#### Parallel Preconditioning Method for III-Conditioned Problems

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#### Large-scale Simulations by Parallel FEM Procedures

- Unstructured grid with irregular data structure
- Large-scale sparse matrices
- Preconditioned parallel iterative solvers
- "Real-world" ill-conditioned problems





#### What are ill-conditioned problems ?

- Various ill-conditioned problems
  - For example, matrices derived from coupled NS equations are ill-conditioned even if meshes are uniform.
- In this work, we are focusing on 3D solid mechanics applications with:
  - heterogeneity
  - contact conditions
  - BILU/BIC
- Ideas can be extended to other fields.

#### **III-Conditioned Problems** Heterogeneous Fields, Distorted Meshes



#### Contact Problems in Simulations of Earthquake Generation Cycle



#### Preconditioning Methods (of Krylov Iterative Solvers) for Real-World Applications

- are the most critical issues in scientific computing
- are based on
  - Global Information: condition number, matrix properties etc.
  - Local Information: properties of elements (shape, size ...)
- require knowledge of
  - background physics
  - applications

#### Technical Issues of "Parallel" Preconditioners in FEM

- Block Jacobi type Localized Preconditioners
- Simple problems can easily converge by simple preconditioners with excellent parallel efficiency.
- Difficult (ill-conditioned) problems cannot easily converge
  - Effect of domain decomposition on convergence is significant, especially for ill-conditioned problems.
    - Block Jacobi-type localized preconditioiners
    - More domains, more iterations
  - There are some remedies (e.g. deep fill-ins, deep overlapping), but they are not efficient.
  - ASDD does not work well for really ill-conditioned problems.

#### Technical Issues of "Parallel" Preconditioners for Iterative Solvers



 If domain boundaries are on "stronger" elements, convergence is very bad.

#### **3D Linear Elastic Problem with 20<sup>3</sup> Tri-Linear Hexahedral Elements**



#### Number of Iterations for Convergence BILU(0)-GPBiCG with 8 domains

- - : E=1.00
- 1-processor
  - $\blacksquare$  : E=10<sup>0</sup> , 31 iterations
  - E=10<sup>+3</sup>, 84 iterations
    - Harder, More ill-conditioned
- 8-processors (MPI, no-overlapping)
  - ■: E=10<sup>0</sup>, 52 iter's(×1.68)
  - ■: E=10<sup>+3</sup>, 158 iter's(×1.88)



#### **Remedies: Domain Decomposition**

- Avoid "Strong Elements"
  - not practical
- Extended Depth of Overlapped Elements
  - Selective Fill-ins, Selective Overlapping [KN 2007]
    - adaptive preconditioning/domain decomposition methods which utilize features of FEM procedures
- PHIDAL/HID (Hierarchical Interface Decomposition) [Henon & Saad 2007]
- Extended HID [KN 2009]

#### **Extension of Depth of Overlapping**



Cost for computation and communication may increase



# Number of Iterations for Convergence BILU(0)-GPBiCG, 8-domains (PE's)

Effect of Extended Depth of Overlapping



| Depth of<br>Overlap | E=10 <sup>0</sup> | E=10 <sup>3</sup> |
|---------------------|-------------------|-------------------|
| 0                   | 52                | 158               |
| 1                   | 33                | 103               |
| 2                   | 32                | 100               |
| 3                   | 32                | 97                |
| 4                   | 31                | 82                |
| Single<br>Domain    | 31                | 84                |

#### Final goal of this work

- Development of robust and efficient parallel preconditioning method
- Construction of strategies for optimum selection of preconditioners, partitioning, and related methods/parameters, such as:
  - Selective Fill-ins
  - Selective Overlapping/HID

#### How to get to the final goal ?

- Utilization of both of:
  - global information obtained from derived coefficient matrices
  - very local information, such as information of each mesh in finite-element applications.
- Usually, this type of work mainly focuses on features of derived coefficient matrices (e.g. ILUT)
  - In real applications, convergence of parallel iterative solvers is often affected by local heterogeneity and/or discontinuity of the field, as shown in this presentation.

