Flat MPI and Hybrid Parallel Programming Models for FEM Applications on SMP Cluster Architectures

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Overview

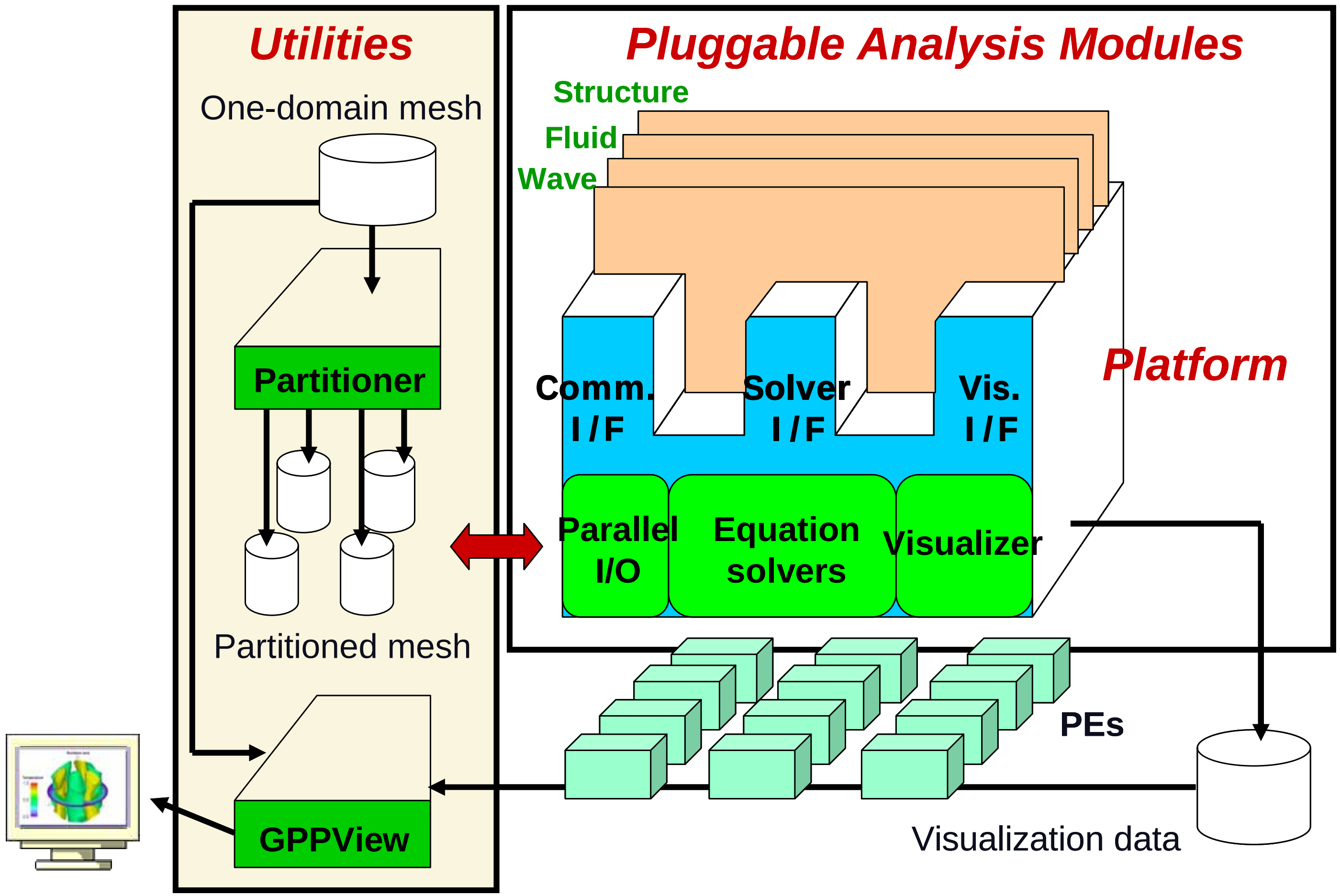
- Background
  - GeoFEM Project & Earth Simulator
  - Preconditioned Iterative Linear Solvers
- Optimization Strategy on the Earth Simulator
  - BIC(0)-CG for Simple 3D Linear Elastic Applications
- Effect of reordering on various types of architectures
  - Contact Problems
  - PGA (Pin-Grid Array)
  - Multigrid
- Summary & Future Works

GeoFEM: FY.1998-2002

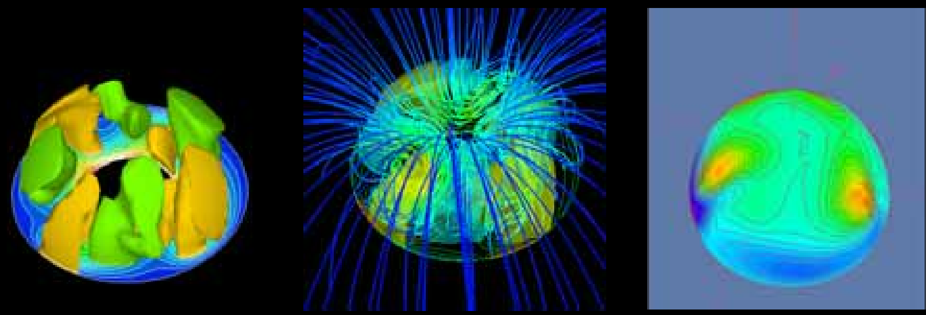
http://geofem.tokyo.rist.or.jp/

- Parallel FEM platform for solid earth simulation.
  - parallel I/O, **parallel linear solvers**, parallel visualization
  - solid earth: earthquake, plate deformation, mantle/core convection, etc.
- Part of national project by STA/MEXT for large-scale earth science simulations using the Earth Simulator.
- Strong collaborations between HPC and natural science (solid earth) communities.
- Current Activity
  - Research Consortium for Solid Earth Simulations on the Earth Simulator (9 sub-groups, >80 members)

