## Reducing Memory Access Latencies using Data Compression in Sparse, Iterative Linear Solvers

An All-College Thesis

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Abstract

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### 1 Introduction

### 2 Background

### 2.1 Conjugate Gradient

Conjugate Gradient is the iterative solver used by HPCG [1]. Symmetric, positive definite matrices will guarantee the converge of Conjugate Gradient to the correct solution within n iterations, where n is the number of dimensions, when using exact algebra [4]. More importantly, Conjugate Gradient can be used as in iterative method, providing a solution,  $\vec{x}$ , where  $\|\mathbf{A}\vec{x} - \vec{b}\|$  is within some tolerance, after significantly fewer than n iterations, allowing it to find solutions to problems where even n iterations is infeasible [5].

To understand the Conjugate Gradient, first consider the quadratic form of  $\mathbf{A}\vec{x} = \vec{b}$ . The quadratic form is a function  $f: \mathbb{R}^n \to \mathbb{R}$  where

$$f(\vec{x}) = \frac{1}{2}\vec{x}^T \mathbf{A}\vec{x} - \vec{b} \cdot \vec{x} + c \tag{1}$$

for some  $c \in \mathbb{R}$ . Note that

$$\nabla f(\vec{x}) = \frac{1}{2} (\mathbf{A} + \mathbf{A}^T) \vec{x} - \vec{b}$$

Then, when **A** is symmetric,

$$\nabla f(\vec{x}) = \mathbf{A}\vec{x} - \vec{b}$$

So, the solution to  $\mathbf{A}\vec{x} = \vec{b}$  is the sole critical point of f [3]. Since  $\mathbf{A}$  is the Hessian matrix of f at the point, if  $\mathbf{A}$  is positive definite, then that critical point is a minimum. Thus, if  $\mathbf{A}$  is a symmetric, positive definite matrix, then the minimum of f is the solution to  $\mathbf{A}\vec{x} = \vec{b}$  [5].

The method of Steepest Decent is useful for understanding Conjugate Gradient, because they both use a similar approach to minimize Equation 1, and thus solve  $\mathbf{A}\vec{x} = \vec{b}$ . This shared approach is to take an initial  $\vec{x}_0$  and move downwards in the steepest direction, within certain constraints, of the surface defined by Equation 1 [3]. Because the gradient at a point is the direction of maximal increase,  $\vec{x}$  should be moved in the opposite direction of the gradient. Thus, to compute the next value of  $\vec{x}$ , use

$$\vec{x}_{i+1} = \vec{x}_i + \alpha_i \vec{r}_i \tag{2}$$

for some  $\alpha_i > 0$  and where  $\vec{r}_i = -\nabla f(\vec{x}_i) = \vec{b} - \mathbf{A}\vec{x}_i$  is the residual of  $\vec{x}_i$ . Since  $\mathbf{A}\vec{x} = \vec{b}$  is the only critical point and a minimum of the quadratic function, f, the ideal value of  $\alpha_i$  is the one that minimizes  $f(\vec{x}_{i+1})$ . Thus, choose  $\alpha_i$  such that

$$0 = \frac{\mathrm{d}}{\mathrm{d}\alpha_{i}} f\left(\vec{x}_{i+1}\right)$$
$$= \frac{\mathrm{d}}{\mathrm{d}\alpha_{i}} f\left(\vec{x}_{i} + \alpha \vec{r}_{i}\right)$$
$$\alpha_{i} = \frac{\vec{r}_{i} \cdot \vec{r}_{i}}{\vec{r}_{i} \cdot \mathbf{A} \vec{r}_{i}}.$$

Note that by using Equation 2, we can derive

$$\vec{r}_{i+1} = \vec{r}_i - \alpha \mathbf{A} \vec{r}_i. \tag{3}$$

Because  $\mathbf{A}\vec{r_i}$  is already computed to find  $\alpha_i$ , using Equation 3 to compute the residual results in one less matrix-vector product per iteration. The steps for the Method of Steepest Decent are

$$\vec{r}_0 = \vec{b} - \mathbf{A}\vec{x}_0$$

$$\alpha_i = \frac{\vec{r}_i \cdot \vec{r}_i}{\vec{r}_i \cdot \mathbf{A}\vec{r}_i}$$

$$\vec{x}_{i+1} = \vec{x}_i + \alpha_i \vec{r}_i$$

$$\vec{r}_{i+1} = \vec{r}_i - \alpha \mathbf{A}\vec{r}_i$$

until  $\|\vec{r}_i\|$  is less than some tolerance [5].

**Example 1.** Consider the linear system

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$$

and use c = 0. Note that the solution is

$$\vec{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$
.

