Experiences in Optimizations of Preconditioned Iterative Solvers for FEM/FVM Applications & Matrix Assembly of FEM using Intel Xeon Phi

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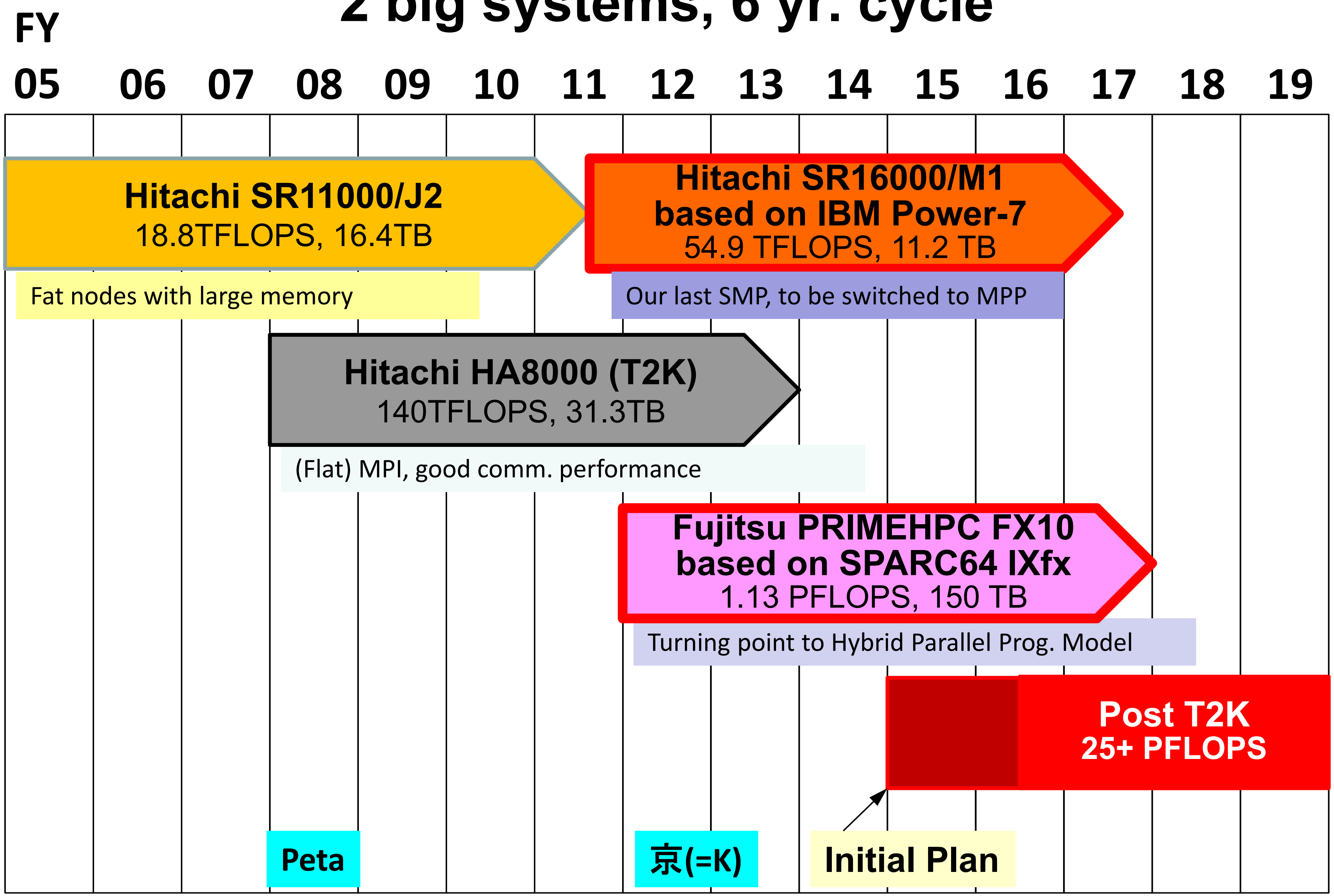
Supercomputers in U.Tokyo

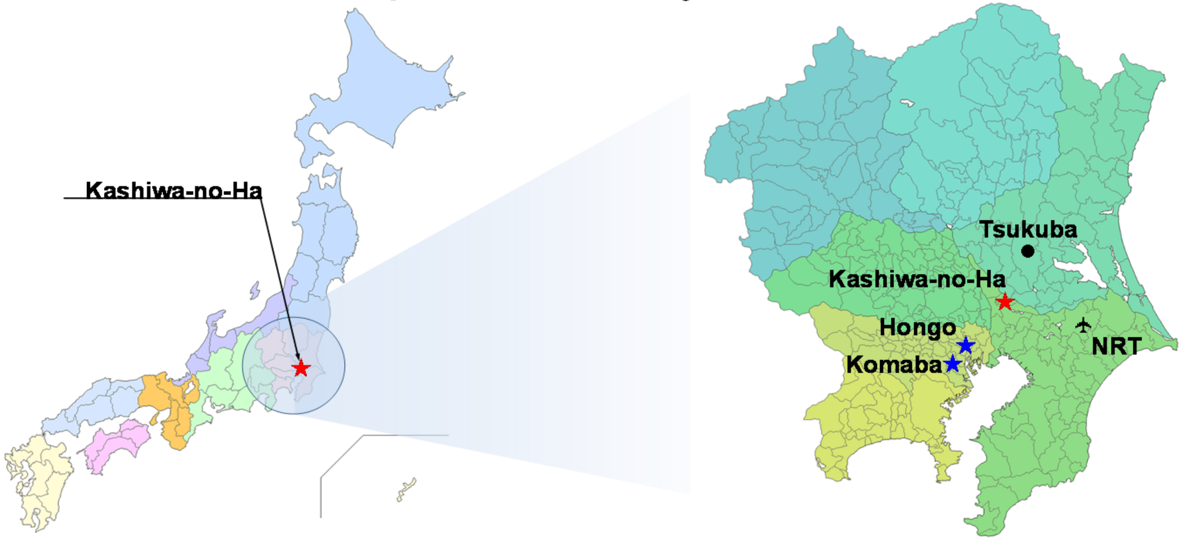
2 big systems, 6 yr. cycle



Post T2K System

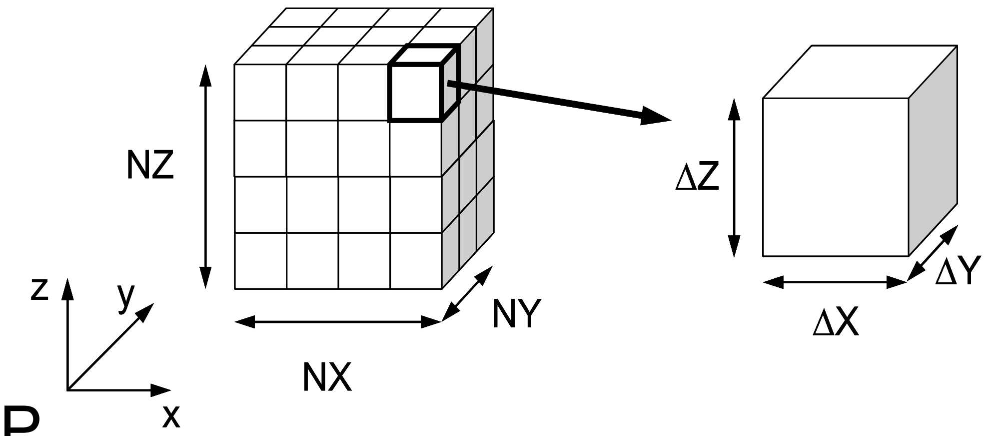
- 25+ PFLOPS, FY. 2016
- Many-core based (e.g. KNL)
- Joint Center for Advanced High Performance Computing (JCAHPC, http://jcahpc.jp/)
  - University of Tsukuba
  - University of Tokyo
    - New system will installed in Kashiwa-no-Ha (Leaf of Oak) Campus/U.Tokyo, which is between Tokyo and Tsukuba

