_0^\circ$, respectively. Renumber the elements of vt_0 according to the rule

$$vt_0(j)(i) \leftarrow permvt_0(vt_0(j)(i))$$

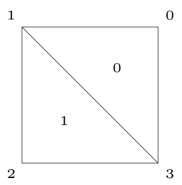
(6) on all partitions, do: redistribute $(x_0 \ldots x_{np-1})$, $(vt_0 \ldots vt_{np-1})$ according to $(px_0 \ldots px_{np-1})$, $(pvt_0 \ldots pvt_{np-1})$ and to the specifications of problem 1 and problem 2 with $perm_d ==$ id.

An algorithm for computing a permutation $perm^\circ$ such that $part \cdot perm^\circ$ is non-decreasing for arbitrary partition functions $part$ can be easily written in terms of relational operations:

Algorithm 7 : order preserving permutation

```
1: $perm^\circ = \text{breadth}(\text{converse}(part))$
Ensure: $\text{is\_non\_decreasing}(\text{compose}(part, perm^\circ))$
```

At line 1 we first compute $part^\circ = \text{converse}(part)$. This is, in general, a relation. It associates to each partition p in $[\,0 \ldots np\,)$ those indexes i in $[\,0 \ldots \text{size}(part)\,)$ for which $part(i) == p$. Notice that the breadth of $part^\circ$ – the concatenation of $part^\circ(0)$, $\ldots part^\circ(np-1)$ – is a permutation of $[\,0 \ldots \text{size}(part)\,)$[8]. Because of the order of concatenation $i < j \Rightarrow part(perm^\circ(i)) \leq part(perm^\circ(j))$ that is $part \cdot perm^\circ$ is non-decreasing. If we apply steps 1)-6) to our simple triangulation 5 with the partition functions given by 6, we obtain "the" following distributed triangulation[9]:



$$
\begin{aligned}
(\, x'_0, x'_1\,) &== ([\,[\,1.0, 1.0\,], [\,0.0, 1.0\,]\,], [\,[\,0.0, 0.0\,], [\,1.0, 0.0\,]\,]) \\
(\, vt'_0, vt'_1\,) &== ([\,[\,3, 0, 1\,]\,], [\,[\,2, 3, 1\,]\,])
\end{aligned} \tag{10}
$$

Steps 1)-6) raise a question and a remark. The question is: how to proceed in case x and vt are already non-trivially distributed (that is, x_p, vt_p are not empty for $p > 0$, for instance as a result of a previous application of steps 1)-6)) and non-trivial distributed partitionings are computed, for instance with ParMetis?

The remark is that, after step 5, one can in fact redistribute $(x_0 \ldots x_{np-1})$, $(vt_0 \ldots vt_{np-1})$ according to an offset-based representation of $(px_0 \ldots px_{np-1})$, $(pvt_0 \ldots pvt_{np-1})$ and therefore to a less general specifications of problem 1 and problem 2.

We are not going to answer the above question in this report. We point out, however, that for solving the problem of redistributing non-trivially distributed functions and relations, the specifications of problem 1 and problem 2 presented in this section

[8]this is because $part$ is a function.

[9]We have not provided a specification of converse that unambiguously defines $part^\circ$ from $part$. Up to this ambiguity, however, the outcome of steps 1)-6) is unique. Here we detail the steps of the computation. Using algorithm (7) and with an implementation of converse with ordered sub-arrays, step 4 yields the following permutations:

$$
\begin{aligned}
permx^\circ_0 &= [\,2, 3, 0, 1\,] \\
permvt^\circ_0 &= [\,1, 0\,]
\end{aligned}
$$

In the first part of step 5, we account for the renumbering of the vertex set in x_0, px_0 and of the triangle set in vt_0, pvt_0. This yields:

$$
\begin{aligned}
x_0 &= [\,[\,1.0, 1.0\,], [\,0.0, 1.0\,], [\,0.0, 0.0\,], [\,1.0, 0.0\,]\,] \\
px_0 &= [\,0, 0, 1, 1\,] \\
vt_0 &= [\,[\,1, 2, 3\,], [\,0, 1, 3\,]\,] \\
pvt_0 &= [\,0, 1\,]
\end{aligned}
$$

In the second part of step 5, we account for the renumbering of the vertex set in vt_0. This yields, with $permx == permx^\circ == [\,2, 3, 0, 1\,]$:

$$
vt_0 = [\,[\,3, 0, 1\,], [\,2, 3, 1\,]\,]
$$

play an important role. This partially answers question Q1. For the purpose of implementing steps 1)-6), it is indeed meaningful to introduce less general specifications. This is what we are going to do next, thereby answering question Q2.

One can think of steps 1)-5) as of pre-processing steps that generate some triangulation file. This file contains a vertex coordinates array x, a vertex-triangles relation vt and two offsets arrays ox and ovt. Steps 1)-6) can be then rephrased as follows:

(1) on all partitions p **in** $[\,0 \ldots np\,)$, initialize an empty vertex coordinates array x_p, an empty vertex-triangles relation vt_p and empty offsets arrays ox_p and ovt_p.
(2) on partition 0, read a vertex coordinates array x, a vertex-triangles relation vt and offsets arrays ox and ovt from some file into x_0, vt_0, ox_0 and ovt_0.
(3) on all partitions, redistribute $(x_0 \ldots x_{np-1})$, $(vt_0 \ldots vt_{np-1})$ according to $(ox_0 \ldots ox_{np-1})$, $(ovt_0 \ldots ovt_{np-1})$.

Implementations of Step 3) are now required to fulfill the following specifications:

3.3.3. *Problem 1'.* Given a distributed representation of a function f and given a partitioning of its source, compute a new distributed representation of f consistent with the given partitioning.

```
Given:
    $(f_0 \ldots f_{np-1}),\ f_p ::\ \mathrm{A(X)}$
    $(o_0 \ldots o_{np-1}),\ o_p ::\ \mathrm{A(Nat)}$
such that:
    i) is_offsets($o_p$)
    ii) size($o_p$) $== np + 1$
    iii) size($f_p$) $== o_p(np)$
find:
    $(f'_0 \ldots f'_{np-1}),\ f'_p ::\ \mathrm{A(X)}$
such that:
    iv) $f'_p ==$ concat $(f''_{p,0} \ldots f''_{p,np-1})$
            where
            $f''_{p,q} = [\, f_q(i) \mid i \ \mathbf{in}\ [\, o_q(p) \ldots o_q(p+1)\,)\,]$
```

3.3.4. *Problem 2'.* Given a distributed representation of a relation R and given a partitioning of its source, compute a new distributed representation of R consistent with the given partitioning.

```
Given:
    $(R_0 \ldots R_{np-1}),\ R_p ::\ \mathrm{A(A(Nat))}$
    $(o_0 \ldots o_{np-1}),\ o_p ::\ \mathrm{A(Nat)}$
such that:
    i) is_offsets($o_p$)
    ii) size($o_p$) $== np + 1$
    iii) source_size($R_p$) $== o_p(np)$
find:
    $(R'_0 \ldots R'_{np-1}),\ R'_p ::\ \mathrm{A(A(Nat))}$
such that:
    iv) $R'_p ==$ concat $(R''_{p,0} \ldots R''_{p,np-1})$
```

where
$R''_{p,q} = [\, R_q(i) \mid i \ \textbf{in} \ [\, o_q(p) \ldots o_q(p+1)\,)\,]$

The problem specifications introduced so far allow one to distribute array-based representations of functions and relations to set up efficient SPMD parallel computations of relation-based algorithms. For our triangle centers example, for instance, as in steps 1-6 above.

We now turn the attention to the problem of actually applying relation-based algorithms and to the specification of the third problem introduced at the end of section 2. Again, we consider our triangle centers computation and the simple triangulation of equation (5). For its distributed representation (10) obtained with steps 1)-6,) we want to compute the centers of the (two) triangles in parallel on partition 0 and on partition 1.

Although we have a distributed representation of (5), we cannot directly apply the relation-based algorithm 2 in parallel on the two partitions. This is because of two reasons. The first reason is that, in order to access the vertex coordinates, we have to *re-scale* the indexes of vt'_p according to the partition number p. The second reason is that, on a given partition, we usually need to access vertex coordinates which are stored in other partitions: in our example these coordinates are, on partition 0, $x'(3)$ and, on partition 1, $x'(0)$. Notice that $x'(0)$ is stored on partition 0 as $x'_0(0)$ and $x'(3)$ is stored on partition 1 as $x'_1(1)$.

Obviously, the indexes of vt'_p have to be rescaled according to the offsets associated with the distributed representation $(\, x'_0, x'_1\,)$ of x'. This means that algorithm 2 has to be modified as follows:

Algorithm 8 : SPMD triangle centers

```
for $j$ in $[\,0 \ldots \mathrm{size}(vt'_p)\,)$ do
    compute center($x'_p(vt'_p(j)(0) - ofs(p))$,
                   $x'_p(vt'_p(j)(1) - ofs(p))$,
                   $x'_p(vt'_p(j)(2) - ofs(p))$)
end for
```

A few remarks are appropriate here: first, notice that the above SPMD version of the triangle centers algorithm 2 is parameterized on the partition number p. This is, in fact, the sense in which the "single program" in the SPMD acronym has to be understood. As the informal descriptions of SPMD parallel computations 1-6 and 1-3 suggest, a SPMD program is not really a "single" program but a family of programs, one for each value of p.

Second, it is clear that, before algorithm 8 can actually be applied, data exchange between partitions has to take place to obtain those vertex coordinates which are needed for the local computation of the center and stored on non-local partitions and to compute the offsets ofs. Obviously, ofs has to be the same on all partitions. In our example we have $ofs(0) == 0$, $ofs(1) == 2$ and $ofs(2) == 4$. Consider the following specification of problem 3:

3.3.5. *Problem 3.* Given a distributed representation of a function f and given, on each partition, a subset d of $\mathrm{dom}(f)$, compute, on each partition, the values of f in d.

```
Given:
    $(f_0 \dots f_{np-1}),\ f_p ::\ \mathrm{A(X)}$
    $(d_0 \dots d_{np-1}),\ d_p ::\ \mathrm{A(Nat)}$
such that:
    i) $\mathrm{max\_elem}(d_p) < ofs(np)$
            where
            $ofs = \mathrm{offsets}(\mathrm{map}(\mathrm{size}, (f_0 \dots f_{np-1})))$
find:
    $(fd_0 \dots fd_{np-1}),\ fd_p ::\ \mathrm{A(X)}$
such that:
    ii) $\mathrm{size}(fd_p) == \mathrm{size}(d_p)$
    iii) $fd_p(i) == f(d_p(i))$
```

Here, the generic function offsets and the function map fulfill:

$$\begin{aligned}
&\mathrm{offsets} ::\ \mathrm{A(Nat)} \longleftarrow \mathrm{Nat}^n\\
&\quad ofs == \mathrm{offsets}(s_0 \dots s_{n-1})\\
&\quad \equiv\\
&\quad \mathrm{size}(ofs) == n+1 \ \wedge\ ofs(0) == 0 \ \wedge\ ofs(p+1) == \textstyle\sum_{k=0}^{k<p+1} s_k
\end{aligned}$$

$$\begin{aligned}
&\mathrm{map} ::\ \mathrm{A(X)} \ \longleftarrow\ (\mathrm{X} \longleftarrow \mathrm{Y}) \times \mathrm{Y}^n\\
&\quad ax == \mathrm{map}\,(f, (y_0 \dots y_{n-1}))\\
&\quad \equiv\\
&\quad ax(k) == f(y_k),\ k = [\,0 \dots n\,)
\end{aligned}$$

With a `dom_complete` program implementing the above specification of problem 3 and with an implementation of algorithm 8, it is easy to write a SPMD program to compute the triangle centers. All we have to do is to:

(1) Apply `dom_complete` and complete the data $\big(x'_0 \dots x'_{np-1}\big)$ on $\big(\,\mathrm{breadth}(vt'_0) \dots \mathrm{breadth}(vt'_{np-1})\,\big)$. This yields the arrays $\big(x''_0 \dots x''_{np-1}\big)$.
(2) Apply algorithm 8 with $x''_p(3*j+i)$ in place of $x'_p(vt'_p(j)(i) - ofs(p))$.