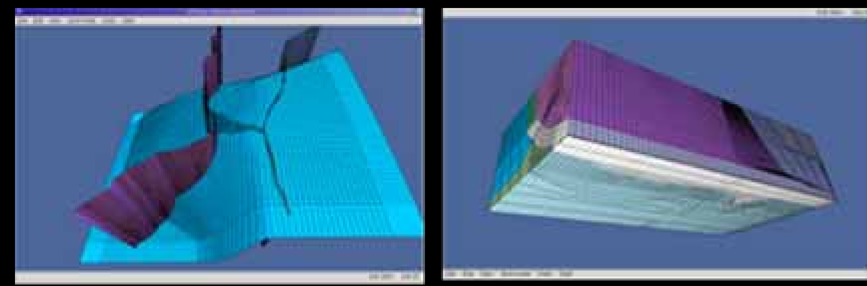
System Configuration of GeoFEM



Results on Solid Earth Simulation



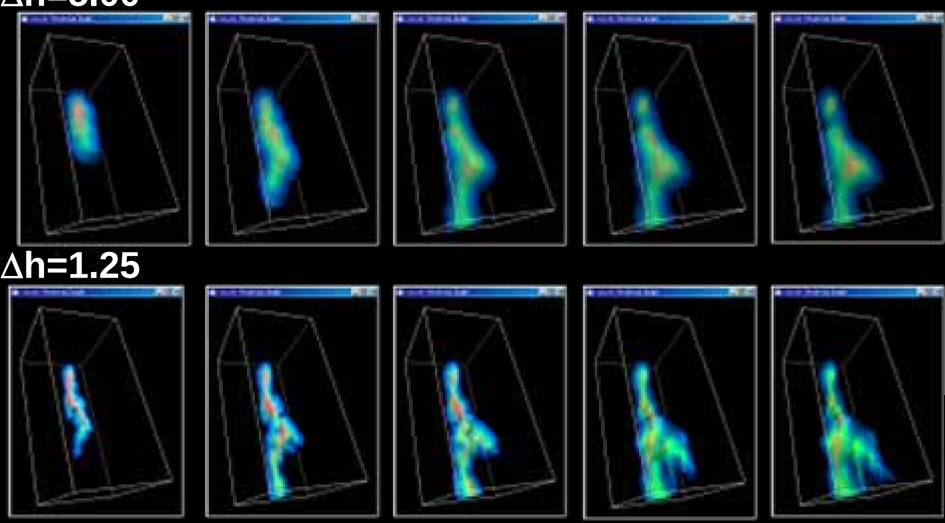
Magnetic Field of the Earth : MHD code



Complicated Plate Model around Japan Islands

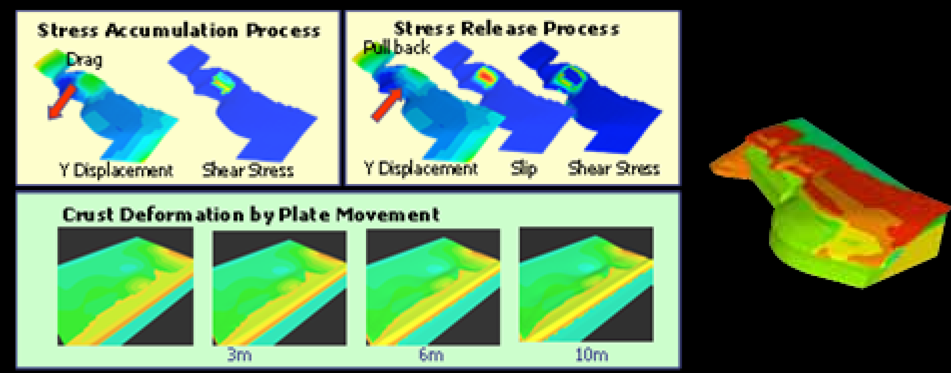
Δh=5.00

Δh=1.25

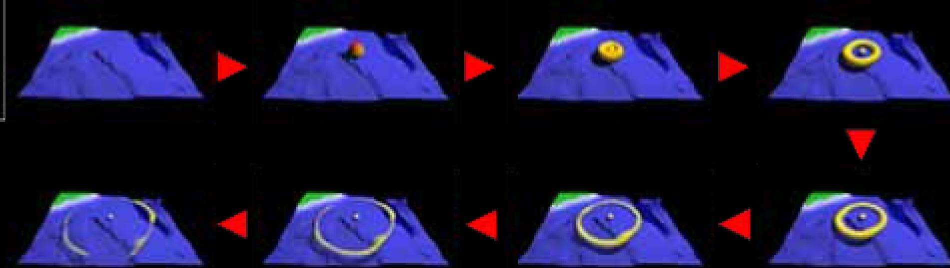


T=100 T=200 T=300 T=400 T=500

Transportation by Groundwater Flow
through Heterogeneous Porous Media

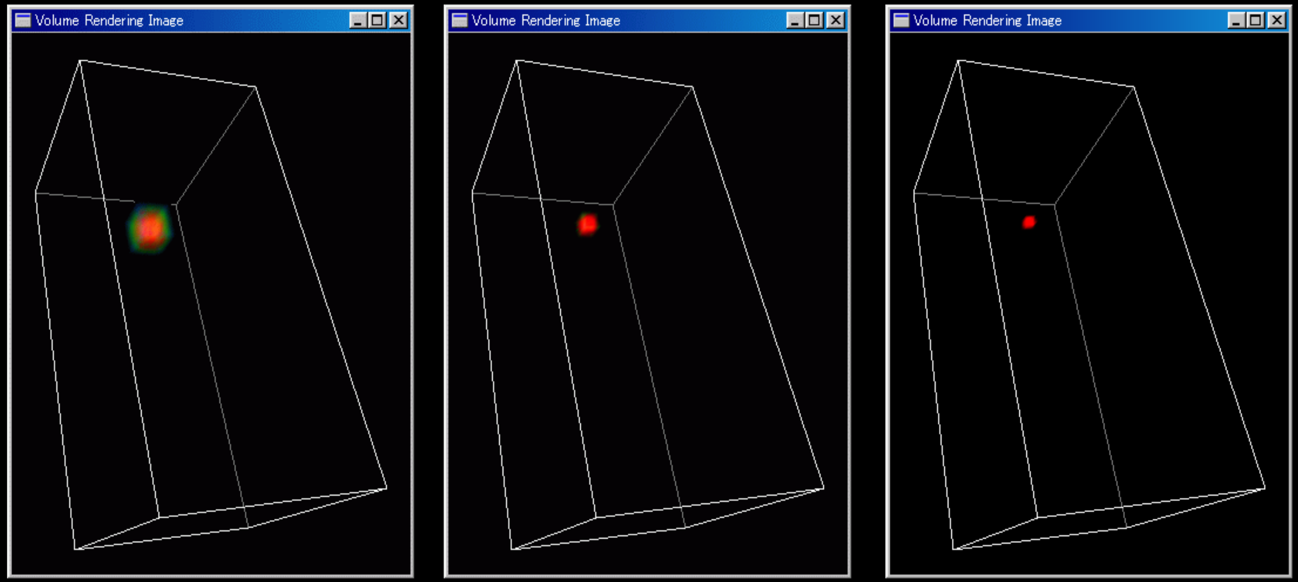


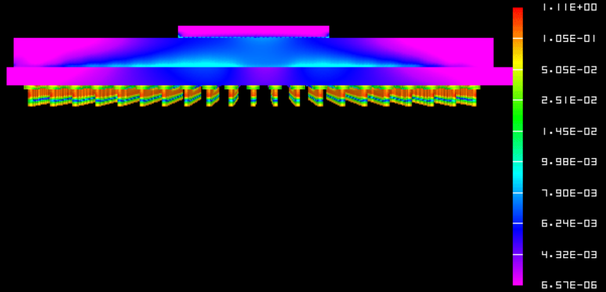
Simulation of Earthquake Generation Cycle
in Southwestern Japan

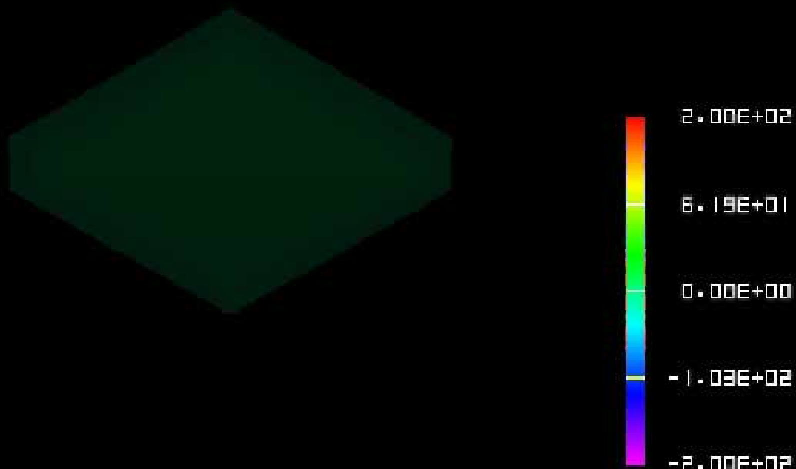


TSUNAMI !!

Results by GeoFEM







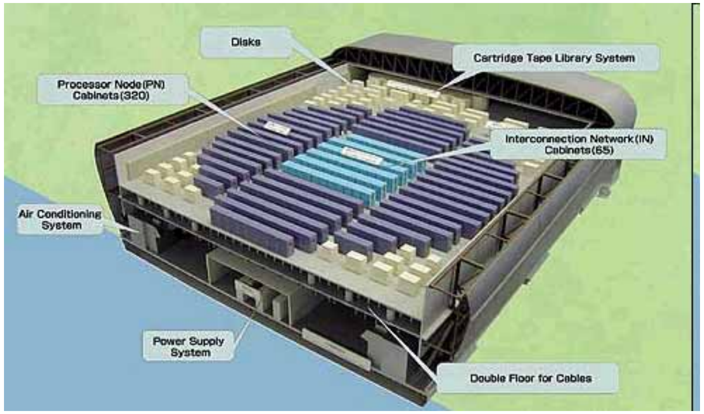
Motivations

- GeoFEM Project (FY.1998-2002)
- Performance evaluation of FEM-type applications with complicated unstructured grids (not LINPACK, FDM …) on the Earth Simulator (ES)
  - Implicit Linear Solvers
    - Preconditioned Iterative Solver
  - Hybrid vs. Flat MPI Parallel Programming Model

Earth Simulator (ES)

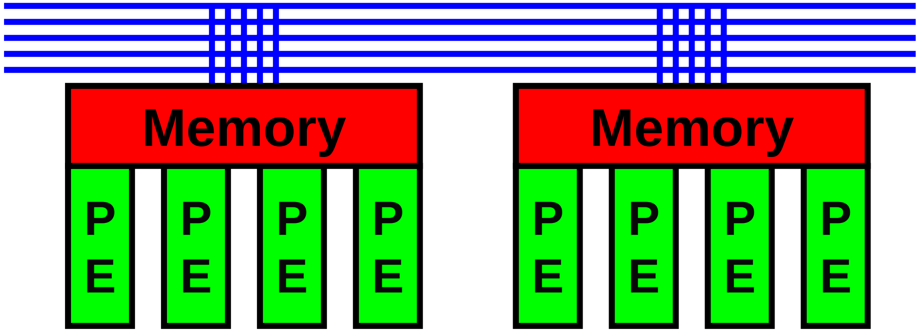
http://www.es.jamstec.go.jp/

- 640×8= 5,120 Vector Processors
  - **SMP Cluster-Type Architecture**
  - 8 GFLOPS/PE
  - 64 GFLOPS/Node
  - 40 TFLOPS/ES
- 16 GB Memory/Node, 10 TB/ES
- 640×640 Crossbar Network
  - 12.3 GB/sec×2
- Memory BWTH with 32 GB/sec.
- **35.6 TFLOPS for LINPACK (2002-March)**
- **26 TFLOPS for AFES (Climate Simulation)**

