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High Performance Grid and Cluster Computing for Some Optimization Problems

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Abstract.
Solving large scale optimization problems requires a huge amount of computational power. The size of optimization problems that can be solved on a few CPUs has been limited due to a lack of computational power. Grid and cluster computing has received much attention as a powerful and inexpensive way of solving large scale optimization problems that an existing single-unit CPU cannot process. The aim of this paper is to show that grid and cluster computing provides tremendous power to optimization methods. The methods that this article picks up are a successive convex relaxation method for quadratic optimization problems, a polyhedral homotopy method for polynomial systems of equations and a primal-dual interior-point method for semidefinite programs. Their parallel implementations on grids and clusters together with numerical results are reported. The article also mentions a grid portal system for optimization problems briefly.

Key words.
Optimization Problem, Parallel Computing, Cluster Computing, Grid Computing, Semidefinite Program, Semidefinite Program Relaxation, Polynomial Equations, Polyhedral Homotopy Method

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1 Introduction

Optimization problems have a variety of practical applications in various fields such as operations research, engineering, science, biology and economics. Many combinatorial and nonconvex optimization problems are known to be $\mathcal{NP}$-hard, which means that there exists no algorithm that finds an optimal solution in polynomial time unless $\mathcal{P} = \mathcal{NP}$. Hence, solving large scale combinatorial and nonconvex optimization problems require a huge amount of computational time and resources, and the size of such problems that we can solve has been limited. As computing resources continue to improve, however, optimal solutions of larger scale optimization problems become more achievable. In particular, grid and cluster computing technology has recently received much attention as a powerful and inexpensive methodology for solving large scale optimization problems that an existing single-unit CPU cannot process.

To solve large scale optimization problems, we need new computing infrastructure which enables us to easily access to computational resources including hardware and software library distributed across a wide area network like the Internet. For example, Applegate et al. [2] implemented the Danzig, Fulkerson and Johnson's cutting plane method for the large scale TSP (traveling salesman problem). They obtained the optimal solution of the TSP that has 15,112 cities (nodes) in Germany. This problem is the largest scale TSPLIB [1] instance that have been solved to date. The computation was executed on a network of 110 processors located at Rice and Princeton Universities. They estimated the total computation time was 22.6 years, scaled to a Compaq EV6(21264) Alpha processor running at 500MHz. A group of researchers at the University of Iowa and Argonne National Laboratory solved the QAP (quadratic assignment problem) instance called NUG30 in QAPLIB [2] using the Condor [3] developed the University of Wisconsin. Condor is a system of daemons and tools to utilize commodity computing resources including idle desktop machines for high-throughput computing. NUG30 is known as a huge scale QAP that would require more than 10 years of computation time by a single CPU. They obtained an optimal solution in just seven days using the Condor system and 653 CPUs on average. See the paper [1] for more details.

In this paper, we present grid and cluster computing for some optimization problems with numerical results. In Section 2 and 3, we focus our attention on GridRPC, which is an RPC system redesigned for Grid applications. Some GridRPC systems such as Netsolve and Ninf are widely used. The Ninf system [11] developed by AIST (National Institute of Advanced Industrial Science and Technology, Japan) employs a client-server model, where server and client machines are connected via a local area network or the Internet. We implemented highly parallel algorithms for some optimization problems and polynomial systems of equations with the use of the Ninf system on several PC clusters connected via a high speed local area network and/or the Internet. In Section 4, we briefly explain the SDPARA (SemiDefinite Programming Algorithm paRAllel version) [16], a parallel implementation of the SDPA [15], and present numerical results on PC clusters. Section 5 presents a Grid Portal system which enables users who have little computational resource for parallel optimization softwares.

