Vector and Parallel Tuning of Solid Earth Simulation Codes

- GeoFEM and Householder QR Decomposition -

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Abstract

In this paper, we discuss vector and parallel tuning of GeoFEM and the Householder QR decomposition process being solid earth simulation codes.

Process of GeoFEM code can be roughly divided into two parts, Matrix Assemble part and Solver part. Currently, GeoFEM's parallel iterative solver has attained good parallel and vector performance, and GeoFEM's Matrix Assemble part has attained good parallel performance too. The remaining problem is vector performance of Matrix Assemble part. In this study, we mainly focused on vector optimization of Matrix Assemble Part and vector performance of whole GeoFEM Test Code. In vector performance of whole GeoFEM Test Code, finally, 45% for peak performance (SX-4 /peak : 2GFlops) was obtained by changing loop structure. In this paper, we describe evaluation of vector/parallel performance of Householder QR decomposition processes in a new geodetic inversion method. Finally, 9.23GFlops was obtained for total performance by 8PE(SX-4/peak : 16Gflops).

Introduction

GeoFEM is being developed as parallel finite element platform for Solid Earth Simulation. In the codes of the finite element method which uses the implicit method/the semi-implicit method, the processing of such kind of finite element method codes can be roughly divided into two parts. First part, is calculates the coefficient of the composition equation(Matrix assemble part). Second part, it solves the system of linear equation(Solver part). In 1998, very large scale linear elastic problem was solved by GeoFEM on University Tokyo's Hitachi SR2201 using 1,000 processors. The two parts of GeoFEM (Matrix assemble part and Solver part) has got at good parallel performance, but single PE performance was very bad[1]. GeoFEM's one of the target machines is the Earth Simulator which is Vector and Parallel machine. Currently, GeoFEM's parallel iterative solver has attained good parallel and vector performance. The remaining problem is vector performance of Matrix Assemble part. We have made a GeoFEM Test Code which have similar GeoFEM Matrix Assemble process and real GeoFEM Solver process. In this study, we mainly focused on vector optimization of Matrix Assemble Part and vector performance of whole GeoFEM Test Code.

We uses Iterative Methd at GeoFEM solver. But people using Dilect Methd solver to solve Solid Earth problems are not few. In order to estimate spatio-temporal distribution of fault slip from time-dependent crustal deformation data, T.Sagiya developed a new geodetic inversion method. In this paper, we describe evaluation of vector/parallel performance of Householder QR decomposition processes in a new geodetic inversion method.

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Vector Optimization of Matrix assemble part in GeoFEM Test Code

Outline of Original code of Matrix assemble part

Loop structure of matrix assemble part for original code is shown in Fig.1.

The outermost 3 loops are 'typewriter scanned' elements loops. 'typewriter scan' is a rectangular sweep for the nested loops consecutively. Jacobian calculating process and element stiffness matrix calculating process are inside the outermost 3 loops. The element stiffness matrix calculating process assembles whole stiffness matrix. This process is constructed from 2 loops which have 8 elements for each loop. This 8 means number of node for hexahedral element. Innermost 3 loops corresponds to integral calculation for each local Coordinates $\xi - \eta - \zeta$ of element.

The integral point for each local coordinate is 2, therefore, we can't get good vector calculation performance for short vector.

Optimization Manner

Strategy for Optimization Manner is loop exchange putting a element loop into innermost loop for getting long vector length. If a elements loop is single loop, a processes of adding up numerical value to same node is produced. This process causes recursive reference for a elements loop. We divided elements loop into some small loops of groups having no recursive reference. Moreover, we divided each groups having no recursive reference into some loops for saving the memory storage of jacobian calculation results. Elements loop was divided finally into 3 loops ,to do dividing for loops of above 2 times.Loop construction is described below(Fig.2).

Outermost loop is a first element loop. Next second loop is a second element loop. We put the jacobian calculating process and the element stiffness matrix calculating process into a second loop. In the jacobian calculating process, we put a third element loop into 3 loops for integral calculation. In the element stiffness matrix calculating process, outer loop is 2 loops (8X8) assembling whole stiffness matrix. We put a loop of integral calculating for ζ coordinate into a outer loop and put a third element loop into a loop of integral calculating for ζ . In a third loop of elements, 2 loops having each 2 elements for integral

calculating for $\xi - \eta$ coordinates were replaced 4 (=2*2) lines operations.

Problem definision

Test problem definision is below.
-Elastic Stracture Analysis for Cube Shape
-50000 Elements
-164000 DOF

Performance

Performance and operation counts of each process is depicted in Fig.2. CPUtime/FLOPS of matrix assembling process was 28.8sec/53.3MFlops(sx-4 /peak : 2GFlops) before vector tuning, and 2.09sec/736.8MFlops(same machine) after tuning. CPUtime/FLOPS of whole test Code was 11.18sec/900.7MFlops(same machine). 4.88sec/2.06GFlops was attained on vpp5000 (peak : 9.6GFlops).