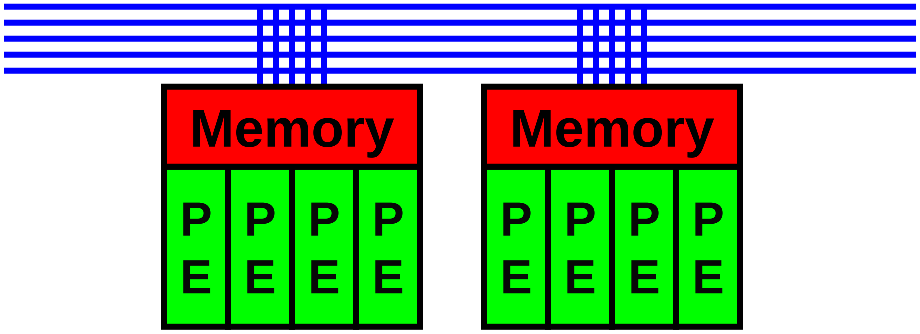


Flat MPI vs. Hybrid

Flat-MPI：Each PE -> Independent



Hybrid：Hierarchal Structure



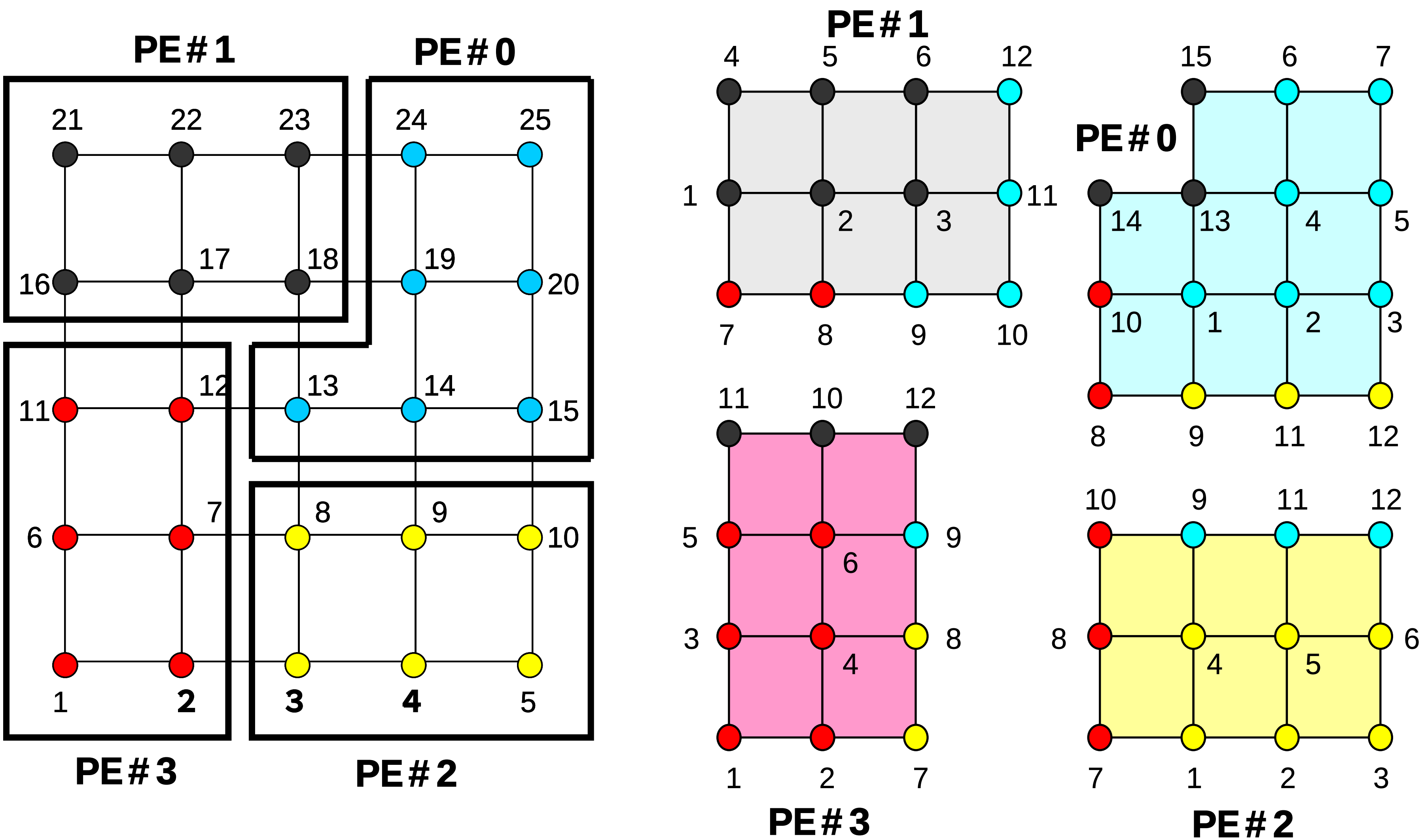
Hybrid vs. Flat-MPI

- “Initial” Motivation for *Hybrid*
  - Block Jacobi-type Localized Parallel Preconditioning
  - Relatively lower convergence rate for many domains (or processors).
  - “Hybrid” may provide better convergence rate (i.e. faster convergence) because domain number is 1/8 of that of Flat-MPI programming model (on ES).

Local Data Structure

Node-based Partitioning

internal nodes - elements - external nodes



Block-Jacobi Type Localized ILU(0) Preconditioning [Nakajima et al. 1999]

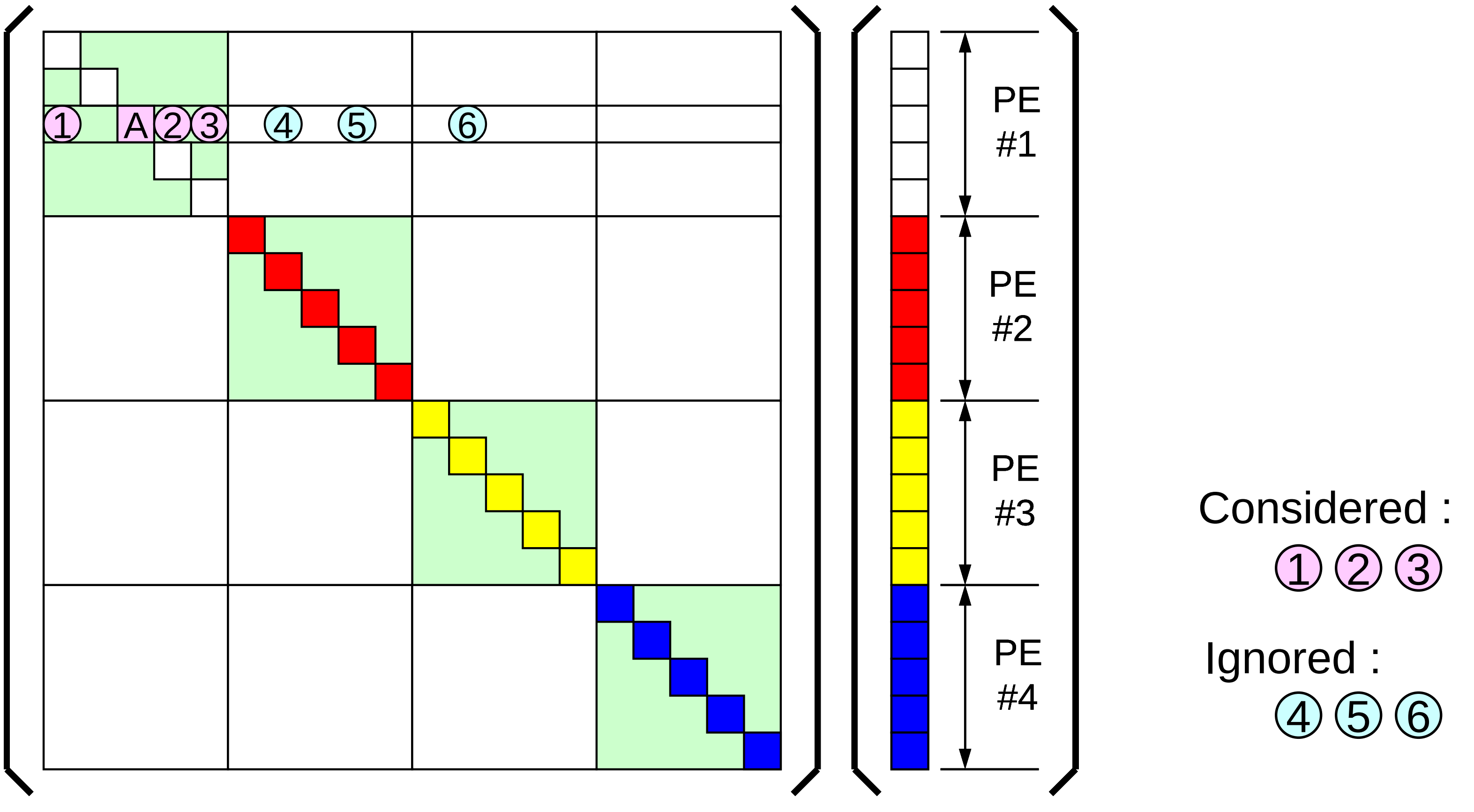
- Global data dependency in ILU preconditioner is not suitable for parallel computing.

$$y_k = b_k - \sum_{j=1}^{k-1} l_{kj} y_j \, (k = 2, \cdots, N)$$

$$x_k = \tilde{d}_k \left(y_k - \sum_{j=k+1}^{N} u_{kj} y_j \right) \quad (k = N, N-1, \cdots, 1)$$

- Ignore the effects by elements which belong to different partition / processor.
- Not as *strong* as original ILU.
  - How bad in many PE cases ?