[1]http://www.iwr.uni-heidelberg.de/iwr/comopt/software/TSPLIB95/
[2]http://www.opt.math.tu-graz.ac.at/qaplib/
[3]http://www.cs.wisc.edu/condor/

2 Parallel Successive Convex Relaxation Method for Nonconvex Quadratic Optimization Problems

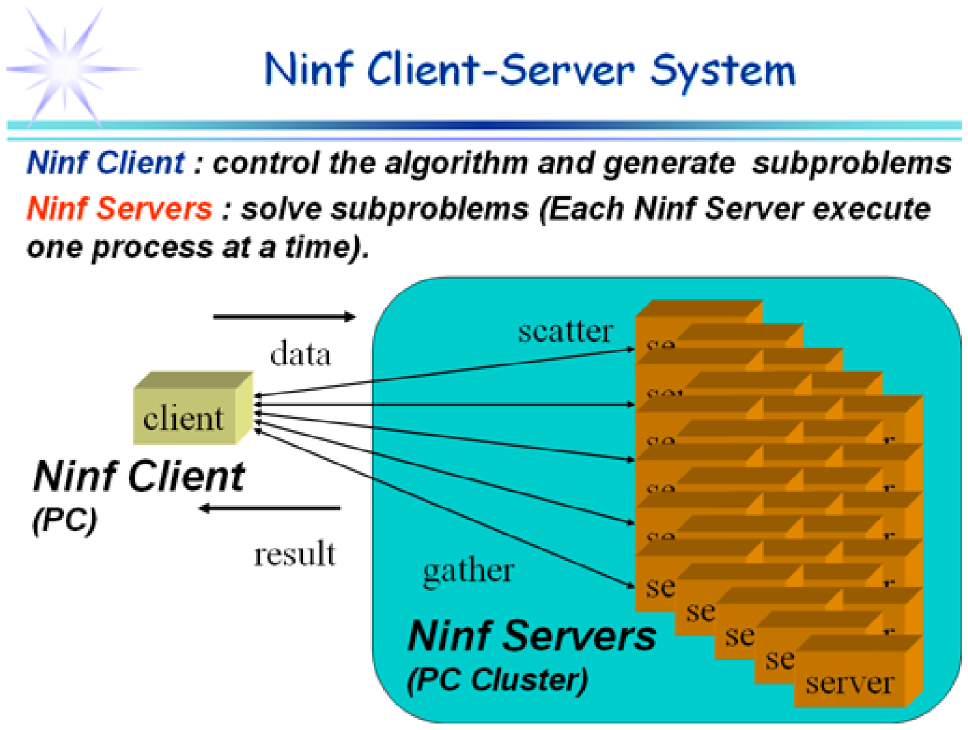

Ninf Client-Server System
Ninf Client : control the algorithm and generate subproblems
Ninf Servers : solve subproblems (Each Ninf Server execute one process at a time).
data
client
Ninf Client
(PC)
result
scatter
gather
Ninf Servers
(PC Cluster)
server

Figure 1: Ninf client-server model

The QOP (Quadratic Optimization Problem) covers various important nonconvex mathematical programs such as 0-1 linear and quadratic integer programs, linear complementarity problems, bilevel quadratic programs, linear and quadratic fractional programs, and so on. Let $\mathbb{R}^n$ and $\mathcal{S}^n$ denote the n-dimensional Euclidean space and the space of $n \times n$ real symmetric matrices, respectively. A general QOP is described in the the following form:

$$\text{(QOP)} \quad \left| \begin{array}{ll} \max & \boldsymbol{c}^T\boldsymbol{x} \\ \text{s.t.} & \gamma_i + 2\boldsymbol{q}_i^T\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{Q}_i\boldsymbol{x} \leq 0 \ (i = 1, \dots m), \end{array} \right. \tag{1}$$

