Development of Scalable Efficient Solvers for Sparse Linear System of Equations

Project report submitted

In fulfilment of the requirement for the degree of

Bachelor of Technology

by

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November, 2016

CERTIFICATE

It is certified that the work contained in the project report titled **"Development of Scalable Efficient Solvers for Sparse Linear System of Equations"**, by **Anshul Goyal** (130103011) and **Kanishk Chaturvedi** (130103035) has been carried out under my supervision and that this work has not been submitted elsewhere for the award of a degree.

7 November , 2016

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DECLARATION

We declare that this written submission represents our ideas in our own words and where others' ideas or words have been included, we have adequately cited and referenced the original sources. We also declare that we have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in our submission. We understand that any violation of the above will be cause for disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

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APPROVAL SHEET

This project report entitled "Development of Scalable Efficient Solvers for Sparse Linear System of Equations" by Anshul Goyal and Kanishk Chaturvedi is approved for the degree of Bachelor of Technology.

Examiners

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Anshul Goyal
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ABSTRACT

The modern era is continuously advancing in the sphere of technology, hence, posing even more complex problems with each step towards a more scientific world. The computations that were earlier possible through direct methods have grown into much larger problems with higher time and space complexities. This calls for a need of further optimization of the pre-existent direct solvers. Hence, certain Iterative solvers like Conjugate Gradient(CG) Method are developed to further satisfy the memory and time constraints of each complex problem.

Although such solvers have experienced a kind of maturation over the past few years, this relatively new sphere of development of Sparse System Solvers is still vulnerable to many undone optimizations and improvements in each particular iteration. If the physical aspects and properties of a mechanical system are exploited in a careful manner, we could reach an even more efficient method of performing calculations on sparse real world problems.

Furthermore, the iterative methods are far more easier to implement on parallel systems like GPU, which helps us to explore the various options of custom modifying the algorithms according to our physical constraints, in order to advance its performance.

Keywords: Sparse Systems, Solvers, Conjugate Gradient, Time & Space Complexities

Nomenclature

A - Stiffness Matrix

x, y, z - Solution Vectors

B, b - Right Hand Vectors

L - Lower Triangular Matrix

U - Upper Triangular Matrix

u, v - Row Vectors

m - number of rows in the matrix **A**

M - an arbit **m x m** matrix

nnz - number of nonzero elements

val, row_ptr, col_ind - Arrays used in CSR format

$\mathbf{p_i}$ **-** direction vectors

$\mathbf{r_k}$ **-** Residual Vector

α, β, k - constants

R,Z - Column Vectors

Contents

Introduction

The finite element method (FEM) is a numerical technique for finding approximate solutions to boundary value problems for partial differential equations. It is also referred to as finite element analysis (FEA). It subdivides a large problem into smaller, simpler parts that are called finite elements. The simple equations that model these finite elements are then assembled into a larger system of equations that models the entire problem. Breaking down of larger elements and summing up the numerous smaller elements requires a high amount of computational time. A modern day CPU with a clock speed as high as 4GHz, will take a huge amount of time solving each iteration one by one. For real life systems this technique might just take ages to solve, thus a different approach is employed to reach a much higher speed of computation. Use of Graphic Processing Units or GPUs serves the purpose of achieving a high speed of computational time. A highly parallel architecture allowed them to do these operations much faster than what was possible on CPUs.

Three traditional ways of making our computers run faster are to increase the clock speed, add more processors, and employ more work per clock cycle. GPUs consists of hundreds of processors which function at the same time. Thus the technique of dividing a problem into smaller parts and then computing the results work efficiently with GPUs as we can compute the smaller problems in parallel thus decreasing the time significantly. This is also termed as General-Purpose Graphic Processing Unit or GPGPU. This can easily be understood by a simple example, choosing 1024 chickens over 2 bulls to plough a field is basically a parallel way of thinking. Thus employing a large number of weak processors results in much better computation than employing a small number of strong processors, with respect to the cost and time both. Parallelism is the way of life these days and we intend to implement it to solve bigger and complex FEM problems by dividing the bigger chunk into smaller chunks and obtain the results in a much faster time.