Block-Jacobi Type Localized ILU(0) Preconditioning [Nakajima et al. 1999]



Matrix components whose columun numbers are outside the processor are ignored (set equal to 0) at Back-Forward Substitution.

Overlapped Additive Schwartz Domain Decomposition Method

Effect of additive Schwartz domain decomposition for solid mechanics example example with $3x44^3$ DOFs 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

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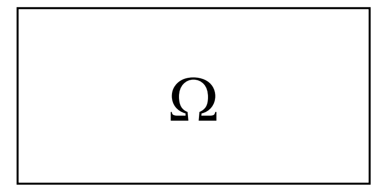
Overlapped Additive Schwartz Domain Decomposition Method

for Stabilizing Localized Preconditioning

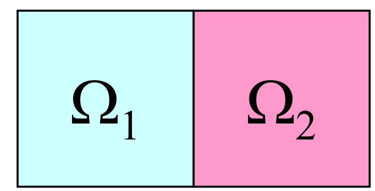
Global Operation

$$Mz = r$$



Local Operation

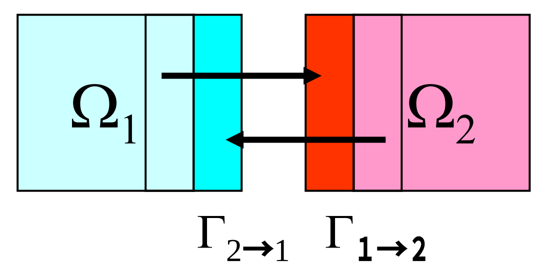
$$M_{\Omega_1} z^n_{\Omega_1} = r_{\Omega_1}, \quad M_{\Omega_2} z^n_{\Omega_2} = r_{\Omega_2}$$



Global Nesting Correction

$$z^n_{\Omega_1} \leftarrow z^{n-1}_{\Omega_1} + M^{-1}_{\Omega_1}\left(r_{\Omega_1} - M_{\Omega_1} z^{n-1}_{\Omega_1} - M_{\Gamma_{2\to1}} z^{n-1}_{\Gamma_{2\to1}}\right)$$

$$z^n_{\Omega_2} \leftarrow z^{n-1}_{\Omega_2} + M^{-1}_{\Omega_2}\left(r_{\Omega_2} - M_{\Omega_2} z^{n-1}_{\Omega_2} - M_{\Gamma_{1\to2}} z^{n-1}_{\Gamma_{1\to2}}\right)$$



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  - “Hybrid” may provide better convergence rate (i.e. faster convergence) because domain number is 1/8 of that of Flat-MPI programming model (on ES).
- Factors for Performance
  - Type of Applications, Problem Size
  - ***Balance*** of H/W Parameters

R. Rabenseifner: *Communication Bandwidth of Parallel Programming Models on Hybrid Architectures*, International Workshop on OpenMP: Experiences and Implementa-tions (WOMPEI 2002), Lecture Notes in Computer Science 2327, pp.437-448, 2002.

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Block IC(0)-CG Solver on the Earth Simulator

- 3D Linear Elastic Problems (SPD)
- Parallel Iterative Linear Solver
  - Node-based Local Data Structure
  - Conjugate-Gradient Method (CG): SPD
  - Localized Block IC(0) Preconditioning (Block Jacobi)
  - Additive Schwartz Domain Decomposition (ASDD)
  - http://geofem.tokyo.rist.or.jp/
- Hybrid Parallel Programming Model
  - OpenMP + MPI
  - Re-Ordering for Vector/Parallel Performance
  - Comparison with Flat MPI

Flat MPI vs. Hybrid

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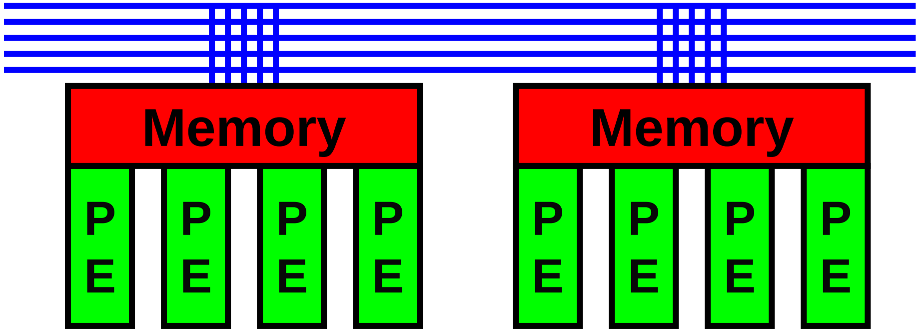

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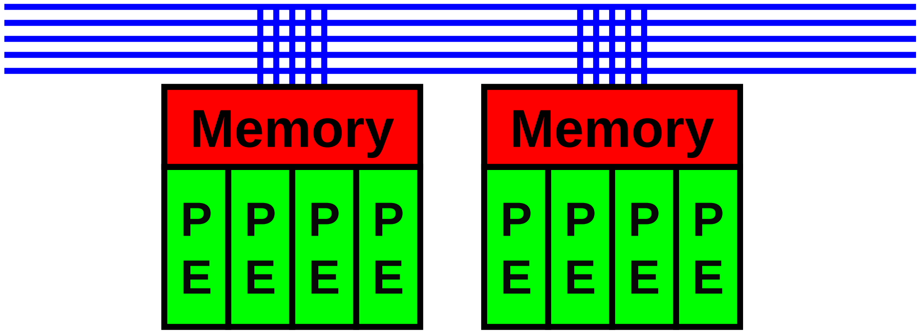

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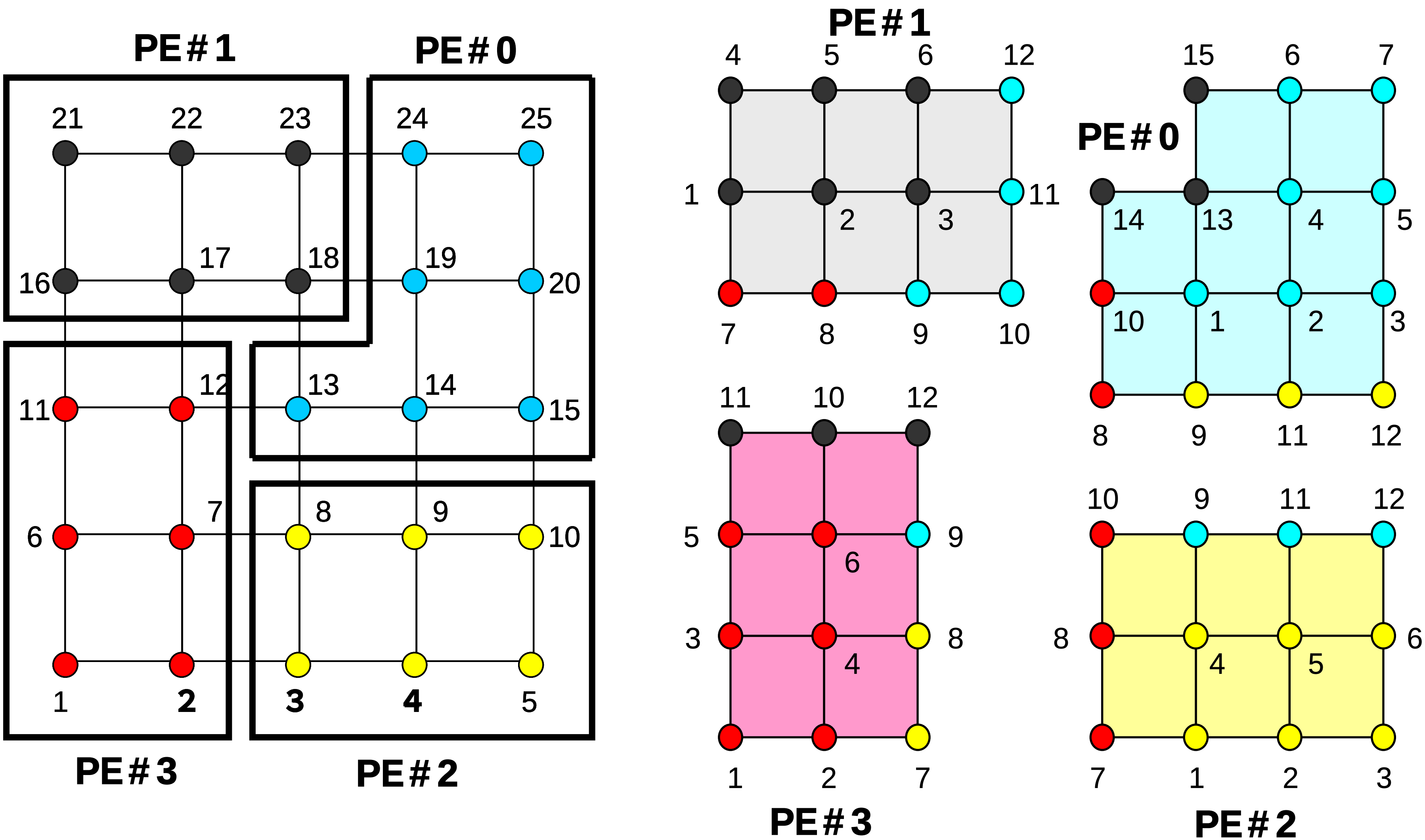
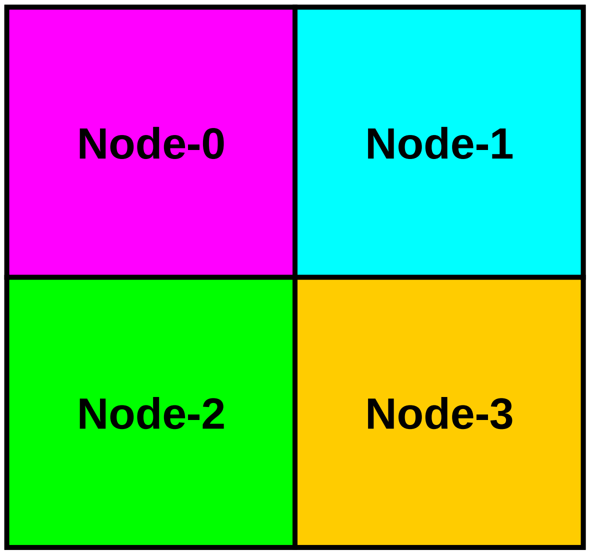
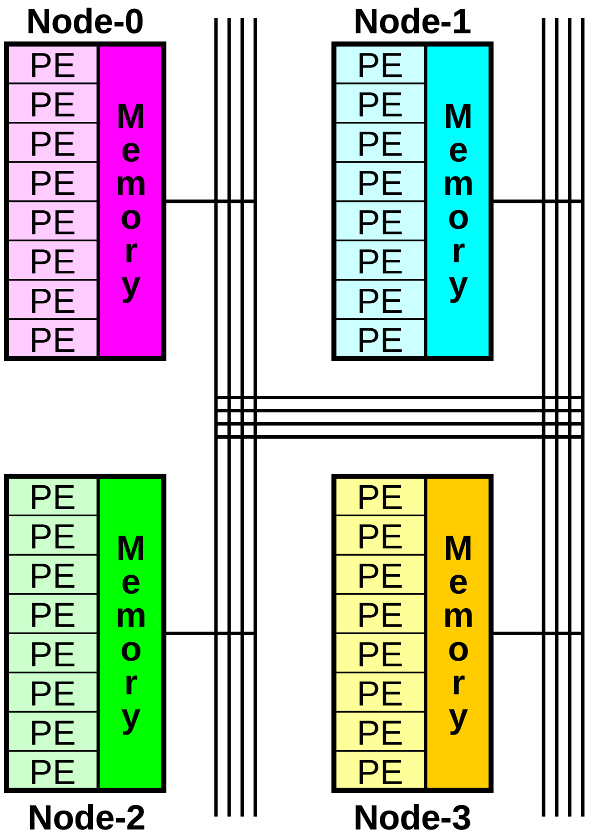