where $\boldsymbol{c} \in \mathbb{R}^n$, $\gamma_i \in \mathbb{R}$, $\boldsymbol{q}_i \in \mathbb{R}^n$ and $\boldsymbol{Q}_i \in \mathcal{S}^n$ $(i = 1, \dots, m)$. When a given QOP has a quadratic objective function such as $\gamma_0 + 2\boldsymbol{q}_0^T\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{Q}_0\boldsymbol{x}$, we can transform it into QOP (1) by replacing the quadratic objective function with a new variable t and adding $-\gamma_0 - 2\boldsymbol{q}_0^T\boldsymbol{x} - \boldsymbol{x}^T\boldsymbol{Q}_0\boldsymbol{x} + t \leq 0$ to the set of inequality constraints. A general QOP is known as one of the most significant nonlinear programming problems. QOPs cover not only economics and engineering applications but also various important nonconvex mathematical programs. Because of their theoretical and computational difficulties, however, solvable QOPs had been limited to convex QOPs where all $\boldsymbol{Q}_i$s are assumed to be positive semidefinite or general QOPs with small size.

The SCRM (Successive Convex Relaxation Method) proposed by Kojima-Tuncel [7] is a powerful numerical method to compute upper bounds of general QOPs by repeated applications of SDP (semidefinite programming) relaxations. The SCRM generates and solves a large number of SDP problems at each iteration. Takeda et al. [12] reported that the SCRM can deal with some larger scale QOPs through numerical experiments on a PC cluster. To get more accurate upper bounds and/or to process larger scale of QOPs, we need more and more computing resources. We implemented a highly parallel SCRM on the Ninf system. Figure 1 shows that a Ninf client-server model. The Ninf client controls the SCRM applied to a QOP and generates a large number of subproblems each of which forms an SDP problem at each iteration. All generated SDP problems are sent to the Ninf server machines. Then each Ninf server solves an SDP problem using the software SDPA [15]. Note that each Ninf server solves only one SDP problem at a time. After finishing the execution of the SDPA, the result is sent back to the Ninf client machine. Takeda et al. [12] also showed computational efficiency of the SCRM by varying the number of Ninf servers. They reported that SDP problems were allocated to each Ninf server in balance and the total computational time consumed by each Ninf server was almost the same. Therefore a good performance and high scalability were attained.

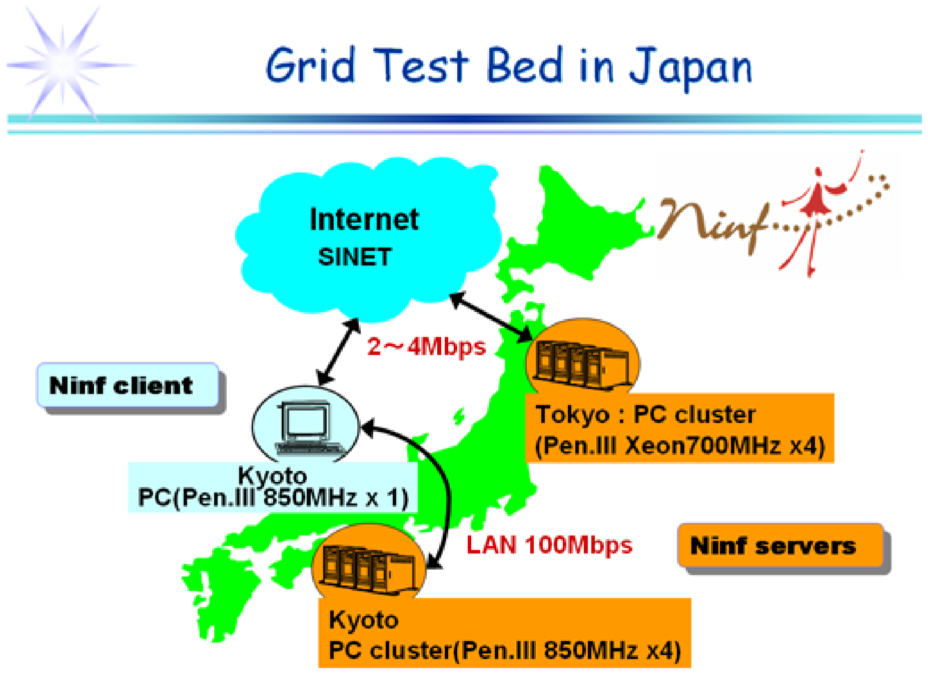


Figure 2: Grid Environment(Kyoto $\Longleftrightarrow$ Tokyo)