In our example, step 1 yields $x''_0 = [\,[\,1.0, 0.0\,], [\,1.0, 1.0\,], [\,0.0, 1.0\,]\,]$ and $x''_1 = [\,[\,0.0, 0.0\,], [\,1.0, 0.0\,], [\,0.0, 1.0\,]\,]$. Step 2) provides the centers $[\,2/3, 2/3\,]$, $[\,1/3, 1/3\,]$ on partitions 0 and 1, respectively. These are indeed the coordinates of the centers of the triangles 0 and 1 of the figure on the left of equation (10).

There are two major problems with the approach outlined above. The first problem is that we are duplicating too much data. Remember that, if we accept to duplicate *a lot* of data, the problem of structuring SPMD parallel computations becomes trivial[10]: we simply store the whole x' on all partitions. Here we increase the memory allocation costs for x' by a factor size(vt')) instead of $np*$size(x'). On large, plane triangulations, however, the number of triangles is about twice the number of nodes and we store three x'-values per triangle. Thus, the ratio between $np *$ size(x') and size(vt')) is about $np/6$. This means that we need at least 6 partitions for our scheme to be competitive with the simple minded, full duplication approach: this is not good.

Notice that, in many applications, the ratio between the memory required to store an x' element and the memory required to store a Nat can be quite large. In our

[10]if we let apart the problem of ensuring the consistency of the duplicated data.

example, x' elements are arrays of 2 doubles. The ratio between `sizeof(double)` and `sizeof`(Nat) is, e.g., on my computing architecture, equal to four. This ratio would be six if the triangulation were embedded in a three-dimensional space.

Also notice that, if we have been able to partition the original triangulations "well", the number of x'-values which are needed for the local triangle centers computation but which are stored on remote partitions will be much smaller than the number of x'-values which are stored locally.

The above remarks suggest a more efficient scheme for storing and accessing the x'-values retrieved from remote partitions. What we want to do is:

(1) *Extend* x'_p with those values of x' which are needed for the local triangle centers computation but which are stored on remote partitions.
(2) Construct an auxiliary *access table* vt''_p such that

$$x'_p(vt''_p(j)(k)) == x'(vt'(j)(k))$$

This approach has been originally proposed in the Janus framework and has been adopted in SCDRC. The second problem that affects triangle centers computations based on the specification of problem 3 given above is more subtle. Although we have not discussed how a `dom_complete` program could be implemented, it is obvious that, in order to compute a tuple $(fd_0 \ldots fd_{np-1})$, the following steps have to be done:

a) on each partition p, do: compute the indexes of d_p (in our example $d_p = \text{breadth}(vt'_p)$) which are in $[\, ofs(q) \ldots ofs(q+1)\,)$ for partitions $q \neq p$.
b) On each partition p, do: compute the indexes of $[\, ofs(p) \ldots ofs(p) + \text{size}(f_p)\,)$ which are in d_q for partitions $q \neq p$.

While the first table can be computed without additional data exchange between partitions[11], the computation of the second table certainly requires communication between partitions. It is only after each partition p knows, for any partition $q \neq p$, which are the indexes whose correspondent f-values have to be sent that such values can actually be exchanged. The cost of computing such *exchange tables* can significantly exceed the cost of exchanging the f-values themselves. The same is true for the cost of computing *access tables* like the auxiliary relation vt''_p discussed above.

These exchange and access tables do not depend on the data to be actually exchanged but only on the set of indexes on which f has to be evaluated on a given partition and, of course, on the partitioning of f itself.

In many practical cases, the parallel computation of relation-based algorithms is required at each step of some iterative procedure in which the values of f change from step to step but the exchange and access tables do not. In our triangle centers example, for instance, the vertex coordinates could change from step to step (e.g. because of forces acting on the triangulation) while the vertex triangle relation and the partitioning of the vertex coordinates stay the same. In the iterative solution of implicit problems (e.g. linear systems of equations) relation-based algorithms that represent the action of some discrete operator on a "vector of unknowns" might be evaluated thousands of times. At each time the values of the "unknowns" would change but the relation and the partitioning scheme for such values would not.

Thus, for many practical cases, it would be very inefficient to recompute, at each iteration step, the tables needed to exchange data between partitions and to efficiently

[11]w.r.t. the data exchange required to compute *ofs*.

access the local data. Therefore it is particularly important to decouple the computation of the exchange and access tables from the actual data exchange. This motivates the specification of the following problem:

3.3.6. *Problem 3'.*

Given:
  $(R_0 \dots R_{np-1}),\ R_p ::\ \mathrm{A(A(Nat))}$
  $(\,ofs \dots ofs\,),\ ofs ::\ \mathrm{A(Nat)}$
such that:
  i) $\mathrm{is\_offsets}(ofs) == \mathrm{true}$
  ii) $\mathrm{max\_elem}(R_p(j)) < ofs(np)$
find:
  $\left(at'_0 \dots at'_{np-1}\right),\ at'_p ::\ \mathrm{A(A(Nat))}$
  $\left(et'_0 \dots et'_{np-1}\right),\ et'_p ::\ \mathrm{A(A(Nat))}$
such that:
  iii) $\forall\ (f_0 \dots f_{np-1}), f_p ::\ \mathrm{A(X)}$
    such that:
      $\mathrm{offsets}(\mathrm{map}(\mathrm{size}, (f_0 \dots f_{np-1}))) == ofs$
    the tuple $\left(f'_0 \dots f'_{np-1}\right)$ obtained with SPMD algorithm 9 satisfies:
      $f'_p(at'_p(j)(k)) == f(R_p(j)(k))$

Algorithm 9 : complete f

```
Require: $ofs(p) \le et'_p(q)(k)\ \wedge\ et'_p(q)(k) < ofs(p+1)$
1: $et''_p = \mathrm{map}(sf'_p, et'_p)$
2:         where
3:         $sf'_p(a) = map(sf_p, a)$
4:         $sf_p(i) = f_p(i - ofs(p))$
5: $f'_p = \mathrm{concat}\left(f_p, \mathrm{breadth}(\mathrm{exchange}\left(et''_0 \dots et''_{np-1}\right)(p))\right)$
```

The input data of problem 3' are, on each partition, a relation R_p and an array of offsets ofs. We omit the index p in ofs to indicate that the array of offsets is is the same on all partitions.

We require ofs to be an offsets array i.e. to satisfy equation (2). Moreover, the largest index appearing in $R_p(j)$ shall not exceed $ofs(np)$. This means that the indexes of $R_p(j)$ are in the source of functions which have been distributed according to ofs.

What is sought in problem 3' are, on each partition, an access table at'_p and an exchange table et'_p. For any functions f distributed according to ofs, $at'_p(j)$ is required to provide, on partition p, access to the values of f at the indexes of $R_p(j)$ through a suitable extension f'_p of f_p.

Algorithm 9 describes how such an extension will be constructed from f_p and from the exchange table et'_p. This represents the table mentioned in step b) on page 22: the array $et'_p(q)$ contains those indexes of R_q which are in $[\,ofs(p) \dots ofs(p+1)\,)$. Since the values of f corresponding to these indexes are stored in partition p (in f_p), we say that $et'_p(q)$ is the "table of requests" issued from partition q.

In the first step of algorithm 9 we compute, for each index of et'_p, the corresponding f-value in et''_p. The pre-condition guarantees that this can be done. In the second step we exchange the table of f values et''_p between partitions. The function exchange plays an outstanding role in SCDRC. Although SCDRC users will almost never call exchange directly, most SCDRC algorithms that require data communication between partitions are designed around this *communication primitive*. We will come back to the implementation of exchange in section 4. Here we provide its specification:

$$\begin{aligned}
&\text{exchange} :: \ \mathrm{A}(\mathrm{A}(\mathrm{X}))^{np} \ \longleftarrow \ \mathrm{A}(\mathrm{A}(\mathrm{X}))^{np} \\
&\quad \big(et'_0 \ldots et'_{np-1}\big) == \text{exchange}(et_0 \ldots et_{np-1}) \\
&\quad \equiv \\
&\quad \text{is\_in}(x, et'_p(q)) == \text{is\_in}(x, et_q(p))
\end{aligned}$$

We read the specification in the following way: x is an element that partition p receives from partition q iff x is an element that partition q sends to partition p.

After having exchanged et''_p between partitions, we obtain, in line 4 of algorithm 9 a tuple of arrays of arrays of elements of the same type of the elements of f. On partition p, the p-th array of the tuple is flattened and concatenated with f_p.

If we have an `exchange` program that implements the specification of exchange, it is easy to write a `complete` program that implements algorithm 9. Also implementing a program `access_exch_table` that fulfills 3' is not difficult if `exchange` is available: tables of requests et_p can be computed locally by sorting the elements of R_p whose f-values are stored on remote partitions according to their correspondent partition number. A call to `exchange` yields then the exchange tables et'_p. The computation of the access tables at'_p is a little bit less straightforward.

Equipped with `access_exch_table` and with `complete`, it is now easy to write a SPMD program for the parallel computation of our triangle centers. In fact, we are now ready to make a further abstraction step and outline a program that, given distributed representations $(f_0 \ldots f_{np-1})$, $(R_0 \ldots R_{np-1})$ of matching f and R and given some “reduction” operator h, implements a SPMD parallel version of our relation-based algorithm 3.

(1) Compute the offsets ofs of $(f_0 \ldots f_{np-1})$.
(2) Compute at'_p, et'_p with `access_exch_table` and $(R_0 \ldots R_{np-1})$, $(\,ofs \ldots ofs\,)$.
(3) Compute f'_p with `complete` and f_p, ofs and et'_p.
(4) Compute algorithm 10.

Algorithm 10 : SPMD distributed RBA evaluation

```
for $j$ in $[\,0 \ldots \text{source\_size}(R_p)\,)$ do
    compute $h(\big[\,f'_p(i) \mid i \text{ in } at'_p(j)\,\big])$
end for
```

Here we have assumed that the RBA is to be evaluated on the whole source of R. Of course, this assumption can be easily weakened. Notice that steps 2-3 could now be embedded in some iteration in which the values of f change from step to step, e.g., as a result of the iteration itself. At each step, only `complete` would be called to extend and synchronize the local partial representations f_p. The computationally expensive and communication intensive computation of the access and exchange tables could be done only once before entering the iteration.

The algorithm outlined above shows how parallel SPMD computations of relation based algorithms can be structured using software components provided by SCDRC. As mentioned in the introduction, these components – e.g. `access_exch_table`, `complete` and components representing RBAs themselves – are designed to support structured user control over communication steps. They allow to distinguish between the kind of communication that takes place in steps 1 and 2 from the communication needed to exchange f-values. However, developers of SCDRC do not need to care about message passing level communication and related synchronization, mutual exclusion, deadlock or race condition problems.

Of course, developers of SCDRC-based, application dependent software are free to hide some of these communication steps and aggregate functionalities in more specific components. For instance, a software component representing a vertex-centered Laplace operator on triangulations could be defined in terms of RBAs in which R and h are fixed. Users could be enabled to construct concrete instances of such Laplace operator by simply passing a distributed function f of the vertexes of the triangulation to suitable constructors. These, in turn, could automatically call RBA constructors and `access_exch_table` functionalities to set up a parallel evaluation of the Laplace operator without further user intervention.

In section 2, we have mentioned the problem of combining grid relations for computing neighborhood relationships and motivated the implementation of simple basic relational operations. We close this section with the specifications of the problems of parallel conversing a distributed relation and of composing two distributed relations.

3.3.7. *Problem 4.* Given a distributed representation of a relation R and of a partitioning of its target, compute a distributed representation of R° consistent with the given partitioning.

