High Performance Multidimensional Scaling for Large High-Dimensional Data Visualization

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Abstract—Technical advancements produces a huge amount of scientific data which are usually in high dimensional formats, and it is getting more important to analyze those large-scale high-dimensional data. Dimension reduction is a well-known approach for high-dimensional data visualization, but can be very time and memory demanding for large problems. Among many dimension reduction methods, multidimensional scaling does not require explicit vector representation but uses pair-wise dissimilarities of data, so that it has a broader applicability than the other algorithms which can handle only vector representation. In this paper, we propose an efficient parallel implementation of a well-known multidimensional scaling algorithm, called SMACOF (Scaling by MAjorizing a COmplicated Function) which is time and memory consuming with a quadratic complexity, via a Message Passing Interface (MPI). We have achieved load balancing in the proposed parallel SMACOF implementation which results in high efficiency. The proposed parallel SMACOF implementation shows the efficient parallel performance through the experimental results, and it increases the computing capacity of the SMACOF algorithm to several hundreds of thousands of data via using a 32-node cluster system.

Index Terms—Multidimensional scaling, Parallelism, Distributed applications, Data visualization.

1 Introduction

Due to the innovative advancements in science and technology, the amount of data to be processed or analyzed is rapidly growing and it is already beyond the capacity of most commodity hardware we are using currently. To keep up with such fast development, study for data-intensive scientific data analyses [1] has been already emerging in recent years. It is a challenge for various computing research communities, such as high-performance computing, database, and machine learning and data mining communities, to learn how to deal with such large and high dimensional data in this data deluged era. Unless developed and implemented carefully to overcome such limits, techniques will face soon the limits of usability. Parallelism is not an optional technology any more but an essential factor for various data mining algorithms, including dimension reduction algorithms, by the result of the enormous size of the data to be dealt by those algorithms (especially since the data size keeps increasing).

Visualization of high-dimensional data in low-dimensional space is an essential tool for exploratory data analysis, when people try to discover meaningful information which is concealed by the inherent complexity of the data, a characteristic which is mainly dependent on the high dimensionality of the data. That is why the dimension reduction algorithms are highly used to do a visualization of high-dimensional data. Among several kinds of dimension reduction algorithms, such as Principle Component Analysis (PCA), Generative Topographic Mapping (GTM) [2], [3], Self-Organizing Map (SOM) [4], Multidimensional Scaling (MDS) [5]–[7], to name a few, we focus on the MDS in our paper due to its wide applicability and theoretical robustness.

The task of visualizing high-dimensional data is getting more difficult and challenged by the huge amount of the given data. In most data analysis with such large and high-dimensional dataset, we have observed that such a task is not only CPU bounded but also memory bounded, in that any single process or machine cannot hold the whole data in its memory any longer. In this paper, we tackle this problem for developing a high performance visualization for large and high-dimensional data analysis by using distributed resources with parallel computation. For this purpose, we will show how we developed a well-known MDS algorithm, which is a useful tool for data visualization, in a distributed fashion so that one can utilize distributed memories and be able to process large and high dimensional datasets.

This paper is an extended version of [8], and this paper shows a slight update of parallel implementation and more experimental analyses in detail. [1] In Section 2, we provide an overview of what the multidimensional scaling (MDS) is, and briefly introduce a well-known MDS algorithm, named SMACOF [9], [10] (Scaling by MAjorizing a COmplicated Function). We explain the details of the proposed parallelized

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version of the SMACOF algorithm, called parallel SMACOF, in Section 3. In the next, we show our performance results of our parallel version of MDS in various compute cluster settings, and we present the results of processing up to 100,000 data points in Section 4 followed by the related work in Section 5. We summarize the conclusion and future works of this paper in Section 6.

2 Multidimensional Scaling (MDS)

Multidimensional scaling (MDS) [5]–[7] is a general term that refers to techniques for constructing a map of generally high-dimensional data into a target dimension (typically a low dimension) with respect to the given pairwise proximity information. Mostly, MDS is used to visualize given high dimensional data or abstract data by generating a configuration of the given data which utilizes Euclidean low-dimensional space, i.e. two-dimension or three-dimension.

Generally, proximity information, which is represented as an $N \times N$ dissimilarity matrix ($\boldsymbol{\Delta} = [\delta_{ij}]$), where N is the number of points (objects) and δ_{ij} is the dissimilarity between point i and j, is given for the MDS problem, and the dissimilarity matrix ($\boldsymbol{\Delta}$) should agree with the following constraints: (1) symmetricity ($\delta_{ij} = \delta_{ji}$), (2) nonnegativity ($\delta_{ij} \geq 0$), and (3) zero diagonal elements ($\delta_{ii} = 0$).

The objective of the MDS technique is to construct a configuration of a given high-dimensional data into low-dimensional Euclidean space, where each distance between a pair of points in the configuration is approximated to the corresponding dissimilarity value as much as possible. The output of MDS algorithms could be represented as an $N \times L$ configuration matrix $\boldsymbol{X}$, whose rows represent each data point x_i ($i = 1, \ldots, N$) in L-dimensional space. It is quite straightforward to compute the Euclidean distance between x_i and x_j in the configuration matrix $\boldsymbol{X}$, i.e. $d_{ij}(\boldsymbol{X}) = \|x_i - x_j\|$, and we are able to evaluate how well the given points are configured in the L-dimensional space by using the suggested objective functions of MDS, called STRESS [11] or SSTRESS [12]. Definitions of STRESS (1) and SSTRESS (2) are following:

$$\sigma(\boldsymbol{X}) = \sum_{i<j\leq N} w_{ij}(d_{ij}(\boldsymbol{X}) - \delta_{ij})^2 \quad (1)$$

$$\sigma^2(\boldsymbol{X}) = \sum_{i<j\leq N} w_{ij}[(d_{ij}(\boldsymbol{X}))^2 - (\delta_{ij})^2]^2 \quad (2)$$

where $1 \leq i < j \leq N$ and w_{ij} is a weight value, so $w_{ij} \geq 0$.

As shown in the STRESS and SSTRESS functions, the MDS problems could be considered to be nonlinear optimization problems, which minimizes the STRESS or the SSTRESS function in the process of configuring an L-dimensional mapping of the high-dimensional data.

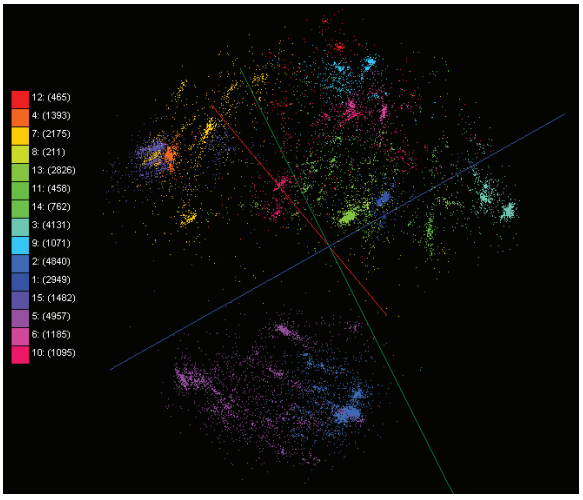


Fig. 1. An example of the data visualization of 30,000 biological sequences by an MDS algorithm, which is colored by a clustering algorithm.

Fig. 1 is an example of the data visualization of 30,000 biological sequence data, which is related to a metagenomics study, by an MDS algorithm, named SMACOF [9], [10] explained in Section 2.1. The colors of the points in Fig. 1 represent the clusters of the data, which is generated by a pairwise clustering algorithm by deterministic annealing [13]. The data visualization in Fig. 1 shows the value of the dimension reduction algorithms which produced lower dimensional mapping for the given data. We can see clearly the clusters without quantifying the quality of the clustering methods statistically.

2.1 SMACOF and its Complexity

There are a lot of different algorithms which could be used to solve the MDS problem, and Scaling by MAjorizing a COmplicated Function (SMACOF) [9], [10] is one of them. SMACOF is an iterative majorization algorithm used to solve the MDS problem with the STRESS criterion. The iterative majorization procedure of the SMACOF could be thought of as an Expectation-Maximization (EM) [14] approach. Although SMACOF has a tendency to find local minima due to its hill-climbing attribute, it is still a powerful method since the algorithm, theoretically, guarantees a decrease in the STRESS (σ) criterion monotonically. Instead of a mathematically detail explanation of the SMACOF algorithm, we illustrate the SMACOF procedure in this section. For the mathematical details of the SMACOF algorithm, please refer to [7].

