Parallel ILU(0)/SGS

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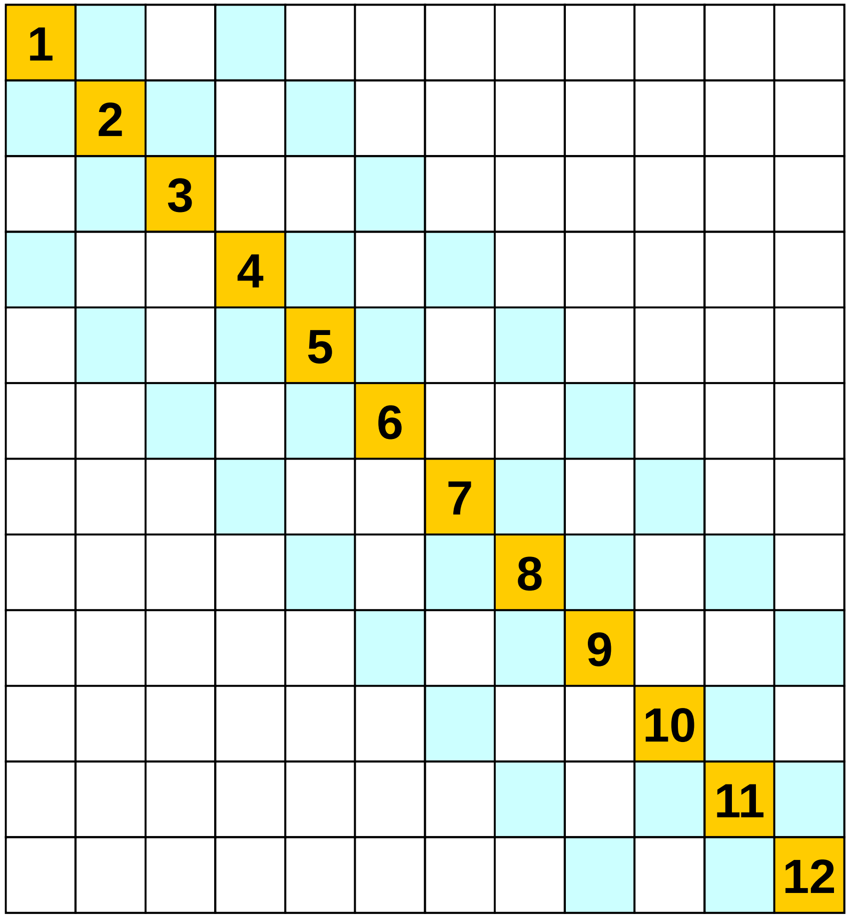
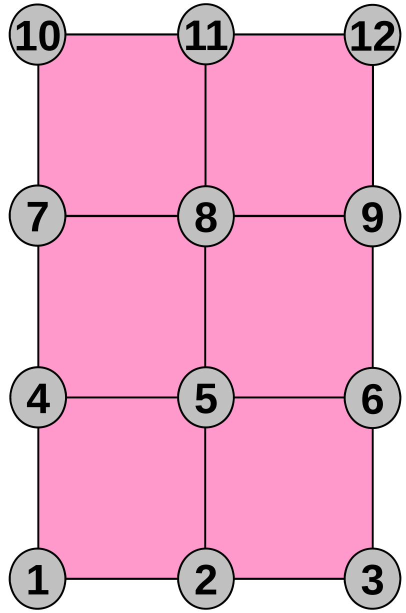
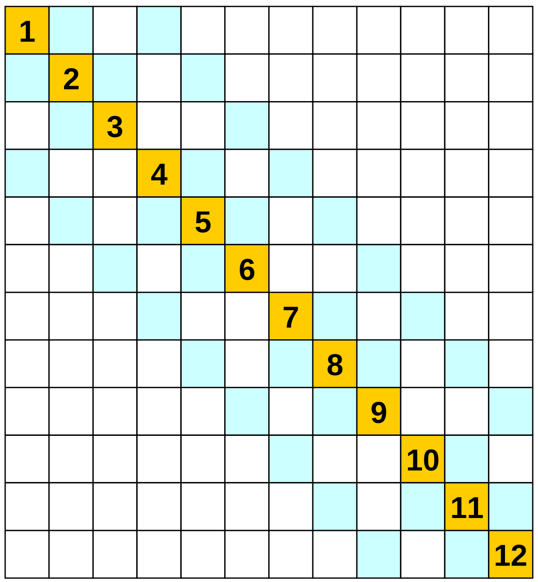
Example: 5-Point Stencil (FDM)

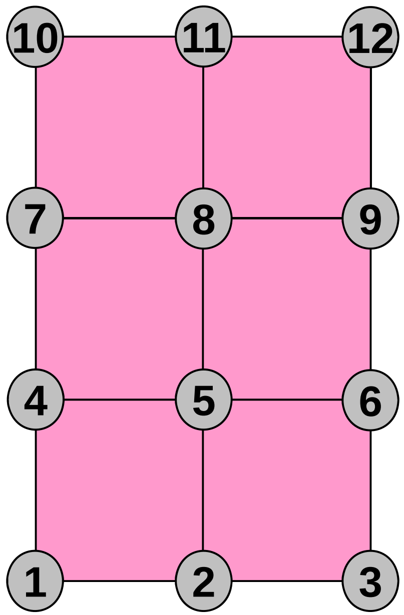




Solution

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00		0.00
−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.00		3.00
0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	3.00		10.00
−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	4.00		11.00
0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	5.00		10.00
0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	6.00	=	19.00
0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	7.00		20.00
0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00	8.00		16.00
0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00	9.00		28.00
0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00	10.00		42.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00	11.00		36.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	12.00		52.00





Complete LU Factorization

type "./lu1"

Original Matrix

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	0.00	6.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−1.00	0.00	−1.00	6.00

LU Factorization

Both of [L] and [U] are shown

Diag. of [L] are "1" (not shown)

fill-in occurs: some of zero components became non-zero.