Given:
$(R_0 \dots R_{np-1}),\ R_p :: \ \mathrm{A}(\mathrm{A}(\mathrm{Nat}))$
$(\,ofs \dots ofs\,),\ ofs :: \ \mathrm{A}(\mathrm{Nat})$
such that:
i) $\mathrm{is\_offsets}(ofs) == \mathrm{true}$
ii) $\mathrm{max\_elem}(R_p(j)) < ofs(np)$
find:
$\big(R^\circ_0 \dots R^\circ_{np-1}\big),\ R^\circ_p :: \ \mathrm{A}(\mathrm{A}(\mathrm{Nat}))$
such that:
iii) $\mathrm{offsets}\ \big(\mathrm{size}(R^\circ_0) \dots \mathrm{size}(R^\circ_{np-1})\big)$
iv) $iRj \ \equiv \ jR^\circ i$

3.3.8. *Problem 5.* Given consistent, distributed representations of relations S and T, compute a consistent, distributed representation of $S \cdot T$.

Given:
$(S_0 \dots S_{np-1}),\ S_p :: \ \mathrm{A}(\mathrm{A}(\mathrm{Nat}))$
$(T_0 \dots T_{np-1}),\ T_p :: \ \mathrm{A}(\mathrm{A}(\mathrm{Nat}))$
such that:
i) $\mathrm{max\_elem}(T_p(j)) < \mathrm{offsets}(\mathrm{map}(\mathrm{source\_size}, (S_0 \dots S_{np-1})))(np)$
find:

$(R_0 \ldots R_{np-1}),\ R_p ::\ \mathrm{A}(\mathrm{A}(\mathrm{Nat}))$
such that:
ii) $\mathrm{source\_size}(R_p) == \mathrm{source\_size}(T_p)$
iii) $iSk \wedge kRj \ \equiv\ iRj$

4. Implementation dependent elements

In this section we present and discuss implementation dependent aspects of SCDRC. In the first part we outline the architecture of SCDRC. In particular, we explain the approach used to represent the two computational environments of SCDRC, we describe the file system structure and the most important SCDRC components and we explain how SCDRC is documented.

In the second part we discuss a small number of data structures and functions in some detail. These functionalities are going to be used in the next and last section to set up a simple SPMD parallel application. As you might have guessed this is the relation-based algorithm example we have been using throughout this report: the computation of the centers of the triangles of a distributed triangulation.

4.1. **Computational environments and namespaces.** In the previous section we have discussed formal specifications for the problems introduced at the end of section 2. The specifications are based on the conceptual model of distributed functions and relations discussed in section 3.2: in this model, distributed functions and relations are represented by tuples of arrays. Accordingly, functions acting on distributed functions and relations take arguments which are tuples of arrays. In general, functions acting of distributed data take tuple arguments.

This is clearly visible in the signature of exchange and has been implicitly assumed for functions like offsets, complete etc. Let us have a closer look at offsets. A specification for this function can be expressed as follows:

$\mathrm{offsets} ::\ \mathrm{A}(\mathrm{Nat})^{np}\ \longleftarrow\ \mathrm{Nat}^{np}$
$(ofs_0 \ldots ofs_{np-1}) == \mathrm{offsets}(s_0 \ldots s_{np-1})$
$\equiv$
$\mathrm{is\_offsets}(ofs_p) == true$
$\wedge$
$ofs_p == ofs_q$
$\wedge$
$ofs(p+1) == \sum_{k=0}^{k<p+1} s_k,\ p\ \mathbf{in}\ [\,0 \ldots np\,)$

With a function exchange fulfilling the specification given in section 4, it is easy to write a SPMD algorithm that implements the above specification:
As usual, the algorithm is parameterized on the partition number p. At line 1 we construct an array et_p of np elements. Each element of et_p is itself an array of Nats of size one and contains the single value s_p. Therefore $et_p(q)(0) == s_p$ independently of q. That is, each partition sends its local size s_p to all other partitions. After exchange, et'_p contains np arrays of Nats of size one. According to the specification of exchange, $et'_p(q)(0) == s_q$ independently of p. This means that et'_p is the same table on all partitions. Thus, in the loop at lines 4-6, the same offset array is computed on all partitions.

Algorithm 11 : offsets

```
1: $et_p = \text{make\_array}(np, \text{make\_array}(1, s_p))$
2: $et'_p = \text{exchange}(et_0 \ldots et_{np-1})(p)$
3: $ofs_p = \text{make\_array}(np + 1, 0)$
4: for $k$ in $[\, 0 \ldots np \,)$ do
5:     $ofs(k + 1) = ofs(k) + et'_p(k)(0)$
6: end for
Ensure: $\text{is\_offsets}(ofs_p) == true$
Ensure: $ofs_p == ofs_q$
Ensure: $ofs(p + 1) == \sum_{k=0}^{k<p+1} s_k,\ p$ in $[\, 0 \ldots np \,)$
```

Notice that steps 2 and the testing of the last two post-conditions requires communication between remote partitions. This is formally indicated by the presence of non-local variables. These are variables with a "partition index" q which is, in general, different from p. Let us consider a SCDRC function `exchange` that implements exchange. As mentioned in the introduction, SCDRC components are C++ programs. Therefore `exchange` is a C++ function.

In the second part of this section we will discuss how exchange is actually implemented. For the moment, it is important to understand that the signature of `exchange` is quite different from the signature of the exchange function it implements:

```
template<typename X>
void
exchange(CRS<X>& t, const CRS<X>& s) /*{
  using local::size;
  using local::pos;
  REQUIRE(size(pos(s)) == n_p() + 1);
  ...
*/};
```

As exchange, the `exchange` function is generic w.r.t. the type of the data to be exchanged `X`. The SCDRC type `CRS<X>` is a compact raw storage representation of arrays of arrays of type `X`. For the purpose of this discussion you can think of an object of type `CRS<X>` as of an object of type `Array<Array<X>>`[12]. In contrast to exchange, however, `exchange` does not take as arguments tuples of arrays of arrays and does not "return" a tuple objects. Instead, `exchange` simply takes a "local" array of arrays s and returns a "local" array of arrays t.

The apparent contradiction between the signature of exchange and the signature of the correspondent implementation `exchange` is typical in the SPMD distributed computational model. In this model, np copies of a program are executed in parallel. Each copy has an associated local memory space and local data. The program is parameterized on a program id p and there is a *computational environment* that associates to each copy of the program a different value of p in $[\, 0 \ldots np \,)$.

In the SPMD computational model, only local data – data in the local memory space – appear in function signatures. This makes the signature of SPMD functions

[12]In C++, expressions involving text like `Array<Array<X>>` yield syntax errors because the double closing angular brackets are interpreted as the "right-shift" operator. In this report we do not care about this problem and freely write `Array<Array<X>>` to denote the type of arrays of arrays of some type `X`.

similar to their SPSD (single program single data) sequential counterpart. In the SPMD computational model, the visibility of local data is controlled by the same scoping rules as in the SPSD model. SPMD functions, however, can also access non-local data via communication between remote partitions. This can be done because the computational environment provides, beside the local program id p, the total number of program copies np and suitable communication primitives.

The absence of explicit representation of non-local argument data in the signature of SPMD functions is often a source of ambiguity and confusion. It makes it challenging to design software which is easily understandable.

Consider a simple size function that computes the size of an array. In a SPSD computational environment size has the following signature:

(11) $\text{size} :: \text{ Nat} \longleftarrow \text{A(X)}$

In a SPMD computational environment one can think of two size functions. One with signature as in 11 and one with signature

(12) $\text{size} :: \text{ Nat} \longleftarrow \text{A(X)}^{np}$

The latter function is understood to take a distributed array argument and to compute its size. This is the sum of the sizes of the tuple elements. SPMD implementations of 12 obviously require data exchange between partitions and are different from implementations of 11. As explained above, however, SPMD implementations of 12 would have exactly the same signature as SPMD implementations of 11, namely:

```
template<typename X>
Nat
size(Array<X>& a);
```

Thus, one of the first problems a design has to face is that of developing an unambiguous naming scheme for functions that appear both in the SPSD and, possibly in two flavors, in the SPMD computational environment. A related problem is that of representing the computational environment itself and of avoiding the erroneous usage of SPMD features in a SPSD program and vice-versa.

To understand the possible consequences of mixing up SPSD and SPMD functions in the same program consider the role of pre- and post-conditions. In SCDRC, pre- and post-conditions play an important role in code-level documentation. A pre-condition example can be seen in the signature of `exchange` given above: `REQUIRE(size(pos(s)) == n_p() + 1);`. Here `s` is an object of type `CRS<X>`. For such objects, `size(pos(s))` returns a natural number equal to the size of the array of arrays `s` represents. In SCDRC and in the SPMD computational environment, `REQUIRE(expr)` checks, on partition 0, that the value of `expr` is `true` on all partitions[13]. A necessary condition for `REQUIRE` to work is that it is called on *all* partitions. Obviously it would be a mistake to call a SPMD `REQUIRE` in a SPSD program. It also would be a mistake to use `REQUIRE`, in a SPMD program, to check a pre-condition of a function that is not called on all partitions !

Because of the fact that even simple functions like size and pre- and post conditions have implementations that depend on the computational environment (and, in the SPMD environment possibly come in two flavors), all or almost all SCDRC components *depend* on the computational environment.

[13]What happens on other partitions and why `REQUIRE` has "tuple-semantics" on partition 0 is not relevant for the present discussion.

Thus, if the computational environment were represented by some type, possibly a *singleton*, all SCDRC types and functions would be parameterized on such type or take an extra "environment" argument. Beside being very cumbersome, this approach would be of little help in preventing inconsistent mixtures of SPSD and SPMD features.

In SCDRC, we represent computational environments by means of C++ namespaces. In contrast to (static) classes, C++ namespaces can be defined and extended in files which can be compiled separately. Thus, namespaces are very suitable for accounting for dependencies that affect all software components. This can be done through *embedding*: a given component – for instance our `size` function – can be made behave in two different ways – for instance according to two different definitions of pre- and post-conditions – by embedding it into two different namespaces.

The SPSD and the SPMD distributed computational environment are represented by the namespaces `SPSD` and `SPMD_Distributed`[14]. A namespace `SPMD_Shared` might be added as a further development to represent a SPMD shared computational environment. Programs that use SCDRC usually include either `SPSD` or `SPMD_Distr` components. These are accessed via standard `using` declarations like in the following example:

```
1   #include <numeric_types/src_cc/Nat.h>
2   #include <spmd_distr/src_cc/SPMD_Distr.h>
3   #include <spmd_distr_ops/src_cc/SPMD_Distr_ops.h>
4   #include <spmd_distr_array/src_cc/SPMD_Distr_Array.h>
5   #include <spmd_distr_array/src_cc/SPMD_Distr_Array_ops.h>
6   #include <spmd_distr_iter/src_cc/SPMD_Distr_Interval_Iter.h>
7   #include <spmd_distr_iter/src_cc/SPMD_Distr_Interval_Iter_ops.h>
8
9   using namespace SPMD_Distr;
10
11  int main(int argc, char **argv) {
12
13    initialize(argc, argv);
14    const Nat sz = p() + 1;
15    Array<Nat> ofs;
16    offsets(ofs, sz);
17    VERIFY(local::is_offsets(ofs));
18    VERIFY(ofs[n_p()] == local::sum(local::interval_iter(n_p())));
19    finalize();
20    return 0;
21  }
```

At lines 1-7 we include standard SCDRC components. The file `Nat.h` provides a type for positive integer numbers. `SPMD_Distr.h`, `SPMD_Distr_ops.h`, `SPMD_Distr_Array.h` and `SPMD_Distr_Array_ops.h` provide the SPMD distributed computational environment, a set of related operations – in this case `offsets` – arrays and array operations. The last two header files provide iterators over zero-based integer intervals and related operations.