When starting at the origin, the iteration of Method of Steepest Decent becomes

$$\vec{x}_{0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \vec{r}_{0} = \begin{bmatrix} 5 \\ 5 \end{bmatrix} \qquad \alpha_{0} = 2/7$$

$$\vec{x}_{1} = \begin{bmatrix} 10/7 \\ 10/7 \end{bmatrix} \qquad \vec{r}_{1} = \begin{bmatrix} 5/7 \\ -5/7 \end{bmatrix} \qquad \alpha_{1} = 2/3$$

$$\vec{x}_{2} = \begin{bmatrix} 40/21 \\ 20/21 \end{bmatrix} \qquad \vec{r}_{2} = \begin{bmatrix} 5/21 \\ 5/21 \end{bmatrix} \qquad \alpha_{2} = 2/7$$

$$\vec{x}_{3} = \begin{bmatrix} 290/147 \\ 50/49 \end{bmatrix} \qquad \vec{r}_{3} = \begin{bmatrix} 5/147 \\ -5/147 \end{bmatrix} \qquad \alpha_{3} = 2/3$$

$$\vdots \qquad \vdots \qquad \vdots$$

The  $\vec{x}_i$ 's are plotted with a contour graph of the quadratic form in Figure 1.  $\square$ 

The Conjugate Directions family of linear solvers, of which Conjugate Gradient is a member of, attempts to improve on the number of iterations needed by Steepest Decent. [5]. Note that, in Example 1, the directions of  $\vec{r}_0$  and  $\vec{r}_2$  are the same and the directions of  $\vec{r}_1$  and  $\vec{r}_3$  are the same. Thus, the same direction has to be traversed multiple times. Additionally, note that the two sets of residual directions are perpendicular to each other. Conjugate Directions attempts

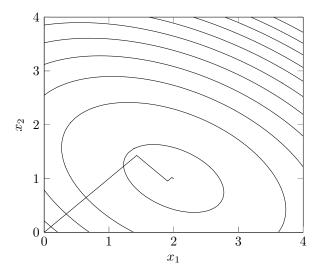


Figure 1: Contour graph of the quadratic function and the first six values of  $\vec{x}$  produced by steepest decent for Example 1

to improve on this, by making the search directions,  $\vec{d_0}, \vec{d_1}, \ldots$ , **A**-orthogonal to each other and only moving  $\vec{x}$  once in each search direction. Two vectors,  $\vec{u}, \vec{v}$  are **A**-orthogonal, or conjugate, if  $\vec{u}^T \mathbf{A} \vec{v} = 0$ . The requirement for Conjugate Directions is to make  $\vec{e}_{i+1}$  **A**-orthogonal to  $\vec{d_i}$ , where  $\vec{e}_i = \vec{x_i} - \mathbf{A}^{-1} \vec{b}$  is the error of  $\vec{x_i}$ . The computation of  $\alpha_i$  changes to find the minimal value along  $\vec{d_i}$  instead of  $\vec{r_i}$ .

$$\alpha_i = \frac{\vec{d}_i^T \vec{r}_i}{\vec{d}_i^T \mathbf{A} \vec{d}_i}.$$

Conjugate Gradient is a form of Conjugate Directions where the residuals are made to be **A**-orthogonal to each other. This is done using the Conjugate Gram-Schmidt Process. To do this, each search direction,  $\vec{d_i}$  is computed by taking  $\vec{r_i}$  and removing any components that are not **A**-orthogonal to the previous  $\vec{d'}$ s. So, let  $\vec{d_0} = \vec{r_0}$  and for i > 0 let

$$\vec{d_i} = \vec{r_i} + \sum_{k=0}^{i-1} \beta_{(i,k)} \vec{d_k}$$

with  $\beta_{(i,k)}$  defined for i > k. Then, solving for  $\beta_{(i,k)}$  gives

$$\beta_{(i,k)} = -\frac{\vec{r}_i \cdot \mathbf{A} \vec{d}_i}{\vec{d}_j \cdot \mathbf{A} \vec{d}_j}.$$

Note that each residual is orthogonal to the previous search directions, and thus the previous residuals. So, it can be shown that  $\vec{r}_{i+1}$  is **A**-orthogonal to

all previous search directions, except  $\vec{d_i}$  [5]. Then,  $\beta_{(i,k)} = 0$  for  $i - 1 \neq k$ . To simplify notation, let  $\beta_i = \beta_{(i,i-1)}$ . So, each new search direction can then be computed by

$$\vec{d_i} = \vec{r_i} + \beta_i \vec{d_{i-1}}.$$

This results in the following steps for Conjugate Gradient

$$\begin{split} \vec{d}_0 &= \vec{r}_0 = \vec{b} - \mathbf{A} \vec{x}_0 \\ \alpha_i &= \frac{\vec{r}_i \cdot \vec{r}_i}{\vec{d}_i \cdot \mathbf{A} \vec{d}_i} \\ \vec{x}_{i+1} &= \vec{x}_i + \alpha_i \vec{d}_i \\ \vec{r}_{i+1} &= \vec{r}_i - \alpha \mathbf{A} \vec{d}_i \\ \beta_{i+1} &= \frac{\vec{r}_{i+1} \cdot \vec{r}_{i+1}}{\vec{r}_i \cdot \vec{r}_i} \\ \vec{d}_{i+1} &= \vec{r}_{i+1} + \beta_{i+1} \vec{d}_i \end{split}$$

continuing the iteration until  $\|\vec{r}_i\|$  is less than the specified tolerance.