Vector/Parallel Optimization of Householder QR Decomposition

Outline of Householder QR Decomposition

Composition matrix is rectangular matrix in the householder QR decomposition for the new geodetic inversion method. The householder QR decomposition algorithm have 3 loops. First loop is j1 loop,and second loop is j3 loop(Fig.3). Innermost loop is i1 loop, and contains 3 processes. A first process is sum of squares for row elements, second process is to exchange pivot between 2 rows, and third is main QR Decomposition process depicting Fig.3. A third process is constructed by calculating inner product ,and calculating of addition/subtraction for vector.

Optimization Manner

First manner is to divide 1 loop into pivoting process loop and main process loop. Second manner is to change access manner for array data of main process from Indirect Access manner to Direct Access manner. Third manner is to parallelize sum of squares process and main process. Both pivoting and main processes has no dependency in calculating for loop data, and these processes can be parallelized for calculation of loop data. In this study, our target machine is sx-4 having 1 node by 8PEs shared memory machine. We used directive parallelized maner, because simple coding can be possible in the shared memory machine.

Performance

Matrix size of the Housholder QR decomposition is 4284*1070. CPUtime/FLOPS of Housholder QR decomposition process was 260.3sec/51.8MFlops(Alpha 21164 533MHz) before tuning, and 9.9sec/1.36Glops(sx-4 /peak : 2GFlops) after tuning. In parallel performance, 99.0% was obtained by 2PE, 92.7% was obtained by 4PE, 84.8% was obtained by 8PE. 9.23GFlops was obtained of total performance by 8PE. (Table 2).

```
do kk1= 1, NZ
 do jj1= 1, NY
  do ii1= 1, NX
   |-jacobian calculate
   do ie= 1, 8
    do je= 1, 8
     do kpn= 1, 2
      do jpn= 1, 2
       do ipn= 1, 2
        |-stiffness matrix calculate
       enddo
      enddo
     enddo
    enddo
   enddo
  enddo
 enddo
enddo
```

Fig.1 Loop structure of matrix assemble part
for original code

```
do loer = 1,50
 do lpn = 1,numlp+1
  do kp=1,2
   do jp=1,2
    do ip=1,2
     do ijk = 1,llnum
      |-jacobian calculate
     enddo
    enddo
   enddo
  enddo
  do ie= 1, 8
   do je= 1, 8
    do kpn= 1, 2
     do ijk = 1,llnum
      |-stiffness matrix calculate
     enddo
     do ijk = 1,llnum
      |-stiffness matrix calculate
     enddo
    enddo
   enddo
  enddo
 enddo
enddo
```

Fig.2 Loop structure of matrix assemble part
for tuned code

Process	Operation Count(Flop)	Dec		SX-4		VPP5000	
		Cputime	Mflops	Cputime	Mflops	Cputime	Mflops
Bounbary condition Matrix Assemble Solver Pre Process	1.54G	0.54 11.85 0.07	123.6	0.19 1.73 0.17	736.8	0.04 0.76 0.11	1692.3
Solver	8.53G	197.10	43.3	9.09	938.4	3.97	2148.6
Total	10.07G	209.56	48.1	11.18	900.7	4.88	2063.5

Table1 Performance and operation counts of each process

$$(Q_kA)_j = \mathbf{a}_j - \alpha\left(\mathbf{w}^T \bullet \mathbf{a}_j\right)\mathbf{w}$$
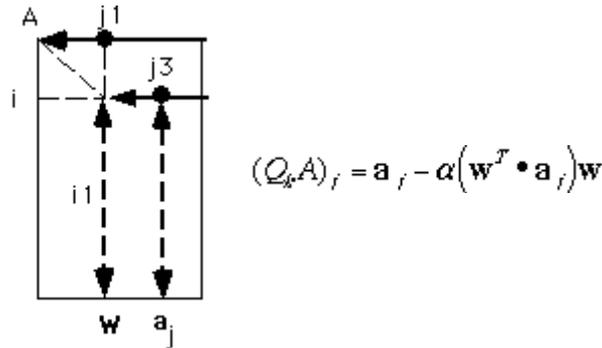
Fig.3 Housholder QR Decomposition process

	DEC	SX-4 1PE	SX-4 2PE	SX-4 4PE	SX-4 8PE
Operation count	13460Mflop				
Cputime(sec)	260.3	9.9	5.00	2.67	1.46
Parallel performance			99.0%	92.7%	84.8%
Total Performance (Mflops)	52	1360	2690	5040	9230

Table2 Performance of Householder QR Decomposition

Acknowledgments

References

[1] K.Garatani,H.Nakamura,H.Okuda,G.Yagawa,GeoFEM:High Performance Parallel FEM for Solid Earth,Proceedings of 7th High-Performance Computing and Networking(HPCN Europe'99),LNCS-1593,133-140,1999.