We now show some numerical experiments of the SCRM on a Grid environment. Figure 2 illustrates that we have two PC clusters which are located in Kyoto and Tokyo. The Kyoto cluster has 4 nodes which are connected to a Ninf client PC through LAN (100BASE-TX). The Tokyo cluster has 4 nodes which are connected to the Ninf client PC through the Internet called SINET. We estimate the average network speed of the SINET between Kyoto and Tokyo to be about 2 to 4 Mbps. Table 1 shows that numerical results of the SCRM on the grid environment illustrated in Figure 2. The first row "# subproblems" denotes that the total number of SDP problems which the Ninf servers in the Kyoto cluster and the Tokyo cluster solved, respectively. The second row denotes that the total execution time of the SDPA in each cluster. The total execution time of the Kyoto cluster is almost the same as that of the Tokyo cluster. Note also that the total transmitting time between the Ninf client and Ninf servers is extremely small. ¿From the Table 1, we can say that the SCRM is well paralleled in the grid environment.

Table 1: Numerical results on grid environments

Prob. name	LC80-144		BLevel20-3	
Ninf Server	Kyoto	Tokyo	Kyoto	Tokyo
# subproblems	1795	1333	883	597
total execution time(sec.)	16486.5	16395.6	1053.6	984.2
total trans. time C $\rightarrow$ S(sec.)	0.150	0.117	0.046	0.028
total trans. time C $\leftarrow$ S(sec.)	0.275	0.069	0.130	0.182

3 Parallel Polyhedral Homotopy Method

Polynomial systems have various applications in many fields of science and engineering. The software package "PHoM" [6] is designed to find all isolated (real and complex) solutions of a polynomial system of equations $f(x) = 0$ (such as the cyclic n problem, see Table 2) using a polyhedral homotopy method. The package consists of three modules. The first module which we call "StartSystem" constructs a family of polyhedral-linear homotopy functions. Takeda et al. [13] implemented a highly paralleled StartSystem using the Ninf. The second module traces the homotopy paths to compute all isolated solutions of a polynomial system of equations. The Ninf servers trace the homotopy paths by applying the predictor-corrector method. The third module verifies whether all isolated solutions of the polynomial system of equations have been computed correctly.

Table 2: cyclic n problem

$$\begin{array}{l}
x_1 + x_2 + \cdots + x_n = 0 \\
x_1x_2 + x_2x_3 + \cdots + x_nx_1 = 0 \\
x_1x_2x_3 + \cdots + x_nx_1x_2 = 0 \\
\ldots \\
x_1x_2x_3\cdots x_n - 1 = 0,
\end{array}$$

Table 3: noon-9 problem

$$\begin{array}{l}
x_1x_2^2 + x_1x_3^2 + \cdots + x_1x_9^2 - 1.1x_1 + 1 = 0 \\
x_2x_1^2 + x_2x_3^2 + \cdots + x_2x_9^2 - 1.1x_2 + 1 = 0 \\
\ldots \\
x_9x_1^2 + x_9x_2^2 + \cdots + x_9x_8^2 - 1.1x_9 + 1 = 0
\end{array}$$

We also employ the Ninf client-server system, illustrated in Figure 1, for the parallel implementation of the first and second modules of the PHoM. Table 4 shows numerical results of the first and second modules for the noon-9 problem. This problem has 19,665

Table 4: Numerical results of the homotopy method (noon-9 problem)