Objective: 1) Implementation of FEM Solver on CPU(Central Processing Unit).

2) Comparison of pre-existing library with our own implementation in CPU.

3) Implementation of FEM solver on GPU(Graphics Processing Unit).

4) Comparison of pre-existing library with our own implementation in GPU.

Problem Statement

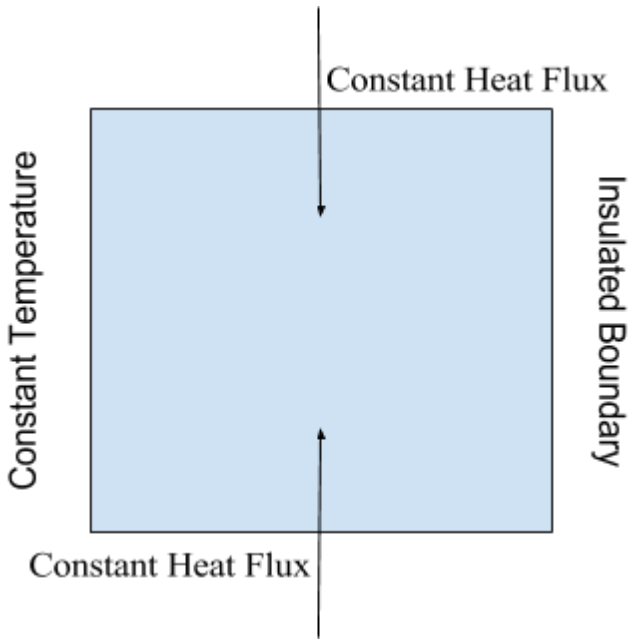
For the primitive testing of our code and implementation we chose a simple two dimensional Thermal Conduction problem, where Temperature is one and only index which we assume to change. Thus it makes it a one-degree of freedom problem which is quite easy to solve using the concepts of FEM.

The Problems Parameters are as follows,

1) Problem consists of a square shaped two-dimensional body, where we can manually specify the division of nodes and elements as per our will
2) The scenario is a One-Degree of Freedom problem where each element is a four noded quadrilateral.

The Boundary Conditions are as follows,

1) Constant heat flux of 1 W/m^2 at top and bottom edge of square body.
2) Constant Temperature of 1^0C at the left edge of square body.
3) Insulated boundary condition at right edge of square body.
4) No Heat Generation per unit volume involved.



The following problem was picked, as because it had less complexity involved and was perfect to start with. Us being new to this field required something which was less typical and easy to compare and run our code, and thus this was selected.

We had access to a MATLAB code for the following problem which helped us to generate solutions for the desired number of elements. The number of elements could be easily changed inside the code and subsequently run to get the solution for it. The code also generates the stiffness matrix and the right hand matrix for the subsequent iterations. We generated many such combinations and ran these different cases for our code. Our code generated answers with high precision and optimum time which we again compared with a solution from the pre-existing library **Eigen.** We will be exploring the results and comparisons later in this report.

Literature Review

To solve the linear system of equations **Ax = B**, one of the popular methods of computation has been the Direct Solver in the form of **Gaussian Elimination**. The Gaussian Elimination(GE) procedure primarily involves two steps of computation:

1) Decomposing the matrix **A** into the product of two matrices: **L** and **U** matrices.

2)Solving **Ly = B** and **Uz = y** by forward and backward substitutions respectively.