1 SMP node => 1 domain for Hybrid Programming Model

MPI communication among domains





Basic Strategy for Parallel Programming on the Earth Simulator

- Hypothesis
  - Explicit ordering is required for unstructured grids in order to achieve higher performance in factorization processes on SMP node and vector processors.

$$M = (L+D)D^{-1}(D+U)$$

$\underline{Mz = r}$ need to solve this equation

$$D^{-1}(D+U) = z_1$$

Forward Substitution

$$(L+D)z_1 = r \;:\; z_1 = D^{-1}(r - Lz_1)$$

Backward Substitution

$$(I + D^{-1}U)z_{NEW} = z_1$$

$$z = z - D^{-1}Uz$$

Basic Strategy for Parallel Programming on the Earth Simulator

- Hypothesis
  - Explicit ordering is required for unstructured grids in order to achieve higher performance in factorization processes on SMP node and vector processors.

Forward Substitution

$(L+D)z= r \;:\; z= D^{-1}(r-Lz)$

```
do i= 1, N
  WVAL= R(i)
  do j= 1, INL(i)
    WVAL= WVAL -  AL(i,j) * Z(IAL(i,j))
  enddo
  Z(i)= WVAL / D(i)
enddo
```

$M = (L+D)D^{-1}(D+U)$

L,D,U: A

Backward Substitution

$(I+ D^{-1} U)z_{new}= z_{old} \;:\; z= z - D^{-1}Uz$

```
do i= N, 1, -1
  SW  = 0.0d0
  do j= 1, INU(i)
    SW= SW + AU(i,j) * Z(IAU(i,j))
  enddo
  Z(i)= Z(i) – SW / D(i)
enddo
```

Dependency…
You need the most recent value of “z” of connected nodes. Vectorization/parallelization is difficult.

Reordering:
Directly connected nodes do not appear in RHS.

Basic Strategy for Parallel Programming on the Earth Simulator

- Hypothesis
  - Explicit ordering is required for unstructured grids in order to achieve higher performance in factorization processes on SMP node and vector processors.
- Re-Ordering for Highly Parallel/Vector Performance
  - Local operation and no global dependency
  - Continuous memory access
  - Sufficiently long loops for vectorization

Basic Strategy for Parallel Programming on the Earth Simulator

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  - Explicit ordering is required for unstructured grids in order to achieve higher performance in factorization processes on SMP node and vector processors.
- Re-Ordering for Highly Parallel/Vector Performance
  - Local operation and no global dependency
  - Continuous memory access
  - Sufficiently long loops for vectorization
- 3-Way Parallelism for Hybrid Parallel Programming
  - Inter Node : MPI
  - Intra Node : OpenMP
  - Individual PE : Vectorization

Re-Ordering Technique for Vector/Parallel Architectures

Cyclic DJDS(RCM+CMC) Re-Ordering
(Doi, Washio, Osoda and Maruyama (NEC))

1. RCM (Reverse Cuthil-Mckee)
2. CMC (Cyclic Multicolor)

Vector
SMP Parallel

3. DJDS re-ordering

Vector

4. Cyclic DJDS for SMP unit

SMP Parallel

These processes can be substituted by **traditional multi-coloring (MC).**

Re-Ordering Technique for Vector/Parallel Architectures

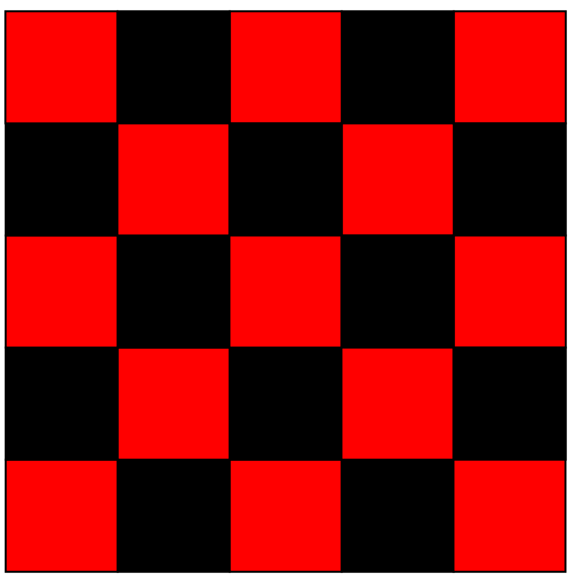
Cyclic DJDS(RCM+CMC) Re-Ordering
(Doi, Washio, Osoda and Maruyama (NEC))

K.Nakajima, “Parallel Iterative Solvers of GeoFEM with Selective Blocking Preconditioning for Nonlinear Contact Problems on the Earth Simulator“
SC2003 Technical Session, Phoenix, Arizona, 2003.[

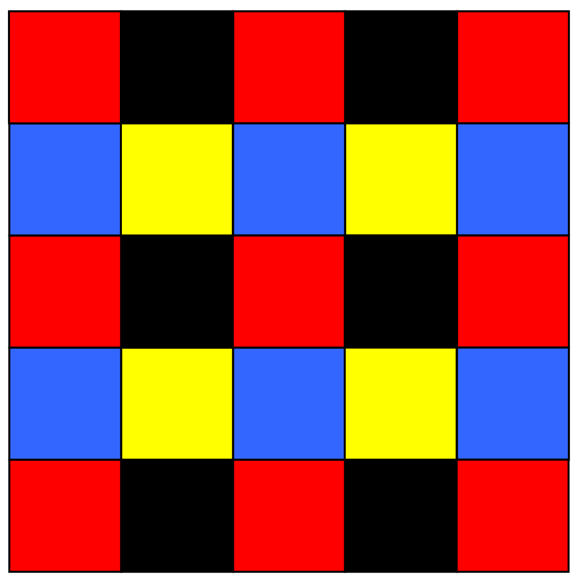
http://www.sc-conference.org/sc2003/paperpdfs/pap155.pdf