JCAHPC



Target Applications
Sparse Matrices = Memory Bound

- GeoFEM Cube
  - 3D FEM
  - Solid Mechanics & Heat Transfer
  - Preconditioned Iterative Solver (PCG, Point Jacobi)
  - Performance
    - PCG Solver & Matrix Assembly
- Poisson3D-OMP
  - 3D FVM
  - Steady Poisson Eq.
  - Performance
    - ICCG Solver
- Codes
  - Simple Geometries
  - Fortran 90, MPI + OpenMP



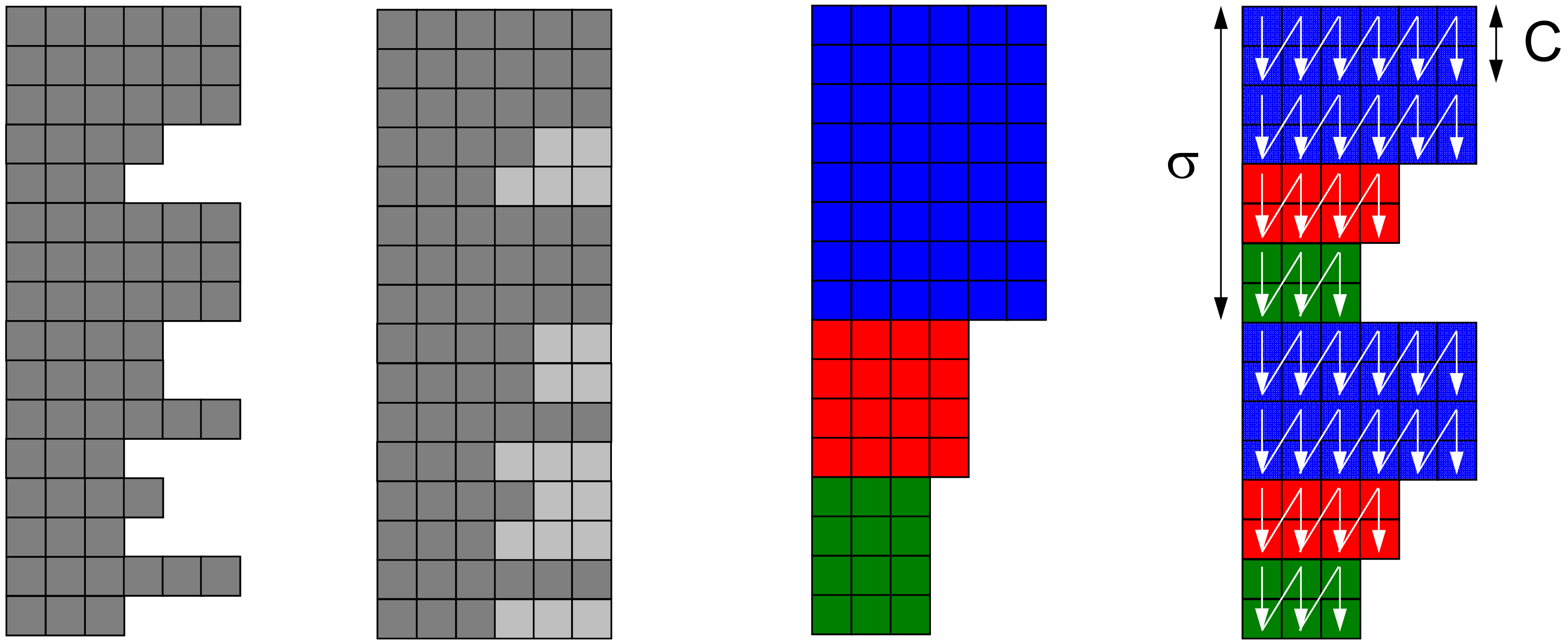
H/W: Single Node/Socket

Code Name	FX10	MIC	IvyB
Architectures	**Fujitsu SPARC64 IX fx**	**Intel Xeon Phi 5110P (Knights Corner)**	**Intel Xeon E5-2680 v2 (Ivy-Bridge-EP)**
Frequency (GHz)	1.848	1.053	2.80
Core # (Thread #)	16 (16)	60 (240)	10 (20)
Memory Type	DDR3	GDDR5	DDR3
Peak Performance (GFLOPS)	236.5	1,010.9	224.0
RAM (GB)	32	8	64
Peak Memory Bandwidth (GB/s)	85.1	320	59.7
STREAM Triad (GB/s)	64	159	49
Cache	L1:32KB/core L2:12MB/socket	L1:32KB/core L2:512KB/core	L1:32KB/core L2:256KB/core L3:25MB/socket

What to be evaluated ?

- Effects of formats for storing sparse matrices in PCG/ICCG Solvers

[Kreutzer, Hager, Wellein 2014]



CRS | ELL | Sliced ELL | SELL-C-σ (SELL-2-8)

- Effects of Vectorization, !$omp simd

- **PCG: GeoFEM Cube/Heat**
- ICCG: Poisson3D-OMP
- Matrix Assembly: GeoFEM Cube/Solid

Example: SELL-4-σ GeoFEM Cube/Heat: SpMV

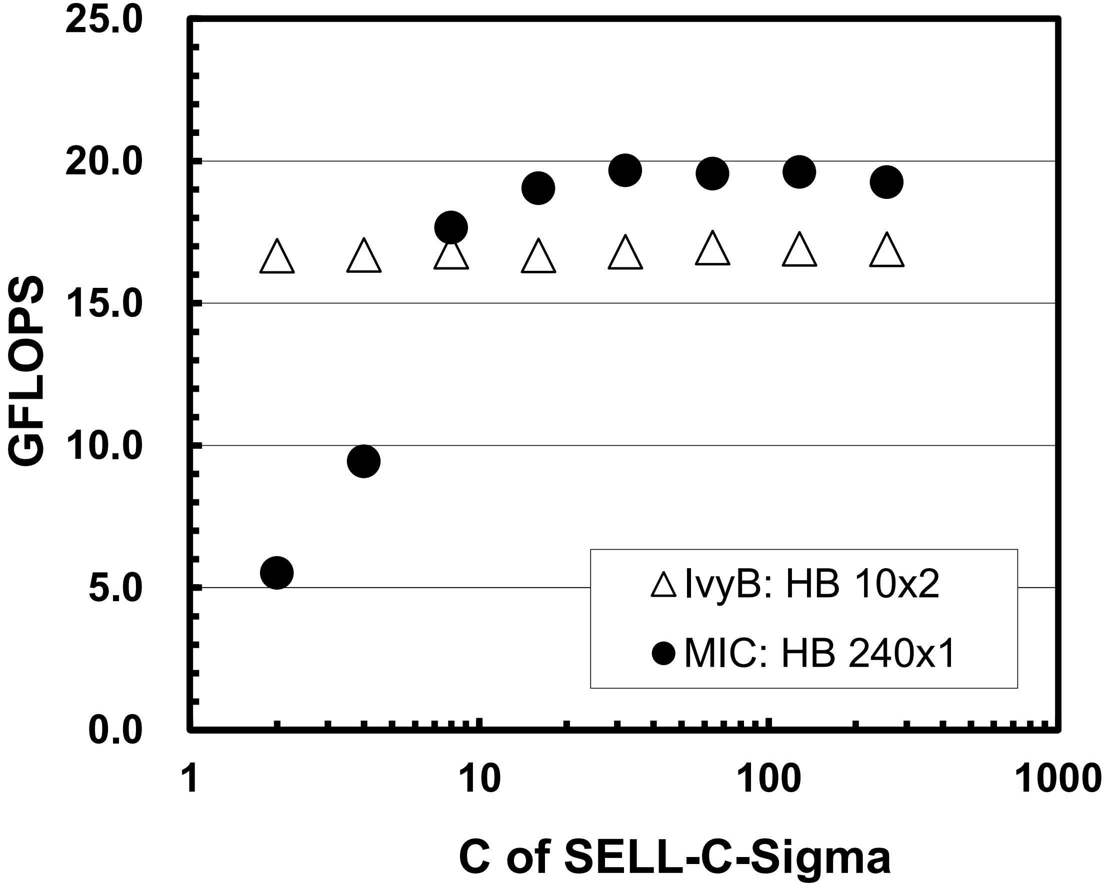
```
!$omp parallel do
      do i= 1, N/2
        Y(2*(i-1)+1)= D(2*(i-1)+1) * X(2*(i-1)+1)
        Y(2*(i-1)+2)= D(2*(i-1)+2) * X(2*(i-1)+2)
      enddo

!$omp parallel do
      do i= 1, N/4
      do j= 1, NCOL(i)
!$omp simd
      do k= 1, 4
        Y(4*(i-1)+k)= Y(4*(i-1)+k) + AMAT(CS(i-1)+(j-1)*4+k)      &
                                   * X(COL(CS(i-1)+(j-1)*4+k))
      enddo
      enddo
      enddo
```