The above procedure, as a result ,had to store **L** and **U** matrices for carrying out the respective substitutions and hence, comprised of a storage requirement of order of square of **m**. The fallout of such an approach was that for matrices of a greater size(such as order of 10^9) , the computations tend to become redundant and slower due to large storage spaces required even for the NULL values and hence, the huge sizes of the matrix **A**.
Hence, to cope up with the real time and space constraints and maintain the efficiency of our solver , we settled on the Iterative Conjugate Gradient Method(CG) as the best approach to tackle such a problem involving multiple computations with large Sparse Matrices having most of its elements as NULL values(zeroes). Moreover, our coefficient matrix **A** is symmetric and positive definite(SPD), hence making it possible to utilize the CG approach.With regards to the time complexity among the various techniques, we observed that the CG method is better than every other optimal steepest descent method as the former converges to a solution point faster with every iteration of the algorithm , owing to the utilization of the scalar preconditioner variable Beta(elaborated later) which improves the direction of convergence of the solution after every iteration in the CG technique.

The iterative CG method is the best for implementation of our future algorithm on GPU parallel systems as they are inexpensive in memory and much time efficient in computations than the direct solvers similar to GE. This was made possible by the incorporation of a sparse storage technique known as Compressed Row Storage(CRS) method into our Conjugate Gradient algorithm.

The most important measure of the efficiency of our algorithm has been the comparison with the standard & recognized library for employing CG method in sparse matrices, namely : EIGEN.

Eigen is a C++ template library for linear algebra: matrices, vectors, numerical solvers, and related algorithms. Computations were performed for sparse coefficient matrices with sizes varying from (4X4) to (3600X3600), corresponding to number of elements varying from 2 to 50 respectively, in each of the mutually perpendicular 2-dimensional direction, and the resulting efficiency and correctness was compared between our own implementation and the Eigen library.

Compressed sparse row format

The **Compressed Sparse Row** (CSR) format represents a matrix **M** by three (one-dimensional) arrays, that respectively contain nonzero values, the extents of rows, and column indices. This format allows fast row access and matrix-vector multiplications (M*y*). The CSR format stores a sparse matrix **M** in row form using three (one-dimensional) arrays namely **"val, row_ptr, col_ind"**. Let **"nnz"** denote the number of nonzero entries in **M**.

The array **"val"** is of length **"nnz"** and holds all the nonzero entries of **M** in left-to-right top-to-bottom ("row-major") order.

The array **"row_ptr"** is of length ***m*** + 1. It is defined by this recursive definition:

- **row_ptr**[0] = 0
- **row_ptr**[*i*] = **row_ptr**[*i* − 1] + number of nonzero elements on the (*i* − 1)-th row in the original matrix
- Thus, the first ***m*** elements of **row_ptr** store the index into **val** of the first nonzero element in each row of **M**, and the last element **row_ptr**[***m***] stores **nnz**, the number of elements in **val**.

The third array, **col_ind**, contains the column index in **M** of each element of **val** and hence is of length **nnz** as well.

Using the following format of storage of sparse matrices, we were able to reduce the total number of multiplications to a large extent, as this particular method takes care of neglecting the multiplications done with **zero-elements** present in the stiffness matrix, thus reducing the time and computation.

The algorithm used for multiplying matrices stored in CSR format is as below :

Initialize Vector R to {0}

m = number of rows in Matrix A

Iterate i from 0 to m

Iterate j from row_ptr[i] to row_ptr[i+1]

R[i,0]=R[i,0]+val[j]*Z[col_ind[j],0]

Solver's CPU Implementation

As discussed above, we have deduced why **Conjugate Gradient** or **CG** method is best for our scenario and our above stated problem statement. In this section we will discuss how did we implement the following method to solve the above-said problem.

Conjugate Gradient Method as discussed above is often implemented as an iterative algorithm where we derive subsequent results from the previous ones.
Just to start with an overview, if we want to solve a system of linear equations,

$$\mathbf{A\,x=b}$$

for the vector x where the known $n \times n$ matrix **A** is **symmetric**, **positive definite**, and **real**, and **b** is known as well. We denote the unique solution of this system by **x**.