Reordering = Coloring

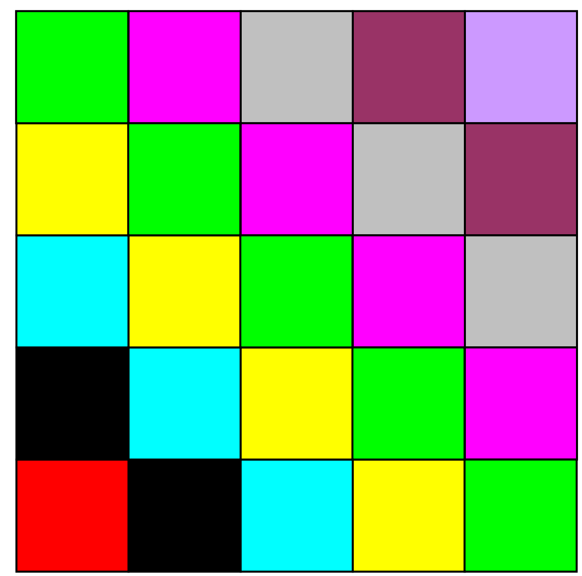
- **COLOR**: Unit of independent sets.
- Elements grouped in the same “color” are independent from each other, thus parallel/vector operation is possible.
- Many colors provide faster convergence, but shorter vector length.: **Trade-Off !!**



Red-Black (2 colors)



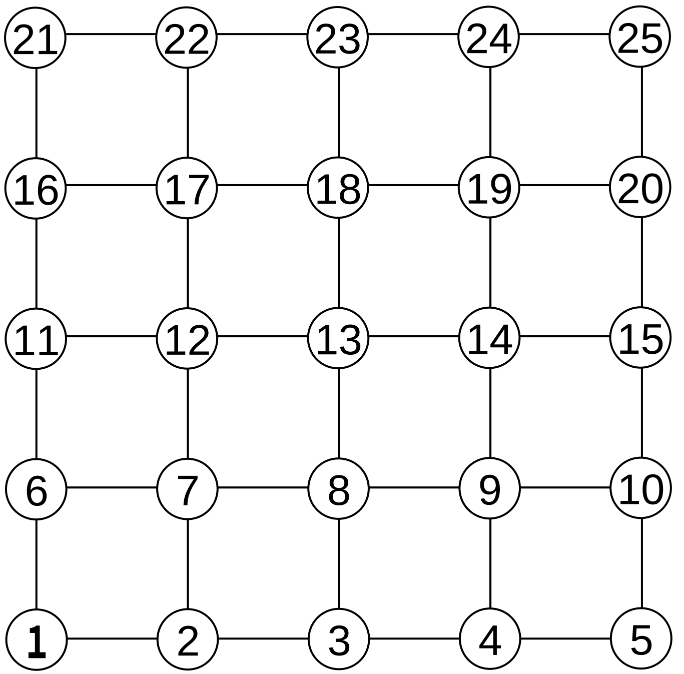
4 colors

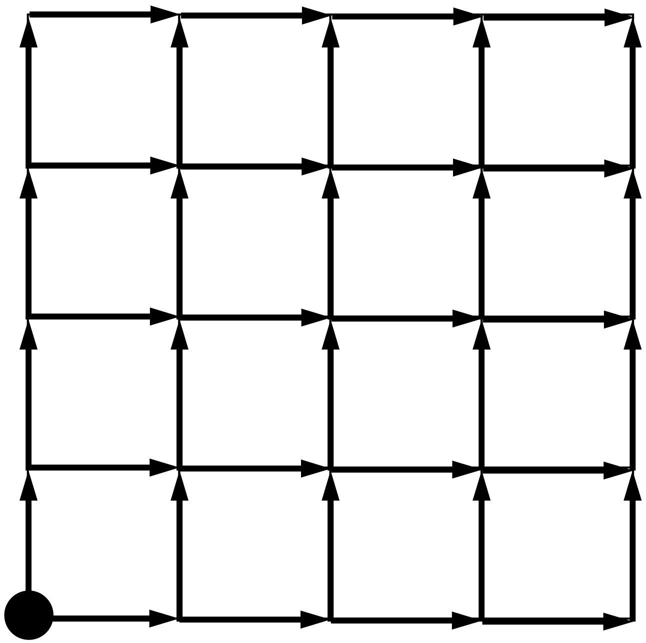


Multicolor

Colors & Iterations Incompatible Nodes

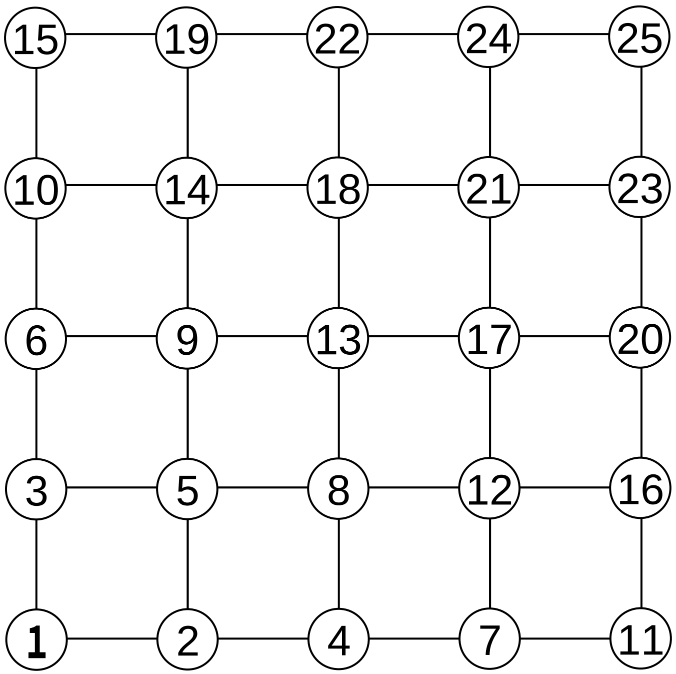
Doi, S. (NEC) et al.

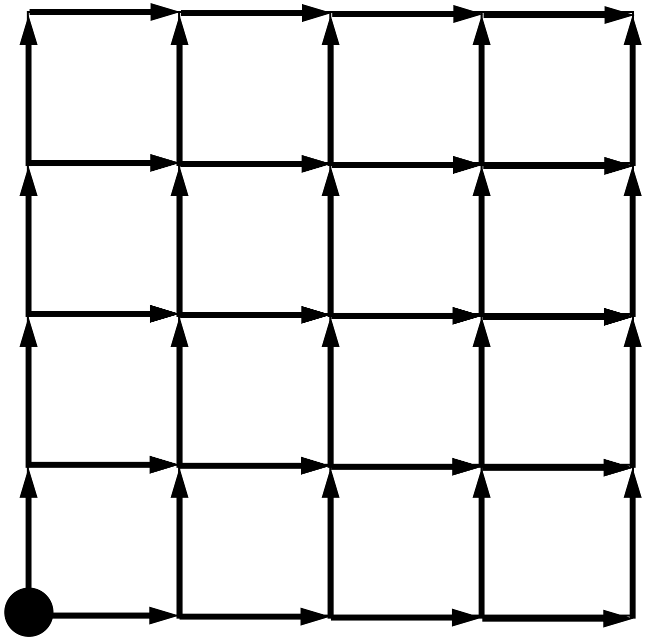




“Incompatible nodes” are not affected by other nodes. System with fewer incompatible nodes provides faster convergence.