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63

Incomp. LU fact. with no fill-in's

type "./lu2"

Incomplete LU Factorization without fill-in's

Both of [L] and [U] are shown

Diag. of [L] are "1" (not shown)

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

LU Factorization

Both of [L] and [U] are shown

Diag. of [L] are "1" (not shown)

fill-in occurs: some of zero components became non-zero.

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63

Slightly “Inaccurate” Solution

Incomplete LU

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	→	0.92
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		1.75
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00		2.76
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00		3.79
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00		4.46
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00		5.57
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00		6.66
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00		7.25
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00		8.46
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00		9.66
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00		10.54
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65		11.83

Complete LU

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	→	1.00
−0.17	5.83	−1.00	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		2.00
0.00	−0.17	5.83	−0.03	−0.17	−1.00	0.00	0.00	0.00	0.00	0.00	0.00		3.00
−0.17	−0.03	0.00	5.83	−1.03	0.00	−1.00	0.00	0.00	0.00	0.00	0.00		4.00
0.00	−0.17	−0.03	−0.18	5.64	−1.03	−0.18	−1.00	0.00	0.00	0.00	0.00		5.00
0.00	0.00	−0.17	0.00	−0.18	5.64	−0.03	−0.18	−1.00	0.00	0.00	0.00		6.00
0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01	−1.00	0.00	0.00		7.00
0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03	−0.18	−1.00	0.00		8.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63	−0.03	−0.18	−1.00		9.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	−0.03	−0.01	5.82	−1.03	−0.01		10.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	−0.03	−0.18	5.63	−1.03		11.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.63		12.00

ILU(0), IC(0)

- “Incomplete” factorization without fill-in’s
  - Reduced memory, computation
- Solving equations by ILU(0)/IC(0) factorization provides slightly “inaccurate” solution, although it’s not far from exact one.
  - “Accurateness” depends on problems (feature of equations).

Full LU and ILU(0)/IC(0)

Full LU

```
do i= 2, n
  do k= 1,  i-1
    a_ik := a_ik/a_kk
    do j= k+1, n
      a_ij := a_ij - a_ik*a_kj
    enddo
  enddo
enddo
```

ILU(0) : keep non-zero pattern of the original coefficient matrix

```
do i= 2, n
  do k= 1,  i-1
    if ((i,k)∈ NonZero(A)) then
      a_ik := a_ik/a_kk
    endif
    do j= k+1, n
      if ((i,j)∈ NonZero(A)) then
        a_ij := a_ij - a_ik*a_kj
      endif
    enddo
  enddo
enddo
```

Deep Fill-in: ILU(p)/IC(p)

p: level of fill-in. If “p” increases, ILU(p)/IC(p) become closer to complete ILU/IC and provide more robust preconditioners, but become more expensive: <u>trade-off</u>

```
LEV_ij=0 if ((i,j)∈ NonZero(A)) otherwise LEV_ij= p+1

do i= 2, n
  do k= 1,  i-1
    if (LEV_ik≦p) then
      a_ik := a_ik/a_kk
    endif
    do j= k+1, n
      if (LEV_ij = min(LEV_ij, 1+LEV_ik+ LEV_kj)≦p) then
        a_ij := a_ij - a_ik*a_kj
      endif
    enddo
  enddo
enddo
```

LU Gauss-Seidel (LU-GS)
LU Symmetric GS (LU-SGS)
in this class

- ILU(0)

```
do i= 2, n
    do k= 1,  i-1
      if ((i,k)∈ NonZero(A)) then
        a_ik := a_ik/a_kk
      endif
      do j= k+1, n
        if ((i,j)∈ NonZero(A)) then
          a_ij := a_ij - a_ik*a_kj
        endif
      enddo
    enddo
  enddo
```

LU Gauss-Seidel (LU-GS)
LU Symmetric GS (LU-SGS)
in this class

- More Simplified Version of ILU(0)

```
do i= 2, n
    do k= 1,  i-1
      if ((i,k)∈ NonZero(A)) then
        a_ik := a_ik/a_kk
      endif
      do j= k+1, n
        if ((i,j)∈ NonZero(A)) then
          a_ij := a_ij - a_ik*a_kj
        endif
      enddo
    enddo
  enddo
```

Only do this

LU Gauss-Seidel (LU-GS)
LU Symmetric GS (LU-SGS)
in this class

- More Simplified Version of ILU(0)

$$
\begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
l_{21} & 1 & 0 & \cdots & 0 \\
l_{31} & l_{32} & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
l_{n1} & l_{n2} & l_{n3} & \cdots & 1
\end{pmatrix}
=
\begin{pmatrix}
1 & 0 & 0 & \cdots & 0 \\
a_{21}/a_{22} & 1 & 0 & \cdots & 0 \\
a_{31}/a_{33} & a_{32}/a_{33} & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_{n1}/a_{nn} & a_{n2}/a_{nn} & a_{n3}/a_{nn} & \cdots & 1
\end{pmatrix}
$$

$$
\begin{pmatrix}
u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\
0 & u_{22} & u_{23} & \cdots & u_{2n} \\
0 & 0 & u_{33} & \cdots & u_{3n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & u_{nn}
\end{pmatrix}
=
\begin{pmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
0 & a_{22} & a_{23} & \cdots & a_{2n} \\
0 & 0 & a_{33} & \cdots & a_{3n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & a_{nn}
\end{pmatrix}
$$

```
do i= 2, n
  do k= 1, i-1
    if ((i,k)∈ NonZero(A)) then
      a_ik := a_ik/a_kk
    endif
    do j= k+1, n
      if ((i,j)∈ NonZero(A)) then
        a_ij := a_ij - a_ik*a_kj
      endif
    enddo
  enddo
enddo
```