Now before entering into the actual algorithm, few terms are to be defined here,

*A **symmetric matrix** is a square **matrix** that is equal to its transpose.*

$$\mathbf{A^T=A}$$

A positive definite matrix is a symmetric matrix with all positive eigenvalues.

$$\mathbf{uAu^T}>0$$

Two non-zero vectors are said to be conjugate with respect to **A** *if,*

$$\mathbf{u^TAv}=0$$

From the above, since **A** is symmetric and positive definite, the left-hand side defines an inner product.

$$\mathbf{\langle u,v\rangle_A := \langle Au,v\rangle = \langle u,A^Tv\rangle = \langle u,Av\rangle = uA^Tv}$$

Two vectors are conjugate if and only if they are orthogonal with respect to this inner product. Being conjugate is a symmetric relation: if **u** is conjugate to **v**, then **v** is conjugate to **u**.
Now that we have defined the necessary terms we will first know how does the solution set depends upon a set of particular directions which are mutually conjugate to each other. Let us suppose that $P=\{\mathbf{p_1},\mathbf{p_2}, \dots , \mathbf{p_n}\}$ are mutually conjugate vectors.Now they form the basis for R_n, and we may express the solution $\mathbf{x}_*$ of **A x = b** in this basis :

$$\mathbf{x}_* = \sum_{i=1}^{n} \alpha_i \mathbf{p}_i$$

Based on this expansion we calculate:

$$\mathbf{A}\mathbf{x}_* = \sum_{i=1}^{n} \alpha_i \mathbf{A}\mathbf{p}_i$$

$$\mathbf{p}_k^T \mathbf{A}\mathbf{x}_* = \sum_{i=1}^{n} \alpha_i \mathbf{p}_k^T \mathbf{A}\mathbf{p}_i$$

$$\mathbf{p}_k^T \mathbf{b} = \sum_{i=1}^{n} \alpha_i \langle \mathbf{p}_k, \mathbf{p} \rangle_A$$

$$\langle \mathbf{p}_k, \mathbf{b} \rangle = \alpha_k \langle \mathbf{p}_k, \mathbf{p} \rangle_A$$

$$\alpha_k = \langle \mathbf{p}_k, \mathbf{b} \rangle / \langle \mathbf{p}_k, \mathbf{p} \rangle_A$$

This gives the following method for solving the equation **Ax** = **b**: find a sequence of *n* conjugate directions, and then compute the coefficients α_k.

If we choose the conjugate vectors $\mathbf{p}_k$ carefully, then we may not need all of them to obtain a good approximation to the solution $\mathbf{x}_*$. So, we want to regard the conjugate gradient method as an iterative method. This also allows us to approximately solve systems where *n* is so large that the direct method would take too much time.

We denote the initial guess for $\mathbf{x}_*$ by $\mathbf{x}_0$. We can assume without loss of generality that $\mathbf{x}_0 = \mathbf{0}$. Starting with $\mathbf{x}_0$ we search for the solution and in each iteration we need a metric to tell us whether we are closer to the solution $\mathbf{x}_*$ (that is unknown to us). This metric comes from the fact that the solution $\mathbf{x}_*$ is also the unique minimizer of the following quadratic function;

$$\mathbf{f(x)} = \tfrac{1}{2} \mathbf{x}^T \mathbf{A}\mathbf{x} - \mathbf{x}^T \mathbf{b}$$

This suggests taking the first basis vector p_0 to be the negative of the gradient of **f(x)** at $x = x_0$. The gradient of **f(x)** equals **Ax** − **b**. Starting with a "guessed solution" x_0 (we can always guess $x_0 = 0$), this means we take $\mathbf{p_0} = \mathbf{b} - \mathbf{A}\mathbf{x_0}$. The other vectors in the basis will be conjugate to the gradient, hence the name *conjugate gradient method*. Let $\mathbf{r}_k$ be the residual at the *k*th step:

$$\mathbf{r_k} = \mathbf{b} - \mathbf{A}\mathbf{x_k}$$

Note that r_k is the negative gradient of **f(x)** at $x = x_k$, so the gradient descent method would be to move in the direction r_k. Here, we insist that the directions p_k be conjugate to each other.