RCM Ordering

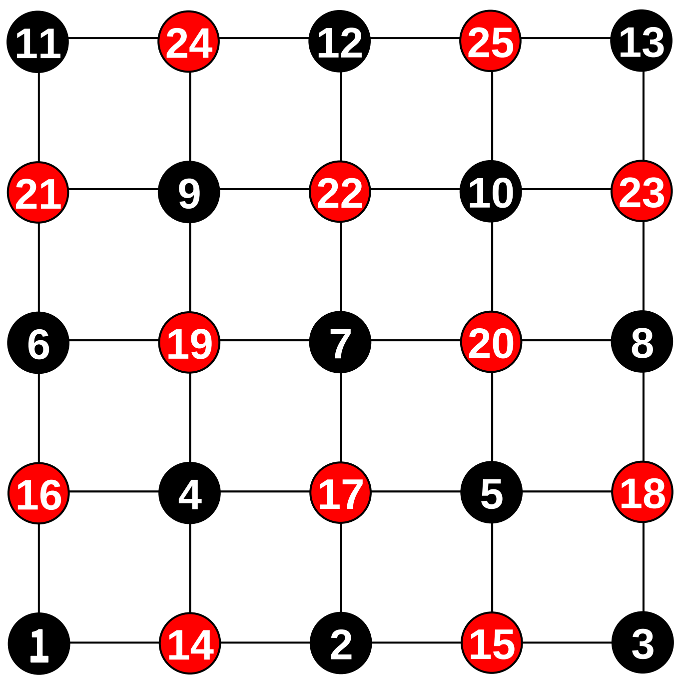


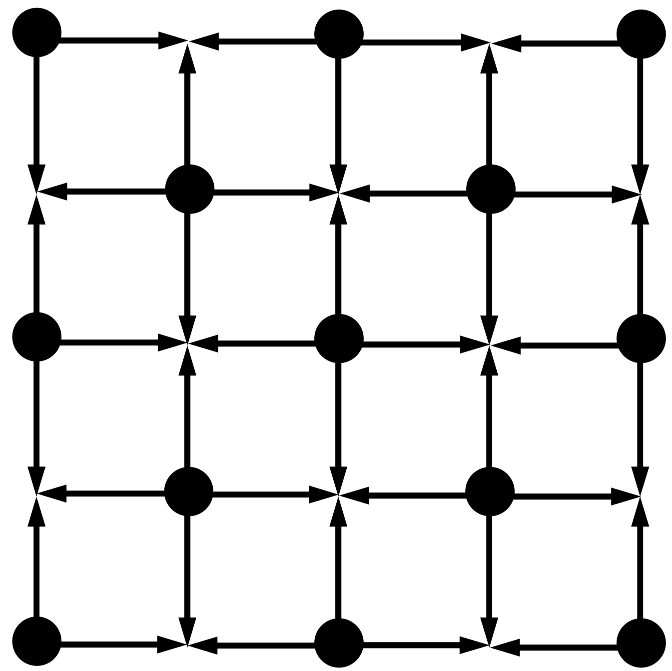


Red-Black Ordering

Highly Parallelized: Large Loop Length

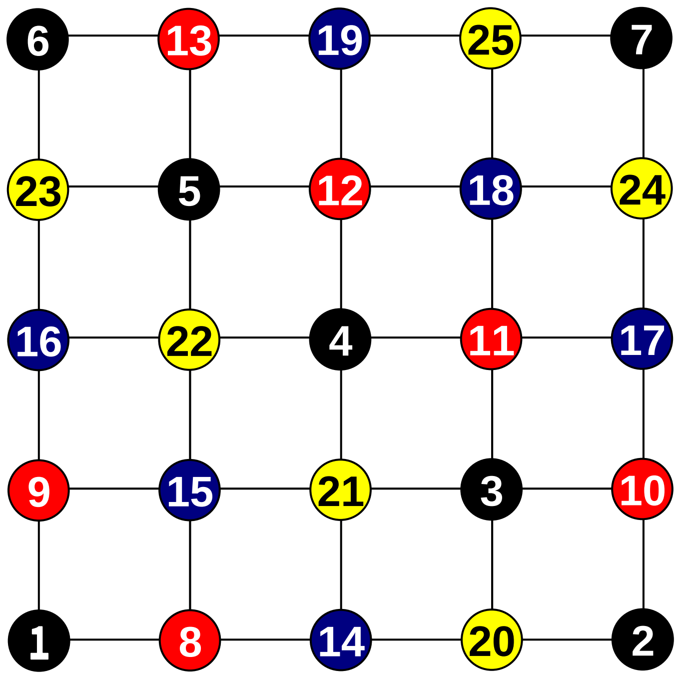
Many Incompatible Nodes: Slow Convergence

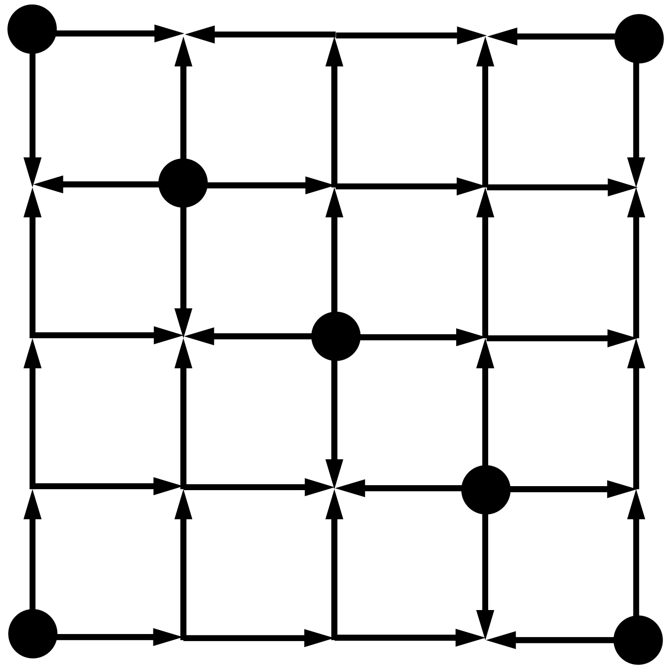




Four-Color Ordering

Fairly Parallelized: Shorter Loop Length
Fewer Incompatible Nodes: Faster Convergence





Cyclic DJDS(RCM+CMC)

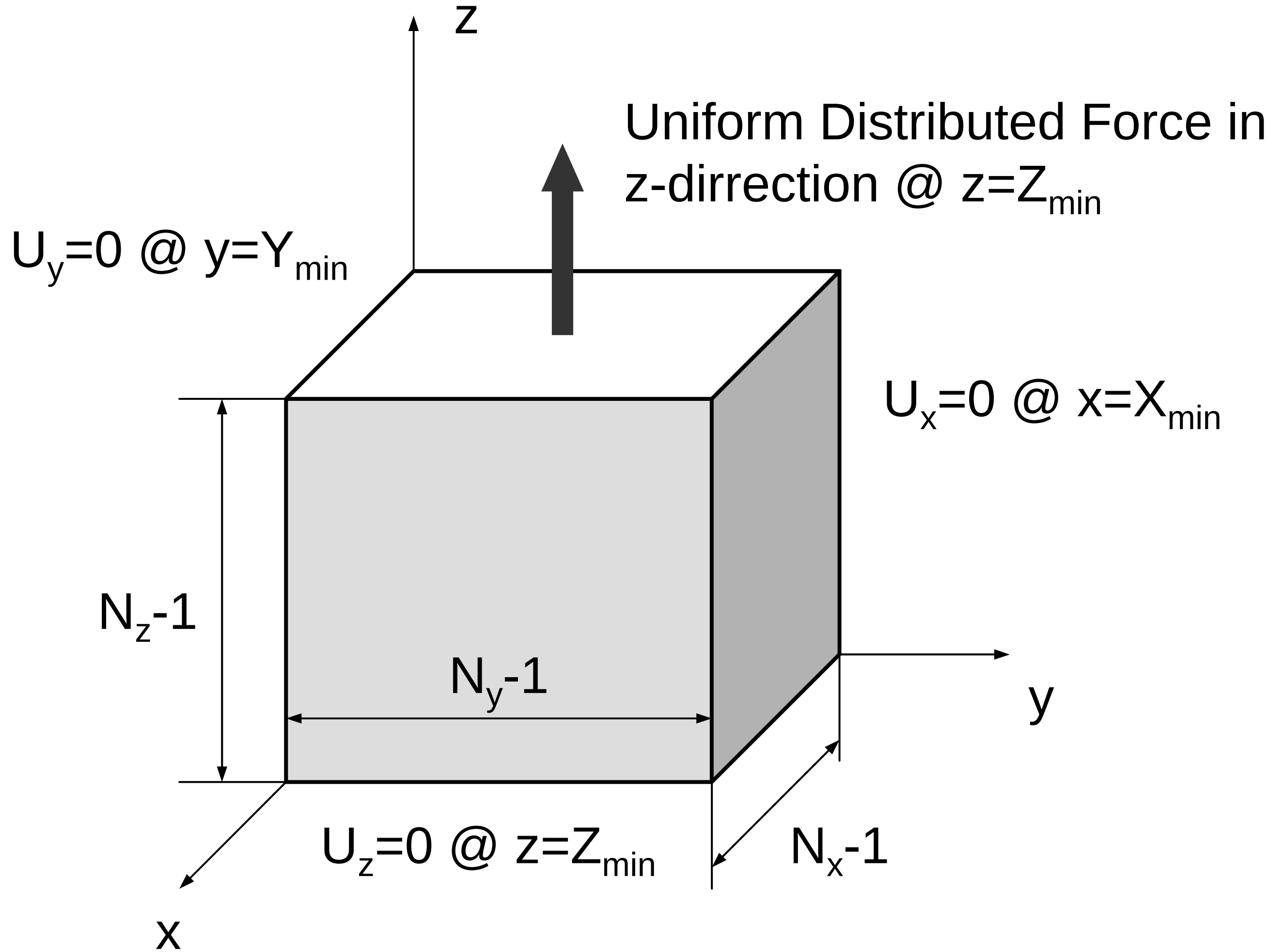
for Forward/Backward Substitution in BILU Factorization

SMP parallel

Vectorized

```
do iv= 1, NCOLORS
!$omp parallel do private (iv0,j,iS,iE,i,k,kk etc.)
do ip= 1, PEsmpTOT
  iv0= STACKmc(PEsmpTOT*(iv-1)+ip- 1)
  do j= 1, NLhyp(iv)
    iS= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip-1)
    iE= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip  )
!CDIR NODEP
    do i= iv0+1, iv0+iE-iS
      k= i+iS - iv0
      kk= IAL(k)
      (Important Computations)
    enddo
  enddo
enddo
enddo
```