ILU, LU-GS

type “./lu3”

Incomplete LU Factorization without Fill-in’s

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

LU-GS without Fill-in’s

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.17	6.00	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	6.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00

Solution is more "inaccurate"

ILU(0)

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	5.83	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	5.66	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.18	5.65	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	5.83	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.17	5.65	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.18	0.00	−0.18	5.65

→

0.92
1.75
2.76
3.79
4.46
5.57
6.66
7.25
8.46
9.66
10.54
11.83

LU-GS

6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	6.00	0.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00	0.00
−0.17	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00	0.00
0.00	−0.17	0.00	−0.17	6.00	−1.00	0.00	−1.00	0.00	0.00	0.00	0.00
0.00	0.00	−0.17	0.00	−0.17	6.00	0.00	0.00	−1.00	0.00	0.00	0.00
0.00	0.00	0.00	−0.17	0.00	0.00	6.00	−1.00	0.00	−1.00	0.00	0.00
0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	−1.00	0.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	0.00	0.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	0.00	6.00	−1.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00	−1.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	−0.17	0.00	−0.17	6.00

→

0.86
1.60
2.60
3.54
3.99
5.09
6.26
6.52
7.73
9.22
9.70
10.96

Forward/Backward Substitution in LU-GS

$$[M]\{z\} = [\tilde{L}\tilde{U}]\{z\} = \{r\}$$

$$\{z\} = [\tilde{L}\tilde{U}]^{-1}\{r\} \rightarrow \begin{array}{l} [\tilde{L}]\{y\} = \{r\} \\ [\tilde{U}]\{z\} = \{y\} \end{array}$$

$$[\tilde{L}] = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ a_{21}/a_{22} & 1 & 0 & \cdots & 0 \\ a_{31}/a_{33} & a_{32}/a_{33} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1}/a_{nn} & a_{n2}/a_{nn} & a_{n3}/a_{nn} & \cdots & 1 \end{pmatrix}$$

$$[\tilde{U}] = \begin{pmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ 0 & 0 & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix}$$

$$[\overline{L}]=\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ a_{21} & 0 & 0 & \cdots & 0 \\ a_{31} & a_{32} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & 0 \end{pmatrix}$$

$$[\overline{U}]=\begin{pmatrix} 0 & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & 0 & a_{23} & \cdots & a_{2n} \\ 0 & 0 & 0 & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

$$[\overline{D}]=\begin{pmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ 0 & a_{22} & 0 & \cdots & 0 \\ 0 & 0 & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix}$$

$$[M]=[\tilde{L}][\tilde{U}]=[\overline{L}+\overline{D}][\overline{D}^{-1}][\overline{D}+\overline{U}]=[\overline{L}\,\overline{D}^{-1}+I][\overline{D}+\overline{U}]$$

$$[\overline{L}\,\overline{D}^{-1}]+[I]=\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ a_{21}/a_{22} & 0 & 0 & \cdots & 0 \\ a_{31}/a_{33} & a_{32}/a_{33} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1}/a_{nn} & a_{n2}/a_{nn} & a_{n3}/a_{nn} & \cdots & 0 \end{pmatrix}+\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}$$

$$=\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ a_{21}/a_{22} & 1 & 0 & \cdots & 0 \\ a_{31}/a_{33} & a_{32}/a_{33} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n1}/a_{nn} & a_{n2}/a_{nn} & a_{n3}/a_{nn} & \cdots & 1 \end{pmatrix}=[\tilde{L}]$$

$$[\overline{D}]+[\overline{U}]=\begin{pmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ 0 & a_{22} & 0 & \cdots & 0 \\ 0 & 0 & a_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix}+\begin{pmatrix} 0 & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & 0 & a_{23} & \cdots & a_{2n} \\ 0 & 0 & 0 & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}=\begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ 0 & 0 & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix}=[\tilde{U}]$$

For/Backward Subst. in LU-GS

$$[M]=[\tilde{L}][\tilde{U}]=[\bar{L}+\bar{D}][\bar{D}^{-1}][\bar{D}+\bar{U}]=[\bar{L}\bar{D}^{-1}+I][\bar{D}+\bar{U}]$$

Forward Substitution

$$[\bar{L}+\bar{D}]\{y\}=\{r\}\Rightarrow\{y\}=[\bar{D}^{-1}](\{r\}-[\bar{L}]\{y\})\Rightarrow y_i=\bar{D}_{ii}^{-1}\left(r_i-\sum_{j=1}^{i-1}\bar{L}_{ij}y_j\right)$$

Backward Substitution

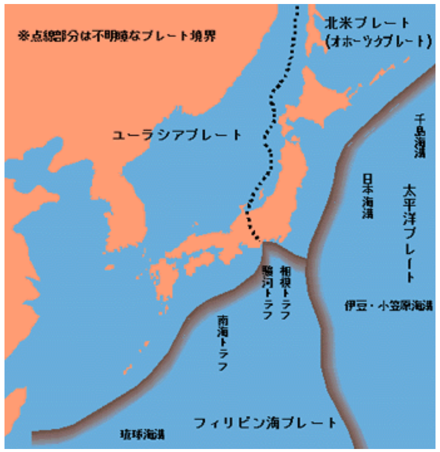
$$[I+\bar{D}^{-1}\bar{U}]\{z\}=\{y\}\Rightarrow\{z\}=\{y\}-[\bar{D}^{-1}][\bar{U}]\{z\}\Rightarrow z_i=y_i-\bar{D}_{ii}^{-1}\left[\sum_{j=i+1}^{N}\bar{U}_{ij}z_j\right]$$