[14]In order to avoid ugly line breaking in code listings, in the remaining of this report we use `Distr`, `distr`, `Tri`, `Rect`, `Coord`, `Sys`, `iter` instead of `Distributed`, `distributed`, `Triangulation`, `Rectangular`, `Coordinate`, `System`, `iterator` respectively.

With the `using` declaration at line 9 we bring the names of `SPMD_Distr` in the local scope. These are, among others: `initialize`, `p`, `Array`, `offsets`, `n_p` and `finalize` and `local`. The latter is the name of a namespace embedded in `SPMD_Distr`. Most of the names in `SPMD_Distr::local` are function names. The correspondent functions do not have "tuple semantics" and only act on the local arguments. Thus, in the `SPMD_Distr` namespace, there is a function `size` implementing (12) and a function `local::size` that implements (11). If we were in the SPSD computational environment, there would be only a `size` function.

The functions `initialize`, `p`, `n_p` and `finalize` are all declared in `SPMD_Distr.h`. The call to `initialize` at line 13 initializes the computational environment. From line 13 and up to the end of `finalize` at line 19, *np* copies of the program are running in parallel on *np* partitions. Program copies and partitions have id numbers from zero to $np-1$. The local id number is provided by the function `p`. The value of *np* depends on how the program has been started and is provided, by `n_p`.

At line 14 we store `p()+1` in `sz`. Thus, `sz` is equal to 1 on partition 0, 2 on partition 1 and so on. An empty array of `Nats ofs` is initialized at line 15. The SCDRC type `Array` is declared in `SPMD_Distr_Array.h`. `Array` is essentially an STL (Standard Template Library) `vector` with overridden element access operators for bounds checking. Of course, bounds checking is implemented with pre-conditions and, as seen above, the implementation of pre-conditions depends on the computational environment. Therefore we have, in SCDRC, `SPSD` and `SPMD_Distr` arrays.

At line 16, `ofs` and `sz` are passed as arguments to a function `offsets`. This is declared in `SPMD_Distr_ops.h` and is a C++ implementation of algorithm 11. At line 17 we verify that the local result `ofs` is actually an offsets array. The function `local::is_offsets` is defined in `SPMD_Distr_Array_ops.h` and is particularly simple:

```
template<typename A>
inline
bool
is_offsets(const Array<Nat, A>& a) {
  using local::size;
  using local::is_non_decreasing;
  return (size(a) > 0 && a[0] == 0 && is_non_decreasing(a));
}
```

Notice that, if `offsets` is an implementation of algorithm 11, the assertion at line 17 should always evaluate to true since it corresponds to the first post-condition of the algorithm. At line 18 we check that the value of the last component of `ofs` is in fact the sum of the sizes which have been passed to the `offsets` function. We compute this sum by first constructing an object of type `Interval_Iter`. This type is provided by `SPMD_Distr_Interval_Iter.h`. The correspondent "ops" header file provides the *factory* function `interval_iter`.

Factory functions are "global" functions that return an object of a given type `X` by simply calling a constructor of `X`. They can be effectively used to avoid complicated type declaration where lightweight objects can be constructed "on the fly" and passed by value to functions like `sum`. In SCDRC this is often the case when working with iterators. To appreciate the gains in readability that can be achieved by systematic usage of factory functions, compare the program fragments:

```
return sum(filter_iter(e8, map_iter(f, array_iter(a))));
```

```
Array_Iter<int> ia(a);
```

```
Map_Iter<F, Array_Iter<Nat> > ifa(f, ia);
Filter_Iter<Eq, Map_Iter<F, Array_Iter<int> > > iffa(e8, ifa);
return sum(iffa);
```

```
return sum(Filter_Iter<Eq, Map_Iter<F, Array_Iter<int> > >
                      (e8, Map_Iter<F, Array_Iter<int> >
                                  (f, Array_Iter<int>(a))));
```

While the first fragment is both terse and readable the same can hardly be said of the other two[15]. The `interval_iter` factory function takes a natural number n and constructs an object of type `Interval_Iter`. Iterator objects can be advanced with a `next` command, queried with `is_end` and dereferenced with the standard star operator. `sum` is a generic function that adds the values visited by its iterator argument to the value of an initial default argument. `sum` is implemented in `SPMD_Distr_Iter_ops.h`:

```
template<class Iter>
inline
typename Iter::value_type
sum(Iter iter, typename Iter::value_type initial = 0) {
  using local::begin;
  using local::is_end;
  using local::next;
  typename Iter::value_type result = initial;
  begin(iter);
  while(!is_end(iter)) {
    result += *iter;
    next(iter);
  }
  return result;
}
```

4.2. **Components, files, directories.** While the two computational environments supported by SCDRC are implemented through C++ namespaces, most software components are implemented as classes or collections of functions.

In SCDRC names for variables, functions, namespaces, classes, files and directories, single words are separated by underscores. Variable, function and directory names are written in lower case like in `is_non_decreasing`. In names of namespaces and classes, the first character of single words starts in uppercase like in `Nat`. The other characters are usually written in lowercase. Exceptions are class and namespace names which contain acronyms. They are written as in `CRS_Rel` where CRS means “compact row storage”.

As explained above, most SCDRC names are embedded either in the `SPSD` or in the `SPMD_Distr` namespace. As you can see from the code examples, the namespace name appears as a prefix of both file and of the directory names. Thus, a relation based on a compact row storage representation is implemented, in the SPSD computational environment, in the class `SPSD::CRS_Rel`. This is declared in the file `SPSD_CRS_Rel.h` which is found in the `spsd_relation/src/` directory.

[15]We are thankful to Dr. Andreas Priesnitz for suggesting the usage of factory functions in SCDRC.

Header files usually contain the declaration of a single class or of a set of functions. In the second case, such functions are often operations involving a particular type. Then, the corresponding file is named after the involved type and carries the `ops` extension as in `SPSD_CRS_Rel_ops.h`. Directories usually contains more than one file. In `spsd_relation/src/`, for instance, you will also find `SPSD_Reg_Rel.h`, `SPSD_CRS_Rel_ops.h` and `SPSD_Reg_Rel_ops.h`. The following scheme shows the most important components and the file structure of SCDRC:

```
math/         numeric_types/      run_time_error/
  src/          src/                src/
    math.h        Nat.h Real.h        run_time_error.h

spsd/                             spmd_distr/
  src/                              src/
    SPSD.h                            SPMD_Distr.h
    SPSD.cc                           SPMD_Distr.cc
                                      SPMD_Distr_MPI.h
spsd_array/                           SPMD_Distr_MPI.cc
  src/
    SPSD_Array.h                  spmd_distr_array/
    SPSD_Array_ops.h                src/
                                      SPMD_Distr_Array.h
                                      SPMD_Distr_Array_ops.h

spsd_iter/                        spmd_distr_iter/
  src/                              src/
    SPSD_Iter_ops.h                   SPMD_Distr_Iter_ops.h
    SPSD_Array_Iter.h                 SPMD_Distr_Array_Iter.h
    SPSD_Array_Iter_ops.h             SPMD_Distr_Array_Iter_ops.h
    SPSD_Filter_Iter.h                SPMD_Distr_Filter_Iter.h
    SPSD_Filter_Iter_ops.h            SPMD_Distr_Filter_Iter_ops.h
    SPSD_Interval_Iter.h              SPMD_Distr_Interval_Iter.h
    SPSD_Interval_Iter_ops.h          SPMD_Distr_Interval_Iter_ops.h
    SPSD_Map_Iter.h                   SPMD_Distr_Map_Iter.h
    SPSD_Map_Iter_ops.h               SPMD_Distr_Map_Iter_ops.h
    SPSD_Slist_Iter.h                 SPMD_Distr_Slist_Iter.h
    SPSD_Slist_Iter_ops.h             SPMD_Distr_Slist_Iter_ops.h

spsd_metis/                       spmd_distr_metis/
  src/                              src/
    SPSD_metis.h                      SPMD_Distr_metis.h

spsd_ops/                         spmd_distr_ops/
  src/                              src/
    SPSD_ops.h                        SPMD_Distr_exch.h
                                      SPMD_Distr_ops.h
                                      SPMD_Distr_ops.cc

spsd_rba/                         spmd_distr_rba/
```

```
    src/                              src/
      SPSD_RBA.h                        SPMD_Distr_RBA.h
                                        SPMD_Distr_RBA_ops.h

  spsd_relation/                    spmd_distr_relation/
    src/                              src/
      SPSD_CRS_Rel.h                    SPMD_Distr_CRS_Rel.h
      SPSD_CRS_Rel_ops.h                SPMD_Distr_CRS_Rel_ops.h
      SPSD_Reg_Rel.h                    SPMD_Distr_Reg_Rel.h
      SPSD_Reg_Rel_ops.h                SPMD_Distr_Reg_Rel_ops.h

  spsd_slist/                       spmd_distr_slist/
    src/                              src/
      SPSD_Slist.h                      SPMD_Distr_Slist.h
      SPSD_Slist_ops.h                  SPMD_Distr_Slist_ops.h

  spsd_vector/                      spmd_distr_vector/
    src/                              src/
      SPSD_Vector.h                     SPMD_Distr_Vector.h
```

4.3. **Interfaces, class operations, contracts and documentation.** The SCDRC components listed above have been conceived on the basis of the formal specifications presented in section 3. Those specification are part of the documentation of SCDRC.

In the process of designing and implementing such components, we had to make choices that cannot be motivated on the basis of the specifications alone. In section 4.1 we have discussed one such choices: how to represent computational environments in implementations. From that discussion it is obvious that the motivation for selecting namespace-based representations instead of singleton parameterization was motivated by language specific considerations.

4.3.1. *Interfaces.* Another choice that has a deep impact on how SCDRC components look like is that of how interfaces are designed. There are, in C++, essentially two possibilities.

One possibility is to represent interfaces explicitly by means of abstract classes. Concrete classes that implement that interface – in Haskell, types that *are instances of* that *type class*, see [17] – inherit from the abstract (interface) class. This approach is often called, in C++, dynamic polymorphism, see [15]. In this context, dynamic polymorphism means that objects of (the types of) concrete classes can be manipulated through pointers or references of (the type of) the interface class. Using dynamic polymorphism, a single program, e.g. to converse relations, can be used to compute the converse of a number of concrete relation types. This approach allows one to write generic programs and to avoid code duplication. This, in turn, improves code correctness, documentation and maintainability. In this approach, a function `f` that takes as argument an object of type (castable to a) reference to an abstract class `Rel` can be read as a generic rule of the kind: "for all types which are instances of `Rel`, `f` does ...".

Dynamic polymorphism has two main drawbacks. The first one is efficiency. The second one is fragility. The possibility to manipulate concrete objects via references to abstract classes implies some extra storage requirements. Moreover, the access to concrete objects necessarily takes place via a (virtual) pointer (table). This fact together with limitation in compiler implementation effectively prevent inlining of function calls. Extra storage and potentially slower access are negligible if the data structures and the function call they affect are not atomic. Otherwise they are unacceptable. In our examples it would be unacceptable if, in a concrete implementation of a relation, the access to the indexes which are in relation with a given source index would take place via virtual pointer table.

The second drawback of dynamic polymorphism is that it leads to deep and possibly stiff class hierarchies. It also tends to lead to "fat" interfaces if multiple inheritance is not systematically used. Systematic use of multiple inheritance is not, in turn, without problems, see [15].

Another possibility of representing interfaces in C++ is implicitly by means of parameterization. This approach is called *static* (or compile-time) polymorphism. In this approach, any parameterized data structure implicitly defines a set of requirements. For instance, the template function `sum` listed at page 31 implicitly defines the following set of requirements for the type `Iter` of argument object:

(1) `Iter` must export the type `value_type`.
(2) A `void` function `local::begin` must be defined for objects of type `Iter`.
(3) A function `local::is_end` of type castable to `bool` must be defined for objects of type `Iter`.
(4) A `void` function `local::next` must be defined for objects of type `Iter`.
(5) A (dereferencing) `operator*` of type `Iter::value_type` must be defined for objects of type `Iter`.
(6) `operator+=` must be defined for objects of type `Iter::value_type`.