**Example 2.** Consider the linear system used in Example 1 where

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}.$$

The result of applying Conjugate Gradient is

$$\vec{x}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \vec{r}_0 = \begin{bmatrix} 5 \\ 5 \end{bmatrix} \qquad \vec{d}_0 = \begin{bmatrix} 5 \\ 5 \end{bmatrix} \qquad \alpha_0 = 2/7$$

$$\vec{x}_1 = \begin{bmatrix} 10/7 \\ 10/7 \end{bmatrix} \qquad \vec{r}_1 = \begin{bmatrix} 5/7 \\ -5/7 \end{bmatrix} \qquad \beta_1 = 1/49 \qquad \vec{d}_1 = \begin{bmatrix} 40/49 \\ -30/49 \end{bmatrix} \qquad \alpha_1 = 7/10$$

$$\vec{x}_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \qquad \vec{r}_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Note that after two iterations,  $\vec{x}$  reaches the exact solution, compared to the iterations of Steepest Decent in Example 1. Figure 2 shows the values of  $\vec{x}$  with the contour graph of the quadratic function.

One way to improve the Conjugate Gradient method is to precondition the system [4]. Instead of solving the original system,  $\mathbf{A}\vec{x} = \vec{b}$ , Conjugate Gradient solves  $\mathbf{M}^{-1}\left(\mathbf{A}\vec{x} - \vec{b}\right) = 0$  instead, where  $\mathbf{M}^{-1}$  is the preconditioner. Note that  $\mathbf{M}$  should be similar to  $\mathbf{A}$ , but  $\mathbf{M}^{-1}$  should be easier to compute than  $\mathbf{A}^{-1}$ . Algorithm 1 shows the preconditioned variant of the Conjugate Gradient.

### 2.2 Multigrid Preconditioner with Gauss-Seidel Step

Multigrid solvers are a class of methods designed for solving discretized partial differential equations (PDEs) and take advantage of more information that just

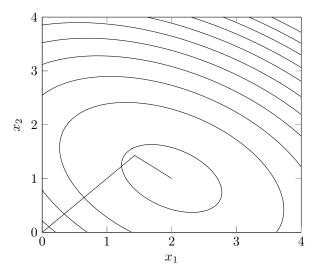


Figure 2: Contour graph of the quadratic function and the each value of  $\vec{x}$  produced by Conjugate Gradient for Example 2

the coefficient matrix and the right hand side [4]. In particular, the solvers use discretizations with different mesh sizes to improve performance of relaxation based solvers. In HPCG, a multigrid solver with high tolerance is used as the preconditioner [1]. Because the solver provides an approximation to  $\mathbf{A}^{-1}$ , the preconditioned matrix is an approximation of  $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$ . This reduces the condition number of the linear system, and so, reduces the number of iterations needed for Conjugate Gradient to converge [4].

The multigrid method works by using meshes of different sizes to allow a relaxation style iterative solver to make the best progress at different levels of meshes [4]. Most relaxation type iterative solvers are able to quickly reduce the components of the residual in the direction of eigenvectors associated with large eigenvalues for the iteration matrix. Such eigenvectors are called high frequency modes. The other components, in the direction of eigenvectors called low frequency modes, are difficult to reduce with standard relaxation. However on a courser mesh, many of these low frequency modes are mapped to high frequency modes [4]. Thus, by applying a relaxation type iterative solver at various mesh sizes, the various components of the residual can be reduced quickly.