Alg. 1 illustrates the SMACOF algorithm for the MDS solution. The main procedure of the SMACOF are its iterative matrix multiplications, called the *Guttman transform*, as shown in Line 8 in Alg. 1, where

Algorithm 1 SMACOF algorithm

1: $\boldsymbol{Z} \Leftarrow \boldsymbol{X}^{[0]}$;
2: $k \Leftarrow 0$;
3: $\varepsilon \Leftarrow$ small positive number;
4: $MAX \Leftarrow$ maximum iteration;
5: Compute $\sigma^{[0]} = \sigma(\boldsymbol{X}^{[0]})$;
6: **while** $k = 0$ or ($\Delta\sigma > \varepsilon$ and $k \leq MAX$) **do**
7: $k \Leftarrow k + 1$;
8: $\boldsymbol{X}^{[k]} = \boldsymbol{V}^{\dagger}\boldsymbol{B}(\boldsymbol{X}^{[k-1]})\boldsymbol{X}^{[k-1]}$
9: Compute $\sigma^{[k]} = \sigma(\boldsymbol{X}^{[k]})$
10: $\boldsymbol{Z} \Leftarrow \boldsymbol{X}^{[k]}$;
11: **end while**
12: **return** $\boldsymbol{Z}$;

$\boldsymbol{V}^{\dagger}$ is the Moore-Penrose inverse [15], [16] (or pseudo-inverse) of matrix $\boldsymbol{V}$. The $N \times N$ matrices $\boldsymbol{V}$ and $\boldsymbol{B}(\boldsymbol{Z})$ are defined as follows:

$$\boldsymbol{V} = [v_{ij}] \tag{3}$$

$$v_{ij} = \begin{cases} -w_{ij} & \text{if } i \neq j \\ \sum_{i \neq j} w_{ij} & \text{if } i = j \end{cases} \tag{4}$$

$$\boldsymbol{B}(\boldsymbol{Z}) = [b_{ij}] \tag{5}$$

$$b_{ij} = \begin{cases} -w_{ij}\delta_{ij}/d_{ij}(\boldsymbol{Z}) & \text{if } i \neq j \\ 0 & \text{if } d_{ij}(\boldsymbol{Z}) = 0, i \neq j \\ -\sum_{i \neq j} b_{ij} & \text{if } i = j \end{cases} \tag{6}$$

If the weights are equal to one ($w_{ij} = 1$) for all pairwise dissimilarities, then $\boldsymbol{V}$ and $\boldsymbol{V}^{\dagger}$ are simplified as follows:

$$\boldsymbol{V} = N\left(I - \frac{\boldsymbol{e}\boldsymbol{e}^t}{N}\right) \tag{7}$$

$$\boldsymbol{V}^{\dagger} = \frac{1}{N}\left(I - \frac{\boldsymbol{e}\boldsymbol{e}^t}{N}\right) \tag{8}$$

where $\boldsymbol{e} = (1, \ldots, 1)^t$ is one vector whose length is N. In this paper, we generate mappings based on the equal weights weighting scheme and we use (8) for $\boldsymbol{V}^{\dagger}$.

As in Alg. 1, the computational complexity of the SMACOF algorithm is $\mathcal{O}(N^2)$, since the Guttman transform performs a multiplication of an $N \times N$ matrix and an $N \times L$ matrix twice, typically $N \gg L$ ($L = 2$ or 3), and the computation of the STRESS value, $\boldsymbol{B}(\boldsymbol{X}^{[k]})$, and $\boldsymbol{D}(\boldsymbol{X}^{[k]})$ also take $\mathcal{O}(N^2)$. In addition, the SMACOF algorithm requires $\mathcal{O}(N^2)$ memory because it needs several $N \times N$ matrices, as in Table 1. Due to the trends of digitization, data sizes have increased enormously, so it is critical that we are able to investigate large data sets. However, it is impossible to run SMACOF for a large data set under a typical single node computer due to the memory requirement increases in $\mathcal{O}(N^2)$. In order to remedy the shortage of memory in a single node, we illustrate how to parallelize the SMACOF algorithm via message passing interface (MPI) for utilizing distributed-memory cluster systems in Section 3.

TABLE 1
Main matrices used in SMACOF

Matrix	Size	Description
$\boldsymbol{\Delta}$	$N \times N$	Matrix for the given pairwise dissimilarity $[\delta_{ij}]$
$\boldsymbol{D}(\boldsymbol{X})$	$N \times N$	Matrix for the pairwise Euclidean distance of mappings in target dimension $[d_{ij}]$
$\boldsymbol{V}$	$N \times N$	Matrix defined by the value v_{ij} in (3)
$\boldsymbol{V}^{\dagger}$	$N \times N$	Matrix for pseudo-inverse of $\boldsymbol{V}$
$\boldsymbol{B}(\boldsymbol{Z})$	$N \times N$	Matrix defined by the value b_{ij} in (5)
$\boldsymbol{W}$	$N \times N$	Matrix for the weight of the dissimilarity $[w_{ij}]$
$\boldsymbol{X}^{[k]}$	$N \times L$	Matrix for current L-dimensional configuration of N data points $\boldsymbol{x}_i^{[k]}(i = 1, \ldots, N)$
$\boldsymbol{X}^{[k-1]}$	$N \times L$	Matrix for previous L-dimensional configuration of N data points $\boldsymbol{x}_i^{[k-1]}(i = 1, \ldots, N)$

3 High Performance Multidimensional Scaling

We have observed that processing a very large dataset is not only a *cpu-bounded* but also a *memory-bounded* computation, in that memory consumption is beyond the ability of a single process or even a single machine, and that it will take an unacceptable running time to run a large data set even if the required memory is available in a single machine. Thus, running machine learning algorithms to process a large dataset, including MDS discussed in this paper, in a distributed fashion is crucial so that we can utilize multiple processes and distributed resources to handle very large data. The memory shortage problem becomes more obvious if the running OS is 32-bit which can handle at most 4GB virtual memory per process. To process large data with efficiency, we have developed a parallel version of the MDS by using a Message Passing Interface (MPI) fashion. In the following, we will discuss more details on how we decompose data used by the MDS algorithm to fit in the memory limit of a single process or machine. We will also discuss how to implement an MDS algorithm, called SMACOF, by using MPI primitives to get some computational benefits of parallel computing.

3.1 Parallel SMACOF

Table 1 describes frequently used matrices in the SMACOF algorithm. As shown in Table 1, the memory requirement of the SMACOF algorithm increases quadratically as N increases. For the small dataset, memory would not be any problem. However, it turns out to be a critical problem when we deal with a

large data set, such as hundreds of thousands or even millions. For instance, if $N = 10,000$, then one $N \times N$ matrix of 8-byte double-precision numbers consumes 800 MB of main memory, and if $N = 100,000$, then one $N \times N$ matrix uses 80 GB of main memory. To make matters worse, the SMACOF algorithm generally needs six $N \times N$ matrices as described in Table 1, so at least 480 GB of memory is required to run SMACOF with 100,000 data points without considering two $N \times L$ configuration matrices in Table 1 and some required temporary buffers.

If the weight is uniform ($w_{ij} = 1, \forall i, j$), we can use only four constants for representing $N \times N$ $\boldsymbol{V}$ and $\boldsymbol{V}^\dagger$ matrices in order to saving memory space. We, however, still need at least three $N \times N$ matrices, i.e. $\boldsymbol{D}(\boldsymbol{X})$, $\boldsymbol{\Delta}$, and $\boldsymbol{B}(\boldsymbol{X})$, which requires 240 GB memory for the above case, which is still an unfeasible amount of memory for a typical computer. That is why we have to implement a parallel version of SMACOF with MPI.

To parallelize SMACOF, it is essential to ensure load balanced data decomposition as much as possible. Load balance is important not only for memory distribution but also for computational distribution, since parallelization implicitly benefits computation as well as memory distribution, due to less computing per process. One simple approach of data decomposition is that we assume $p = n^2$, where p is the number of processes and n is an integer. Though it is a relatively less complicated decomposition than others, one major problem of this approach is that it is a quite strict constraint to utilize available computing processors (or cores). In order to release that constraint, we decompose an $N \times N$ matrix to $m \times n$ block decomposition, where m is the number of block rows and n is the number of block columns, and the only constraint of the decomposition is $m \times n = p$, where $1 \leq m, n \leq p$. Thus, each process requires only approximately $1/p$ of the full memory requirements of SMACOF algorithm. Fig. 2 illustrates how we decompose each $N \times N$ matrix with 6 processes and $m = 2, n = 3$. Without a loss of generality, we assume $N\%m = N\%n = 0$ in Fig. 2.

A process $P_k, 0 \leq k < p$ (sometimes, we will use P_{ij} for matching M_{ij}) is assigned to one rectangular block M_{ij} with respect to the simple block assignment equation in (9):

$$k = i \times n + j \tag{9}$$

where $0 \leq i < m, 0 \leq j < n$. For $N \times N$ matrices, such as $\boldsymbol{\Delta}, \boldsymbol{V}^\dagger, \boldsymbol{B}(\boldsymbol{X}^{[k]})$, and so on, each block M_{ij} is assigned to the corresponding process P_{ij}, and for $\boldsymbol{X}^{[k]}$ and $\boldsymbol{X}^{[k-1]}$ matrices, $N \times L$ matrices where L is the target dimension, each process has a full $N \times L$ matrix because these matrices have a relatively smaller size, and this results in reducing the number of additional message passing routine calls. By scattering decomposed blocks throughout the distributed memory, we are now able to run SMACOF with as huge a data set as the distributed memory will allow, via paying the cost of message passing overheads and a complicated implementation.

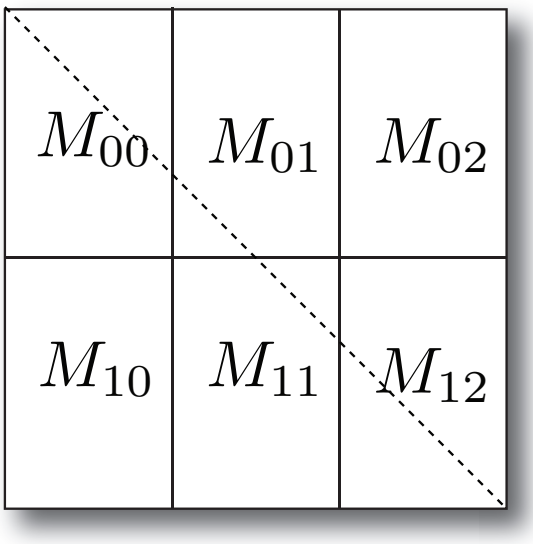


Fig. 2. An example of an $N \times N$ matrix decomposition of parallel SMACOF with 6 processes and 2×3 block decomposition. Dashed line represents where diagonal elements are.