We also require that the next search direction be built out of the current residue and all previous search directions, which is reasonable enough in practice.

This results in the following expression,

$$\mathbf{p_k = r_k - \sum_{i<k} (p_i^T A r_k / p_i^T A p_i) * p_i}$$

Following this direction, the next optimal location is given by,

$$\mathbf{x_{k+1} = x_k + \alpha_k p_k} \text{ , and}$$

$$\alpha_k = \mathbf{(p_k^T r_{k-1}) / (p_k^T A p_k)}$$

A closer analysis of the algorithm shows that r_{k+1} is orthogonal to p_i for all $i < k$, and therefore only r_k, p_k, and x_k are needed to construct r_{k+1}, p_{k+1}, and x_{k+1}.

Thus the final algorithm is as follows,

r_0 := b - Ax_0

p_0 := r_0

k :=0

repeat

$\alpha_k := \mathbf{(r_k^T r_k) / (p_k^T A p_k)}$

$\mathbf{x_{k+1} = x_k + \alpha_k p_k}$

$\mathbf{r_{k+1} = r_k - \alpha_k A p_k}$

if r_{k+1} is sufficiently small then exit loop

$\beta_k = \mathbf{(r_{k+1}^T r_{k+1}) / (r_k^T r_k)}$

$\mathbf{p_{k+1} = r_{k+1} + \beta_k p_k}$

k=k+1

end repeat

The result is x_{k+1}

Graphs and Analytical Data

The above drawn table of data has the following parameters :

Number of Elements	Size of Matrix	Time1 (in sec)	N1 iterations	Time2 (in sec)	N2 iterations
2	4	0	1	0	0
3	9	0.001	9	0.001	2
4	16	0.001	16	0.002	4
5	25	0.001	25	0.002	5
6	36	0.004	36	0.011	12
7	49	0.006	49	0.019	12
8	64	0.011	64	0.061	24
9	81	0.014	81	0.074	17
10	100	0.023	100	0.21	34
11	121	0.034	121	0.28	31
12	144	0.051	144	0.67	51
13	169	0.064	169	0.648	37
14	196	0.079	196	1.423	62
15	225	0.101	225	1.468	47
16	256	0.152	256	2.864	72
17	289	0.152	289	2.843	55
18	324	0.214	324	5.009	82
19	361	0.314	361	4.826	63
20	400	0.357	400	8.541	92
21	441	0.528	441	8.373	71
22	484	0.568	484	14.172	102
23	529	0.739	529	14.63	79
24	576	0.863	576	22.827	113
25	625	0.995	625	22.254	87
26	676	1.284	676	33.669	122
27	729	1.245	729	31.278	101
28	784	1.498	784	48.313	132
29	841	1.623	841	44.256	102
30	900	2.089	900	69.749	142
31	961	2.126	961	61.735	109
32	1024	2.723	1024	95.379	152
33	1089	2.182	1089	81.579	117
34	1156	3.228	1156	126.542	162
35	1225	3.235	1225	110.37	123
36	1296	10.707	1296	171.505	172
37	1369	4.465	1369	146.789	131
38	1444	5.339	1444	226.119	181
39	1521	5.967	1521	209.805	149
40	1600	6.09	1600	281.078	191
41	1681	7.29	1681	271.081	157
42	1764	15.805	1764	477.94	201
43	1849	13.655	1849	408.021	153
44	1936	12.12	1936	552.622	211
45	2025	10.187	2025	437.038	173
46	2116	12.314	2116	595.934	220
47	2209	12.157	2209	491.537	167
48	2304	14.192	2304	789.347	247
49	2401	16.049	2401	604.858	174
50	2500	16.988	2500	1337.75	240
51	2601	17.234	2601	738.372	181
52	2704	34.965	2704	1472.2	249
53	2809	28.313	2809	1225.64	188
54	2916	24.895	2916	3089.49	258
55	3025	34.324	3025	1499.81	213
56	3136	29.286	3136	2075	268
57	3249	39.7	3249	1870.35	220
58	3364	38.47	3364	2968.33	300
59	3481	40.82	3481	2392.05	229
60	3600	48.927	3600	3054.83	287

Column 1: Number of Elements in the Sparse Coefficient Matrix in one orthogonal direction, which varies from 2 to 60 in our experimental data.