#### Overview

#### Background

- Selective Blocking
- More General Problems
  - Extension of Overlapped Zones
- Preconditioning/Partitioning Methods
  - Target Application
  - Selective Fill-ins, Selective Overlapping
- HID
  - Hierarchical Interface Decomposition
- Extended HID
- Fields with Heterogeneity

#### Initial Motivation: Contact Problems in Simulations of Earthquake Generation Cycle

- Quasi-static stress accum. process at plate boundaries
- Non-linear contact problems with Newton-Raphson iter's
- Ill-conditioned linear equations due to penalty constraint by ALM (Augmented Lagrangean).
- Parallel FEM with domain decomposition (GeoFEM)



#### **Contact Problems in Simulations of Earthquake Generation Cycle**

- Assumptions (GeoFEM: <u>http://geofem.tokyo.rist.or.jp/</u>)
  - Infinitesimal deformation, static contact relationship.
    - Location of nodes is in each "contact pair" is identical.
    - "Consistent" node number and position
- Large-scale problems
  - Parallel preconditioned iterative solvers
- Special preconditioning : Selective Blocking.
  - provides robust and smooth convergence in 3D solid mechanics simulations for geophysics with contact.
- Special partitioning

Contact

Surface

# Special Method for Contact Problem

Strongly coupled nodes are put into the same diagonal block. Full LU factorization for each block.



#### **More General Problems**

- Moving boundaries due to large slip conditions
- Inconsistent node number (and location) at boundary surfaces
  - Assembly structure for machine parts.
    - where meshes for each part are separately generated.
  - Commercial FEM codes (e.g. ABAQUS, NASTRAN) can treat problems for this type of "inconsistent" cases. (single PE, direct method for linear equations).







#### Example of Assembly Structure Jet Engine



## More General Problems

#### **Inconsistent Number of Nodes at Boundary Surfaces**

- Difficult to apply "selective blocking"
  - Size of each "selective block" may be too large for full LU factorization
- Difficult to apply "special partitioning"
- Remedy
  - Higher-order fill-in's
  - Extension of overlapped zones for parallel computing







# Number of Iterations for Convergence BILU(0)-GPBiCG, 8-domains (PE's)

Effect of Extended Depth of Overlapping



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- Background
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  - More General Problems
    - Extension of Overlapped Zones
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# Robust and efficient preconditioning for parallel iterative solvers in more general cases

- Selective fill-ins for serial & parallel computing
- Selective overlapping for parallel computing
- Features of individual element are utilized.

### **Example for "Inconsistent" Cases**

This model simulates contact problem in assembly structure



- Each block is discretized into cubic tri-linear elements
  elastic material: E= 1.00, Poisson ration= 0.25
- Each block is connected through elastic truss elements generated on each node on contact surfaces.
  - Truss elements are crossing.

### **Example for "Inconsistent" Cases**

This model simulates contact problem in assembly structure



- Elastic coefficient of truss elements is set to 10<sup>3</sup> times as large as that of solid elements.
  - This condition simulates constraint boundary conditions for contact.
- Distributed uniform force at z=z<sub>max</sub> surface

- u=0@x=0, v=0@y=0, w=0@z=0

#### **Selective Fill-ins [KN 2007]**

- Apply higher order of fill-ins between nodes which connect to truss-type elements.
  - Similar concept as "selective blocking"
- In this work: **BILU(1+)** 
  - BILU(2) for these special nodes (2nd order fill-ins)
  - BILU(1) for general nodes (1st order fill-ins)
- Cost is similar to that of BILU(1), but effect of preconditioning is expected to be competitive with that of BILU(2).

#### Idea of "Selective Fill-ins": ILU(1+)



- 2nd order fill-in's are considered for these nodes
- 2nd order fill-in's are NOT considered for these nodes
- 2nd order fill-in's are NOT considered for these nodes

#### Summary of Problem Setting Single Core

- Problem Size
  - 32,768 elements (except truss's) 117,708 DOF
- Preconditioned GPBiCG [Zhang, 1997]
  - for general matrices, although the matrices are SPD
    - BILU(0,1,2), Selective Fill-in (BILU(1+))
- Environment
  - dual-core AMD Opteron 275 (2.2GHz)
  - F90 + MPI

#### **Results: Single Core** 107,811 DOF, λ=10<sup>3</sup>, ε=10<sup>-8</sup>







#### Selective Overlapping [KN 2007]

- Same rules in "selective fill-ins" are applied to extention of overlapping zones.
  - Similar concept as "selective blocking"
- In selective overlapping, extension of overlapping for nodes that are not connected to special elements for contact conditions is *delayed*.
- The increase in cost for computation and communication by extension of overlapped elements is suppressed.

#### **Internal Nodes for Partitioning**





#### One-Layer Overlapping (d=0/1)

Internal Nodes
External Nodes
Overlapped Elements



This is the general configuration of local data set for parallel FEM (one-layer of overlapping).