Algorithm 2 Pseudo-code for block row and column assignment for each process for high load balance.

```
Input: pNum, N, myRank
1: if N%pNum = 0 then
2:    nRows = N / pNum;
3: else
4:    if myRank ≥ (N%pNum) then
5:       nRows = N / pNum;
6:    else
7:       nRows = N / pNum + 1;
8:    end if
9: end if
10: return nRows;
```

Although we assume $N\%m = N\%n = 0$ in Fig. 2, there is always the possibility that $N\%m \neq 0$ or $N\%n \neq 0$. In order to achieve a high load balance under the $N\%m \neq 0$ or $N\%n \neq 0$ cases, we use a simple `modular` operation to allocate blocks to each process with at most ONE row or column difference between them. The block assignment algorithm is illustrated in Alg. 2.

At the iteration k in Alg. 1, the application should acquire up-to-date information of the following matrices: $\boldsymbol{\Delta}$, $\boldsymbol{V}^\dagger$, $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$, $\boldsymbol{X}^{[k-1]}$, and $\sigma^{[k]}$, to implement Line 8 and Line 9 in Alg. 1. One good feature of the SMACOF algorithm is that some of matrices are invariable, i.e. $\boldsymbol{\Delta}$ and $\boldsymbol{V}^\dagger$, through the iteration. On

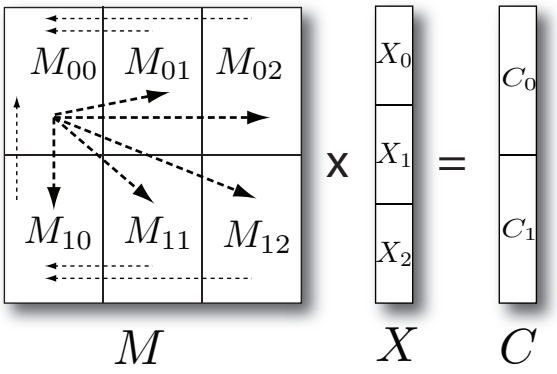


Fig. 3. Parallel matrix multiplication of $N \times N$ matrix and $N \times L$ matrix based on the decomposition of Fig. 2

the other hand, $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$ and STRESS ($\sigma^{[k]}$) value keep changing at each iteration, since $\boldsymbol{X}^{[k-1]}$ and $\boldsymbol{X}^{[k]}$ are changed in every iteration. In addition, in order to update $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$ and the STRESS ($\sigma^{[k]}$) value in each iteration, we have to take the $N \times N$ matrices' information into account, so that related processes should communicate via MPI primitives to obtain the necessary information. Therefore, it is necessary to design message passing schemes to do parallelization for calculating the $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$ and STRESS ($\sigma^{[k]}$) values as well as the parallel matrix multiplication in Line 8 in Alg. 1.

Computing the STRESS (Eq. (10)) can be implemented simply by a partial error sum of $\boldsymbol{D}_{ij}$ and $\boldsymbol{\Delta}_{ij}$ followed by an `MPI_Allreduce`:

$$\sigma(\boldsymbol{X}) = \sum_{i<j\leq N} w_{ij}(d_{ij}(\boldsymbol{X}) - \delta_{ij})^2 \qquad (10)$$

where $1 \leq i < j \leq N$ and w_{ij} is a weight value, so $w_{ij} \geq 0$. On the other hand, calculation of $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$, as shown at Eq. (5), and parallel matrix multiplication are not simple, especially for the case of $m \neq n$.

Fig. 3 depicts how parallel matrix multiplication applies between an $N \times N$ matrix $\boldsymbol{M}$ and an $N \times L$ matrix $\boldsymbol{X}$. Parallel matrix multiplication for SMACOF algorithm is implemented in a three-step process of message communication via MPI primitives. Block matrix multiplication of Fig. 3 for acquiring C_i ($i = 0, 1$) can be written as follows:

$$C_i = \sum_{0\leq j<3} M_{ij} \cdot X_j. \qquad (11)$$

Since M_{ij} of $N \times N$ matrix is accessed only by the corresponding process P_{ij}, computing $M_{ij} \cdot X_j$ part is done by P_{ij}. Each computed sub-matrix by P_{ij}, which is $\frac{N}{2} \times L$ matrix for Fig. 3, is sent to the process assigned M_{i0}, and the process assigned M_{i0}, say P_{i0}, sums the received sub-matrices to generate C_i by one collective MPI primitive call, such as `MPI_Reduce` with the `Addition` operation. Then P_{i0} sends C_i block to P_{00} by one collective MPI call, named

Algorithm 3 Pseudo-code for distributed parallel matrix multiplication in parallel SMACOF algorithm

Input: $\boldsymbol{M}_{ij}, \boldsymbol{X}$

1: /* $m =$ `Row Blocks`, $n =$ `Column Blocks` */
2: /* $i =$ `Rank-In-Row`, $j =$ `Rank-In-Column` */
3: /* $rowComm_i$: `Row Communicator` of row i, $rowComm_i \in P_{i0}, P_{i1}, P_{i2}, \ldots, P_{i(n-1)}$ */
4: /* $colComm_0$: `Column Communicator` of column 0, $colComm_0 \in P_{i0}$ where $0 \leq i < n$ */
5: $\boldsymbol{T}_{ij} = \boldsymbol{M}_{ij} \cdot \boldsymbol{X}_j$
6: **if** $j \neq 0$ **then**
7: /* Assume `MPI_Reduce` is defined as `MPI_Reduce(data, operation, root)` */
8: Send $\boldsymbol{T}_{ij}$ to P_{i0} by calling `MPI_Reduce` ($\boldsymbol{T}_{ij}$, `Addition`, P_{i0}).
9: **else**
10: Generate $\boldsymbol{C}_i$ = `MPI_Reduce` ($\boldsymbol{T}_{i0}$, `Addition`, P_{i0}).
11: **end if**
12: **if** $i == 0$ and $j == 0$ **then**
13: /* Assume `MPI_Gather` is defined as `MPI_Gather(data, root)` */
14: Gather $\boldsymbol{C}_i$ where $i = 0, \ldots, m-1$ by calling `MPI_Gather` (C_0, P_{00})
15: Combine $\boldsymbol{C}$ with $\boldsymbol{C}_i$ where $0 \leq i < m$
16: Broadcast $\boldsymbol{C}$ to all processes
17: **else if** $j == 0$ **then**
18: Send $\boldsymbol{C}_i$ to P_{00} by calling `MPI_Gather`(C_i, P_{00})
19: Receive $\boldsymbol{C}$ Broadcasted by P_{00}
20: **else**
21: Receive $\boldsymbol{C}$ Broadcasted by P_{00}
22: **end if**

`MPI_Gather`, as well. Note that we are able to use `MPI_Reduce` and `MPI_Gather` instead of `MPI_Send` and `MPI_Receive` by establishing row- and column-communicators for each process P_{ij}. `MPI_Reduce` is called under an established row-communicator, say $rowComm_i$ which is constructed by P_{ij} where $0 \leq j < n$, and `MPI_Gather` is called under defined column-communicator of P_{i0}, say $colComm_0$ whose members are P_{i0} where $0 \leq i < m$. Finally, P_{00} combines the gathered sub-matrix blocks C_i, where $0 \leq i < m$, to construct $N \times L$ matrix $\boldsymbol{C}$, and broadcasts it to all other processes by `MPI_Broadcast` call.

Each arrow in Fig. 3 represents message passing direction. Thin dashed arrow lines describes message passing of $\frac{N}{2} \times L$ sub-matrices by either `MPI_Reduce` or `MPI_Gather`, and message passing of matrix $\boldsymbol{C}$ by `MPI_Broadcast` is represented by thick dashed arrow lines. The pseudo code for parallel matrix multiplication in SMACOF algorithm is in Alg. 3

For the purpose of computing $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$ in parallel, whose elements b_{ij} is defined in (6), the message passing mechanism in Fig. 4 should be applied under

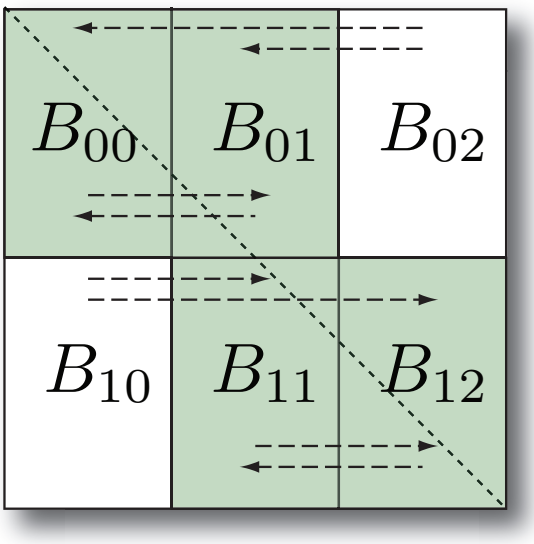


Fig. 4. Calculation of $\boldsymbol{B}(\boldsymbol{X}^{[k-1]})$ matrix with regard to the decomposition of Fig. 2.