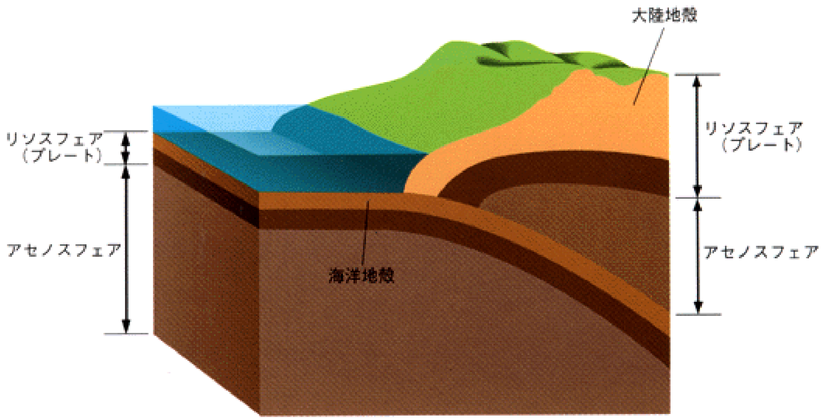
$$[\bar{L}\bar{D}^{-1}]+[I]=\begin{pmatrix}0&0&0&\cdots&0\\a_{21}/a_{22}&0&0&\cdots&0\\a_{31}/a_{33}&a_{32}/a_{33}&0&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\a_{n1}/a_{nn}&a_{n2}/a_{nn}&a_{n3}/a_{nn}&\cdots&0\end{pmatrix}+\begin{pmatrix}1&0&0&\cdots&0\\0&1&0&\cdots&0\\0&0&1&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\0&0&0&\cdots&1\end{pmatrix}=\begin{pmatrix}1&0&0&\cdots&0\\a_{21}/a_{22}&1&0&\cdots&0\\a_{31}/a_{33}&a_{32}/a_{33}&1&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\a_{n1}/a_{nn}&a_{n2}/a_{nn}&a_{n3}/a_{nn}&\cdots&1\end{pmatrix}$$

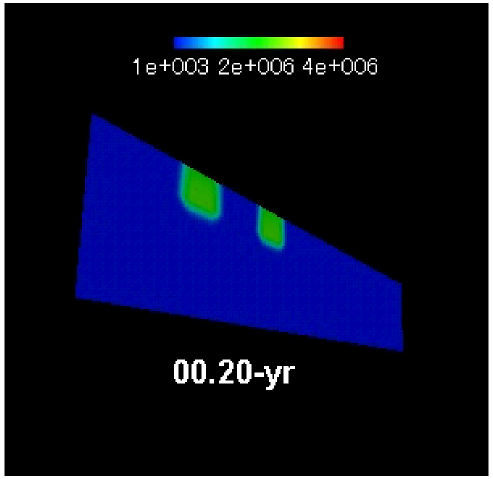
$$[\bar{D}]+[\bar{U}]=\begin{pmatrix}a_{11}&0&0&\cdots&0\\0&a_{22}&0&\cdots&0\\0&0&a_{33}&\cdots&0\\\vdots&\vdots&\vdots&\ddots&\vdots\\0&0&0&\cdots&a_{nn}\end{pmatrix}+\begin{pmatrix}0&a_{12}&a_{13}&\cdots&a_{1n}\\0&0&a_{23}&\cdots&a_{2n}\\0&0&0&\cdots&a_{3n}\\\vdots&\vdots&\vdots&\ddots&\vdots\\0&0&0&\cdots&0\end{pmatrix}=\begin{pmatrix}a_{11}&a_{12}&a_{13}&\cdots&a_{1n}\\0&a_{22}&a_{23}&\cdots&a_{2n}\\0&0&a_{33}&\cdots&a_{3n}\\\vdots&\vdots&\vdots&\ddots&\vdots\\0&0&0&\cdots&a_{nn}\end{pmatrix}$$

Preconditioning Method for Contact Problems

- Contact Problems for Simulations of Earthquake Simulation Cycle
  - Quasi-Static Stress Accumulation Process at Plate Boundaries
  - Non-Linear Contact Problems, Newton-Raphson Method
  - Constraint Conditions through Augmented Lagrangean Method (ALM): Penalty Terms



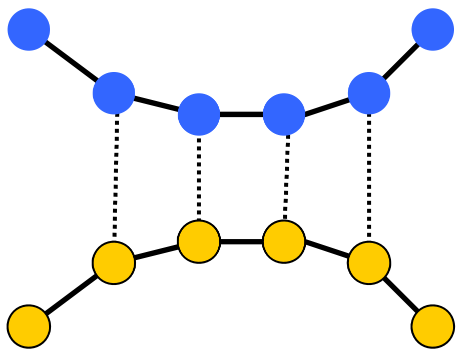




Preconditioning Method for Contact Problems (cont.)