In HPCG, a symmetric Gauss-Seidel iteration is used as the relaxation iteration solver at each level of coarseness [1]. The symmetric Gauss-Seidel iteration consists of a forward Gauss-Seidel iteration followed by a backward Gauss-Seidel iteration. Letting  ${\bf A}={\bf L}+{\bf D}+{\bf U}$  where  ${\bf L}$  is strictly lower triangular,  ${\bf D}$  is

### Algorithm 1 Preconditioned Conjugate Gradient [4]

```
\begin{split} \vec{r_0} \leftarrow \vec{b} - \mathbf{A} \vec{x}_0 \\ \vec{z_0} \leftarrow \mathbf{M}^{-1} \vec{r}_0 \\ \vec{d_0} \leftarrow \vec{z}_0 \\ \text{for } i = 0, 1, \dots \text{ until } \|\vec{r_i}\| \leq \epsilon \text{ do} \\ \alpha_i \leftarrow \frac{\vec{r_i} \cdot \vec{z}_i}{\vec{d_i} \cdot \mathbf{A} \vec{d_i}} \\ \vec{x}_{i+1} \leftarrow \vec{x}_i + \alpha_i \vec{d_i} \\ \vec{r}_{i+1} \leftarrow \vec{r}_i + \alpha_i \mathbf{A} \vec{d_i} \\ \vec{z}_{i+1} \leftarrow \mathbf{M}^{-1} \vec{r}_{i+1} \\ \beta_{i+1} \leftarrow \frac{\vec{r}_{i+1} \cdot \vec{z}_{i+1}}{\vec{r}_i \cdot \vec{z}_i} \\ \vec{d}_{i+1} \leftarrow \vec{z}_{i+1} + \beta_{i+1} \vec{d_i} \\ \text{end for} \end{split}
```

diagonal and U is strictly upper case, the iteration can be represented by

$$\vec{x}_i^* = \mathbf{D}^{-1} \left( \vec{b} - \mathbf{L} \vec{x}_i^* - \mathbf{U} \vec{x}_i \right)$$
$$\vec{x}_{i+1} = \mathbf{D}^{-1} \left( \vec{b} - \mathbf{U} \vec{x}_{i+1} - \mathbf{L} \vec{x}_i^* \right).$$

Note that while  $\vec{x}_i^*$  and  $\vec{x}_{i+1}$  are on both sides of the equation where they are respectively computed, they can be computed with this formulation by computing the entries in order as they become available for the product with L and U respectively.

# 2.3 Problem Setup of High Performance Conjugate Gradient

The problem used to create the linear system used by HPCG, and thus by this project, is a three dimensional partial differential equation (PDE) model [1]. This problem is approximating the function u(x, y, z) over the three dimensional rectangular region  $\Omega \in \mathbb{R}^3$  such that

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0,$$

with u(x, y, z) = 1 along the boundaries of  $\Omega$ . Note that the solution is u(x, y, z) = 1 over  $\Omega$ . The linear system is created by using the finite difference method with a 27-point stencil on the PDE over a rectangular grid with nodes of fixed distance. The matrix's diagonal consists of the value 26, and -1's fill the entries for the row's 26 grid neighbors. The right hand side of the equation has a value of 14 for corner points, 12 for edge points, 9 for side points and 0 for interior points [2]. The solution vector consists of all 1's.

HPCG uses an implementation of Conjugate Gradient algorithm with a multigrid preconditioner variant [1]. As HPCG is designed to emulate the performance characteristics of real world problems with out needing to be a robust

Strategy	Vector Values	Matrix Values	Matrix Indices
Single Precision	Yes	Yes	Not Able
Mixed Precision	Yes	Not Able	Not Able
1 Bit	Not Able	Yes	Not Able
Squeeze (SZ)	Yes	Yes	Yes
ZFP	Yes	Yes	No
Elias Gamma	Not Able	Not Able	Yes
Elias Delta	Not Able	Not Able	Yes
Huffman	Not Able	No	Yes
Op Code	Not Able	Not Able	Yes

Figure 3: Overview of Compression Strategies

solver, it only uses 3 levels of grid coarseness with only a since smoother pass at the coarsest grid level. The smoother used by the multigrid is based on a symmetric Gauss-Seidel step, however each process uses the old value for entries located on other processes. The restriction operation simply samples half the points in dimension, resulting in a reduction of grid size by a factor of eight in each level of coarseness. To prolong the coarse grids, each coarse point is added to the fine point in was sampled from. The zero vector is used as the overall initial guess for x, as well as the initial guess for each grid level in the multigrid cycle.

# 2.4 Data Access Patterns of High Performance Conjugate Gradient

#### 2.5 Compression Strategies

Numerous compression strategies were considered for this project. Figure 3 lists the compressions tried for each main data structure. Note that most compression methods were only used with one or two of the data types, even if able to be reasonably used within the constraints of additional data.

- 2.5.1 Restrictions on Compression Strategies
- 2.5.2 Single and Mixed Precision Floating Point Numbers
- 2.5.3 1 bit Compression
- 2.5.4 Squeeze (SZ) Compression
- 2.5.5 ZFP Compression
- 2.5.6 Elias Gamma Coding and Delta Coding
- 2.5.7 Op-Code Compression
- 2.5.8 Huffman Coding
- 2.5.9 Combined Compression Strategies

### 3 Test Results

### 4 Conclusions and Future Work

### 5 References

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