The above set of requirement could be interpreted as a refinement of an iterator *concept* in the STL sense. In general, however, sets of requirements implicitly defined by parameterized data structures cannot be easily re-conducted to useful concepts. Implicit interfaces tend to reflect more the way types are actually used than the concepts they represent.

Implicit interfaces are more efficient and more flexible than explicit ones but they also have serious drawbacks. Some drawbacks are of practical nature and reflect the state of the art in C++ compiler technology: error messages after failures in instantiations of heavily parameterized data structures are known for their poor readability. Other drawbacks are typical of the C++ implementation of templates: constrained genericity – expressing conditions like "for all types `Iter` such that ..." – is not directly supported in C++. Complex schemes for mimicking "type-class instance relationships" with static polymorphism in C++ have been proposed, among other, by Barton-Nackman [2] and Kothari and Sulzmann [13]. A more systematic approach is proposed in [16].

In SCDRC, all interfaces are represented statically and are therefore implicit. We have tried to document the intended usage of parameterizes data structures with careful choices of template argument (type) names. The above definition of `sum`, for instance, suggests that the first argument is expected to be an iterator. Of course, every type fulfilling the requirements 1-6 can be used as an argument of `sum`. We have not been able to systematically apply Barton-Nackman or "enable_if"-like approaches to constrain generic template parameters in SCDRC.

4.3.2. *Class operations.* For a given SCDRC type, a certain number of operations are declared in the corresponding `ops` files. Some operations are implemented for almost all SCDRC types. These are those operations that correspond to the type's member functions and output operations. Examples of operations corresponding to a type's member functions are the already seen factory functions. They correspond to calls of a type's constructor. The `map_iter` function used above, for instance, is defined as follows:

```
template<class Fun, class Forward_Iter>
inline
Map_Iter<Fun, Forward_Iter>
map_iter(const Fun& f, const Forward_Iter iter) {
  return Map_Iter<Fun, Forward_Iter>(f, iter);
}
```

Other standard functions corresponding to a type's member functions are `size`, `is_empty`, `begin`, `end` for arrays and lists and `is_end`, `next` for iterators. A version of `operator<<` to output an object's value is implemented for almost all SCDRC types. Notice that the names standard functions corresponding to some type's member functions are necessarily heavily overloaded. Of course, heavily overloaded names negatively affect compile time. On the other hand, they allow to achieve a higher *uniformity of notation* than the more conventional mixture of member and global functions. A comparison of the following code fragments shows that uniformity of notation can, in fact, significantly improve readability:

```
REQUIRE(target_size(t) <= back(offsets(source_size(s))));
```

```
REQUIRE(t.target_size() <= offsets(s.source_size()).back());
```

4.3.3. *pre- and post-conditions and documentation.* An important aspect of the design of SCDRC is the systematic usage of contracts as a documentation element. Consider, for instance, the following code fragment:

```
template<typename A>
inline
Array<Nat>
invert_permutation(const Array<Nat, A>& p) {
  using local::require;
  using local::ran_size;
  using local::source_size;
  using local::is_in_normal_form;
  using local::compose;
  using local::ensure;
  REQUIRE(ran_size(p) == source_size(p));
  REQUIRE(is_in_normal_form(p));
  const Nat sz = source_size(p);
  Array<Nat> result(sz);
  for(Nat i = 0; i < sz; i++)
    result[p[i]] = i;
  ENSURE(compose(result, p) == id(sz));
  ENSURE(compose(p, result) == id(sz));
  return result;
}
```

The function `invert_permutation` takes an array of natural numbers `p` and returns an array of natural number `result`. `p` is understood to represent a permutation of $[\,0\ldots\mathrm{size}(\mathtt{p})\,)$. Therefore the first *pre-condition* of `invert_permutation` requires the size of the range of `p` to coincide with the size of `p`[16]. The second pre-condition requires `p` to be in normal form. The query function `is_in_normal_form` is declared as follows:

```
template<class A>
inline
bool
is_in_normal_form(const Array<Nat, A>& a) /*{
  using local::is_empty;
  using local::min_max_elem;
  using local::ran_size;
  using local::target_size;
  using local::ensure;
  ...
  ENSURE(result == (ran_size(a) == target_size(a)));
  return result;
}*/
```

The *post-condition* of `is_in_normal_form` shows that the pre-conditions of `invert_permutation` actually require:

$$\mathtt{target\_size}(\mathtt{p}) == \mathtt{ran\_size}(\mathtt{p}) == \mathtt{source\_size}(\mathtt{p})$$

For non empty arrays of natural numbers, the size of the target is defined to be equal to one plus the maximal element of the array. Thus, the first equality implies that `p` is surjective on $[\,0\ldots\mathtt{max\_elem}(\mathtt{p})\,)$. The second equality guarantees that `p` is bijective: if there were distinct indexes `i` and `j` in $[\,0\ldots\mathtt{source\_size}(\mathtt{p})\,)$ with $\mathtt{p}(\mathtt{i}) == \mathtt{p}(\mathtt{j})$, the size of the range of `p` could be, at most, equal to $\mathtt{source\_size}(\mathtt{p}) - 1$. Thus, the pre-conditions of `invert_permutation` require `p` to be a permutation. The post-conditions require the result of `invert_permutation` to be the inverse permutation of `p`: composition of `result` with `p` (and of `p` with `result`) shall yield the identity. The SCDRC function `id` is another example of a factory function.

The discussion above shows that consistent usage of contracts and sensible naming schemes can significantly improve code understandability and documentation. Of course, contracts cannot, in general, express full problem specifications and for many SCDRC we have not been able to derive suitably implementable post-conditions. Contracts and pre-conditions in particular, however, can be extremely useful in documenting the intended usage of functions. As an example we list the pre-conditions on the "in" arguments of `partition_recursive`, a subset of the the SCDRC interface to Metis for partitioning the source of symmetric, anti-reflexive relations with minimal edge cut:

```
template<class Rel>
void
partition_recursive(Array<Nat>& part,
                    Nat& n_cuts,
```

[16]In SCDRC, `size` and `source_size` are, for arrays, the same function. Both return the *length* (the number of elements) of the array. We use `size` and `source_size` for container and function arguments, respectively.

```
                     const Rel& r,
                     const Nat n_partitions,
                     const Array<Nat>& elem_weights = Array<Nat>(0),
                     const Array<Nat>& pair_weights = Array<Nat>(0),
                     const Array<Nat>& options = Array<Nat>(0)) {
  ...
  REQUIRE(is_symmetric(r));
  REQUIRE(is_anti_reflexive(r));
  REQUIRE(n_partitions <= source_size(r));
  REQUIRE(size(elem_weights) == 0 ||
          size(elem_weights) % source_size(r) == 0);
  REQUIRE(size(pair_weights) == 0 ||
          size(pair_weights) == size(r));
  REQUIRE(size(pair_weights) == 0 ||
          is_symmetric_weights(pair_weights, r));
  REQUIRE(size(options) == 0 || size(options) == 5);
  REQUIRE(size(options) == 0 || options[0] == 0 || options[0] == 1);
  REQUIRE(size(options) == 0 ||
          (options[0] == 1 &&
           (options[1] == 1 || options[1] == 2 || options[1] == 3)));
  REQUIRE(size(options) == 0 ||
          (options[0] == 1 && options[2] == 1));
  REQUIRE(size(options) == 0 ||
          (options[0] == 1 && options[3] == 1));
  REQUIRE(size(options) == 0 ||
          (options[0] == 1 && options[4] == 0));
  ...
}
```

At the present state of development, the SCDRC approach towards source-level documentation is based on contracts and on a set of naming rules. In addition to the rules discussed in section 4.2, we have used the following conventions:

- Function names:
  - Boolean queries start with `is` or `are` followed by the queried feature as in `is_empty`, `is_initialized`, `are_subarrays_nubbed`.
  - Feature queries are named after the queried feature, usually a noun as in `size`, `breadth`, `back`.
  - Commands use imperative forms as in `invert_permutation`, `compose`, `converse`.
- Variable names:
  - Cardinalities (the number of dimensions, the number of partitions) are prefixed with `n` as in `n_dims`, `n_partitions`, `n_triangles`.
  - Function arguments, in particular constructor arguments, are spelled in length as in `CRS(const Array<T>& breadth, const Array<Nat>& pos)`.

4.4. **Iterators.** Iterators play an important role in SCDRC. As we will see in the next section, all SCDRC relations implement a common interface. This interface essentially consists of five iterators. Examples of SCDRC functions acting on iterators or producing iterators are the factory functions discussed in section 4.1.

As in the standard template library, SCDRC iterators act as a link between generic algorithms and a variety of *traversable* data structures. However, SCDRC iterators are different from STL iterators in many ways, being more similar to Boost ranges. In SCDRC, a type `Iter` represents an iterator if:

- `Iter` exports the type `value_type`. This means that `Iter` contains a public `typedef` declaration where `value_type` appears as the second argument of `typedef` as in `typedef Nat value_type;` in the SCDRC class `Interval_Iter`.
- `Iter`s can be dereferenced with `operator*`.
- `Iter`s can be queried with `is_end`.
- `Iter`s can be incremented with `next`.

Because the state of SCDRC iterators can be queried with `is_end`, traversable data structures can be visited with a single iterator and there is no need to operate with "begin" and "end" iterator pairs as in STL. A second important difference between STL and SCDRC iterators is that SCDRC iterators can be used to represent lazily evaluated computational rules. Consider, for instance, the program fragment:

```
Map_Iter<F, Array_Iter<Nat> > ifa(f, ia);
```

Here `ifa` is an object of type `Map_Iter`. It is constructed with a function `f` of type `F` and with an iterator over arrays of natural numbers. We can step through and dereference `ifa` with the iterator interface, for instance as in:

```
while(!is_end(ifa)) {
  if(is_odd(*ia))
    cout << *ifa << endl;
  next(ia);
  next(ifa);
}
VERIFY(is_end(ia));
```

The program fragment prints the values of `f` at the odd elements of the array iterated by `ia`. The evaluation of `f` takes place where `ifa` is dereferenced. This means that `ifa` represents the mapping of `f` on `ia` *lazily*: if the natural numbers visited by `ia` are all even, `f` is never evaluated.

A small set of basic iterator classes is implemented, in SCDRC, in `spsd_iter` and `spmd_distr_iter`: `Interval_Iter`, `Array_Iter`, `Slist_Iter`, `Map_Iter` and `Filter_Iter`. These operators extend the above interface with the command `begin`, the query `size` and with the random access operator `operator[]`.

4.5. **Relations.** As explained in 4.3.1, SCDRC interfaces are implicit. As for iterators, there is no abstract class from which concrete relation classes are derived and we use the expression relation interface to denote a set of functionalities that any concrete SCDRC relation `Rel` has to implement. These are:

- Public definitions of five nested iterator classes:
  - `Lambdas_Iter`
  - `Lambda_Sizes_Iter`
  - `Lambda_Offsets_Iter`
  - `Graph_Ran_Iter`
  - `Graph_Dom_Iter`

  Each class implements the basic iterator functionalities of the previous section.

- Public definition of five void constant `Rel` member functions: `lambdas`, `lambda_sizes`, `lambda_offsets`, `graph_ran` and `graph_dom`. The return types of these functions correspond with the types of the nested classes.
- Definition of five factory functions `lambdas`, `lambda_sizes`, `lambda_offsets`, `graph_ran` and `graph_dom`. These functions take (constant references) `Rel` arguments and return types correspondent to those of the nested classes. They simply call the correspondent member function on the argument. For instance, `lambdas` is defined as follows:

```
inline
Rel::Lambdas_Iter
lambdas(const Rel& r) {
  return r.lambdas();
}
```

In `Lambdas_Iter`, the value of `value_type` is `Array_Iter<const Nat>`: this is the type of the objects which are obtained by dereferencing the output of `lambdas`. If `r` is a SCDRC object representing some relation R, `lambdas(r)[j]` returns an iterator over the indexes of $R(j)$.