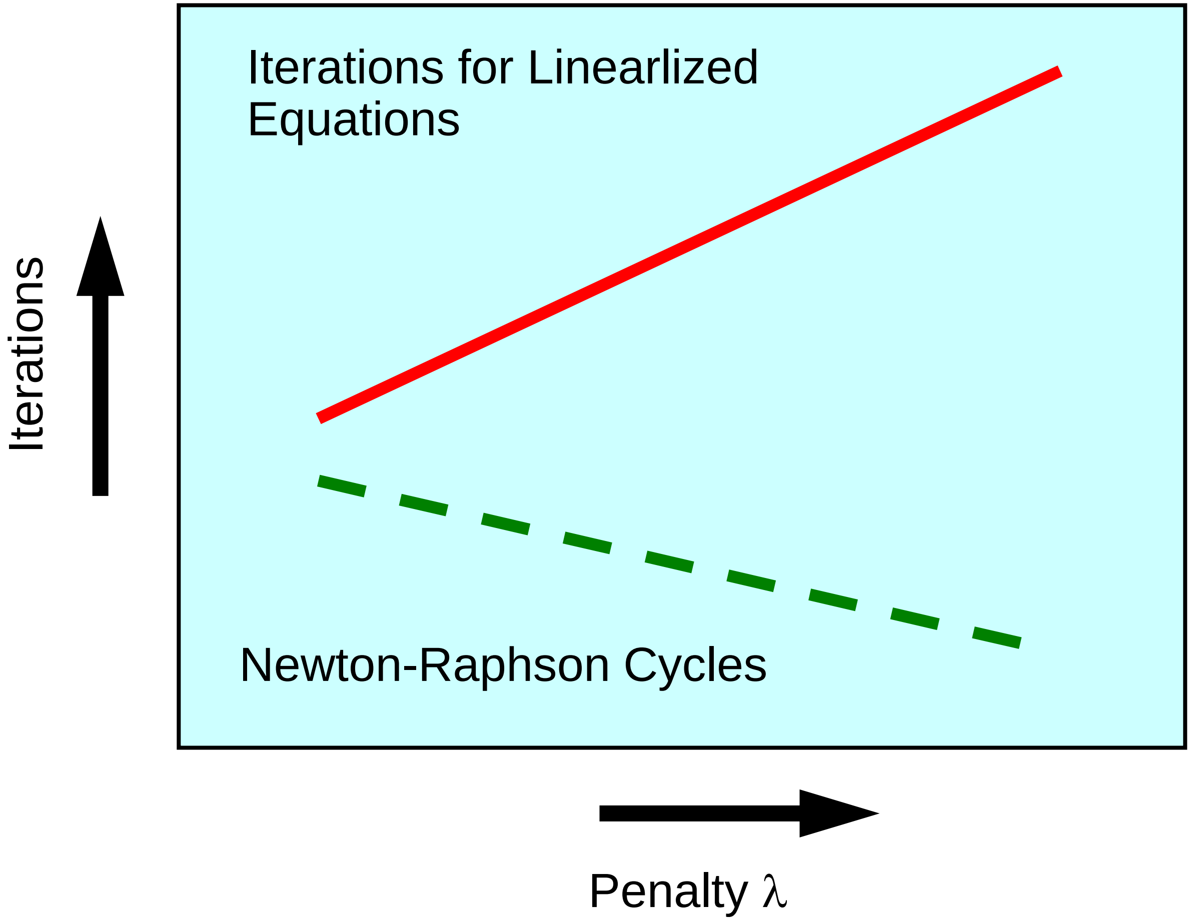
- Assumption
  - Infinitesimal Deformation Theory, Static Contact Condition (contact conditions not changed)
  - No friction: symmetric coefficient matrices
- Special preconditioning method: ***Selective Blocking.***
  - Suitable for 3D contact problems

- Computations
  - Hitachi SR2201: 2001-2002
  - Earth Simulator: 2002-2003
  - IBM SP-3: 2003-2005



Augmented Lagrangean

Newton-Raphson / Iterative Solver



If penalty number becomes larger, number of Newton-Raphson cycles is smaller because of higher accuracy for contact conditions.

But, linearlized equations are worse-conditioned.

Preliminary Results

Elastic Problems with Penalty Constraint

27,888 nodes, 83,664 DOFs, $\varepsilon=10^{-8}$

Single PE case (Xeon 2.8MHz)

<u>GeoFEM's Original Solvers (Scalar Version)</u>

Preconditioning	λ	Iterations	Set-up (sec.)	Solve (sec.)	Set-up+Solve (sec.)	Single Iteration (sec.)	Memory Size (MB)
Diagonal Scaling	10^2	1531	<0.01	75.1	75.1	0.049	119
	10^6	No Conv.	-	-	-	-	
IC(0) (Scalar Type)	10^2	401	0.02	39.2	39.2	0.098	119
	10^6	No Conv.	-	-	-	-	
BIC(0)	10^2	388	0.02	37.4	37.4	0.097	59
	10^6	2590	0.01	252.3	252.3	0.097	
BIC(1)	10^2	77	8.5	11.7	20.2	0.152	176
	10^6	78	8.5	11.8	20.3	0.152	
BIC(2)	10^2	59	16.9	13.9	30.8	0.236	319
	10^6	59	16.9	13.9	30.8	0.236	
SB-BIC(0)	10^0	114	0.10	12.9	13.0	0.113	67
	10^6	114	0.10	12.9	13.0	0.113	

Ill-Conditioned Problems

- Generally, direct methods have been used for ill-conditioned linear equations.
- But, it is difficult to “parallelize” direct method for large-scale problems
- Robust preconditioning is required

- Remedies
  - Similar to Direct Method with Higher Order of Fill-in’s
  - Blocking
  - Reordering

Higher Order of Fill-in’s

- Closer to Direct Method
- More Expensive (Memory, Computation)

Blocking in For/Backward Sub.

$$[M]=[\tilde{L}][\tilde{U}]=[\bar{L}+\bar{D}][\bar{D}^{-1}][\bar{D}+\bar{U}]=[\bar{L}\bar{D}^{-1}+I][\bar{D}+\bar{U}]$$

<u>Forward Substitution</u>

$$[\bar{L}+\bar{D}]\{y\}=\{r\}\Rightarrow\{y\}=[\bar{D}^{-1}](\{r\}-[\bar{L}]\{y\})\Rightarrow y_i=\bar{D}_{ii}^{-1}\left(r_i-\sum_{j=1}^{i-1}\bar{L}_{ij}y_j\right)$$