Width of Chunk: l_i (Number of Non-Zero Off Diagonals: **`CL(i)`**)

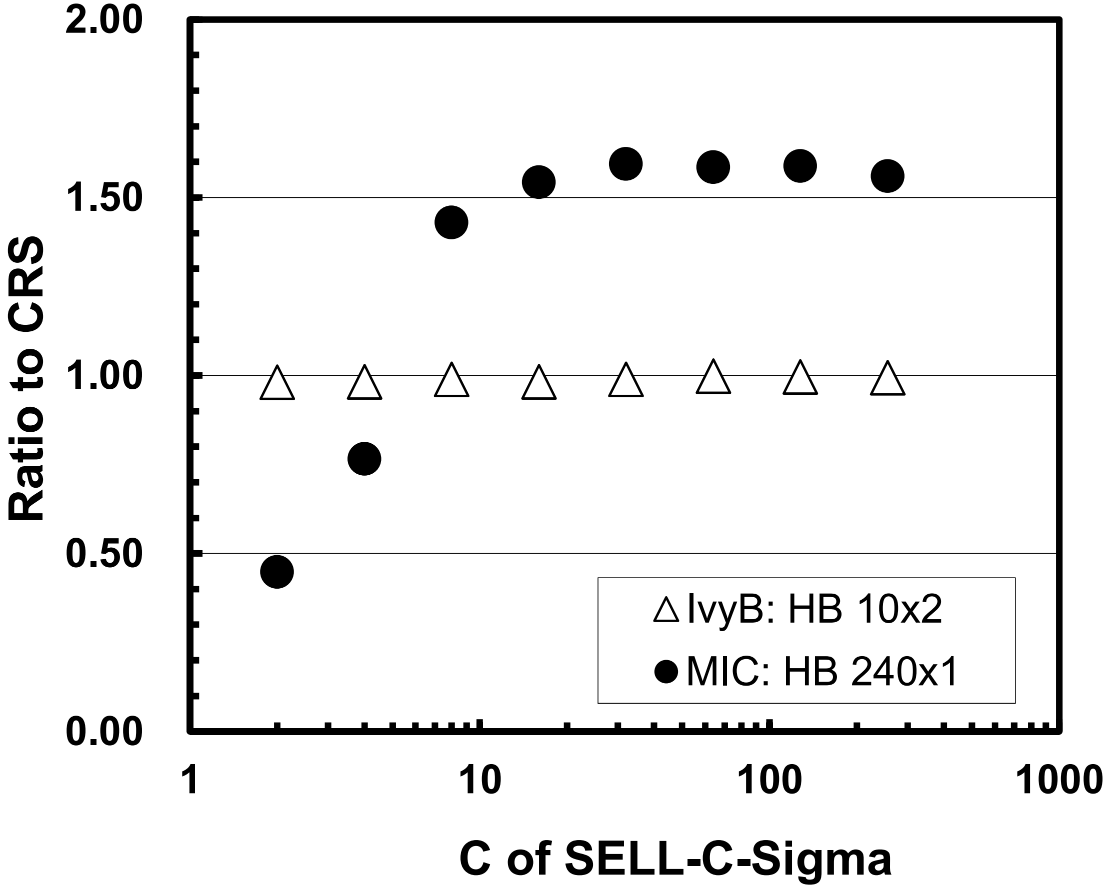
PCG in GeoFEM Cube/Heat GFLOPS Rate

MIC：Low Performance if C（Chunk Size）< 8



- IvyB
  - 10 threads x 2 soc.
- MIC
  - 240 threads x 1
  - SIMD幅512bit
  - 64bit×8

PCG in GeoFEM Cube/Heat Ratio to CRS (Original)

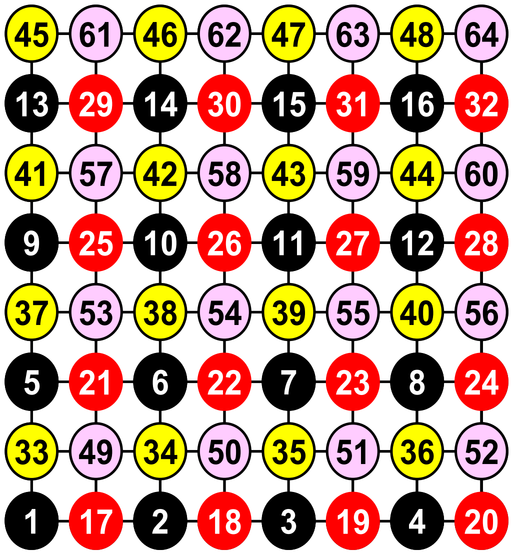


- IvyB
  - No effects by SELL-C-Sigma/ELL
  - Out-of-Order ?

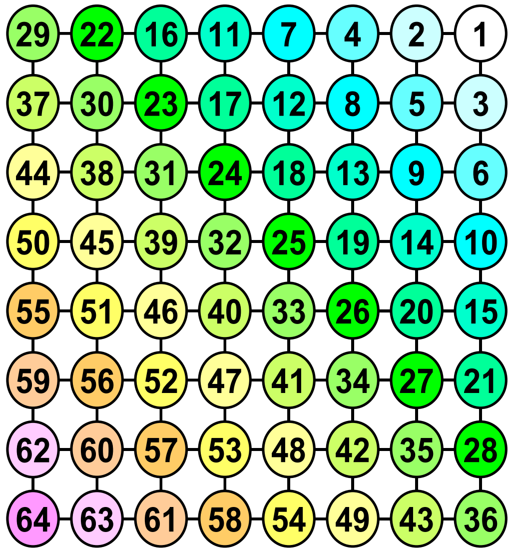
- PCG: GeoFEM Cube/Heat
- **ICCG: Poisson3D-OMP**
- Matrix Assembly: GeoFEM Cube/Solid

Elimination of Data Dependency in ICCG

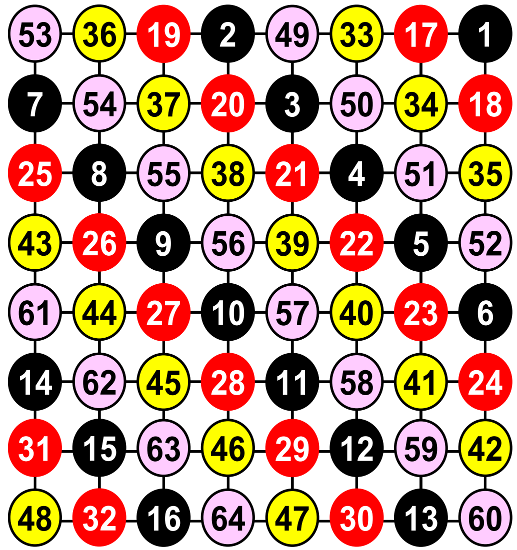
- Coloring + Reordering
- More colors, better convergence/larger sync. overhead
  - MC: good parallel performance, bad convergence
  - RCM: good convergence, many colors
  - **CM-RCM: combinations of MC + RCM**