In the other nested classes, the value of `value_type` is `Nat`. `lambda_sizes(r)[j]` and `lambda_offsets(r)[j]` provide access to the size and to the offset associated to $R(j)$. For `j` in `[0...source_size(r))`, they fulfill:

$$\texttt{size}(\texttt{lambda\_sizes}(\texttt{r})) == \texttt{source\_size}(\texttt{r})$$

$$\wedge$$

$$\texttt{size}(\texttt{lambda\_offsets}(\texttt{r})) == \texttt{source\_size}(\texttt{r}) + 1$$

$$\wedge$$

$$\texttt{lambda\_offsets}(\texttt{r})[0] == 0$$

$$\wedge$$

$$\texttt{lambda\_offsets}(\texttt{r})[\texttt{j} + 1] == \texttt{lambda\_offsets}(\texttt{r})[\texttt{j}] + \texttt{lambda\_sizes}(\texttt{r})[\texttt{j}]$$

The iterators returned by `graph_ran` and by `graph_dom` allow traversing a relation as a set of pairs. This is particularly useful in the implementation of relational operations like `converse` and `compose`.

At the present stage, SCDRC provides two data structures for relations: `CRS_Rel` and `Reg_Rel<n>`. The first class is useful for *irregular* relations i.e. for relations for which the size of $R(j)$ is not constant. The second class is useful for *regular* relations such as the vertex-triangle relation of our example. The template `Nat` value `n` represents the size of the $R(j)$.

Both `CRS_Rel` and `Reg_Rel<n>` use, internally, arrays of `Nat`s to store the elements of $R(j)$ and guarantee access to these elements in asymptotically constant time. As mentioned in section 2, efficient access to $R(j)$ is crucial for the implementation of relation-based algorithms.

In many important applications, however, implementations of $R(j)$ in terms of arrays are sub-optimal. For neighborhood relations on structured grids, for instance, functions like $R(j)$ can be written in terms of simple analytical expression. In this case, it would be computationally inefficient to represent such relations with `Reg_Rel<n>`s or with `CRS_Rel`s. Using the examples of `CRS_Rel` and `Reg_Rel<n>`, it is easy to extend SCDRC with lightweight types which are optimized for particular classes of relations.

As far as the new types implement the interface described above, they can be used in relation-based computations in the same way as `CRS_Rel` and `Reg_Rel<n>`. We plan to provide such extensions upon user's demand.

4.6. **Relation-based algorithms.** In section 2 we have introduced relation-based algorithms as generic computational rules defined in terms of a relation R, of a functions f taking values in the target of R and of a "reduction" operator h. In section 4 we have seen that, in order to apply parallel SPMD relation-based algorithms, auxiliary data structures and functionalities are in general needed. These can be described in terms of suitable exchange and access tables and in terms of functionalities to complete local array-based partial representations of f.

In SCDRC, relation-based algorithms are implemented as specializations of a generic type RBA:

```
template<class H,
         class F,
         class R,
         Nat h_arity = H::arity,
         Nat f_arity = F::arity>
class
RBA;
```

Objects of type `RBA` can be easily constructed by passing objects of type `H`, `F` and `R` to the `RBA` constructor as in

```
RBA<H, F, R> tca(triangle_center,
                 vertex_coordinates(tri),
                 vertex_triangle(tri));
```

`H` is, in general, a user-defined type. It is required to export the type `return_type`, the constant `Nat` value `arity` and to implement a generic function call operator `operator()`. For the case `arity` $==1$, `operator()` is required to have the following signature:

```
template<class Random_Access_Data>
return_type
operator()(Random_Access_Data& x) const;
```

In most practical cases, `H` is a user defined wrapper of some specific, problem dependent computational rule. In the example given above, for instance, `H` represents a rule for computing the triangle centers. As mentioned in section 2, this rule depends on application specific *aspects* like the kind of triangles (plane, spherical), the coordinate system associated with the triangle vertexes etc. In our triangle centers example, for instance, `H` is defined as follows:

```
typedef Triangle_Area<Coordinate_System> H;

template<class Coordinate_System>
class Triangle_Center {
public:
  typedef Vector<Real, Coordinate_System::n_crds> return_type;
  static const Nat arity = 1;
  template<class Random_Access_Data>
  Vector<Real, Coordinate_System::n_crds>
  operator()(Random_Access_Data& x) const {
      return Coordinate_System::triangle_center(x[0], x[1], x[2]);
    }
  };
```

In many practical cases, F is an array of a type matching the type of the arguments of the specific rule wrapped by H, in our example triangle_center. However, F could be an RBA itself. This allows relation-based algorithms to be composed to express complex computational patterns. The type R is an SCDRC relation. As discussed above, SCDRC provides, at the present stage, two relation types: CRS_Rel and Reg_Rel<n>.

In the SPSD computational environment, relation-based algorithms can be evaluated right after construction. The triangle center algorithm object tca of out example, for instance, could be evaluated on the triangles of tri with the simple loop:

```
  for(Nat i = 0; i < source_size(vertex_triangle(tri)); i++)
    cout << tca(i) << endl;
```

In the SPMD distributed computational environment, and for the case in which F is an array, the auxiliary access and exchange tables have to be computed and the local arrays f have to be completed before relation based algorithms can be evaluated. The SPMD distributed computational environment supports these computations with two functions. They can be called with relation-based algorithm arguments as follows:

```
  init_access_exch_tables(tca);
  complete_f(tca);
```

As discussed in section 3.3, these functions allow users to set up parallel computations of distributed relation-based algorithms without having to care about message passing level communication and related synchronization, mutual exclusion, deadlock or race condition problems. At the same time, init_access_exch_tables and complete_f support the optimization of computational procedures in which complete_f has to be called at each step of some iteration, init_access_exch_tables, however, only once at the beginning of the iteration. In scientific computing, such iterative procedures are found, e.g. in the numerical integration of (partial) differential equations, in linear algebra and in the solution of optimization problems.

4.7. **Communication primitives, exchange and MPI interface.** In the next and last section of this report, we show how to setup a parallel computation of the centers of the triangles of a distributed triangulation. We are going to use some of the SCDRC data structures discusses in this section, functionalities like init_access_exch_tables and complete_f and primitives for redistributing distributed arrays and relations.

As mentioned in section 3, all SCDRC functionalities that require data communication between partitions have been designed on the top of a single communication primitive called exchange. An implementation of exchange is provided, in the SPMD distributed computational environment by the function SPMD_Distr::exch. This function is implemented, internally, in terms of the MPI primitive MPI_Alltoallv. This is one of the few MPI functionalities used by SCDRC. In SCDRC, most MPI entities are accessed via a small interface. This is implemented as a MPI namespace embedded in SPMD_Distr. SPMD_Distr::MPI contains:

- The type Comm (MPI_Comm).
- The constant values:
  - INT (MPI_INT).

  - `CHAR` (`MPI_CHAR`).
  - `communicator` (`MPI_COMM_WORLD`).
- The functions:
  - `initialize`, implemented in terms of `MPI_Init`.
  - `is_initialized`, implemented in terms of `MPI_Initialized`.
  - `finalize`, implemented in terms of `MPI_Finalize`.
  - `is_finalized`, implemented in terms of `MPI_Finalized`.
  - `get_rank`, implemented in terms of `MPI_Comm_rank`.
  - `get_size`, implemented in terms of `MPI_Comm_size`.

Other MPI entities used in SCDRC are the already mentioned `MPI_Alltoallv` and `MPI_Abort` and `MPI_Allgather`. `MPI_Alltoallv` is used only in the implementation of `exch`. The other two MPI primitives are used only in the implementation of contracts in the SPMD distributed environment. Thus, the dependency of SCDRC on MPI is limited to a few primitives and confined to very few files.

5. Preliminary results, outlook

In this section we show how SCDRC can be used to set up a parallel computation of the center of the areas of a triangulation and present some preliminary results. We close this report with an outlook on future activities.

5.1. **Center of area computations.**

In this example we set up a parallel computation of the center of the areas of a triangulation. The computation is embedded in a time stepping procedure. On each partition and at each iteration step, the coordinates of the vertexes of the triangulation are displaced according to a simple rule and a new center is computed. The computation of the center is based on two relation-based algorithms, one for computing the centers and one for computing the areas of the triangles. The coordinates of the center of the triangulation and of its total area are accumulated in local variables `c` and `a`. At the end of the iteration, the average center coordinates and the average areas are collected, together with simple computation metrics, on partition zero. Here the average center is computed and the results are sent to the standard output.

Beside the SCDRC functionalities discussed in section 4, we use simple components for representing surface triangulations and basic rules for geometrical computations in a three-dimensional Cartesian coordinate system. These components are not part of SCDRC. The type `Tri`, in particular, just wraps a vertex-triangle relation and a vertex coordinates array in a data structure. For this data structure, basic input-output functionalities are provided in different data formats, e.g. for visualization.

In setting up the computation, we assume, as discussed at the end of the specification of problem 2 in section 3, that the triangulation, together with correspondent offsets for the vertex coordinates and for the vertex-triangle relation, are stored in files which are given as arguments on the command line. This is consistent with steps 1-3 of page 18. This means that, in a pre-processing step, we have already computed a partitioning of the triangles and of the vertexes of the triangulation and we have renumbered the original vertex-triangle relation and the vertex coordinates array accordingly. The output of these computations, a "new" triangulation and the correspondent offsets arrays, is the input of our example. We interleave the listing of the program with remarks.

```
1   #include <numeric_types/src_cc/Nat.h>
```

```
 2  #include <run_time_error/src_cc/run_time_error.h>
 3  #include <spmd_distr/src_cc/SPMD_Distr.h>
 4  #include <spmd_distr_ops/src_cc/SPMD_Distr_ops.h>
 5  #include <spmd_distr_array/src_cc/SPMD_Distr_Array.h>
 6  #include <spmd_distr_array/src_cc/SPMD_Distr_Array_ops.h>
 7  #include <spmd_distr_relation/src_cc/SPMD_Distr_Reg_Rel.h>
 8  #include <spmd_distr_relation/src_cc/SPMD_Distr_Reg_Rel_ops.h>
 9  #include <spmd_distr_iter/src_cc/SPMD_Distr_Interval_Iter.h>
10  #include <spmd_distr_iter/src_cc/SPMD_Distr_Interval_Iter_ops.h>
11  #include <spmd_distr_iter/src_cc/SPMD_Distr_Map_Iter.h>
12  #include <spmd_distr_iter/src_cc/SPMD_Distr_Map_Iter_ops.h>
13  #include <spmd_distr_rba/src_cc/SPMD_Distr_RBA.h>
14  #include <spmd_distr_rba/src_cc/SPMD_Distr_RBA_ops.h>
```

At lines 1-2, we include the header files for natural numbers and contracts. These do not depend on the computational environment. Subsequently, we include the SPMD distributed computational environment, its operations, distributed arrays, relations, iterators and relation-based algorithms with the respective operations.

```
15  #include <spmd_distr_geometry/src_cc/SPMD_Distr_Rect_Coord_Sys.h>
16  #include <spmd_distr_triangulation/src_cc/SPMD_Distr_Tri.h>
17  #include <spmd_distr_triangulation/src_cc/SPMD_Distr_Tri_ops.h>
18  #include <spmd_distr_geometry/src_cc/SPMD_Distr_Triangle.h>
19  #include <spmd_distr_io_ascii/src_cc/SPMD_Distr_io_ascii.h>
20  #include <fstream>
21  #include <iostream>
22  #include <string>
23
24  using namespace SPMD_Distr;
25  using namespace std;
26  using local::operator<<;
```