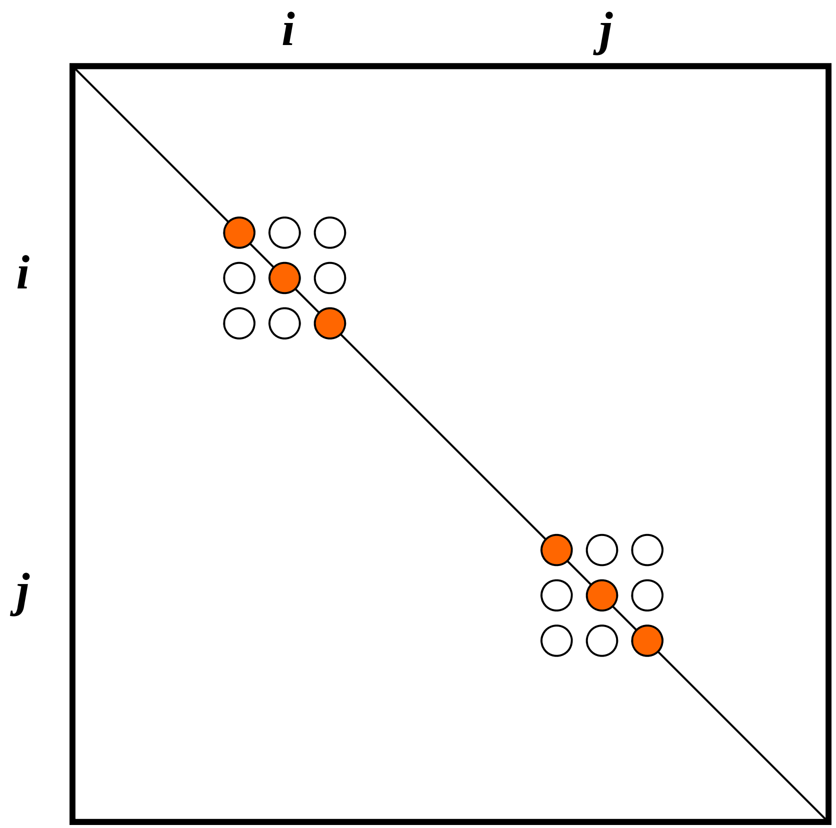
<u>Backward Substitution</u>

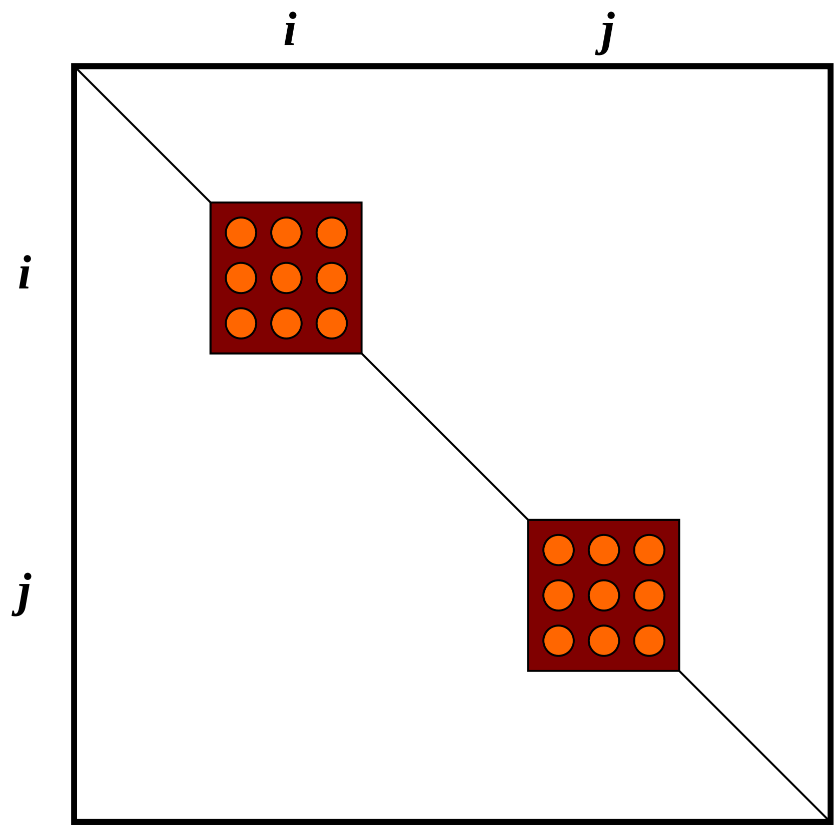
$$[I+\bar{D}^{-1}\bar{U}]\{z\}=\{y\}\Rightarrow\{z\}=\{y\}-[\bar{D}^{-1}][\bar{U}]\{z\}\Rightarrow z_i=y_i-\bar{D}_{ii}^{-1}\left[\sum_{j=i+1}^{N}\bar{U}_{ij}z_j\right]$$

- Full LU factorization of 3x3 diagonal block in stead of diagonal scaling for the process of “multiplying D^{-1}”.
  - 3D solid mechanics
  - 3 strongly coupled components on each node
  - Smaller indirect access, more efficient

Storing 3x3 Block (3/3)

- Stabilization of Computation
  - Instead of division by diagonal components, full LU factorization of 3x3 Diagonal Block is applied.
  - Effective for ill-conditioned problems





Results in the Benchmark

27,888 nodes, 83,664 DOFs, $\varepsilon=10^{-8}$

Single PE case (Xeon 2.8MHz)

Effect of Blocking/Fill-in

Preconditioning	λ	Iterations	Set-up (sec.)	Solve (sec.)	Set-up+Solve (sec.)	Single Iteration (sec.)	Memory Size (MB)
Diagonal Scaling	10^2	1531	<0.01	75.1	75.1	0.049	119
	10^6	No Conv.	-	-	-	-	
IC(0) (Scalar Type)	10^2	401	0.02	39.2	39.2	0.098	119
	10^6	No Conv.	-	-	-	-	
BIC(0)	10^2	388	0.02	37.4	37.4	0.097	59
	10^6	2590	0.01	252.3	252.3	0.097	
BIC(1)	10^2	77	8.5	11.7	20.2	0.152	176
	10^6	78	8.5	11.8	20.3	0.152	
BIC(2)	10^2	59	16.9	13.9	30.8	0.236	319
	10^6	59	16.9	13.9	30.8	0.236	
SB-BIC(0)	10^0	114	0.10	12.9	13.0	0.113	67
	10^6	114	0.10	12.9	13.0	0.113	

Blocking and Higher Order of Fill-in's improved robustness.