Column 2: Size of the coefficient matrix which is (N X N), where N varies from (4 to 3600).

Column 3: Time (T1) in seconds required for the developed solver to achieve the results for a given matrix size n.

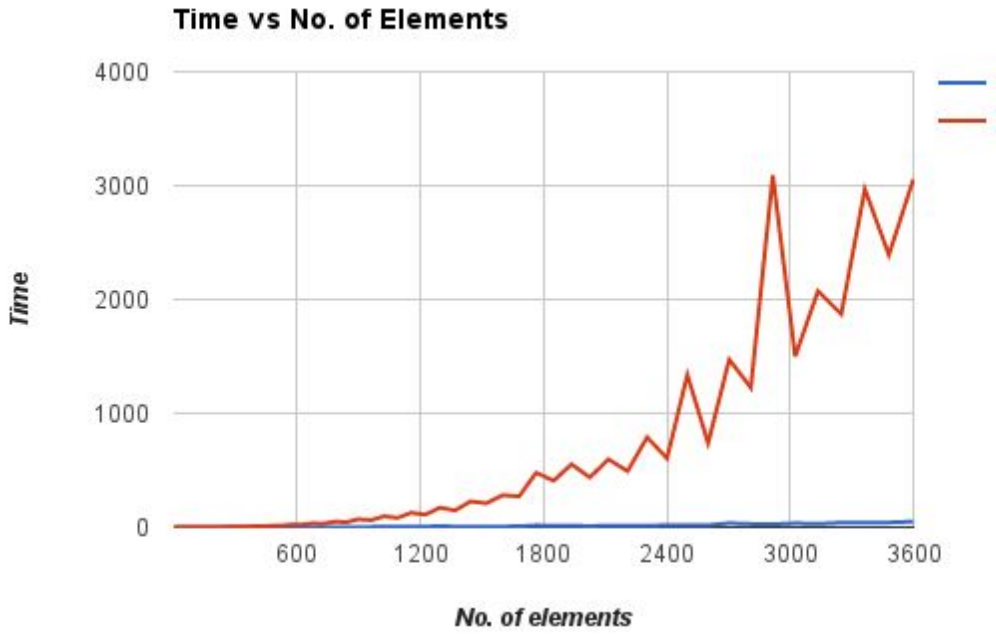
Column 4: Number of Iterations N1 of the developed algorithm to achieve the final solution with optimum accuracy for a given input matrix size N.

Column 5: Time (T2) in seconds required for the standard Eigen solver to achieve the results for a given matrix size N.