a 2×3 block decomposition, as in Fig. 2. Since $b_{ss} = -\sum_{s \neq j} b_{sj}$, a process P_{ij} assigned to $\boldsymbol{B}_{ij}$ should communicate a vector $\boldsymbol{s}_{ij}$, whose element is the sum of corresponding rows, with processes assigned sub-matrix of the same block-row P_{ik}, where $k = 0, \ldots, n-1$, unless the number of column blocks is 1 ($n == 1$). In Fig. 4, the diagonal dashed line indicates the diagonal elements, and the green colored blocks are diagonal blocks for each block-row. Note that the definition of *diagonal blocks* is a block which contains at least one diagonal element of the matrix $\boldsymbol{B}(\boldsymbol{X}^{[k]})$. Also, dashed arrow lines illustrate the message passing direction. The same as in parallel matrix multiplication, we use a collective call, i.e. `MPI_Allreduce` of row-communicator with `Addition` operation, to calculate row sums for the diagonal values of $\boldsymbol{B}$ instead of using pairwise communicate routines, such as `MPI_Send` and `MPI_Receive`. Alg. 4 shows the pseudo-code of computing sub-block B_{ij} in process P_{ij} with MPI primitives.

Algorithm 4 Pseudo-code for calculating assigned sub-matrix $\boldsymbol{B}_{ij}$ defined in (6) for distributed-memory decomposition in parallel SMACOF algorithm

Input: $\boldsymbol{M}_{ij}, \boldsymbol{X}$

```
/* m = Row Blocks, n = Column Blocks */
/* i = Rank-In-Row, j = Rank-In-Column */
/* We assume that sub-matrix B_ij is assigned to process P_ij */
Find diagonal blocks in the same row (row i)
if B_ij ∉ diagonal blocks then
    compute elements b_st of B_ij
    Send a vector s_ij, whose element is the sum of corresponding rows, to P_ik, where B_ik ∈ diagonal blocks. For simple and efficient implementation, we use MPI_Allreduce call for this.
else
    compute elements b_st of B_ij, where s ≠ t
    Receive a vector s_ik, whose element is the sum of corresponding rows, where k = 1,...,n from other processes in the same block-row, and sum them to compute a row-sum vector by MPI_Allreduce call.
    Compute b_ss elements based on the row sums.
end if
```

4 Performance Analysis of the Parallel SMACOF

For the performance analysis of parallel SMACOF discussed in this paper, we have applied our parallel SMACOF algorithm for high-dimensional data visualization in low-dimension to the dataset obtained from the PubChem database[2], which is an NIH-funded repository for over 60 million chemical molecules. It provides their chemical structure fingerprints and biological activities, for the purpose of chemical information mining and exploration. Among 60 Million PubChem dataset, in this paper we have used 100,000 randomly selected chemical subsets and all of them have a 166-long binary value as a fingerprint, which corresponds to the properties of the chemical compounds data.

In the following, we will show the performance results of our parallel SMACOF implementation with respect to 6,400, 12,800, 50,000 and 100,000 data points having 166 dimensions, represented as 6400, 12800, 50K, and 100K datasets, respectively.

In addition to the PubChem dataset, we also use a biological sequence dataset for our performance test. The biological sequence dataset contains 30,000 biological sequence data with respect to the metagenomics study based on pairwise distance matrix. Using these data as inputs, we have performed our experiments on our two decent compute clusters as summarized in Table 2.

Since we focus on analyzing the parallel performance of the parallel SMACOF implementation but not mapping quality in this paper, every experiment in this paper is finished after 100 iterations without regard to the stop condition. In this way, we can measure parallel runtime performance with the same number of iterations for each data with different experimental environments.

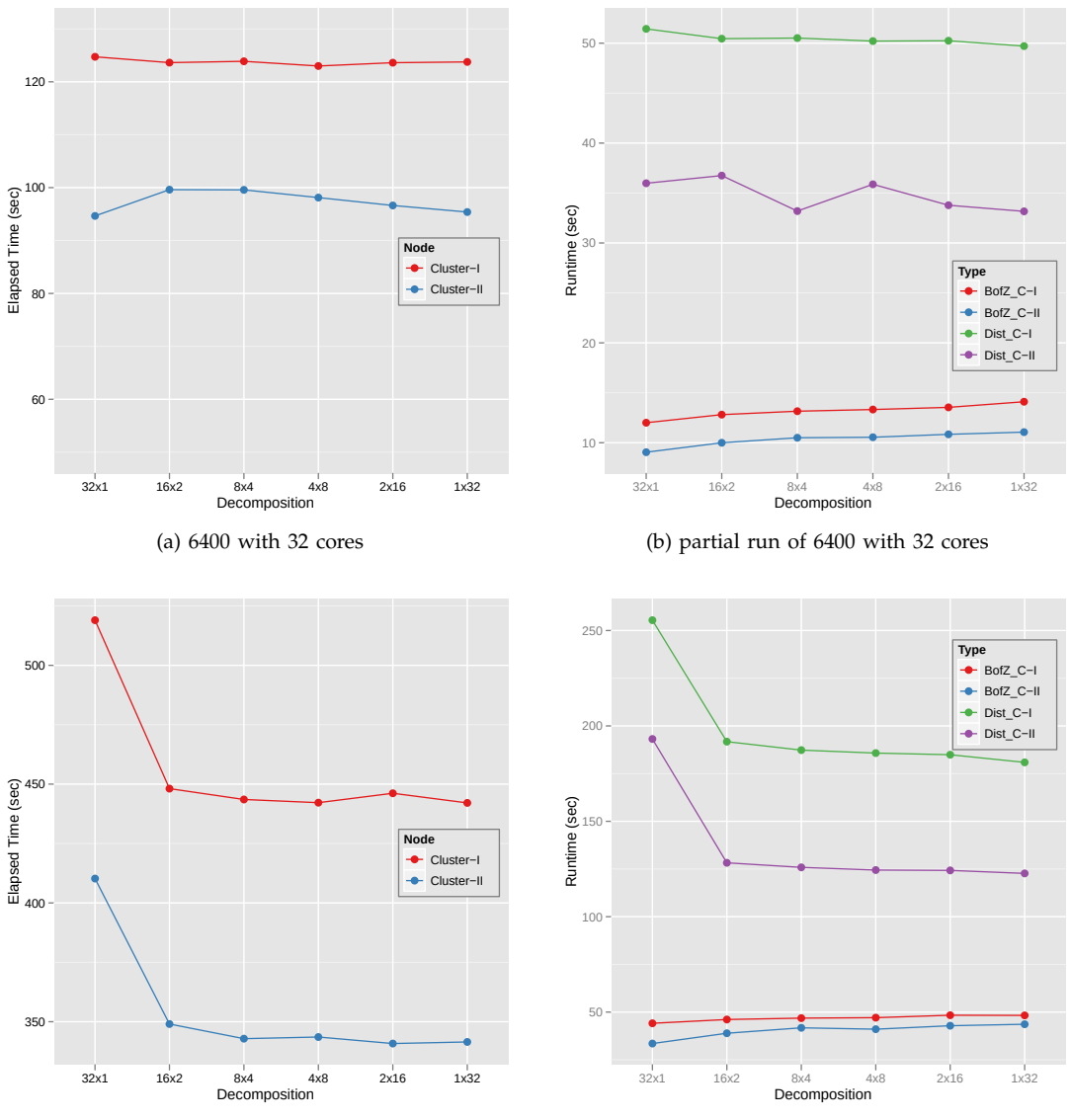
4.1 Performance Analysis of the Block Decomposition

Figure 5-(a) and (c) show the overall elapsed time comparisons for the 6400 and 12800 PubChem data

2. PubChem,http://pubchem.ncbi.nlm.nih.gov/

TABLE 2
Cluster systems used for the performance analysis

Features	Cluster-I	Cluster-II
# Nodes	8	32
CPU	AMD Opteron 8356 2.3GHz	Intel Xeon E7450 2.4 GHz
# CPU / # Cores per node	4 / 16	4 / 24
Total Cores	128	768
L1 (data) Cache per core	64 KB	32 KB
L2 Cache per core	512 KB	1.5 MB
Memory per node	16 GB	48 GB
Network	Giga bit Ethernet	20 Gbps Infiniband
Operating System	Windows Server 2008 HPC Edition (Service Pack 2) - 64 bit	Windows Server 2008 HPC Edition (Service Pack 2) - 64 bit



(a) 6400 with 32 cores

(b) partial run of 6400 with 32 cores

(c) 12800 with 32 cores

(d) partial run of 12800 with 32 cores

Fig. 5. Overall Runtime and partial runtime of parallel SMACOF for 6400 and 12800 PubChem data with 32 cores in Cluster-I and Cluster-II w.r.t. data decomposition of $N \times N$ matrices.

sets with respect to how to decompose the given $N \times N$ matrices with 32 cores in Cluster-I and Cluster-II. Also, Fig. 5-(b) and (d) illustrate the partial runtime related to the calculation of $\boldsymbol{B}(\boldsymbol{X})$ and the calculation

of $\boldsymbol{D}(\boldsymbol{X})$ of 6400 and 12800 PubChem data sets. An interesting characteristic of Fig. 5-(a) and (c) is that matrix data decomposition does not much affect the execution runtime for a small data set (here 6400 points, in Fig. 5-(a)), but for a large data set (here 12800 points, in Fig. 5-(c)), row-based decomposition, such as $p \times 1$, is severely worse in performance compared to other data decompositions. Fig. 5-(c) and (d) describe that the overall performance with respect to data decomposition is highly connected to the calculation of the distance matrix runtime.