Preconditioned Iterative Solver

e.g. CG method (Conjugate Gradient)

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

- Dot products
- Matrix-vector multiplication
- Preconditioners
- DAXPY

Localized SGS/SSOR Preconditioning

- SGS/SSOR: Global Operations (Forward/Backward Substitution)
  - NOT suitable for parallel computing
- Ignoring effects of external points for preconditioning
  - Block-Jacobi Localized Preconditioning
- WEAKER than original SGS/SSOR
  - More PE's, more iterations

$$(L)\{z\}=\{r\}$$

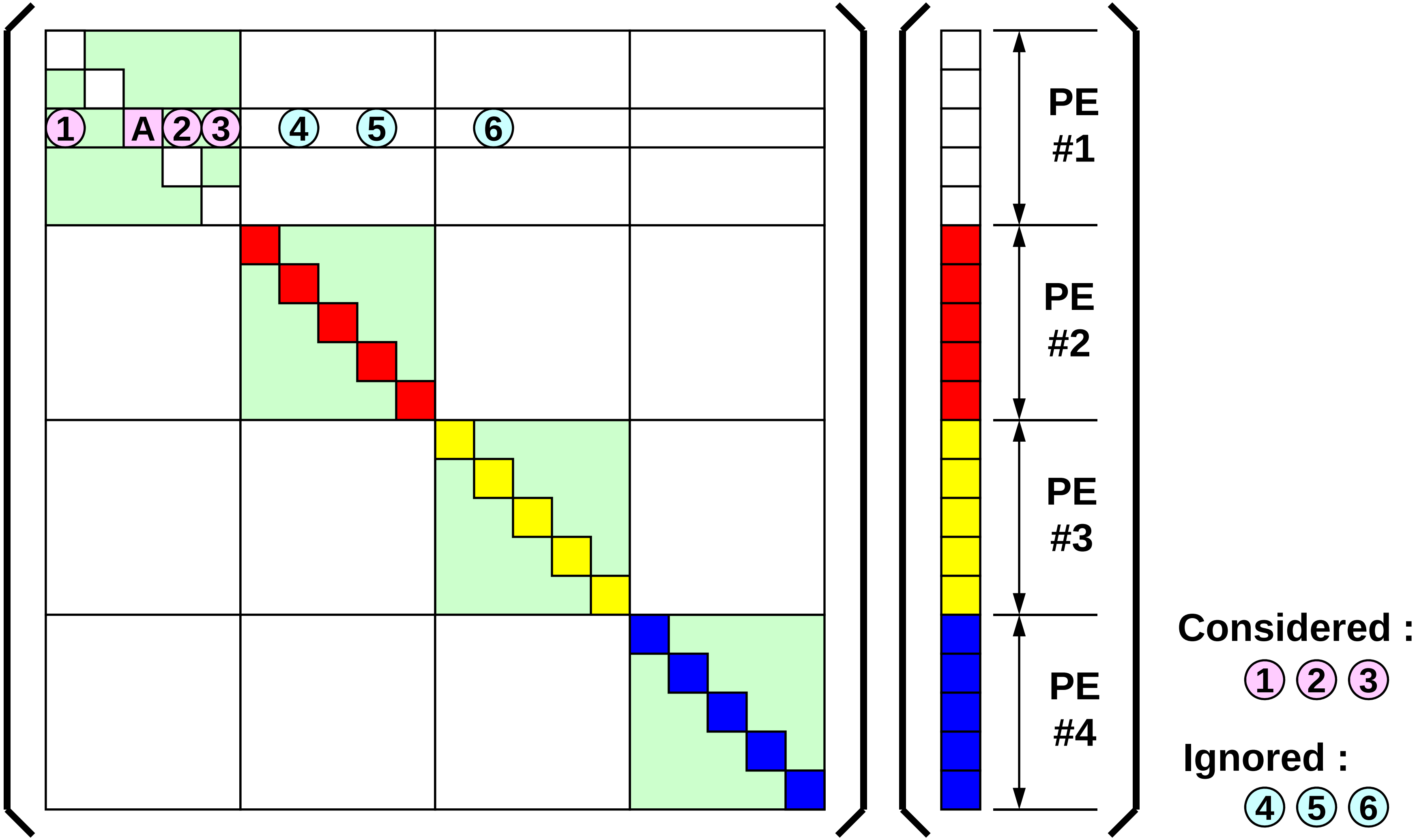
$$(U)\{z\}=\{z\}$$

```
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do i= 1, N
        WVAL= W(i,Z)
        do k= indexL(i-1)+1, indexL(i)
          WVAL= WVAL -  AL(k) * W(itemL(k),Z)
        enddo
        W(i,Z)= WVAL / D(i)
      enddo

      do i= N, 1, -1
        SW  = 0.0d0
        do k= indexU(i), indexU(i-1)+1, -1
          SW= SW + AU(k) * W(itemU(k),Z)
        enddo
        W(i,Z)= W(i,Z) - SW / D(i)
      enddo
!C===
```