Next, we include non-SCDRC components for geometrical rules, triangulations and IO in ASCII format. This is the format in which the triangulation and the offset arrays are stored in the input files. At line 24, we bring all the names of the SPMD distributed computational environment in the global scope. At line 26, we inject `local::operator<<` in the global scope. As mentioned earlier, most SCDRC data structures can be processed by `operator<<`. At the present, we have not implemented any version of `operator<<` with "tuple-semantics". The implemented `operator<<` act on local data and are therefore embedded, in the SPMD distributed computational environment, in the `local` namespace. Since there is no ambiguity in the usage of these operators, we make them available in the global scope.

```
27  int
28  main(int argc, char** argv) {
29
30    if(argc < 4) {
31      cerr << "Usage: "
32           << argv[0]
33           << " tri vofs tofs"
34           << endl;
35      exit(0);
36      }
37
38      initialize(argc, argv);
```

At line 38, after the number of command line arguments check, we issue the first SPMD function call: `initialize` starts the SPMD distributed computational environment. From line 38 and up to the call to `finalize` at line 135, `n_p()` copies of the program are running in parallel on `n_p()` partitions.

```
39      Reg_Rel<3> vt;
40      Array<Vector<Real, 3> > vx;
41      Array<Nat> vtofs(n_p() + 1, 0);
42      Array<Nat> vxofs(n_p() + 1, 0);
43
44      if(p() == 0) {
45        typedef Rect_Coord_Sys<3> Coord_Sys;
46        typedef Tri<Coord_Sys> T;
47        T tri;
48        string tri_file = argv[1];
49        local::read_ascii(tri, tri_file);
50        vt = tri.vertex_triangle();
51        vx = tri.vertex_coordinates();
52        string vofs_file = argv[2];
53        local::read_ascii(vxofs, vofs_file);
54        string tofs_file = argv[3];
55        local::read_ascii(vtofs, tofs_file);
56        local::VERIFY(local::is_offsets(vxofs));
57        local::VERIFY(local::size(vxofs) == n_p() + 1);
58        local::VERIFY(local::target_size(vt) == local::back(vxofs));
59        local::VERIFY(local::is_offsets(vtofs));
60        local::VERIFY(local::size(vtofs) == n_p() + 1);
61        local::VERIFY(local::source_size(vt) == local::back(vtofs));
62      }
```

First we initialize, on each partition, an empty vertex-triangle regular relation `vt`, an empty array of vertex coordinates `vx` and trivial partitioning offsets `vtofs` and `vxofs` for the source of `vt` and for the source of `vx`, respectively. These variables correspond to vt_p, x_p, ovt_p and ox_p of steps 1-3 of page 18.

Then, on partition 0, we initialize an empty triangulation `tri` in a three-dimensional rectangular (Cartesian) coordinate system (lines 45-47), we read `tri` from the file given on the command line (lines 48-49) and we initialize `vt` and `vx` with the vertex-triangle relation and with the vertex coordinates array of `tri`.

At lines 52-61, we read the offsets arrays and we verify the consistency of the input data. In particular, we check that `vtofs` and `vxofs` are indeed offsets arrays of proper size and that they represent non-decreasing partitioning functions for `vt` and `vx`, respectively. Notice the `local` qualifier in front of the `VERIFY` macros and in their argument expressions.

```
63      Reg_Rel<3> vtp;
64      redistribute_after_offsets(vtp, vt, vtofs);
65      Array<Vector<Real, 3> > vxp;
66      redistribute_after_offsets(vxp, vx, vxofs);
```

```
67      Array<Nat> ofs;
68      offsets(ofs, vxp.size());
69      typedef Rect_Coord_Sys<3> Coord_Sys;
70      typedef Triangle_Area<Coord_Sys> TA;
71      typedef Triangle_Center<Coord_Sys> TC;
72      typedef Array<Vector<Real, 3> > F;
73      typedef Reg_Rel<3> R;
74      TA triangle_area;
75      TC triangle_center;
76      RBA<TA, F, R> taa(triangle_area, vxp, vtp, ofs);
77      RBA<TC, F, R> tca(triangle_center, vxp, vtp, ofs);
```

At this point, we are ready to set up a parallel computation of the center of the areas of `tri`. We first redistribute `vt` and `vx` according to `vtofs`, `vxofs`. This is done at lines 64-67 and yields, on each partition, a new distributed vertex-triangle relation `vtp` and a new vertex coordinates array `vxp`.

Notice the usage of `redistribute_after_offsets`: this is an overloaded function (it is used, at lines 65 to redistribute a `Reg_Rel<3>` relation and, at line 67, to redistribute an array) which implements the specifications of problem 2' and 1' of section 3.3. Therefore, `redistribute_after_offsets` has "tuple-semantics" although, as explained in section 4.1, only local data formally appear as "function" arguments.

`redistribute_after_offsets` is an example of how SCDRC supports structuring parallel computations by providing communication primitives that relieve the user from the burden of low-level data transferring. As explained in the introduction, however, SCDRC does not attempt to hide the underlying distributed data model to the user. This model is visible in the offsets array arguments that "high-level" SCDRC primitives like `redistribute_after_offsets` require.

The offsets arrays `vtofs` and `vxofs` describe, on each partition, which chunks of `vt` and `vx` have to be sent to which partition. In order to efficiently initialize the relation-based algorithms, it is useful to compute, on each partition, the offsets that describe how the new distributed vertex coordinates array `vxp` is actually distributed. This is done at lines 67 and 68.

Lines 69 to 77 is where the relation-based algorithms `taa` and `tca` for triangle areas and centers are actually constructed. The `typedef`s instructions just introduce convenient type synonyms; the RBA constructors are called in the last two lines. Notice that both `taa` and `tac` use the same "f" function `vxp` and the same "R" relation `vtp`. The "h" functions of `taa` and `tca` are `triangle_area` and `triangle_center`, respectively. These rules are provided by non-SCDRC components. As the example shows, RBAs are quite flexible generic types: users can define their own "h" functions to construct ad hoc RBA objects.

```
78      init_access_exch_tables(taa);
79      init_access_exch_tables(tca);
80      const Nat n_iter = 10000;
81      const Real alpha = 0.1;
82      const Real omega = 1.0;
83      Array<Vector<Real, 3> > vx0(vxp);
84      Real a = 0.0;
85      Vector<Real, 3> c = Vector<Real, 3>(0.0);
86      for(Nat iter = 0; iter < n_iter; iter++) {
 87      const Real t = 2.0 * Real_PI * Real(iter) / Real(n_iter - 1);
 88      for(Nat i = 0; i < vx0.size(); i++)
 89        vxp[i] = vx0[i] * (1.0 + alpha * sin(omega * t));
 90      complete_f(taa);
 91      complete_f(tca);
 92      for(Nat j = 0; j < local::source_size(vtp); j++) {
 93        const Real area = taa(j);
 94        const Vector<Real, 3> center = tca(j);
 95        a += area;
 96        c += area * center;
 97      }
 98    }
 99    a /= Real(n_iter);
100    c /= Real(n_iter);
```

Since we are in the SPMD computational environment and the "*f*" function of taa and tca is represented by a distributed array, the auxiliary access and exchange tables have to be computed and the local arrays f have to be completed before taa and tca can actually be evaluated.

The computation of the access and exchange tables is done at lines 78 and 79. This is outside the main iteration (lines 86 to 98) because the tables only depend on the vertex-triangle relation and on the offsets of the vertex coordinate arrays. In contrast to the vertex coordinates, the relation and the offsets do not change during the iteration. As explained in section 3.3, the computation of the access and exchange table is computationally demanding and it would be very inefficient to recompute such tables every time we need to complete the local vertex coordinates arrays.

At lines 80-82 we initialize the number of iterations n_iter, the amplitude alpha and the frequency omega. Amplitude and the frequency are used at line 89 to impose a simple periodic motion on the vertexes of the triangulation. At lines 83-85 we initialize an auxiliary array of vertex coordinates vx0 and the variable a and c. We use a and c to accumulate the sums of the areas and of the centers of the triangulation.

Inside the iteration we first compute an "iteration time" t and move the vertexes of the triangulation. Then, at lines 90-91, we complete the local vertex coordinate array with the "new" values. As for the access and exchange table computations discussed above, SCDRC users are supposed to know that, at each iteration step, vertex coordinates have to be exchanged between partitions. However, SCDRC users do not need to know the details of which data have to be exchanged and of how this can be done. They simply call the SCDRC primitives init_access_exch_tables and complete_f. After these calls, all partitions have enough data to compute the areas and the centers of the triangles independently of each other: the loop at lines 92-97 can be done in parallel. This loop is where the computational work is actually done: for each triangle, we compute the triangle area with taa and the triangle center with tca. These results are stored in the loop variables area and center. These are used to increment a and c at lines 95 and 96. At lines 99-100, a and c are divided by the number of iteration thus yielding the average area and triangulation center.

```
135    finalize();
136    return 0;
137  }
```

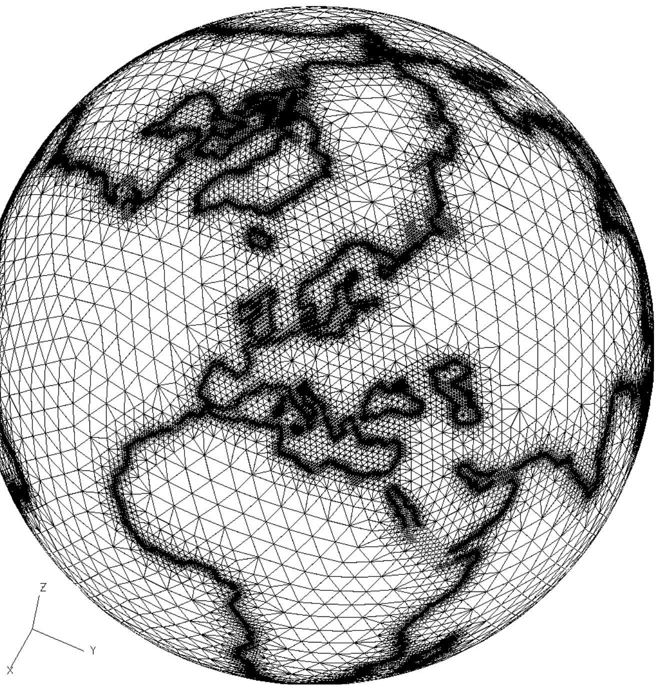


FIGURE 1. Earth surface triangulation

We do not list program lines 101-134. These contain instructions for collecting the partial results on partition zero and for printing global results and are not relevant for the present discussion. The last interesting SCDRC function call is at line 135: here we finalize the SPMD distributed computational environment. From here on, only one copy of the program is left running. We terminate the computation at line 136.

5.2. **Preliminary results.** We have used the center of areas program discussed above to set up a test parallel computation. In spite of its simplicity, the parallel computation of the center of areas is representative in terms of computational complexity for an important set of applications, for example matrix-vector multiplications and approximation of integrals of fluxes in FVMs.

As source data, we used the earth surface triangulation shown in figure 1.

This triangulation has been computed by 8 adaptive refinement steps starting from a simple icosahedron. We have used a version of the red-green local mesh adaptation algorithm developed by D. Hempel and described in [11]. At each step, we have marked for refinement those triangles which are cut by the level set $z = 0$. Here z represents the altitude above or below the mean sea-level. All triangles are *plane* triangles. All vertexes lie in a piecewise bilinear approximation to the earth surface. This is computed with the etopo20 earth surface dataset[17].

The triangulations have been partitioned into 2, 4, 8, 16, 32 and 64 subtriangulations using the SCDRC interface to Metis described in section 2.2.