Also, Fig. 6-(a) and (c) show the overall elapsed time comparisons for the 6400 and 12800 PubChem data sets with respect to how to decompose the given $N \times N$ matrices with 64 cores in Cluster-I and Cluster-II. Fig. 6-(b) and (d) illustrate the partial runtimes related to the calculation of $\boldsymbol{B}(\boldsymbol{X})$ and the calculation of $\boldsymbol{D}(\boldsymbol{X})$ of 6400 and 12800 PubChem data sets, the same as Fig. 5. Similar to Fig. 5, the data decomposition does not make a substantial difference in the overall runtime of the parallel SMACOF with a small data set. However, row-based decomposition, in this case a 64×1 block decomposition, takes much longer for running time than the other decompositions, when we run the parallel SMACOF with the 12800 points data set. If we compare Fig. 6-(c) with Fig. 6-(d), we can easily find that the overall performance with respect to data decomposition is mostly affected by the calculation of the distance matrix runtime for the 64 core experiment.

The performance of overall elapsed time and partial runtimes of the 6400 and 12800 Pubchem data sets based on different decompositions of the given $N \times N$ matrices with 128 cores are experimented in only the Cluster-II system in Table 2. Those performance plots are shown in Fig. 7. As shown in Fig. 5 and Fig. 6, the data decomposition does not have a considerable impact on the performance of the parallel SMACOF with a small data set but it does have a significant influence on that performance with a larger data set.

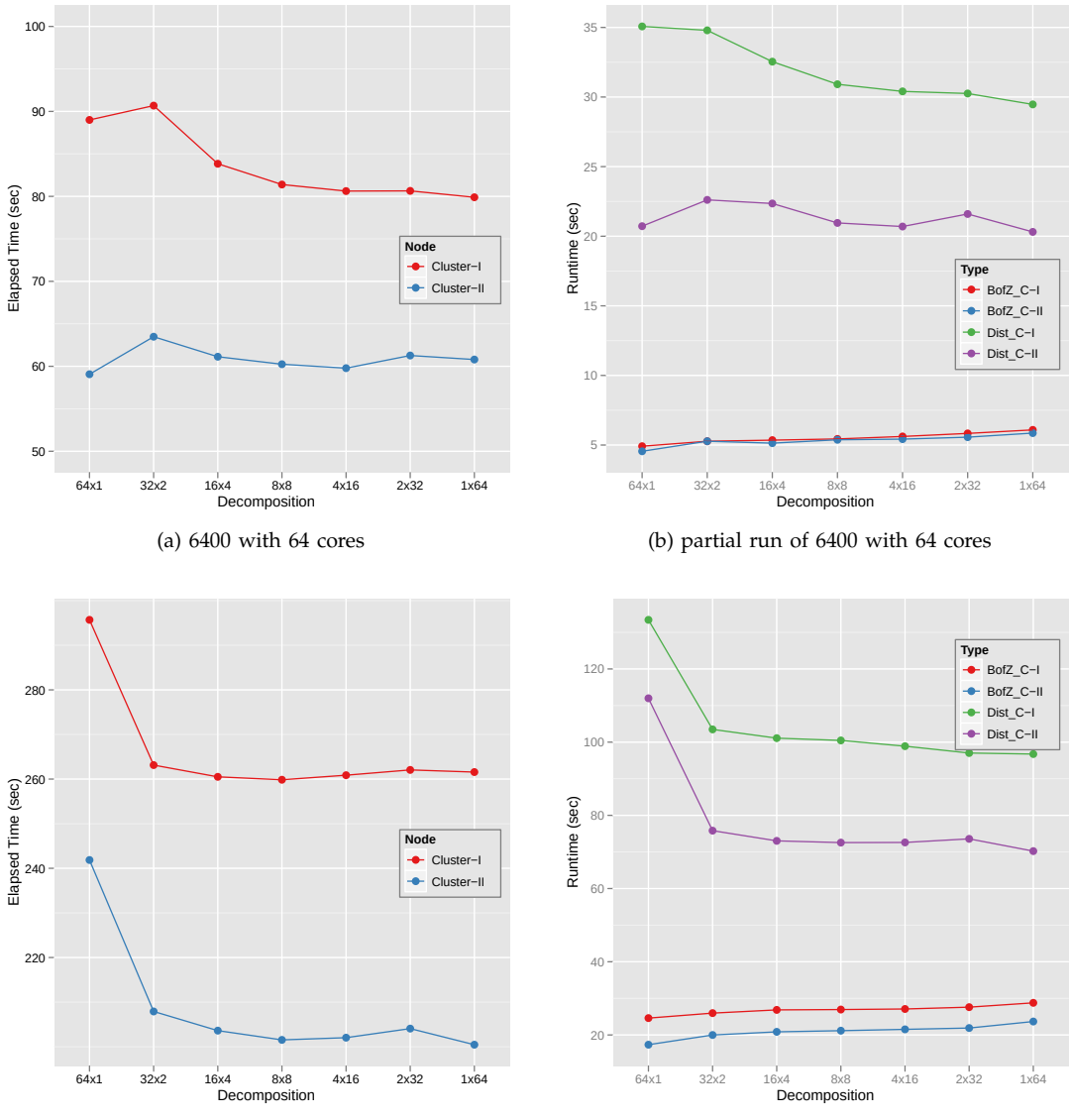
The main reason for the above data decomposition experimental results is the cache line effect that affects cache reusability, and generally balanced block decomposition shows better cache reusability so that it occurs with less cache misses than the skewed decompositions [17], [18]. In the parallel implementation of the SMACOF algorithm, two main components actually access data multiple times so that will be affected by cache reusability. One is the $[N \times N] \cdot [N \times D]$ matrix multiplication part. Since we implement the matrix multiplication part based on the block matrix multiplication method with a 64×64 block for the purpose of better cache utilization, the runtime of matrix multiplication parts is almost the same without regard to data decomposition.

However, the distance matrix updating part is a tricky part. Since each entry of the distance matrix is accessed only once whenever the matrix is updated, it is not easy to think about the entries reusability. Although each entry of the distance matrix is accessed only once per each update, the new mapping points are accessed multiple times for calculation of the distance matrix. In addition, we update the distance matrix row-based direction for better locality. Thus, it is better for the number of columns to be small enough so that the coordinate values of each accessed mapping points for updating the assigned distance sub-matrix remain in the cache memory as much as necessary.

Fig. 5-(b),(d) through Fig. 7-(b),(d) illustrate the cache reusability effect on 6400 points data and 12800 points data. For instance, for the row-based decomposition case, $p \times 1$ decomposition, each process is assigned an $N/p \times N$ block, i.e. 100×6400 data block for the cases of $N = 6400$ and $p = 64$. When $N = 6400$, the runtime of the distance matrix calculation part does not make much difference with respect to the data decomposition. We might consider that, if the number of columns of the assigned block is less than or equal to 6400, then cache utilization is no more harmful for the performance of the distance matrix calculation part of the parallel SMACOF. On the other hand, when $N = 12800$ which is doubled, the runtime of the distance matrix calculation part of row-based decomposition ($p \times 1$), and which is assigned a $12800/p \times 12800$ data block for each process, is much worse than the other data decomposition cases, as in sub-figure (d) of Fig. 5 - Fig. 7. For the other decomposition cases, such as $p/2 \times 2$ through $1 \times p$ data decomposition cases, the number of columns of the assigned block is less than or equal to 6400, when $N = 12800$, and the runtime performance of distance matrix calculation part of those cases are similar to each other and much less than the row-based data decomposition.

We have also investigated the runtime of the $\boldsymbol{B}(\boldsymbol{X})$ calculation, since the message passing mechanism for computing $\boldsymbol{B}(\boldsymbol{X})$ is different based on data decomposition. Since the diagonal elements of $\boldsymbol{B}(\boldsymbol{X})$ are the negative sum of elements in the corresponding rows, it is required to call `MPI_Allreduce` or `MPI_Reduce` MPI APIs for each row-communicator. Thus, the less number of column blocks means faster (or less MPI overhead) processes in computing $\boldsymbol{B}(\boldsymbol{X})$, and even the row-based decomposition case does not need to call the MPI API for calculating $\boldsymbol{B}(\boldsymbol{X})$. The effect of the different message passing mechanisms of $\boldsymbol{B}(\boldsymbol{X})$ in regard to data decomposition is shown in sub-figure (b) and (d) of Fig. 5 through Fig. 7.

In terms of a system comparison between the two test systems in Table 2, Cluster-II performs better than Cluster-I in Fig. 5 through Fig. 7, although the clock speeds of the cores are similar to each other. There are two different factors between Cluster-I and Cluster-II in Table 2. We believe that those factors result in Cluster-II outperforming Cluster-I, i.e. L2 cache size



(a) 6400 with 64 cores

(b) partial run of 6400 with 64 cores

(c) 12800 with 64 cores

(d) partial run of 12800 with 64 cores

Fig. 6. Overall Runtime and partial runtime of parallel SMACOF for 6400 and 12800 PubChem data with 64 cores in Cluster-I and Cluster-II w.r.t. data decomposition of $N \times N$ matrices.

and Networks. The L2 cache size per core is 3 times bigger in Cluster-II than in Cluster-I, and Cluster-II is connected by 20Gbps Infiniband but Cluster-I is connected via 1Gbps Ethernet. Since SMACOF with large data is a memory-bound application, it is natural that the bigger cache size results in the faster running time.