MC (Color#=4)
Multicoloring



RCM
Reverse Cuthill-Mckee

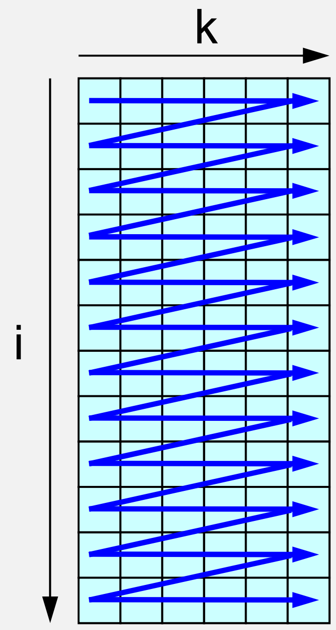


CM-RCM (Color#=4)
Cyclic MC + RCM

ELL: Row-wise

CRS with fixed length
Forward Substitution

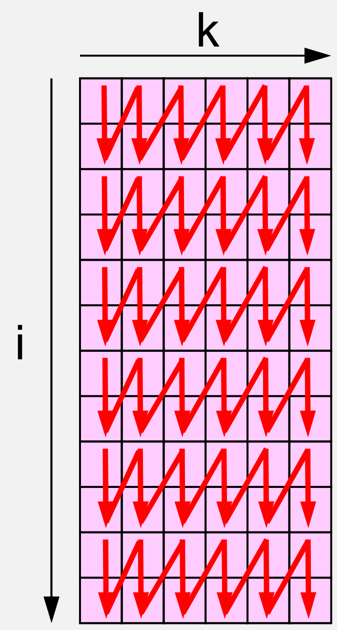
```
!$omp parallel
    do icol= 1, NCOLORtot
!$omp do
    do ip  = 1, PEsmpTOT
      do i= Index(ip-1,icol)+1, Index(ip,icol)
        do k= 1, 6
          Z(i)= Z(i) - AML(k,i)*Z(IAML(k,i))
        enddo
        Z(i)= Z(i) / DD(i)
      enddo
    enddo
    enddo
!omp end parallel
```



ELL: Column-wise

Jagged Diagonal
Forward Substitution

```
!$omp parallel
    do icol= 1, NCOLORtot
!$omp do
    do ip  = 1, PEsmpTOT
      do k= 1, 6
!$omp simd
        do i= Index(ip-1,icol)+1, Index(ip,icol)
          Z(i)= Z(i) + AML (i,k)*Z(IAML(i,k))
        enddo
      enddo
      do i= Index(ip-1,icol)+1, Index(ip,icol)
        Z(i)= Z(i) / DD(i)
      enddo
    enddo
    enddo
!omp end parallel
```



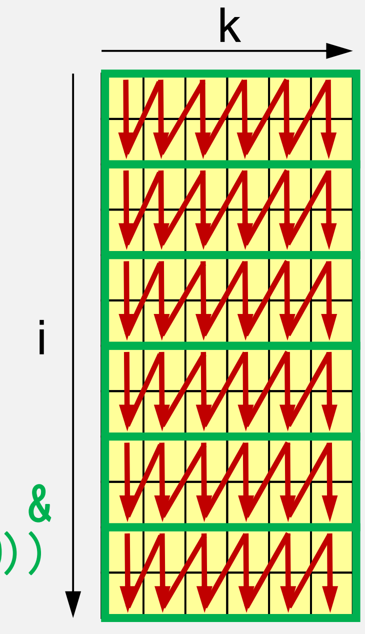
Each Color/Thread

ELL: Column-wise

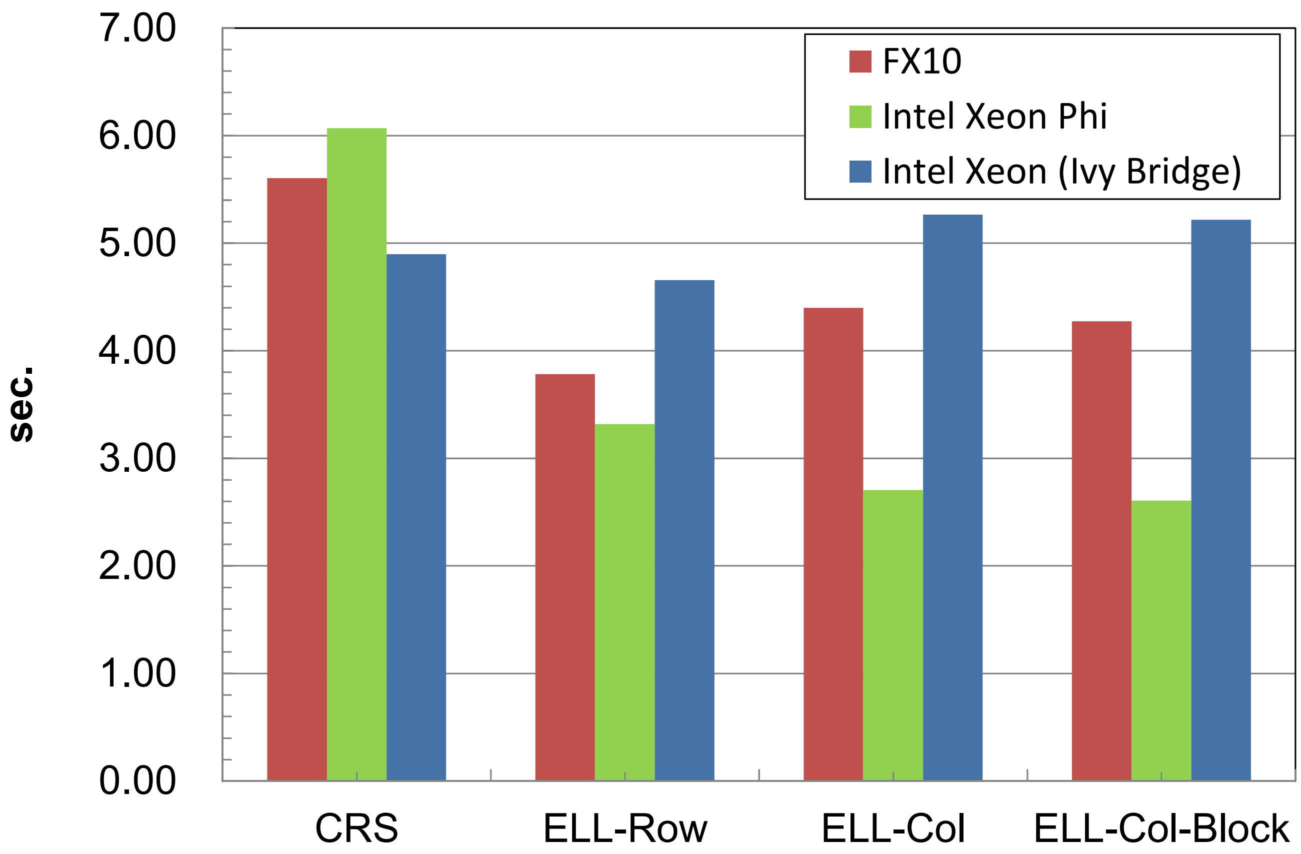
Jagged Diagonal, Blocked Version

Forward Substitution

```
!$omp parallel
    do icol= 1, NCOLORtot
!$omp do
    do ip  = 1, PEsmpTOT
      blkID= (ip-1)*NCOLORtot + ip
      do k= 1, 6
!$omp simd
      do i= IndexB(ip-1,blkID,icol)+1, &
            IndexB(ip  ,blkID,icol)
        locID= i - IndexB(ip-1,blkID,icol)
        Z(i)= Z(i) +                                  &
              AMLb(locID,k,blkID)* X(IAMLb(locID,k,blkID))
      enddo
      enddo
      do i= IndexB(ip-1,blkID,icol)+1, IndexB(ip  ,blkID,icol)
        Z(i)= Z(i) / DD(i)
      enddo
    enddo
    enddo
!omp end parallel
```