#### Extension of Overlapped Zones Internal Nodes (2-layers: d=2)



#### Extension of Overlapped Zones Internal Nodes (d=2 and d=1+)




#### Extension of Overlapped Zones Internal Nodes (d=2 and d=1+)



Selective Overlapping (d=1+) "Delayed" extension for elements which do not include nodes connected to truss-type elements



#### Extension of Overlapped Zones Internal Nodes (d=3 and d=2+)





#### **BILU** with selective fill-in/overlapping

- **BILU** (**p**)-(**d**)
  - **p** level of fill-ins (0, 1, 1+, 2, 2+ ...)
  - **d** depth of overlapping (0, 1, 1+, 2, 2+ ...)

#### Summary of Problem Setting Multiple Cores

- Problem Size
  - Large: 1,000,000 elements (except truss's), 3,152,412 DOF
- Preconditioned GPBiCG [Zhang, 1997]
  - for general matrices, although the matrices are SPD
  - Localized preconditioning (block Jacobi type)
    - BILU(0,1,2), Selective Fill-in (BILU(1+))
- Partitioning
  - GeoFEM-based local data structure: http://geofem.tokyo.rist.or.jp/
  - Recursive Coordinate Bisection (RCB): 8~64
    - <u>Selective Overlapping</u>
- Environment
  - 64-core AMD Opteron 275 (2.2GHz), Infiniband
  - F90 + MPI

#### Domain boundaries are on "truss's"



#### **Results: 64 cores**

3,090,903 DOF,  $\lambda$ =10<sup>3</sup>,  $\epsilon$ =10<sup>-8</sup> Effect of Overlapping

BILU(1)-(d)
 BILU(1+)-(d)
 BILU(2)-(d)





#### **Results: 64 cores**

3,090,903 DOF,  $\lambda$ =10<sup>3</sup>,  $\epsilon$ =10<sup>-8</sup> Effect of Overlapping

BILU(1)-(d)
 BILU(1+)-(d)
 BILU(2)-(d)





#### **Results: 64 cores**

#### 3,090,903 DOF, $\lambda$ =10<sup>3</sup>, $\epsilon$ =10<sup>-8</sup> Effect of Overlapping





#### Summary

- Selective Fill-ins
- Selective Overlapping
  - Features of FEM applications (element-by-element) are utilized
  - Factorization processes are executed according to information of each element
    - much cheaper than ILUT-based methods, where dropping rules are applied after forming entire matrix
- Generally, BILU(1+)-(1+) is robust and efficient
- Significant improvement of convergence if d (depth of overlapping) is 0⇒1⇒1+.

- Background
  - Selective Blocking
  - More General Problems
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- Preconditioning/Partitioning Methods
  - Target Application
  - Selective Fill-ins, Selective Overlapping
- HID
  - Hierarchical Interface Decomposition
- Extended HID
- Fields with Heterogeneity

#### HID: Hierarchical Interface Decomposition [Henon & Saad 2007]

- Multilevel Domain Decomposition
  - Extension of Nested Dissection
- Non-overlapping at each level: Connectors, Separators
- Suitable for Parallel Preconditioning Method



#### Parallel ILU for each Connector at each LEVEL

- The unknowns are reordered according to their <u>level</u> numbers, from the lowest to Level-1
- The block structure of the reordered matrix leads to natural parallelism if ILU/IC decompositions or forward/backward Level-4 substitution processes are applied.



#### Communications at Each Level Forward Substitutions

```
do lev= 1, LEVELtot
  do i= LEVindex(lev-1)+1, LEVindex(lev)
    SW1 = WW(3*i-2,R); SW2 = WW(3*i-1,R); SW3 = WW(3*i,R)
    isL= INL(i-1)+1; ieL= INL(i)
    do j= isL, ieL
      k = IAL(j)
      X1 = WW(3*k-2,R); X2 = WW(3*k-1,R); X3 = WW(3*k,R)
      SW1= SW1 - AL(9*j-8)*X1 - AL(9*j-7)*X2 - AL(9*j-6)*X3
      SW2 = SW2 - AL(9*j-5)*X1 - AL(9*j-4)*X2 - AL(9*j-3)*X3
      SW3 = SW3 - AL(9*i-2)*X1 - AL(9*i-1)*X2 - AL(9*i)*X3
    enddo
    X1 = SW1; X2 = SW2; X3 = SW3
    X2 = X2 - ALU(9*i-5)*X1
    X3= X3 - ALU(9*i-2)*X1 - ALU(9*i-1)*X2
    X3 = ALU(9*i) X3
    X2 = ALU(9*i-4)*(X2 - ALU(9*i-3)*X3)
    X1 = ALU(9*i-8)*(X1 - ALU(9*i-6)*X3 - ALU(9*i-7)*X2)
    WW(3*i-2,R) = X1; WW(3*i-1,R) = X2; WW(3*i,R) = X3
                                                            Additional
  enddo
                                                            Comm.
  call SOLVER SEND RECV 3 LEV(lev,...):
                                          Communications using
                                          Hierarchical Comm. Tables.
enddo
```