4.2 Performance Analysis of the Efficiency and Scalability

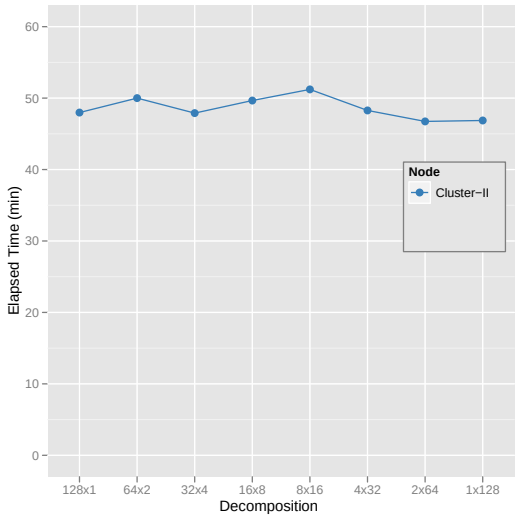
In addition to data decomposition experiments, we measured the parallel scalability of parallel SMACOF in terms of the number of processes p. We investigated the scalability of parallel SMACOF by running with different number of processes, e.g. $p = 64$, 128, 192, and 256. On the basis of the above data decomposition experimental results, the balanced decomposition has been applied to this process scaling experiments. As p increases, the elapsed time should decrease, but linear performance improvement could not be achieved due to the parallel overhead.

We make use of the parallel efficiency value with respect to the number of parallel units for the purpose of measuriing scalability. Eq. (12) and Eq. (13) are the equations of overhead and efficiency calculations:

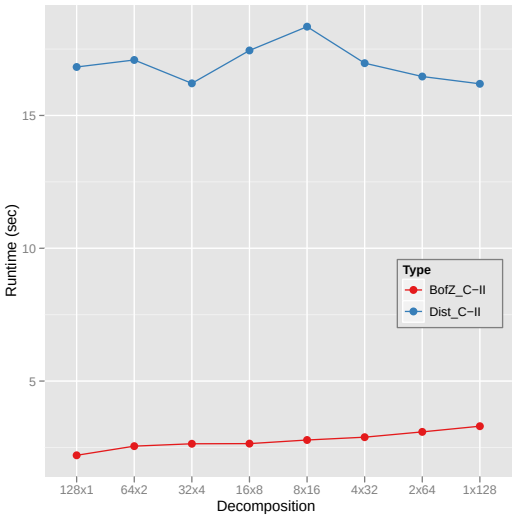
$$f = \frac{pT(p) - T(1)}{T(1)} \tag{12}$$

$$\varepsilon = \frac{1}{1+f} = \frac{T(1)}{pT(p)} \tag{13}$$

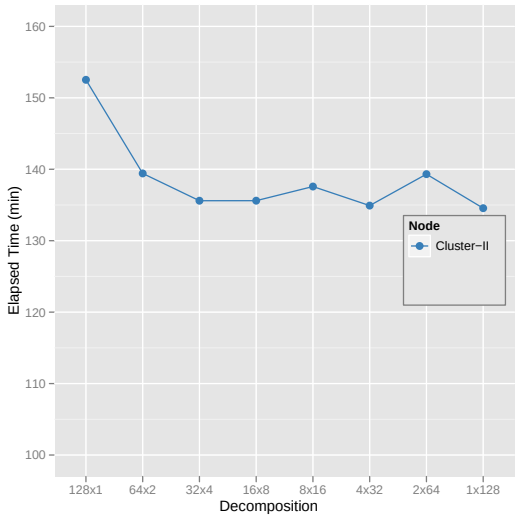
where p is the number of parallel units, $T(p)$ is the



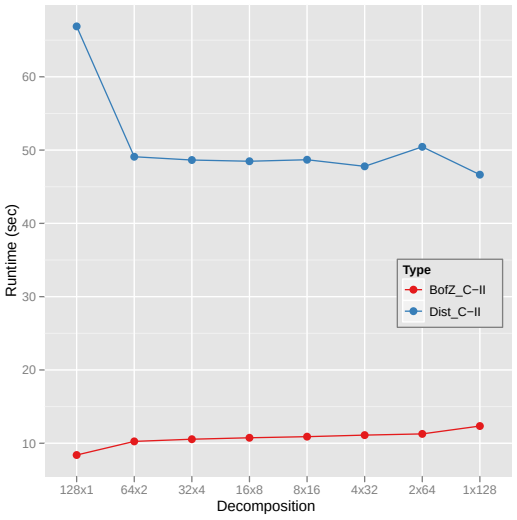
(a) 6400 with 128 cores



(b) partial run of 6400 with 128 cores



(c) 12800 with 128 cores



(d) partial run of 12800 with 128 cores

Fig. 7. Overall Runtime and partial runtime of parallel SMACOF for 6400 and 12800 PubChem data with 128 cores in Cluster-II w.r.t. data decomposition of $N \times N$ matrices.

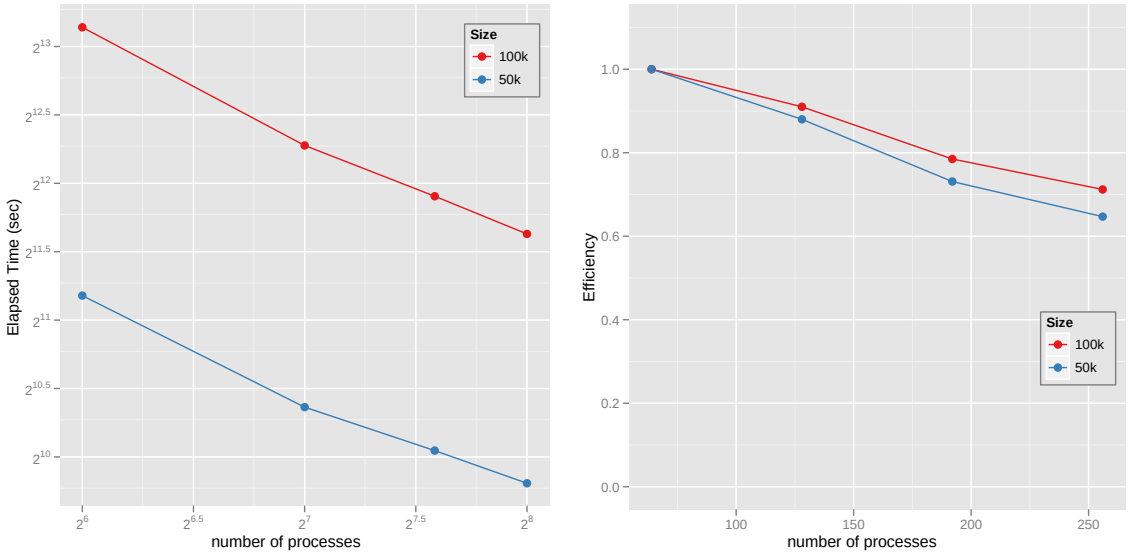
running time with p parallel units, and $T(1)$ is the sequential running time. In practice, Eq. (12) and Eq. (13) can be replaced with Eq. (14) and Eq. (15) as follows:

$$f = \frac{\alpha T(p_1) - T(p_2)}{T(p_2)} \tag{14}$$

$$\varepsilon = \frac{1}{1+f} = \frac{T(p_2)}{\alpha T(p_1)} \tag{15}$$

where $\alpha = p_1/p_2$ and p_2 is the smallest number of used cores for the experiment, so $\alpha \geq 1$. We use Eq. (14) and Eq. (15) in order to calculate the overhead and corresponding efficiency, since it is impossible to run in a single machine for 50k and 100k data sets. Note that we used 16 computing nodes in Cluster-II (total memory size in 16 computing nodes is 768 GB) to perform the scaling experiment with a large data set, i.e. 50k and 100k PubChem data, since the SMACOF algorithm requires 480 GB memory for dealing with 100k data points, as we disscussed in Section 3.1, and Cluster-II can only perform that with more than 10 nodes.

The elapsed time of the parallel SMACOF with two large data sets, 50k and 100k, is shown in Fig. 8-(a), and the corresponding relative efficiency of Fig. 8-(a) is shown in Fig. 8-(b). Note that both coordinates are log-scaled, in Fig. 8-(a). As shown in Fig. 8-(a), the parallel SMACOF achieved performance improvement as the number of parallel units (p) increases. However, the performance enhancement ratio (a.k.a. efficiency) is reduced as p increases, which is demonstrated



(a) large data runtime (b) large data efficiency

Fig. 8. Performance of parallel SMACOF for 50K and 100K PubChem data in Cluster-II w.r.t. the number of processes, i.e. 64, 128, 192, and 256 processes (cores). (a) shows runtime and efficiency is shown at (b). We choose balanced decomposition as much as possible, i.e. 8×8 for 64 processes. Note that both x and y axes are log-scaled for (a).

in Fig. 8-(b). A reason for reducing efficiency is that the ratio of the message passing overhead over the assigned computation per each process is increased due to more message overhead and less computing portion per process as p increases, as shown in Table 3. Another reason for efficiency decrease is the memory bandwidth effect, since we used a fixed number of nodes (16 nodes) for the experiments with the large data sets, due to large memory requirement for large data sets, and have increased the used number of cores per node to increase the parallel units.