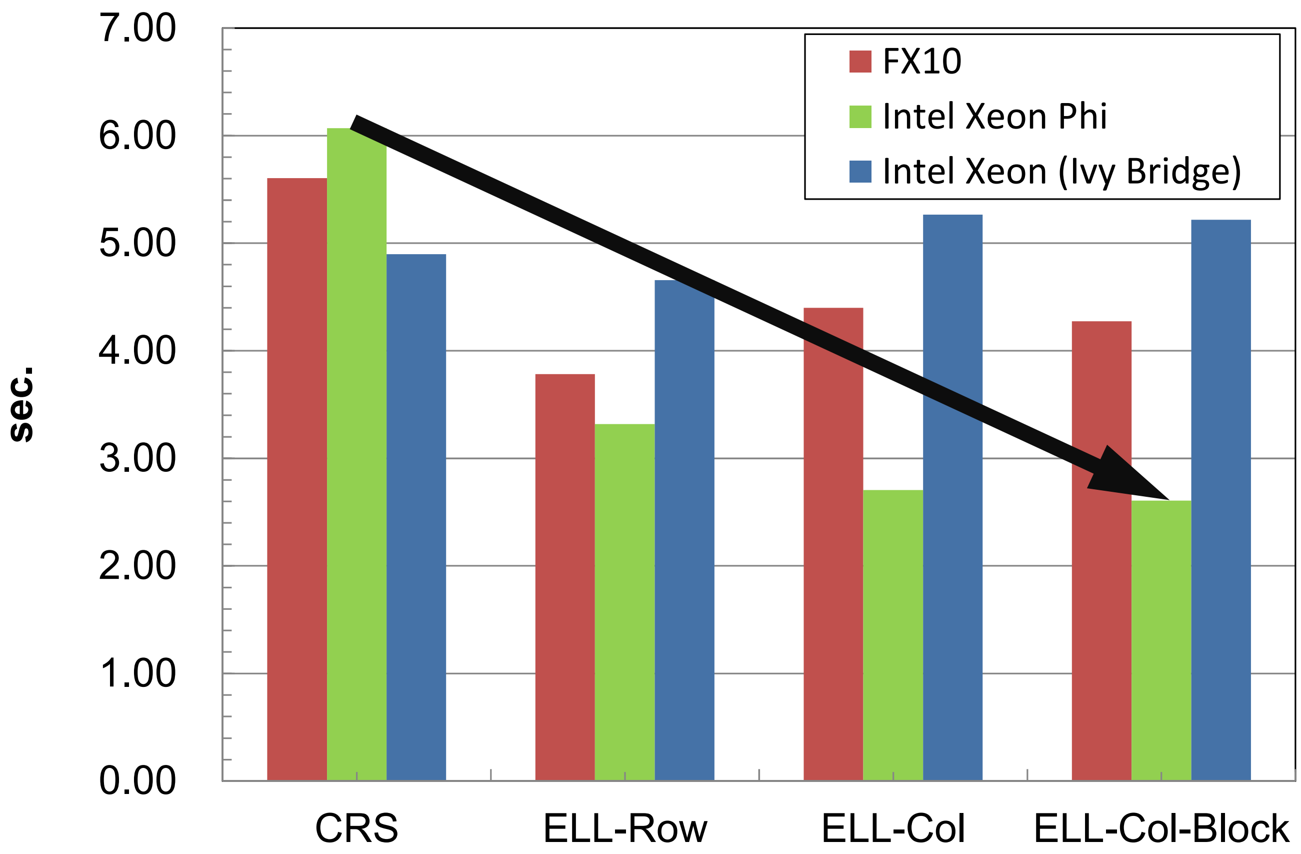


Results (Computation Time for Linear Solver): Down is Good !



- FX10
  - 16 T x 1
- IvyB
  - 10 T x 1
- MIC
  - 240 T x 1

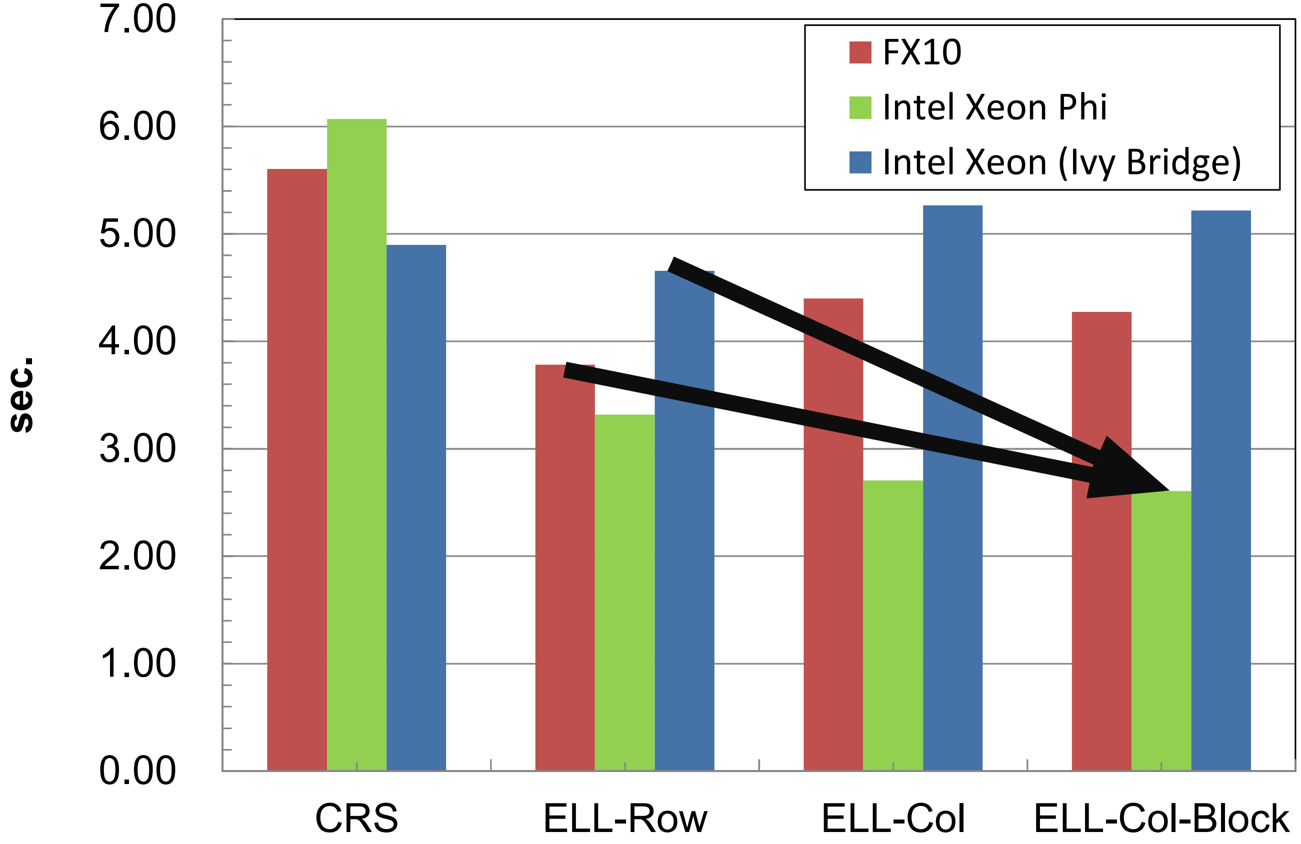
Results (Computation Time for Linear Solver): Down is Good !