	StartSystem		Trace		Total	
# CPUs	time(s.)	sp-up-raito	time(s.)	sp-up-ratio	time(s.)	sp-up-ratio
1	43	1.00	44,119	1.00	44,162	1.00
2	25	1.72	22,192	1.99	22,217	1.99
4	22	1.95	11,109	3.97	11,131	3.97
8	14	3.07	5,548	7.95	5,562	7.94
16	14	3.07	2,822	15.63	2,826	15.57
32	20	2.15	1,435	30.74	1,455	30.35

isolated solutions. All numerical experiments were executed on the Presto I cluster which has 64 nodes (each CPU is Celeron 500MHz). The 'sp-up-ratio' stands for the computation time (# of CPUs is 1) divided by the computation time (# of CPUs is k). If 'sp-up-ratio' is sufficiently close to k, we can regard the software as well paralleled on the Ninf client-server system. Takeda et al. [13] reported that the computation of mixed cells by StartSystem (the first module) is suitable for parallel computation through some numerical experiments. We furthermore observe from Table 4 that tracing all homotopy paths (the second module) is also suitable for parallel computation on the Ninf client-server system. Table 5 also shows numerical results of the second module for the cyclic problems with dimensions $n = 11,\ 12$ and 13. There are many homotopy paths, which can be traced independently in parallel; specifically the cyclic 13 problem has 208,012 homotopy paths, and the above noon-9 problem has 19,665 homotopy paths. We use two PC clusters which are located in Tokyo Institute of Technology. All homotopy paths of the cyclic 11 problem were computed in the Presto I cluster, while all homotopy paths of the cyclic 12 and 13 problems were computed on the Presto III cluster which has 256 nodes and 512 CPUs (each CPU is Athlon 1900+). From Table 5, we observe that the second module of the PHoM is quite suitable for parallel computation on PC clusters. Note that more than 5,000 seconds were required to compute all homotopy paths of the cyclic 13 problem even when we used 256 CPUs simultaneously. Therefore parallel computing is indispensable to process larger scale polynomial systems of equations.

Table 5: Numerical results of tracing homotopy paths (cyclic n problem)

	cyclic-11		cyclic-12		cyclic-13	
# CPUs	time(s.)	sp-up-raito	time(s.)	sp-up-ratio	time(s.)	sp-up-ratio
2	47,345	1.00				
4	23,674	2.00				
8	11,852	3.99				
16	5,927	7.99				
32	2,967	15.96				
64	1,487	31.84	2,592	1.00		
128			1,332	1.95	10,151	1.00
256			703	3.69	5,191	1.95
# paths traced	16,796		41,696		208,012	

4 Parallel Implementation of Semidefinite Programming

In the last decade, SDP problems have been intensively studied in theoretical, numerical and practical aspects in various fields such as interior-point methods, combinatorial optimization, control and systems, robust optimization and quantum chemistry. Let $\mathcal{S}^n$ denote the vector space of $n \times n$ symmetric matrices. For a pair of matrices $\boldsymbol{X}, \boldsymbol{Y} \in \mathcal{S}^n$, the inner product is defined as $\boldsymbol{X} \bullet \boldsymbol{Y} = \sum_{i=1}^n \sum_{j=1}^n X_{ij} Y_{ij}$. We use the notation $\boldsymbol{X} \in \mathcal{S}^n_+$ ($\mathcal{S}^n_{++}$) to indicate that $\boldsymbol{X} \in \mathcal{S}^n$ is positive semidefinite (or positive definite). Given $\boldsymbol{A}_i \in \mathcal{S}^n$ $(i = 0, 1, \ldots, m)$ and $\boldsymbol{b} \in \mathbb{R}^m$, the standard form SDP problem is written as follows:

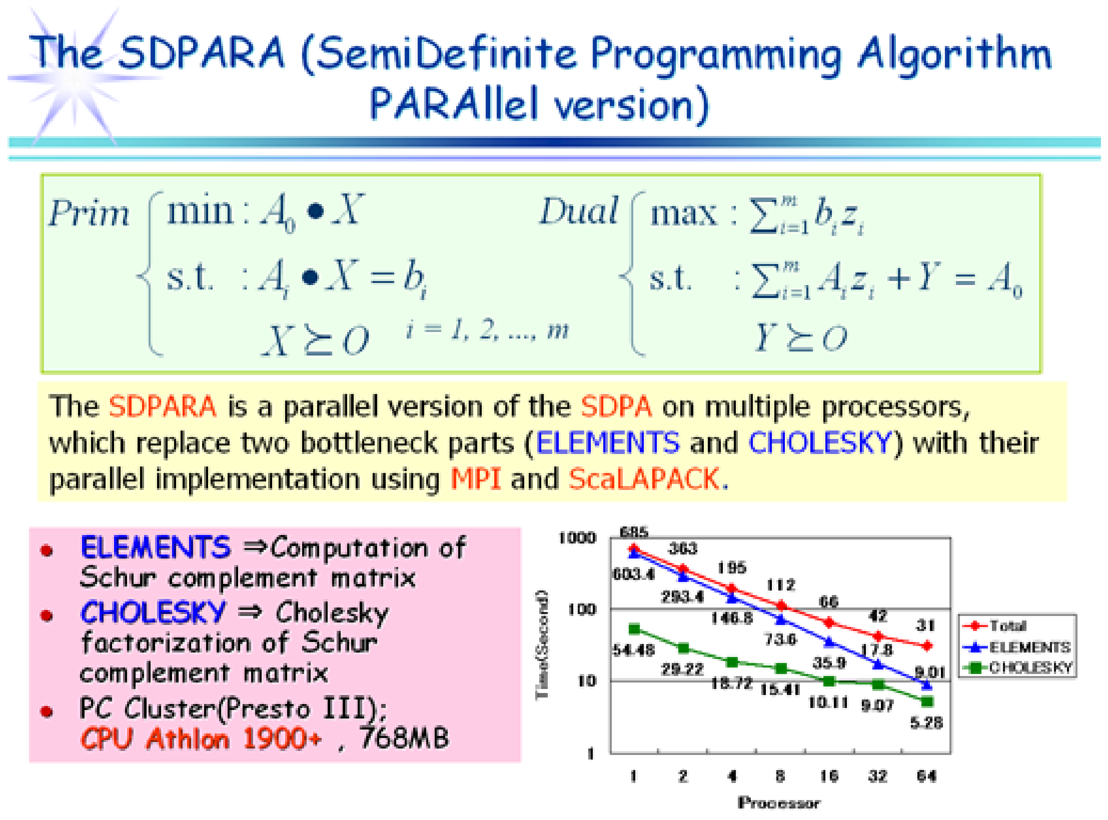
$$\left.\begin{array}{ll} \text{minimize} & \boldsymbol{A}_0 \bullet \boldsymbol{X} \\ \text{subject to} & \boldsymbol{A}_i \bullet \boldsymbol{X} = b_i \ (i = 1, 2, \ldots, m), \ \boldsymbol{X} \in \mathcal{S}^n_+ \end{array}\right\}. \tag{2}$$

The corresponding dual problem is as follows:

$$\left.\begin{array}{ll} \text{maximize} & \displaystyle\sum_{i=1}^m b_i z_i \\ \text{subject to} & \displaystyle\sum_{i=1}^m \boldsymbol{A}_i z_i + \boldsymbol{Y} = \boldsymbol{A}_0, \ \boldsymbol{Y} \in \mathcal{S}^n_+ \end{array}\right\}. \tag{3}$$

It is known that the primal-dual interior point method is capable of solving these problems in polynomial time. The SDPA (SemiDefinite Programming Algorithm) [15] is an optimization software, written by the C++ language, of a PDIPM (primal-dual interior-point method) for solving the standard form SDP problem. The SDPA incorporates a special data structure for handling block diagonal data matrices and an efficient method proposed by Fujisawa, Kojima and Nakata [3] for computing search directions when problems to be solved are large scale and sparse. In many applications, however, SDP problems become too large for SDP software packages including the SDPA to solve on a single processor. It is well-known that the PDIPM for SDP problems has two major time consuming parts at each iteration even if we exploit the sparsity of the date matrices. The first part is the computation of the so-called Schur complement matrix. The second part is the Cholesky factorization of the Schur complement matrix. These two parts are called ELEMENTS and CHOLESKY in Figure 3 below.