Table 3 is the result of the runtime analysis of the parallel matrix multiplication part of the proposed parallel SMACOF implementation which detached the time of the pure block matrix multiplication computation part and the time of the MPI message passing overhead part for parallel matrix multiplication, from the overall runtime of the parallel matrix multiplication part of the parallel SMACOF implementation. Note that **#Procs**, **tMatMult**, **tMM_Computing**, and **tMM_Overhead** represent the number of processes (parallel units), the overall runtime of the parallel matrix multiplication part, the time of the pure block matrix multiplication computation part, and the time of the MPI message passing overhead part for parallel matrix multiplication, respectively.

Theoretically, the **tMM_Computing** portion should be negatively linear with respect to the number of parallel units, if the number of points is the same and the load balance is achieved. Also, the **tMM_Overhead** portion should be increased as the number of parallel units is increased, if the number of points is the same. More specifically, if `MPI_Bcast` is implemented as one of the classical algorithms, such as a binomial tree or a binary tree algorithm [19], in MPI.NET library, then the **tMM_Overhead** portion will follow somewhat $\mathcal{O}(\lceil \lg p \rceil)$ with respect to the number of parallel units (p), since the `MPI_Bcast` routine in Alg. 3 could be the most time consuming MPI method among the MPI routines of parallel matrix multiplication due in part to the large message size and the maximum number of communication participants.

Fig. 9 illustrates the efficiency (calculated by Eq. (15)) of **tMatMult** and **tMM_Computing** in Table 3 with respect to the number of processes. As shown in Fig. 9, the pure block matrix multiplication part shows very high efficiency, which is almost ONE. In other words, the pure block matrix multiplication part of the parallel SMACOF implementation achieves linear speed-up as we expected. Based on the efficiency measurement of **tMM_Computing** in Fig. 9, we could conclude that the proposed parallel SMACOF implementation achieved good enough load balance and the major component of the decrease of the efficiency is the compulsary MPI overhead for implementing parallelism. By contrast, the efficiency of the overall runtime of the parallel matrix multiplication part is decreased to around 0.5, as we expected based on Table 3.

We also compare the measured MPI overhead of the parallel matrix multiplication (**tMM_Overhead**) in Table 3 with the estimation of the MPI overhead with respect to the number of processes. The MPI overhead is estimated based on the assumption that `MPI_Bcast`

TABLE 3
Runtime Analysis of Parallel Matrix Multiplication part of parallel SMACOF with 50k data set in Cluster-II

#Procs	tMatMult	tMM_Computing	tMM_Overhead
64	668.8939	552.5348	115.9847
128	420.828	276.1851	144.2233
192	366.1	186.815	179.0401
256	328.2386	140.1671	187.8749

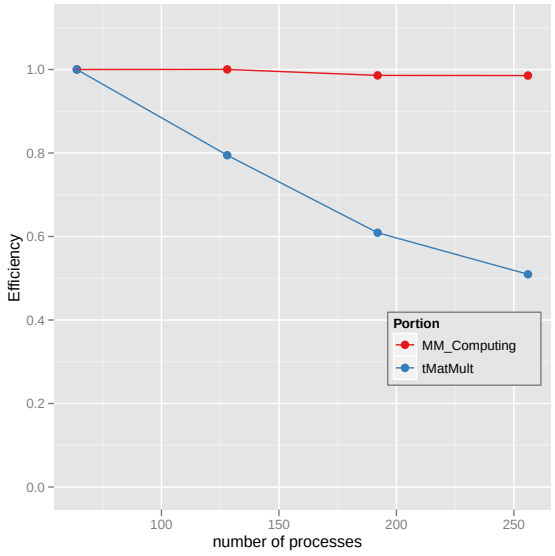


Fig. 9. Efficiency of **tMatMult** and **tMM_Computing** in Table 3 with respect to the number of processes.

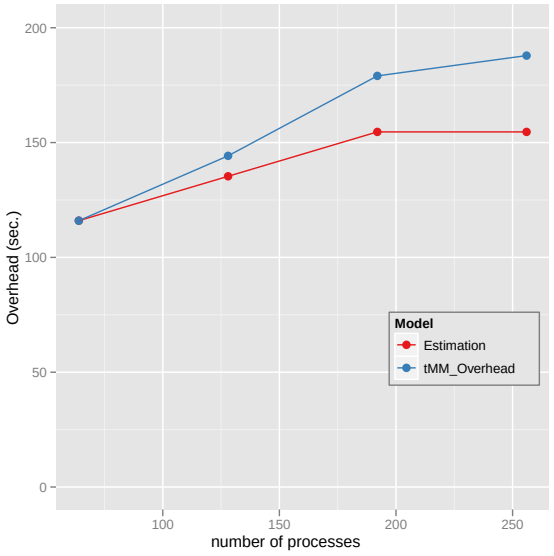


Fig. 10. MPI Overhead of parallel matrix multiplication (**tMM_Overhead**) in Table 3 and the rough Estimation of the MPI overhead with respect to the number of processes.

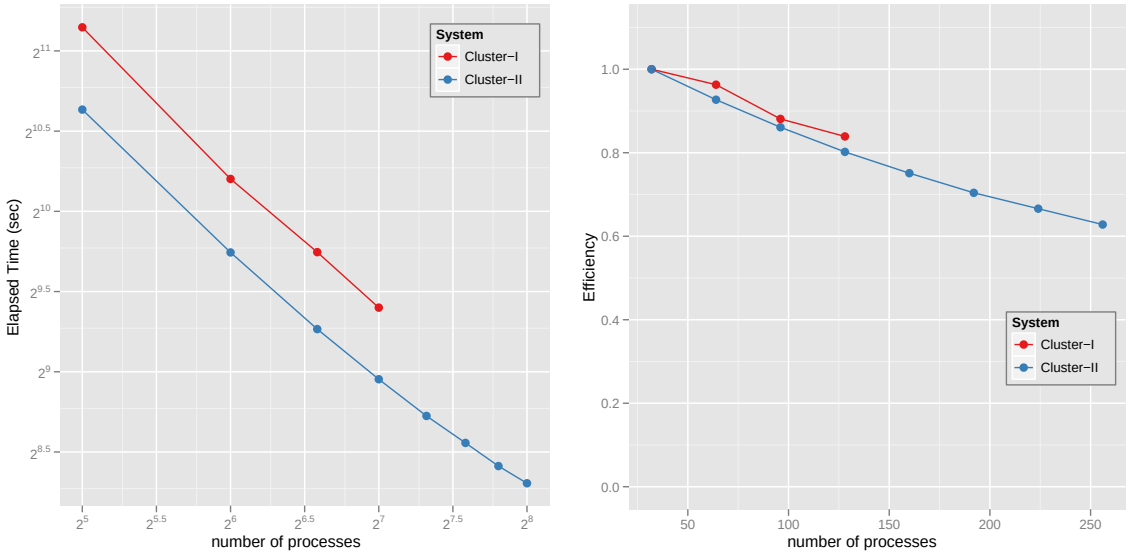
is implemented by a binomial tree or a binary tree algorithm, so that the runtime of `MPI_Bcast` is in $\mathcal{O}(\lceil \lg(p) \rceil)$ with respect to the number of parallel units (p). The result is described in Fig. 10. In Fig. 10, it is shown that the measured MPI overhead of the parallel matrix multiplication part has a similar shape with estimation overhead. We could conclude that the measured MPI overhead of the parallel matrix multiplication part takes the expected amount of time.

In addition to the experiment with pubChem data, which is represented by a vector format, we also experimented on the proposed algorithm with other real data sets, which contains 30,000 biological sequence data with respect to the metagenomics study (hereafter MC30000 data set). Although it is hard to present a biological sequence in a feature vector, researchers can calculate a dissimilarity value between two different sequences by using some pairwise sequence alignment algorithms, like Smith Waterman - Gotoh (*SW-G*) algorithm [20], [21] which we used here.

Fig. 11 shows: (a) the runtime; and (b) the efficiency of the parallel SMACOF for the MC30000 data in Cluster-I and Cluster-II in terms of the number of processes. We tested it with 32, 64, 96, and 128 processes for Cluster-I, and experimented on it with more processes, i.e. 160, 192, 224, and 256 processes, for Cluster-II. Both (a) and (b) sub-figure of Fig. 11 show similar tendencies to the corresponding sub-figure of Fig. 8. In contrast to the experiments of large pubchem data sets, we fixed the number of cores used per node (8 cores per node) in the experiments of MC30000 data set, and increased the number of nodes for the increase of paralle units. Therefore, we may assume that there is no memory bandwidth effect for the decrease of the efficiency related to Fig. 11.