Localized SGS/SSOR Preconditioning

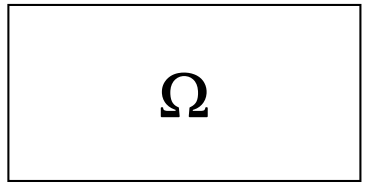


Overlapped Additive Schwartz Domain Decomposition Method

Stabilization of Localized Preconditioning: ASDD

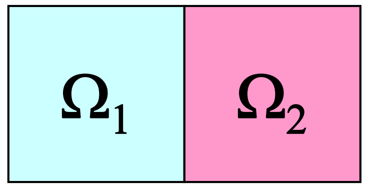
Global Operation

$$Mz = r$$



Local Operation

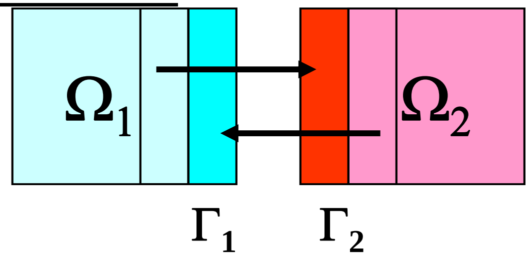
$$z_{\Omega_1} = M_{\Omega_1}^{-1} r_{\Omega_1}, \quad z_{\Omega_2} = M_{\Omega_2}^{-1} r_{\Omega_2}$$



Global Nesting Correction: Repeating -> Stable

$$z_{\Omega_1}^{n} = z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1}(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1})$$

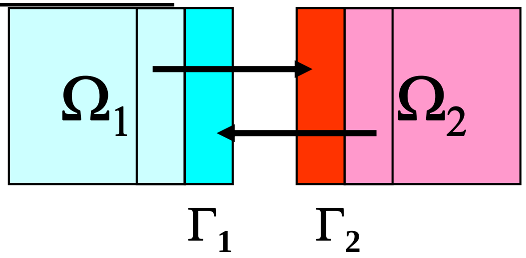
$$z_{\Omega_2}^{n} = z_{\Omega_2}^{n-1} + M_{\Omega_2}^{-1}(r_{\Omega_2} - M_{\Omega_2} z_{\Omega_2}^{n-1} - M_{\Gamma_2} z_{\Gamma_2}^{n-1})$$



Overlapped Additive Schwartz Domain Decomposition Method

Stabilization of Localized Preconditioning: ASDD

Global Nesting Correction: Repeating -> Stable



$$z_{\Omega_1}^{n} = z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1}\left(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1}\right)$$

$$z_{\Omega_2}^{n} = z_{\Omega_2}^{n-1} + M_{\Omega_2}^{-1}\left(r_{\Omega_2} - M_{\Omega_2} z_{\Omega_2}^{n-1} - M_{\Gamma_2} z_{\Gamma_2}^{n-1}\right)$$

$$\Delta r_{\Omega_1} = r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1}$$

$$\Delta z_{\Omega_1} = M_{\Omega_1}^{-1} \Delta r_{\Omega_1} \quad where \quad \Delta z_{\Omega_1} = z_{\Omega_1}^{n} - z_{\Omega_1}^{n-1}$$

$$z_{\Omega_1}^{n} = z_{\Omega_1}^{n-1} + \Delta z_{\Omega_1} = z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1} \Delta r_{\Omega_1} = z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1}\left(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1}\right)$$

Overlapped Additive Schwartz Domain Decomposition Method

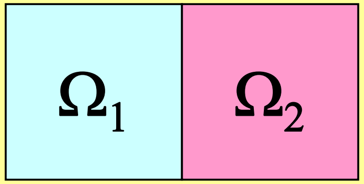
Effect of additive Schwartz domain decomposition for solid mechanics example example with $3\text{x}44^3$ DOF on Hitachi SR2201, Number of ASDD cycle/iteration= 1, $\varepsilon = 10^{-8}$

	NO Additive Schwartz			WITH Additive Schwartz		
PE #	**Iter. #**	**Sec.**	**Speed Up**	**Iter.#**	**Sec.**	**Speed Up**
1	204	233.7	-	144	325.6	-
2	253	143.6	1.63	144	163.1	1.99
4	259	74.3	3.15	145	82.4	3.95
8	264	36.8	6.36	146	39.7	8.21
16	262	17.4	13.52	144	18.7	17.33
32	268	9.6	24.24	147	10.2	31.80
64	274	6.6	35.68	150	6.5	50.07

Overlapped Additive Schwartz Domain Decomposition Method

Stabilization of Localized Preconditioning: ASDD

do iterPRE= 1, iterPREmax



Local Operation (Forward/Backward Substitution)

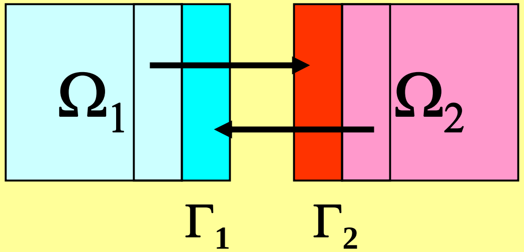
$$calc.\quad M_{\Omega_1}^{-1}(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1})$$

$$calc.\quad M_{\Omega_2}^{-1}(r_{\Omega_2} - M_{\Omega_2} z_{\Omega_2}^{n-1} - M_{\Gamma_2} z_{\Gamma_2}^{n-1})$$

Global Nesting Correction: Repeating -> Stable

$$z_{\Omega_1}^{n} = z_{\Omega_1}^{n-1} + M_{\Omega_1}^{-1}(r_{\Omega_1} - M_{\Omega_1} z_{\Omega_1}^{n-1} - M_{\Gamma_1} z_{\Gamma_1}^{n-1})$$

$$z_{\Omega_2}^{n} = z_{\Omega_2}^{n-1} + M_{\Omega_2}^{-1}(r_{\Omega_2} - M_{\Omega_2} z_{\Omega_2}^{n-1} - M_{\Gamma_2} z_{\Gamma_2}^{n-1})$$



enddo