The SDPARA (SemiDefinite Programming Algorithm PARAllel version) [16] is a parallel version of the SDPA on multiple processors and distributed memory, which replaces these two bottleneck parts mentioned above by their parallel implementation using MPI and ScaLAPACK. The SDPARA reads input data m, n, $\boldsymbol{b}$, $\boldsymbol{A}_0$, $\boldsymbol{A}_1$, $\ldots$, $\boldsymbol{A}_m$ and each processor keeps the memory space for the input data and variables $\boldsymbol{X}$, $\boldsymbol{Y}$, $\boldsymbol{z}$ independent of other processors, while the Schur complement matrix is divided and stored on each processor. The SDPARA can compute each row of the Schur complement matrix independently in parallel and applies a parallel Cholesky factorization provided by ScaLAPACK to the Schur complement matrix. Figure 3 explains the main features of the SDPARA. The SDPARA on a PC cluster attains high scalability for large scale SDP problems. The largest scale problem arising from the quantum chemistry [8] which we can solve involves a $24,503 \times 24.503$ Schur complement matrix. For more details, see the



The SDPARA (SemiDefinite Programming Algorithm PARAllel version)

$$\textit{Prim}\begin{cases}\min : A_0 \bullet X \\ \text{s.t.} \;\; : A_i \bullet X = b_i \\ \qquad X \succeq O \quad i = 1, 2, \ldots, m\end{cases} \qquad \textit{Dual}\begin{cases}\max : \sum_{i=1}^{m} b_i z_i \\ \text{s.t.} \;\; : \sum_{i=1}^{m} A_i z_i + Y = A_0 \\ \qquad Y \succeq O\end{cases}$$

The SDPARA is a parallel version of the SDPA on multiple processors, which replace two bottleneck parts (ELEMENTS and CHOLESKY) with their parallel implementation using MPI and ScaLAPACK.

- ELEMENTS ⇒Computation of Schur complement matrix
- CHOLESKY ⇒ Cholesky factorization of Schur complement matrix
- PC Cluster(Presto III); CPU Athlon 1900+ , 768MB

Figure 3: The SDPARA (SemiDefinite Programming Algorithm PARAlell Version)

Yamashita et al. [16]. Zhao et al. [17] proposed another SDP formulation of the quantum chemistry. The size of the Schur complement matrix of their formulation is not so large, however, the size of matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$ are very large compared with the SDP formulation proposed in [8] (See Table 6). We solved these two problems on the PC cluster which we call ACT-JST cluster. The ACT-JST cluster in Tokyo Denki University has 40 nodes (each node has 1 or 2 GB memory) and 80 CPUs (Athlon 1.2GHz).

Table 6: Large scale problems arising from the quantum chemistry

problem	(1):Nakata et al. [8]	(2):Zhao et al. [17]
size of the Schur complement matrix ($= m$))	24,503	7,230
size of $\boldsymbol{X}$ and $\boldsymbol{Y}$ ($= n$)	630	5,990
time(s.)	4153.5 (64CPUs)	38009.0 (32CPUs)

As we described above, each processor must maintain all input data and variables, whereas the Schur complement matrix is stored on distributed memory. Therefore, the current version of the SDPARA is suitable for a large scale SDP problem which involves a large Schur complement matrix and not so large variables like the SDP problem (1) in Table 6. The SDP problem (2) in Table 6 requires that all processors need more than 1 GB for input data, variables and the distributed Schur complement matrix. AS a given SDP problem to be solved gets larger, it becomes difficult to share common input data and variables with all processors; we eventually need to distribute input data and variables among the processors to save memory in each processor.

We also developed a new software package called SDPA-C to exploit the sparsity structure of large scale SDP problems based on some fundamental results about positive semidefinite matrix completion [5, 9]. The SDPARA-C [10] is an parallel implementation of SDPA-C using the parallel computing techniques including the ones used for the SDPARA. We confirm that SDPARA-C attains high scalability and works efficiently to solve large scale and sparse SDP problems through some numerical experiments on PC clusters.