#### HID: Hierarchical Interface Decomposition [Henon & Saad 2007]

- Multilevel Domain Decomposition
- Non-overlapped Approach
  - see the paper for detailed information
- Suitable for Parallel Preconditioning Method
- Comparison with Selective Overlapping
  - Cost of HID corresponds to that of (d=0) or (d=1), but as robust as (d=1+) or (d=2)
  - More robust than Block Jacobi.

#### Results: 64 cores Contact Problems 3,090,903 DOF





- Background
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  - More General Problems
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#### Weakness of Original HID

- Original HID cannot consider the effects of fill-ins of higher order at boundary nodes.
  - although it's perfect for parallel ILU(0).



#### **Extended Version of HID**

- Extension of Overlapped Elements
- Thicker Layers of Separators

#### Sample Graph

(A) could be referred from (B) for ILU(2) (depends on numbering)



#### Sample Graph

## (A) CANNOT be referred from (B) for ILU(2), because they are at same level and on different domain



level-1 
level-2

#### Domain Decomposition & Local Data Set





Node-based Domain Decomposition (Internal Nodes)



Distributed Local Data (Internal+External Nodes)

#### **Original Local Data Set**

- Original HID
  - NO overlapping/1-layer overlapping
  - cannot consider the effects of fill-ins of higher order for external nodes at same level.
    - Effect of "A" is not considered for "B" in BILU(2)

#### **Distributed Local Data**



B

#### Remedy 1: Extension of Overlapping

level-1

level-2

- Extension of Overlapping
  - 2-layer overlapping
  - can consider the effects of fill-ins of higher order for external nodes at same level.
    - Effect of B can be considered for A in BILU(2)
  - But still localized, Block
     Jacobi approach
    - because the value at "A" is not the most recent one

**Distributed Local Data** 



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Range for "Global" Operations"



#### **Remedy 2: Thicker Separator Layers**

- Thicker Separator
  - <u>HID-new</u>
  - can consider the effects of fill-ins of higher order for external nodes at same level.
    - Effect of "A" can be considered for "B" in BILU(2)
  - In global manner
  - seems to provide more robust convergence than Remedy 1.
  - difficulty for loadbalancing

**Distributed Local Data** 



Range for "Global" Operations"



- Background
  - Selective Blocking
  - More General Problems
    - Extension of Overlapped Zones
- Preconditioning/Partitioning Methods
  - Target Application
  - Selective Fill-ins, Selective Overlapping
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#### **Target Application (1/3)**

• 3D linear elastic problem with locally distorted elements



#### **Target Application (2/3)**

- 3D linear elastic problem with locally distorted elem's
- Initial mesh: cube
  - distortion around Z-axis of each element
- Local Heterogeneity
  - local "intensity" of distortion
  - sequential Gauss algorithm [Deutsch & Journel 1988]





### **Target Application (3/3)**





- 3D linear elastic problem with locally distorted elements
- Very ill-conditioned for significant distortion
  - requires BILU(2) or higher
  - semi indefinite
- Maximum distortion= 200 deg.
- Strong Scaling
  - 128<sup>3</sup> Elements
  - 6,440,067 Unknowns

#### Selective Fill-ins/Overlapping with Threshold

- **BILU**  $(\mathbf{p}, \boldsymbol{\omega})$ - $(\mathbf{d}, \boldsymbol{\alpha})$ 
  - If E >  $\omega$  selective fill-ins is applied
  - If E >  $\alpha$  selective overlapping is applied



•: fill-ins of higher order and extension of overlapping are allowed on these nodes

#### Results: 64 cores Distorted Meshes BILU( $p,\theta$ )-( $d,\alpha$ ) 3,090,903 DOF MAX distortion: 150-deg.

BILU(1)-(d,α) GPBiCG
 BILU(1+,120°)-(d,α)
 BILU(1+, 60°)-(d,α)
 BILU(1+, 30°)-(d,α)
 BILU(2)-(d,α)

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(θ,α)