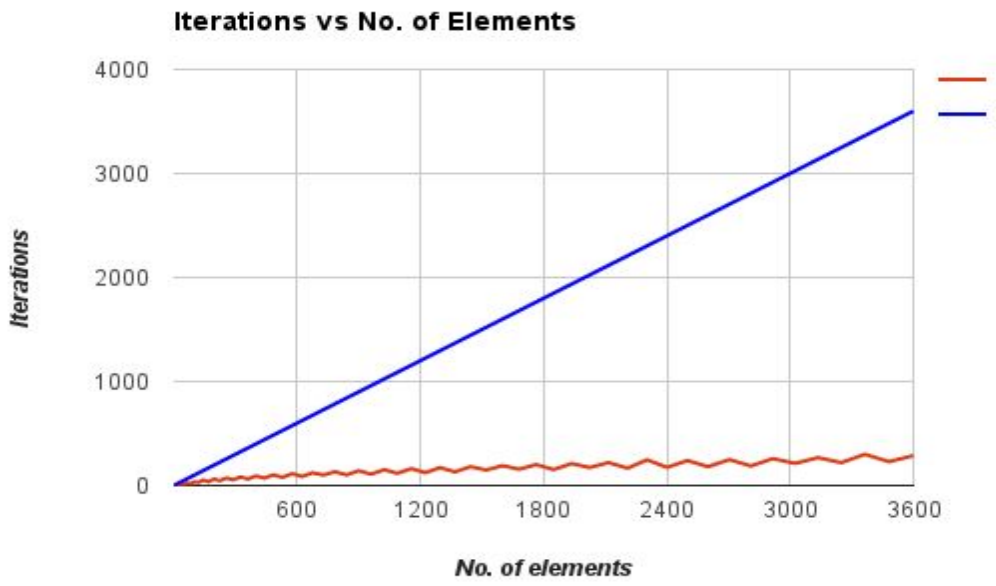
Column 6: Number of Iterations N2 of the standard Eigen algorithm to achieve the final solution for a given input matrix size n.

Keep in mind that in the following graphs, the color Blue is corresponding to our developed Scalable Solver whereas the color Red is corresponding to the standard Eigen Solver.

Graph 1:



Graph 2:



Conclusions

From the obtained graphical data and analysis, we can construe the following experimental conclusions:

1) As observed from Graph 1, the time complexity of both the developed solver and the pre-existent standard Eigen solver increases with the increase in the input size of the sparse coefficient matrix A.

2) From Graph 1, comparing the time complexities of the two, we conclude that the time complexity of our algorithm is better than that of the standard Eigen Library by a factor of order hundred or more for the whole input range varying from SPD(symmetric positive definite) matrices of size(4X4) to (3600X3600).

3) The sparse storage CRS format consists of 3 sparse storage vectors which greatly optimizes the space complexity of our algorithm, corresponding to the **eigen::makeCompressed()** command in the standard library.The conclusion (2) is true despite the fact that the number of iterations performed by our algorithm to reach the end result is far greater(usually by a factor of 100) than the standard library algorithm. It is worth noting that the number of iterations for both the procedures increase with the increase in the input size, in order to reach the final minimum residue solution.

4) Hence, we comfortably manage to maintain the accuracy of our results(cross checked by the results from MATLAB solver and the solutions from the library) within the recommended time and space constraints.Thus, we can finally reach the conclusion that the CG solver developed in our project work achieves the result for the given initial problem maintaining the accuracy till four places of decimal for every numerical element in the solution, and that too within much better time complexity and utilization of greater number of iterations for every input matrix of size(**m x m**), where **m** varies from 4 to 3600 in the experimental data.

5) The much better performance of our solver algorithm within the constraints of the initial value problem can be owed to the multiple optimizations done at each mathematical and storage operation within the iterative technique(for instance, the vector multiplication of sparse matrices), which are handled by our own custom developed optimized functions to carry out particular operations in the solver.

Future Work

Keeping in mind the above drawn conclusions, we can thoroughly map our path to future perspectives such as computation in GPU parallel systems utilizing the Parallel Programming and Computing Platform CUDA . CUDA is a parallel computing platform and application programming interface (API) model created by Nvidia.

Such parallel computations on each elementary step of our CG method greatly improves the time complexity from our benchmark of CPU computations performed till now, and corresponding to our competition with the Eigen Library in CPU systems, puts us in place to further compute even with the more robust Cusp library for GPU parallel systems.Cusp is a library for sparse linear algebra and graph computations and it provides a flexible, high-level interface for manipulating sparse matrices and solving sparse linear systems.

Furthermore, as a future objective, we aim to optimize the CG method according to the parallel computational environment using a particular system of Kernels of synchronous threads depending on the space and time constraints of the calculation, multiplying it with the optimizations of the storage technique CRS(compressed row storage).

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