- FX10
  - 16 T x 1
- IvyB
  - 10 T x 1
- MIC
  - 240 T x 1

2.33x Improvement
CRS -> ELL-Col-Block
Contributions by !$omp simd: 5-10%

Results (Computation Time for Linear Solver): Down is Good !



- FX10
  - 16 T x 1
- IvyB
  - 10 T x 1
- MIC
  - 240 T x 1

1.45x faster than FX10
1.79x faster than IvyB

Compiler Options for MIC: Additional Improvement

ELL-Col-Block	Coalesced		Sequential	
	sec.	GFLOPS	sec.	GFLOPS
-O3 -openmp -mmic -align array64byte (base)	2.654	10.53	**2.603**	**10.74**
-opt-streaming-stores always	3.165	8.832	3.159	8.849
-opt-streaming-cache-evict=0	2.625	10.65	2.600	10.75
-opt-streaming-cache-evict=1	2.639	10.59	2.605	10.73
-opt-streaming-stores always -opt-streaming-cache-evict=0	2.486	11.24	2.539	11.01
-opt-streaming-stores always -opt-streaming-cache-evict=1	2.477	11.29	2.556	10.94
-opt-streaming-stores always -opt-streaming-cache-evict=0 -opt-prefetch-distance=a,b	**2.385 (2,0)**	**11.72**	2.477 (8,1)	11.29
-opt-streaming-stores always -opt-streaming-cache-evict=1 -opt-prefetch-distance=c,d	2.404 (2,0)	11.63	2.487 (16,1)	11.24

Further Optimization by Compiler Options

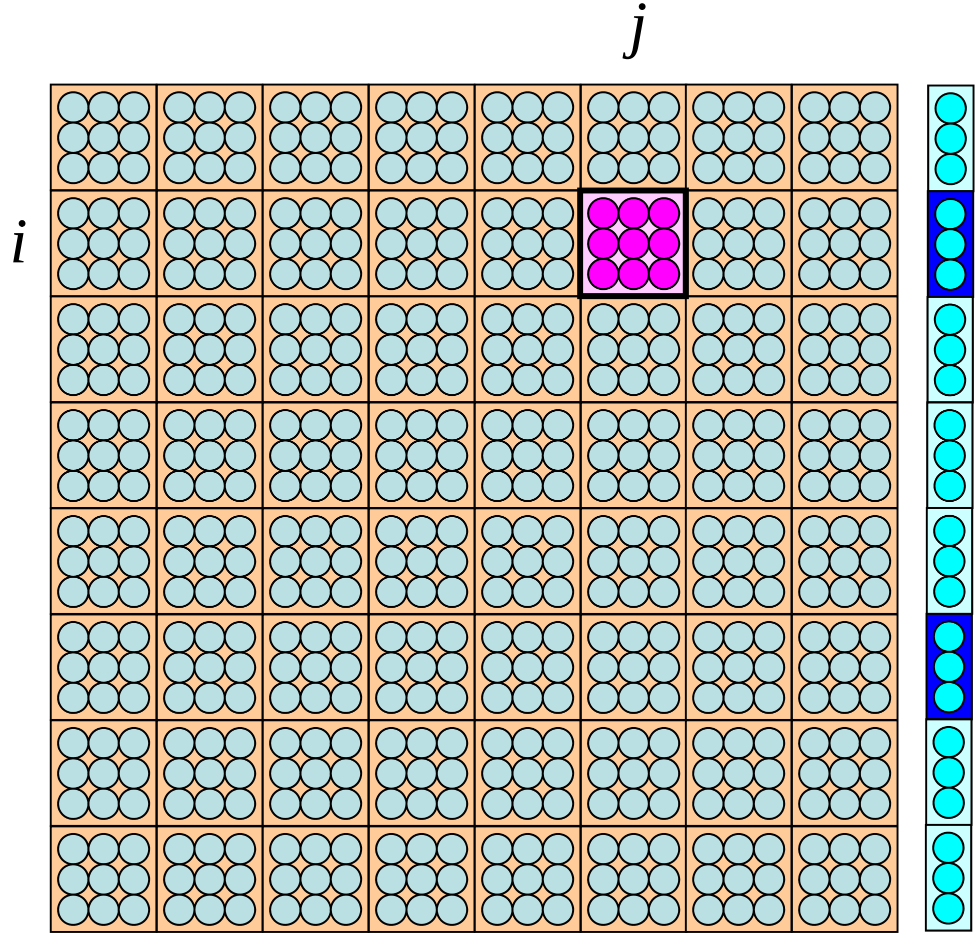
✓-opt-streaming-cache-evict=0	+1.14%
✓-opt-streaming-stores always	+5.60%
✓-opt-prefetch-distance=a,b	+4.56%
	(11.3% total)

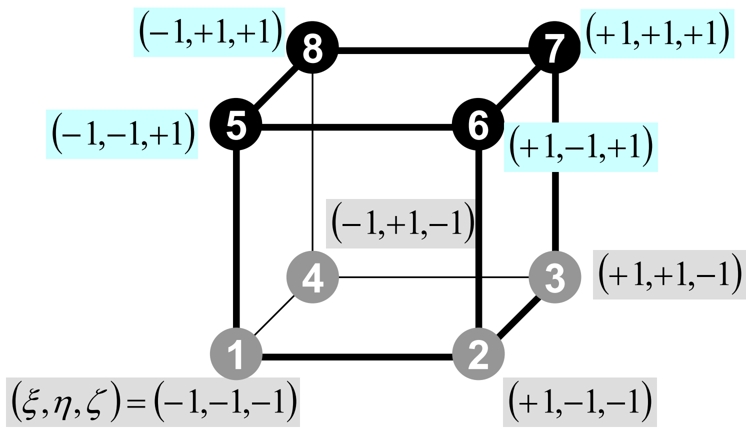
✓Automatic experimental tool for compiler options is now under development

- PCG: GeoFEM Cube/Heat
- ICCG: Poisson3D-OMP
- **Matrix Assembly: GeoFEM Cube/Solid**

Element Matrix: 24x24 Dense Mat.

(u,v,w) components on each node are physically strongly-coupled: these three components are treated in block-wise manner: 8×8 matrix





$$\begin{bmatrix} a_{i_e j_e 11} & a_{i_e j_e 12} & a_{i_e j_e 13} \\ a_{i_e j_e 21} & a_{i_e j_e 22} & a_{i_e j_e 23} \\ a_{i_e j_e 31} & a_{i_e j_e 32} & a_{i_e j_e 33} \end{bmatrix} \left(i_e, j_e = 1 \ldots 8\right)$$