#### Results: 64 cores Distorted Meshes BILU( $p,\theta$ )-( $d,\alpha$ ) 3,090,903 DOF MAX distortion: <u>225-deg.</u>







# Selective Blocking/Overlapping does not work well in this case !

- 150 deg.: BILU(1)-(1)
- 225 deg.: BILU(2)-(2)

#### Software, Linear Solvers

MPI + FORTRAN90 (Hitachi Compiler)

Flat MPI

- NUMA control: Optimum case
  - numactl --cpunodebind=\$SOC --membind=\$SOC
- Finite-Element Method
  - Tri-linear hexahedral elements
- Linear Solver
  - GPBiCG [Zhang 1997]
- Preconditioners
  - Block ILU(2,t): 2nd order of fill-ins, Threshold parameter
  - keep  $m_{ij}$  component of preconditioner [M] if  $m_{ji} > t$ 
    - t=0: Original BILU(2)
  - Optimum value of "t" @512 cores= 0.02~0.03

#### Hardware Environment

- "T2K Open Super Computer (Tokyo)"
  - T2K/Tokyo
  - Total 952 nodes (15,232 cores)
    - each node = 4x AMD Quadcore Opteron Socket (Barcelona)
  - 45th in TOP500 (NOV. 2009)
- up to 32 nodes (512 cores) in this work





#### **Strategies for Domain Decomposition**

- BILU (2,t, loc-**d**)
  - Localized Block Jacobi with extended overlapping
  - d: Depth of overlapping
    - BILU(2,t,loc-1), BILU(2,t,loc-2), BILU(2,t,loc-3)
- BILU (2,t, org-**d**)
  - Original HID (HID-org) with extended overlapping
    - BILU(2,t,org-1), BILU(2,t,org-2)
- BILU (2,t, new-**d**)
  - HID with extended overlapping/thicker separators: HID-new
    - BILU(2,t,new-1), BILU(2,t,new-2)
    - 3 layers for level-2 separators
    - NO special treatment for load-balancing

#### **Strategies for Domain Decomposition**

#### **Original HID**



level-1 ● level-2 ● level-4 ○

#### **HID-new**



level-1 ● level-2 ● level-3 ● ● ● ● level-4 ○
### Strong Scaling, 128<sup>3</sup> elements MAX: 200 deg., Scalability



• Normalized by performance of BILU(2,0.03,new-1) at each core

### Localized Block Jacobi BILU(2,t,loc-d): not robust



- BILU(2,t,loc-2) is the best
  - although BILU(2,t,loc-d)'s do not converge in some cases.
- Performance is generally worse than BILU(2,t,new-1) with HID

Parallel Preconditioning

# Orig. HID with Extended Overlapping BILU(2,t,org-1)



• BILU(2,t,org-1) gets unstable, as core number increase (>128).

Parallel Preconditioning

# Orig. HID with Extended Overlapping BILU(2,t,org-d)



Extended overlapping provides robustness: BILU(2,t,org-d)

Parallel Preconditioning

#### New HID with Extended Overlapping BILU(2,t,new-d)



• BILU(2,t,new-d)'s generally more robust and efficient, if number of cores is larger (BILU(2,t,org-d)'s are better, if core# is smaller).

# Strong Scalability: 32~512 cores

Performance of BILU(2,0.03,new-1) with 32 cores= 32.0



#### **Bottlenecks for Scalability**

- Additional Communications
  Load Imbalance (512 cores) in HID-org/HID-new
  - rate for entire solver time

- - Standard Deviation ( $\sigma$ )
    - BILU(2,t,loc-**d**) 85
    - BILU(2,t,org-**d**) 155



# Summary

- Extended version of HID
  - Extension of overlapped elements between domains
  - Thicker separators
- Extended HID provides more robust and scalable performance than original HID and localized block Jacobi BILU
  - Effect of *thicker separator* is very significant if the number of core is larger.
    - more effective than deeper overlapping
  - Extended HID with thicker separator can introduce effect of external nodes efficiently in factorization and forward/backward substitution processes with higher order of fill-ins.

#### **Future Works**

- Evaluation of feasibility for various types of applications of:
  - Localized Block Jacobi with Extended Overlapping
    - also selective fill-ins, selective overlapping
  - Original HID, New HID
- Development of sophisticated domain partitioner for complicated geometries
  - key technology for practical application of extended HID to real applications.
  - *Thickening* of separator layers should be considered at every level for robust convergence.
    - Only at level-2 layers in the present work
  - Load-balancing for *extend HID* 
    - another big technical issue to be solved in the future.