[17]`http://ferret.wrc.noaa.gov/cgi-bin/dods/nph-dods/data/alh/etopo20.cdf.html`

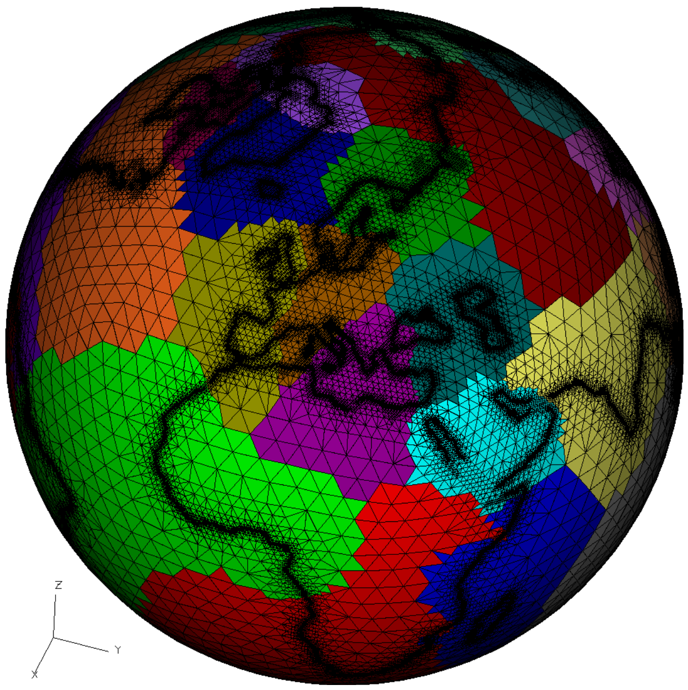


Figure 2. Partitioning of the triangulation into 32 subpartitions.

	2 part.	4 part.	8 part.	16 part.	32 part.	64 part.
total num. triangles	86750	86750	86750	86750	86750	86750
min. triangles per part.	43311	21344	10527	5226	2629	1307
max. triangles per part.	43439	22020	11153	5583	2794	1398
tot. comm. volume	187	406	638	1138	1745	2538
min. comm. volume	77	77	56	53	34	23
max. comm. volume	110	112	92	128	84	65

Table 1. Parallel triangulation center computation metrics.

Figure 2 shows the result of this partitioning into 32 subpartitions and some important metrics associated with different partitionings are summarized in table 1.

In particular, the communication volume for a given partition (table 1) is defined as the number of elements (of the type of the elements of `vx`, `Vector<Real, 3>`) that that partition has to send in a single `complete_f` call.

After `init_access_exch_tables` has been called on a relation-based algorithm, this number and the number of partitions the data have to be sent to (the number of communication peers) can be queried with a SCDRC function.

The computations have been run on an IBM p655 cluster consisting of 30 nodes with 8 Power4 1.1GHz CPUs per node. For computations involving 8 partitions and above, we have used a blocking factor of 8. The blocking factor specifies the way in which processes will be assigned to a node. For a blocking factor of 8, entire nodes

	2 proc.	4 proc.	8 proc.	16 proc.	32 proc.	64 proc.
time (n = 1)	1866	944	485	321	385	784
speedup	1	1.98	3.84	5.81	4.84	2.38
time (n = 10)	1854	919	466	247	144	139
speedup	1	2.01	3.98	7.51	12.88	13.34
time (n = 100)	1890	976	480	241	129	67
speedup	1	1.93	3.94	7.84	14.65	28.21
time (no comm.)	1878	926	458	229	114	57
speedup	1	2.02	4.1	8.2	16.47	32.95

Table 2. Parallel triangulation center computation times.

are reserved for the application. For 2 or 4 tasks and a blocking factor of 2 or 4 respectively, it is guaranteed that the tasks will run on the same node.

Execution times were recorded for several sets of runs and speedup values calculated accordingly. Each run had a fixed number of iterations ($N = 100000$). Speedup is defined here as the ratio between the time taken to run on np processors relative to the time taken with 2 processors. Times have been calculated by calling the MPI_Wtime() function - which returns current wall-clock time - before and after the main execution loop. All processes are synchronized before measurements are taken by calling the MPI_Barrier() function.

We also modified the code to investigate the effect of changing the ratio between computation and communication costs. This was done by changing how often the communication was carried out during a run while keeping the number of computation steps constant. Specifically, this was carried out by changing how often `complete_f` was called inside the main execution loop. Table 2 shows the execution times (in seconds) and speedup values for communication at every step ($n = 1$) and at every 10th ($n = 10$) and 100th ($n = 100$) step and for the case of no communication ($n = 0$).

With the partitioning scheme described above and with no communication, we expect the total run time to halve with each doubling of the number of processors.

Table 2 shows that this is indeed the case. As the frequency of communication increases, and with a greater number of processors, it can be seen that we get much less than this ideal speedup. In the extreme case of 64 processors and communication at every iteration ($n = 1$), the performance is only marginally better than when using just 2 processors.

We will now try to explain the results in table 2 by means of a simple computational cost model. The time taken for a run is the sum of two components, computation time and communication time: $t = t_{comp} + t_{comm}$. As can be seen from table 2 computation time is inversely proportional to the number of processors being used in the no-communication case. We expect this to hold for all communication frequency cases: $t_{comp} = k_1/np$.

The communication time for N iterations is proportional to the number of communication steps, i.e. N/n.

$$t_{comm} = t_1 \cdot \frac{N}{n}$$

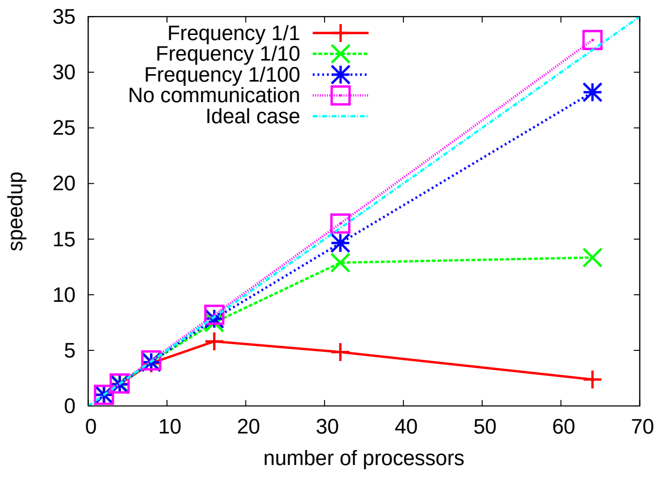


FIGURE 3. Speedup figures with communication at varying frequency

The time for one communication step t_1 depends of course on the amount of data to be communicated. As can be seen from Table 1, this increases with an increasing number of partitions. The relationship between t_1 and np can be estimated as follows:

$$t_1 = c_1 \cdot np \cdot pbs_{np} \tag{13}$$

where pbs_{np} is the average partition boundary size for the case of np partitions. Because the perimeter is proportional to the square root of the surface area:

$$pbs_{np} = c_2 \cdot \sqrt{ps_{np}} \tag{14}$$

As seen from Table 1 we have subdivided the triangulation into roughly equally-sized subtriangulations and therefore

$$ps_{np} = \frac{c_3}{np} \tag{15}$$

From 13, 14 and 15 it follows that

$$t_1 = k_2 \cdot \sqrt{np}$$

with $k_2 = c_1 \cdot c_2 \cdot \sqrt{c_3}$. Thus

$$t = \frac{k_1}{np} + k_2 \cdot \frac{N}{n} \cdot \sqrt{np} \tag{16}$$

This formula can be seen to be similar to the BSP cost model presented in (see [6], section 1.2).

The least-squares method was used determine the parameters k_1 and k_2 from the entire data set in table 2. It can be seen from figure 4 that equation 16 fits well with the observed results for moderate communication frequencies (bottom).

In the case of communication occuring at every step, the fit is rather poorer (figure 4, top left).

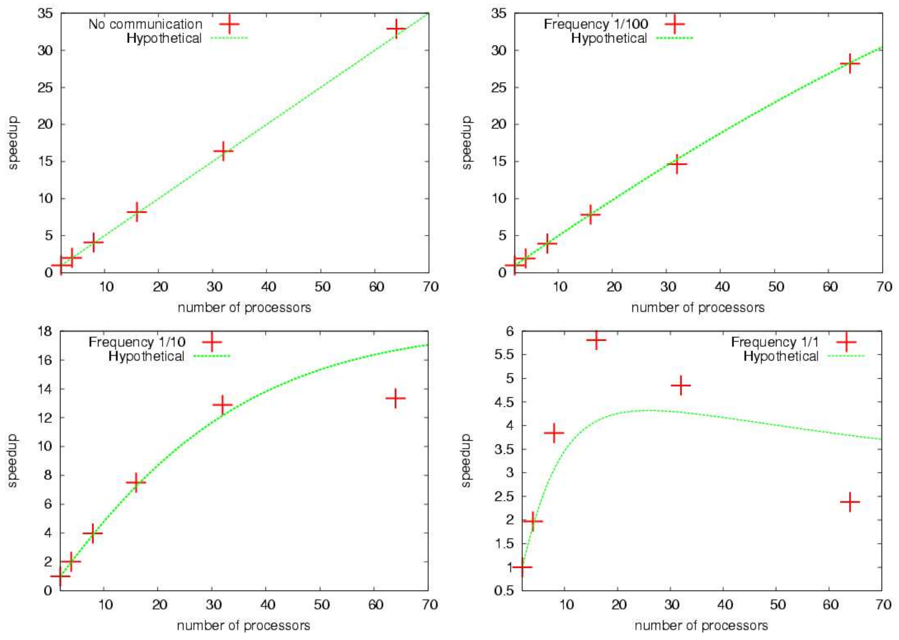


FIGURE 4. Modelling speedup figures

The constants k_1 and k_2 were also determined for each frequency case independently, but there was no improvement in the fit of the curve. This suggests that the relationship between k_2 and np is perhaps not as simple as hypothesized above or that the times taken for computation and communication are not independent of each other. It may be that the high frequency communication has passed some threshold, for example a network buffer is more quickly reaching its maximum capacity when the number of processors is higher.

The experiments showed that it is not necessarily beneficial to increase the number of processors in a parallel computation and therefore it is important, when setting up a parallel computation for a given practical application, to run some preliminary tests to ascertain what a sensible value for np might be. As our experiments show, this will depend dramatically on the computing architecture and the ratio between computation and communication costs.

Despite the limitation of this simple model at high communication frequencies, it can be applied to this preliminary analysis and can guide the design of a parallel application in terms of the number of processors which can be effectively applied to a problem while still achieving a reasonable speedup.

Of course, practical applications might require, at each step of some iterative procedure (e.g. for iteratively solving systems of equations) more or less operations and greater or lesser communication volume than our example. These factors will also play a role in designing the overall structure of a parallel application.

Our model fits well for low numbers of processors at low communication frequencies. Further work would need to be carried out to determine if a greater number of processors at low frequency also display the poor speedup figures we have observed at high frequencies.

5.3. **Outlook.** We have presented a prototype version of SCDRC, a small set of software components for distributed relation-based computations. As explained in the introduction, SCDRC is a thin software layer above message passing libraries and is not meant to be directly used by applications. Applications are expected to use SCDRC indirectly via application dependent components.

The triangulation and geometry components used to write the parallel program for computing the center of a triangulation are simple examples of an application dependent software layer built upon SCDRC. In fact, SCDRC has been written in the framework of a project for developing software components for distributed adaptive finite volume computations[18]. In finite volume computations, relation-based algorithms and relation-based computations play an outstanding role.

Relation-based algorithms and relation-based computations, however, are found in different research areas at the core of many computationally demanding procedures: adaptive stochastic sequential decision processes and Bayesian network inference are two examples.

We plan to use SCDRC to develop prototype application dependent software components for one or more such applications domains. This will provide a natural testbed for our prototype and lead to a stable version of SCDRC, possibly extended with new functionalities for basic relational operations.

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- Metis, `http://www-users.cs.umn.edu/~karypis/metis`.
- ParMetis, `http://www-users.cs.umn.edu/~karypis/metis/parmetis`.
- TVMET, `http://tvmet.sourceforge.net`.
- mpich, `http://www-unix.mcs.anl.gov/mpi/mpich`.
- NetCDF, `http://www.unidata.ucar.edu/software/netcdf`.
- Silo, `http://www.llnl.gov/bdiv/meshtv`.

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