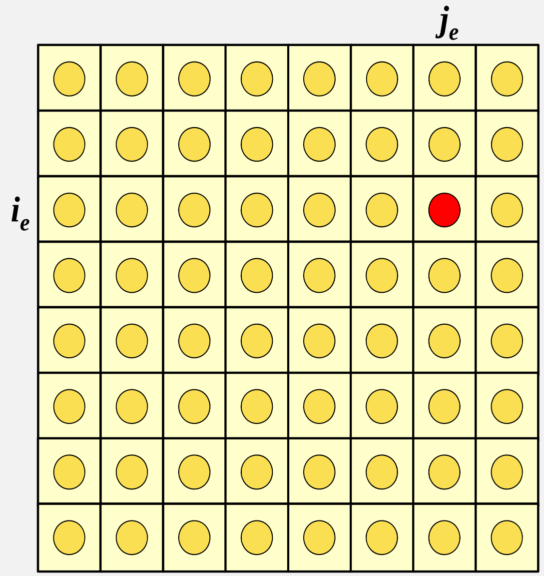
Overview of Matrix Assembling

```
do icel= 1, ICELTOT      Loop for Elements

  <Calculates Jacobian>

  do ie= 1, 8          Local ID
    do je= 1, 8        Local ID
      <Global ID of Nodes: ip, jp>
      <Address of A_ip,jp in sparse matrix: kk>

      do kpn= 1, 2      Gaussian Quad. in ζ
        do jpn= 1, 2    Gaussian Quad. in η
          do ipn= 1, 2  Gaussian Quad. in ξ
            <Calculation of Element Matrices>
          enddo
        enddo
      enddo
    enddo
  enddo
  <Accumulation to Global Matrix>
enddo
```



$$\left[k_{i_e j_e}\right] \quad (i_e, j_e = 1 \sim 8)$$

Assembly of Matrices

- ① Calculations of Jacobian and Grad. of Shape Fn's
- ② Searching of Addresses of Sparse Matrices
- ③ Calculations of Element Matrices
- ④ Accumulations to Global Matrix
  - COLORtot: Number of Colors for Elements (=8)
  - col_index(color): Number of Elements in each Color

```
    do color= 1, COLORtot
!$OMP PARALLEL DO
    do icel= col_index(color-1)+1, col_index(color)
      <① Jacobian & Grad. Shape Fn' s>
      do ie= 1, 8; do je= 1, 8
        <② Address in Sparse Matrix >
        <③ Element Matrices>
        <④ Global Matrix>
      enddo; enddo
    enddo
    enddo
```

Type-A

BLKSIZ: Elem.# in Blocks, NBLK: Block #, icel: Elem. ID

```
!$omp parallel (…)
    do color= 1, COLORtot
!$omp do
    do ip= 1, THREAD_num
      NBLK: calculated by (col_index, color, thread#)
    do ib= 1, NBLK
      do blk= 1, BLKSIZ
        icel: calculated by (col_index, ib, blk)
!$omp simd
        do ie= 1, 8; do je= 1, 8
          <② Address in Sparse Matrix>
        enddo; enddo
      enddo
      do blk= 1, BLKSIZ
        icel: calculated by (col_index, ib, blk)
        <① Jacobian & Grad. Shape Fn’ s>
!$omp simd
        do ie= 1, 8; do je= 1, 8
          <③ Element Matrices >
        enddo; enddo
      enddo
      do blk= 1, BLKSIZ
        icel: calculated by (col_index, ib, blk)
!$omp simd
        do ie= 1, 8; do je= 1, 8
          <④ Global Matrices>
        enddo; enddo
      enddo
    enddo
    enddo
    enddo
!$omp end parallel
```

Type-B

BLKSIZ: Elem.# in Blocks, NBLK: Block #, icel: Elem. ID

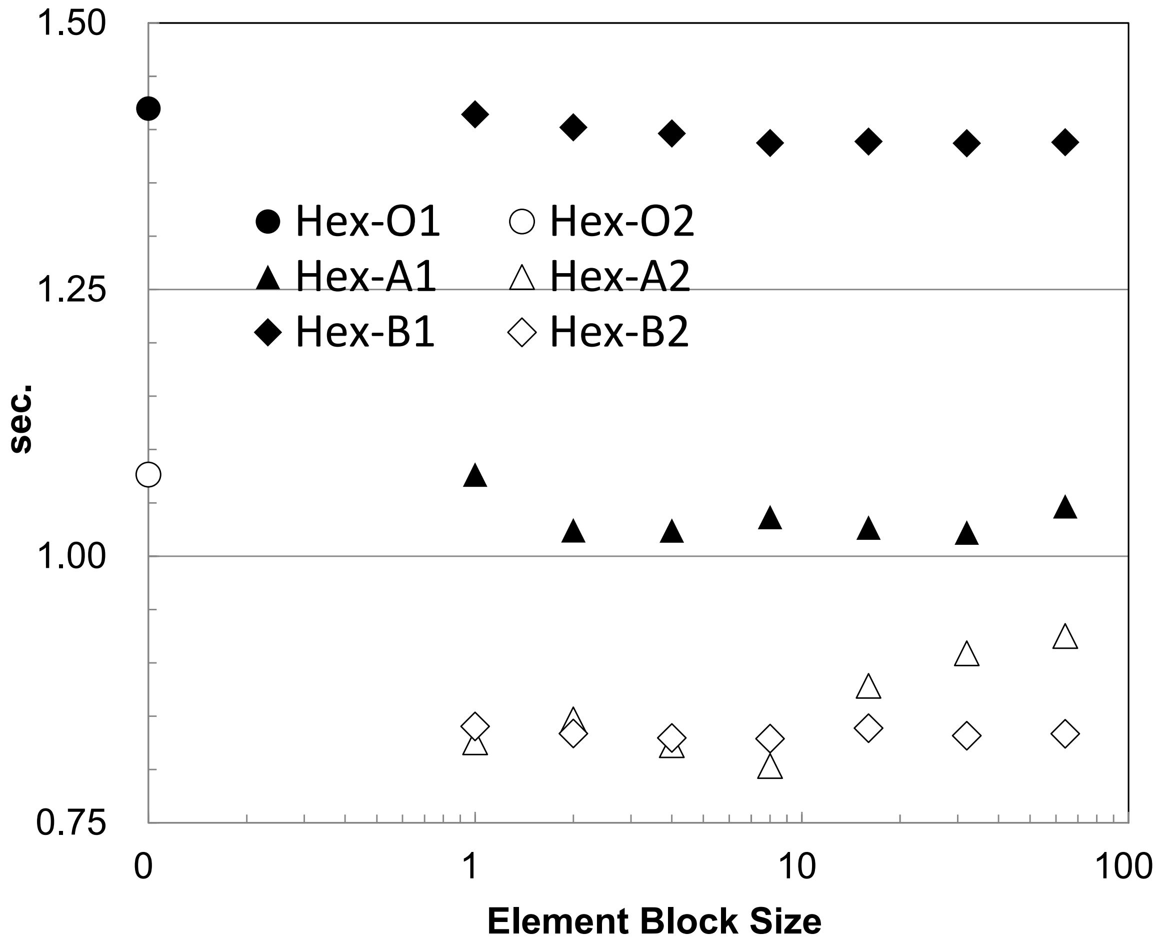
```
!$omp parallel (…)
    do color= 1, COLORtot
!$omp do
    do ip= 1, THREAD_num
      NBLK: calculated by (col_index, color, thread#)
    do ib= 1, NBLK
      do blk= 1, BLKSIZ
        icel: calculated by (col_index, ib, blk)
!$omp simd
        do ie= 1, 8; do je= 1, 8
          <② Address in Sparse Matrix>
        enddo; enddo
      enddo
      do blk= 1, BLKSIZ
        <① Jacobian & Grad. Shape Fn’s>
        icel: calculated by (col_index, ib, blk)
!$omp simd
        do ie= 1, 8; do je= 1, 8
          <③ Element Matrices>
          <④ Global Matrices>
        enddo; enddo
      enddo
    enddo
    enddo
    enddo
!$omp end parallel
```