5 Related Work

As parallel computing is getting important due to the broad distribution of multicore chips and the large-scale datasets, some parallel efforts have been proposed in MDS community. MDS solution by applying Genetic Algorithm (GA) [22] (hereafter called *GA-MDS*) was proposed by Mathar et al. [23], and Varoneckas et. al. [24] applied parallel computing to GA-MDS. In parallel GA-MDS [24], the parallelism is used for the improving the efficiency and the accuracy of GA which is applied to solving MDS by using



(a) MC30000 runtime (b) MC30000 efficiency

Fig. 11. Performance of parallel SMACOF for MC 30000 data in Cluster-I and Cluster-II w.r.t. the number of processes, i.e. 32, 64, 96, and 128 processes for Cluster-I and Cluster-II, and extended to 160, 192, 224, and 256 processes for Cluster-II. (a) shows runtime and efficiency is shown at (b). We choose balanced decomposition as much as possible, i.e. 8×8 for 64 processes. Note that both x and y axes are log-scaled for (a).

multiple populations as proposed in [25], but not for dealing with larger data sets in MDS. Pawliczek et. al. [26] proposed a parallel implementation of MDS method for the purpose of visualizing large datasets of multidimensional data. Instead of using traditional approaches, which utilize minimization methods to find an optimal (or local optimal) mapping of the STRESS function, they proposed a heuristic method based on particle dynamics in [26]. In addition to the above parallel efforts on MDS methods, a threading-based shared memory parallel implementation of SMACOF algorithm was also proposed in [18].

6 Conclusion and Future Work

In this paper, we have described a well-known dimension reduction algorithm, called MDS (SMACOF), and we have discussed how to utilize the algorithm for a huge data set. The main issues involved in dealing with a large amount of data points are not only lots of computations but also huge memory requirements. Parallelization via the traditional MPI approach in order to utilize the distributed memory computing system, which can support much more computing power and extend the accessible memory size, is proposed as a solution for the amendment of the computation and memory shortage so as to be able to treat large data with SMACOF.

As we discussed in the performance analysis, the data decomposition structure is important to maximize the performance of the parallelized algorithm since it affects message passing routines and the message passing overhead as well as the cache-line effect. We look at overall elapsed time of the parallel SMACOF based on data decomposition as well as sub-routine runtimes, such as calculation of BofZ matrix ($\boldsymbol{B}(\boldsymbol{X})$) and distance matrix ($\boldsymbol{D}(\boldsymbol{X})$). The cache reusability affects the performance of updating the distance matrix of the newly generated mappings with respect to the data decomposition if we run a large data set. From the above analysis, balanced data decomposition ($m \times n$) is generally better than skewed decomposition ($p \times 1$ or $1 \times p$) for the parallel MDS algorithm.

In addition to data decomposition analysis, we also analyzed the efficiency and the scalability of the parallel SMACOF. Although the efficiency of the parallel SMACOF is decreased by increasing the number of processes due to the increase of overhead and the decrease of pure parallel computing time, the efficiency is still good enough for a certain degree of parallelism. Based on the fact that the **tMM_Computing** in Table 3 achieved almost linear speedup as in Fig. 9, it is shown that the parallel SMACOF implementation deals with the load balance issue very well and the inevitable message passing overhead for parallelism is the main factor of the reduction of the efficiency.

There are important problems for which the data set sizes are too large for even our parallel algorithms to be practical. Because of this, we developed interpolation approaches for the MDS algorithm, which could be synergied by the proposed parallel SMACOF implementation. Here we run normal MDS (or parallel MDS) with a (random) subset of the dataset

(called *sample data*), and the dimension reduction of the remaining points are interpolated based on the pre-mapped mapping position of the sample data. The detail of the interpolation approach is reported in [27].

In [1], [28], we investigated the overhead of pure MPI and hybrid (MPI-Threading) model with multicore cluster systems. In [1], pure MPI outperforms hybrid model for the application with relatively fast message passing synchronization overhead. However, for the case of high MPI synchronization time, hybrid model outperforms pure MPI model with high parallelism. Since the MPI overhead is grown as the number of processes is increased in Fig. 10, it is worth to investigate hybrid model SMACOF.

REFERENCES

[1] G. Fox, S. Bae, J. Ekanayake, X. Qiu, and H. Yuan, "Parallel data mining from multicore to cloudy grids," in *Proceedings of HPC 2008 High Performance Computing and Grids workshop*, Cetraro, Italy, July 2008.

[2] C. Bishop, M. Svensén, and C. Williams, "GTM: A principled alternative to the self-organizing map," *Advances in neural information processing systems*, pp. 354–360, 1997.

[3] ——, "GTM: The generative topographic mapping," *Neural computation*, vol. 10, no. 1, pp. 215–234, 1998.

[4] T. Kohonen, "The self-organizing map," *Neurocomputing*, vol. 21, no. 1-3, pp. 1–6, 1998.

[5] W. S. Torgerson, "Multidimensional scaling: I. theory and method," *Psychometrika*, vol. 17, no. 4, pp. 401–419, 1952.

[6] J. B. Kruskal and M. Wish, *Multidimensional Scaling*. Beverly Hills, CA, U.S.A.: Sage Publications Inc., 1978.

[7] I. Borg and P. J. Groenen, *Modern Multidimensional Scaling: Theory and Applications*. New York, NY, U.S.A.: Springer, 2005.

[8] J. Y. Choi, S.-H. Bae, X. Qiu, and G. Fox, "High performance dimension reduction and visualization for large high-dimensional data analysis," in *Proceedings of the 10th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGRID) 2010*, May 2010, pp. 331–340.

[9] J. de Leeuw, "Applications of convex analysis to multidimensional scaling," *Recent Developments in Statistics*, pp. 133–145, 1977.

[10] ——, "Convergence of the majorization method for multidimensional scaling," *Journal of Classification*, vol. 5, no. 2, pp. 163–180, 1988.

[11] J. B. Kruskal, "Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis," *Psychometrika*, vol. 29, no. 1, pp. 1–27, 1964.

[12] Y. Takane, F. W. Young, and J. de Leeuw, "Nonmetric individual differences multidimensional scaling: an alternating least squares method with optimal scaling features," *Psychometrika*, vol. 42, no. 1, pp. 7–67, 1977.

[13] T. Hofmann and J. M. Buhmann, "Pairwise data clustering by deterministic annealing," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 19, pp. 1–14, 1997.

[14] A. Dempster, N. Laird, and D. Rubin, "Maximum likelihood from incomplete data via the em algorithm," *Journal of the Royal Statistical Society. Series B*, pp. 1–38, 1977.

[15] E. H. Moore, "On the reciprocal of the general algebraic matrix," *Bulletin of American Mathematical Society*, vol. 26, pp. 394–395, 1920.

[16] R. Penrose, "A generalized inverse for matrices," *Proceedings of the Cambridge Philosophical Society*, vol. 51, pp. 406–413, 1955.

[17] X. Qiu, G. C. Fox, H. Yuan, S.-H. Bae, G. Chrysanthakopoulos, and H. F. Nielsen, "Data mining on multicore clusters," in *Proceedings of 7th International Conference on Grid and Cooperative Computing GCC2008*. Shenzhen, China: IEEE Computer Society, Oct. 2008, pp. 41–49.

[18] S.-H. Bae, "Parallel multidimensional scaling performance on multicore systems," in *Proceedings of the Advances in High-Performance E-Science Middleware and Applications workshop (AHEMA) of Fourth IEEE International Conference on eScience*. Indianapolis, Indiana: IEEE Computer Society, Dec. 2008, pp. 695–702.

[19] J. Pješivac-Grbović, T. Angskun, G. Bosilca, G. Fagg, E. Gabriel, and J. Dongarra, "Performance analysis of mpi collective operations," *Cluster Computing*, vol. 10, no. 2, pp. 127–143, 2007.

[20] T. F. Smith and M. S. Waterman, "Identification of common molecular subsequences," *Journal of molecular biology*, vol. 147, no. 1, pp. 195–197, 1981.

[21] O. Gotoh, "An improved algorithm for matching biological sequences," *Journal of Molecular Biology*, vol. 162, no. 3, pp. 705–708, 1982.

[22] D. Goldberg, *Genetic algorithms in search, optimization, and machine learning*. Addison-wesley, 1989.

[23] R. Mathar and A. Žilinskas, "On global optimization in two-dimensional scaling," *Acta Applicandae Mathematicae*, vol. 33, no. 1, pp. 109–118, 1993.

[24] A. Varoneckas, A. Zilinskas, and J. Zilinskas, "Multidimensional scaling using parallel genetic algorithm," *Computer Aided Methods in Optimal Design and Operations*, pp. 129–138, 2006.

[25] E. Cantu-Paz, *Efficient and accurate parallel genetic algorithms*. Springer, 2000, vol. 1.

[26] P. Pawliczek and W. Dzwinel, "Parallel implementation of multidimensional scaling algorithm based on particle dynamics," in *Parallel Processing and Applied Mathematics*, ser. Lecture Notes in Computer Science, R. Wyrzykowski, J. Dongarra, K. Karczewski, and J. Wasniewski, Eds., vol. 6067. Springer Berlin / Heidelberg, 2010, pp. 312–321.

[27] S.-H. Bae, J. Y. Choi, X. Qiu, and G. Fox, "Dimension reduction and visualization of large high-dimensional data via interpolation," in *Proceedings of the ACM International Symposium on High Performance Distributed Computing (HPDC) 2010*, Chicago, Illinois, June 2010.

[28] J. Qiu, S. Beason, S. Bae, S. Ekanayake, and G. Fox, "Performance of windows multicore systems on threading and mpi," in *2010 10th IEEE/ACM International Conference on Cluster, Cloud and Grid Computing*. IEEE, 2010, pp. 814–819.