5 Future Works

We are planning to apply Grid and Cluster computing to some other optimization problems such as the vehicle routing problem with time windows and more general mixed integer programming problems. So far we have mainly employed the Ninf GridRPC system (which we call Ninf-1). Tanaka et al. [14] have recently redesigned the Ninf and implemented a new GridRPC system called Ninf-G. The Ninf-G is a full re-implementation of the Ninf-1 using Globus Toolkit. This takes advantage of high interoperability with some other Globus-based Grid systems. We have plans to reconstruct our software packages such as the SCRM and the PHoM using the Ninf-G and Globus Toolkit.

We are also developing a grid portal system for some optimization problem softwares including the SDPARA, which enables users to easily perform parallel computation through the Internet. GridLib in Figure 4 developed by AIST (National Institute of Advanced Industrial Science and Technology, Japan) provides a development framework to construct a virtual computer center as ASP (Application Service Provider). For a

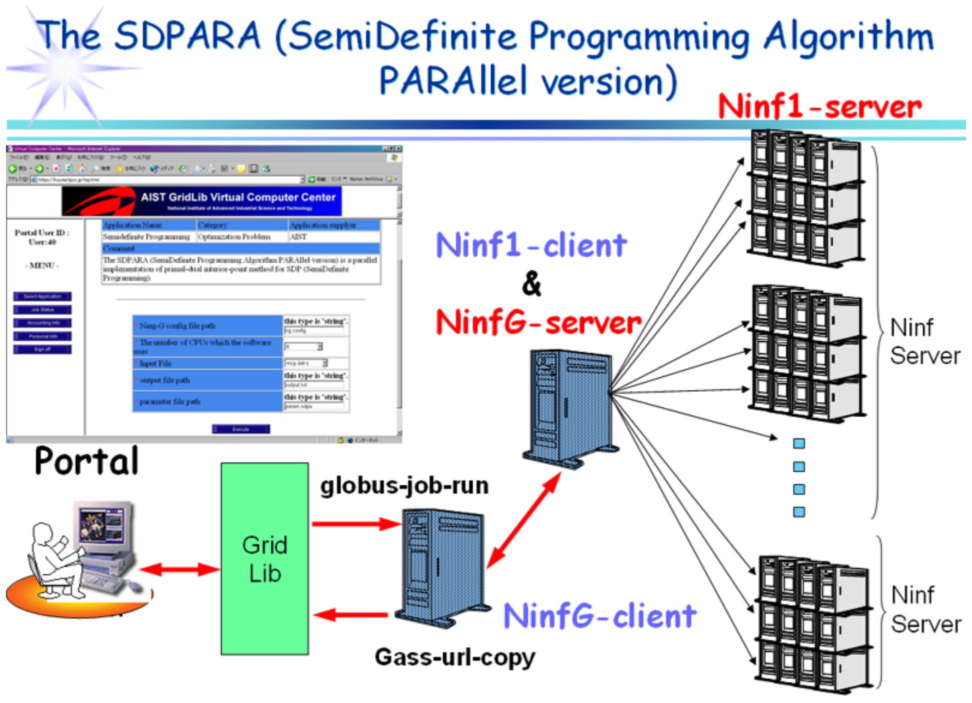


Figure 4: A Grid Portal System for the SDPARA

GridLib user, no particular knowledge about the Web securities and the Web programming is needed. We have already finished making a grid portal system for the SDPARA with a little deal of trouble. We mention that little modification to the SDPARA is necessary to portalize it. The user first access the Web portal site, select an application and a problem to be solved. GridLib starts up a Ninf-G client program associated with the application selected, and send the problem to a Ninf-G server over the Internet. Now the Ninf-G server plays the role of a Ninf-1 client, which calls Ninf-1 servers among a PC cluster to execute the SDPARA. After finishing the execution of the SDPARA, the result is back to the Web portal site following the reverse route.

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