Comp. Time for Matrix Assembly

KNC: 240 Threads x 1

O: Original, A: Type-A, B: Type-B

1: without !$omp simd, 2: with !$omp simd



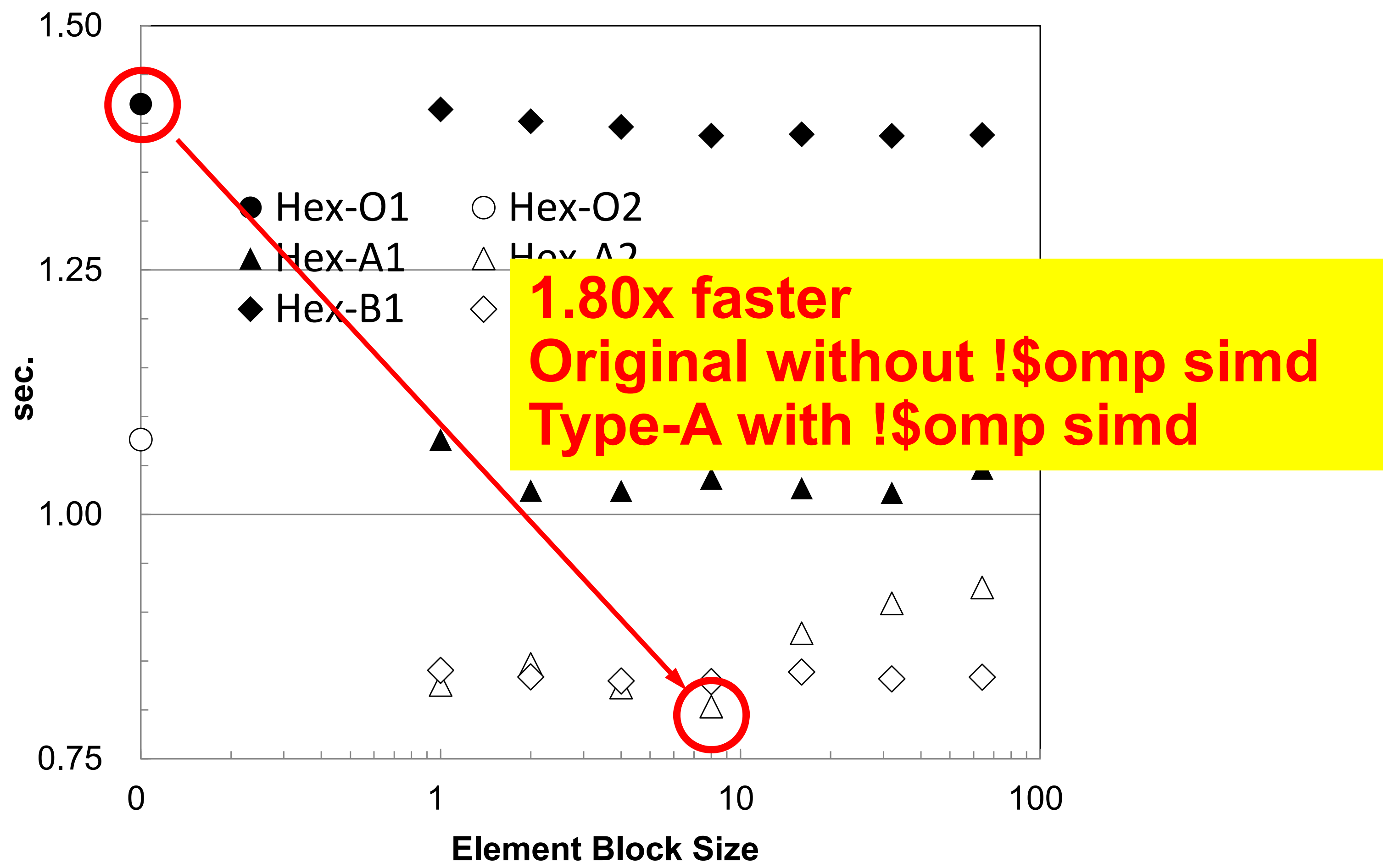
Significant Improvement by !$omp simd

Comp. Time for Matrix Assembly

KNC: 240 Threads x 1

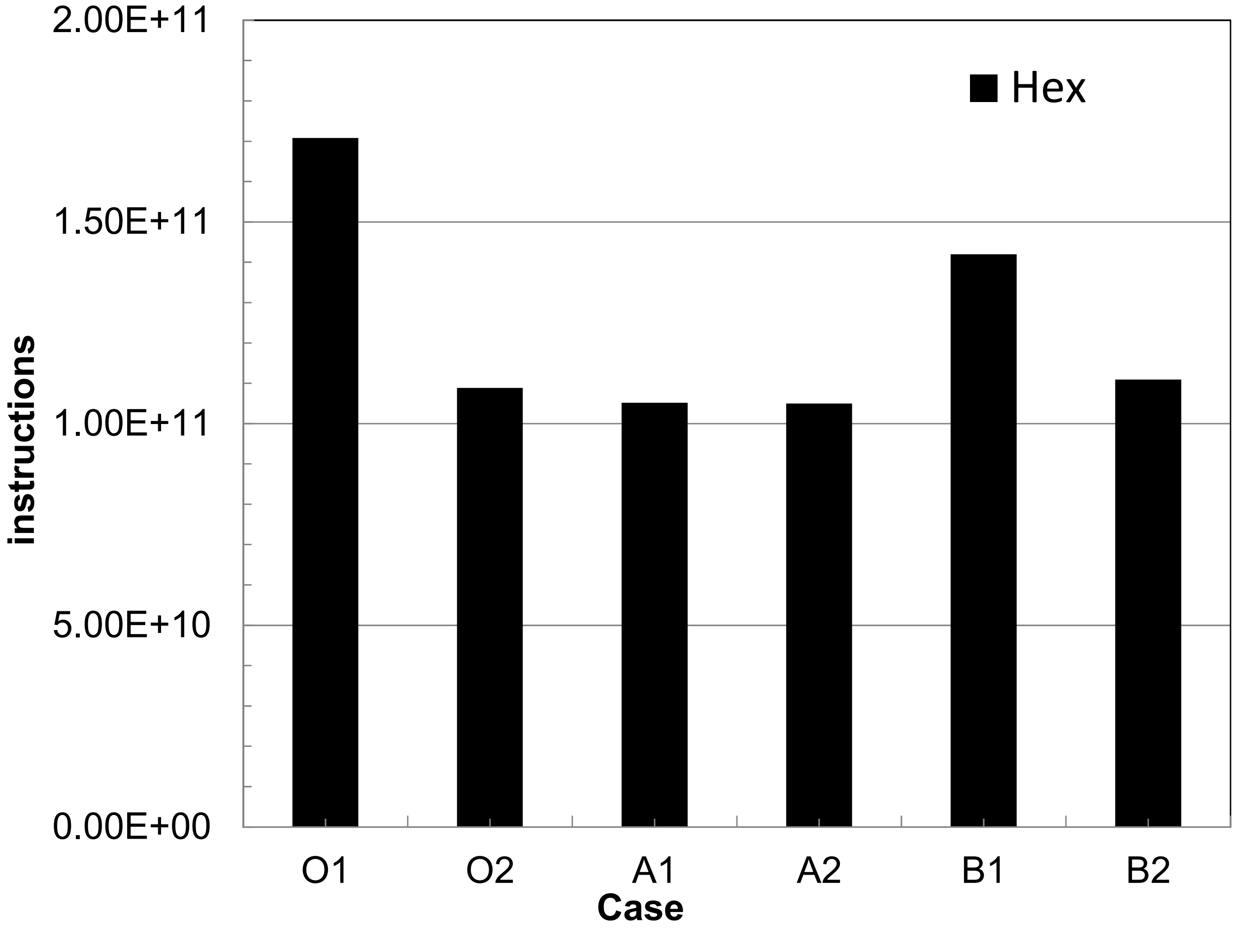
O: Original, A: Type-A, B: Type-B

1: without !$omp simd, 2: with !$omp simd



Instruction # for Matrix Assembly

KNC: 240 Threads x 1, Vtune
O: Original, A: Type-A, B: Type-B
1: without !$omp simd, 2: with !$omp simd



Summary

- Iterative Solvers
  - Format for Storing Sparse Matrices
    - MIC: Significant
    - IvyB: Very small (Out-of-Order architecture?, What’s happening in KNL ?)
  - Vectorization
    - Effects are not so clear in ICCG
    - Future Works: SELL-C-Sigma in ICCG
  - Compile Options
    - Interesting results
    - An automatic tool for experiments under development
- Matrix Assembly
  - Effects of vectorization is significant