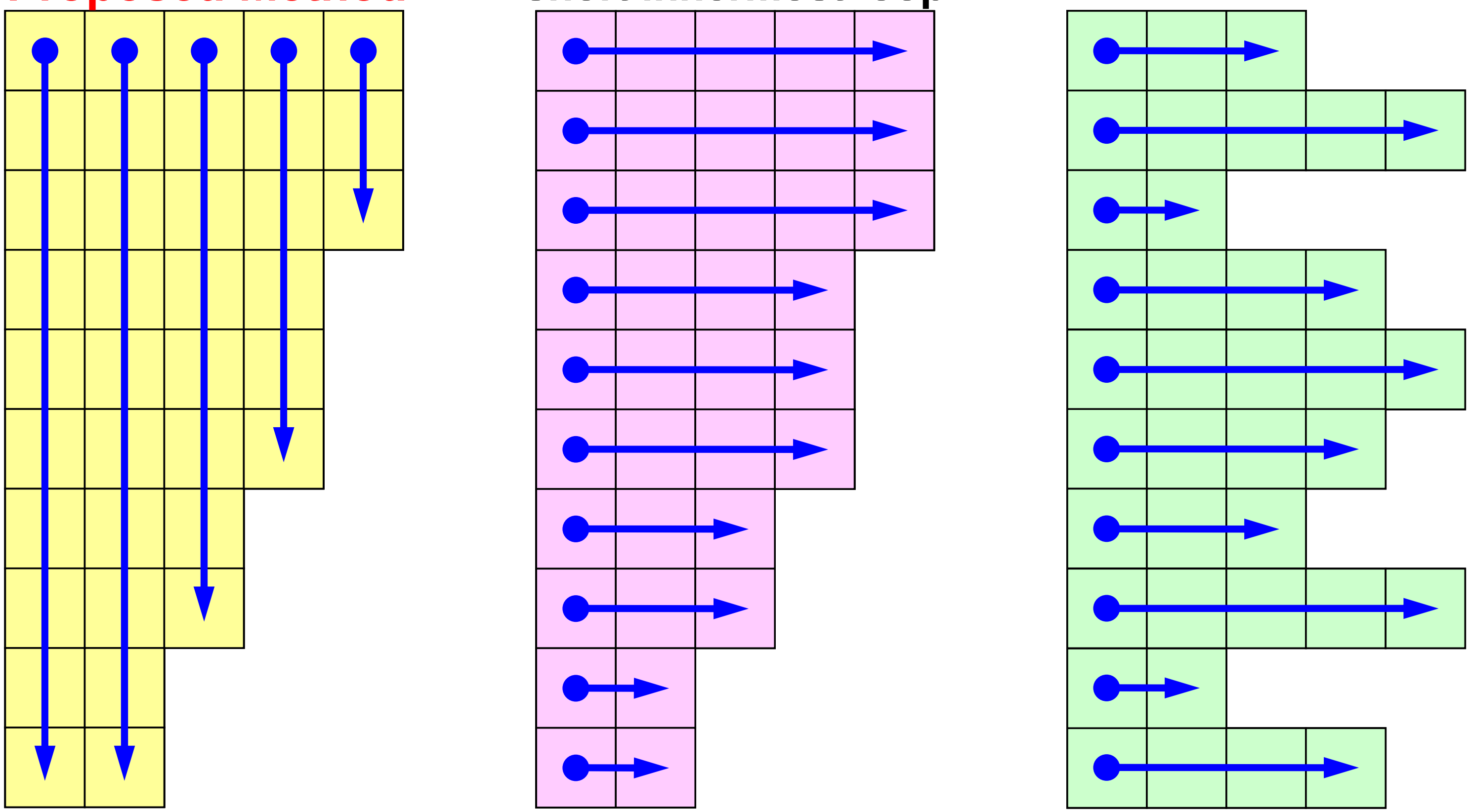
Simple 3D Cubic Model



Effect of Ordering

Effect of Re-Ordering

Long Loops Continuous Access	Short Loops Continuous Access	Short Loops Irregular Access
PDJDS/CM-RCM **Proposed Method**	**PDCRS/CM-RCM** **short innermost loop**	**CRS no re-ordering**

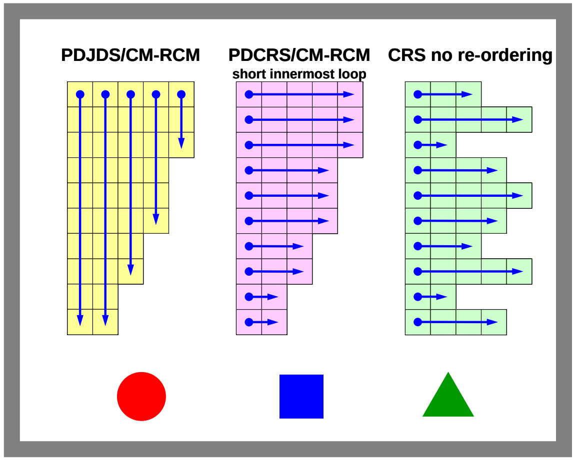


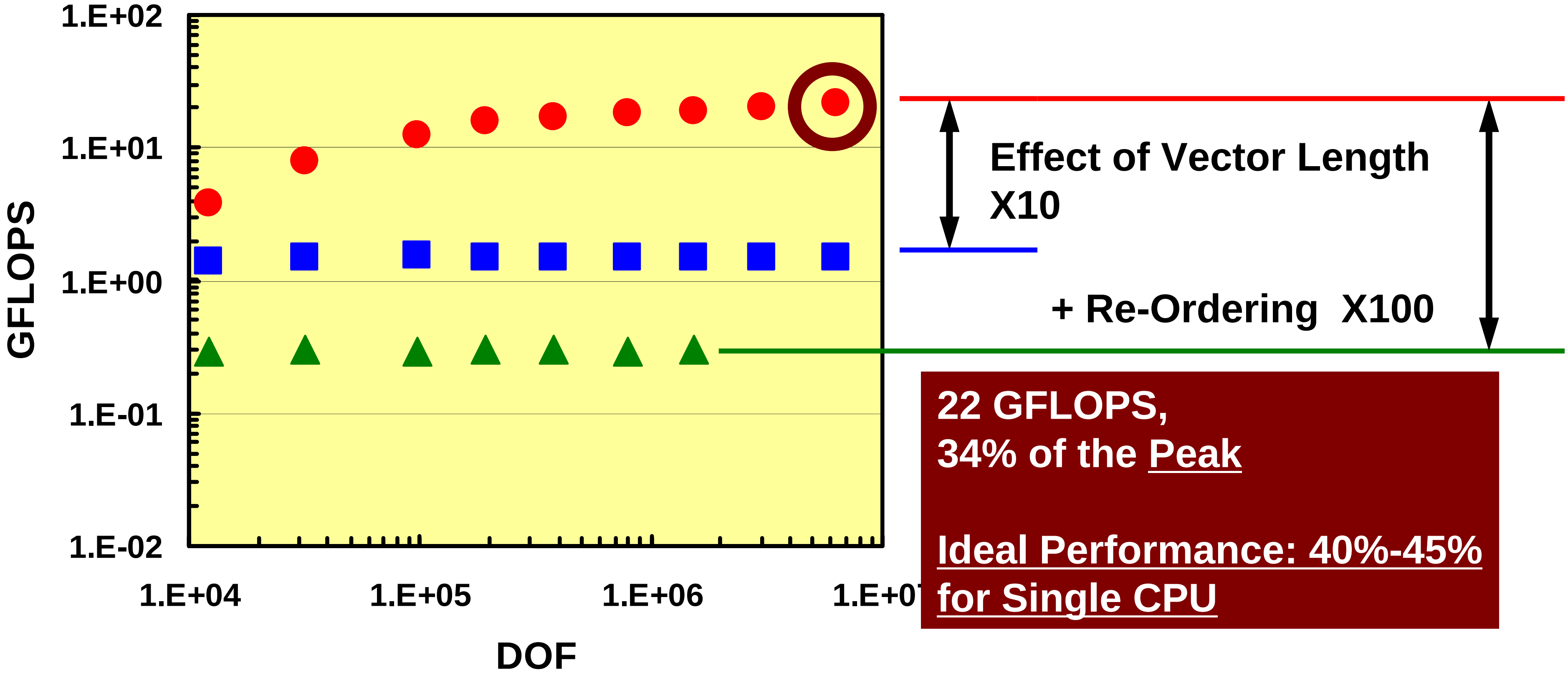
Effect of Re-Ordering

Results on 1 SMP node

Color #: 99 (fixed)

Re-Ordering is REALLY required !!!





22 GFLOPS,
34% of the Peak

Ideal Performance: 40%-45% for Single CPU

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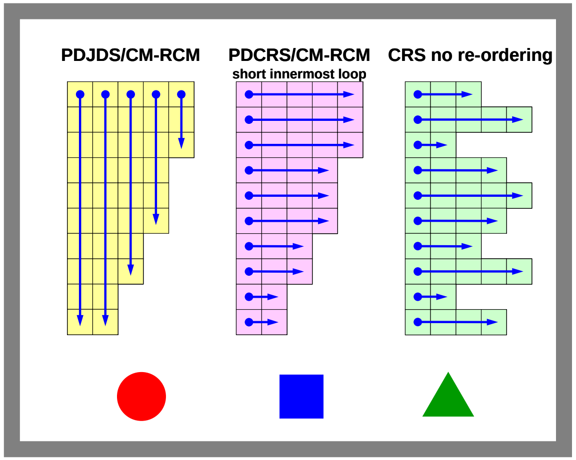
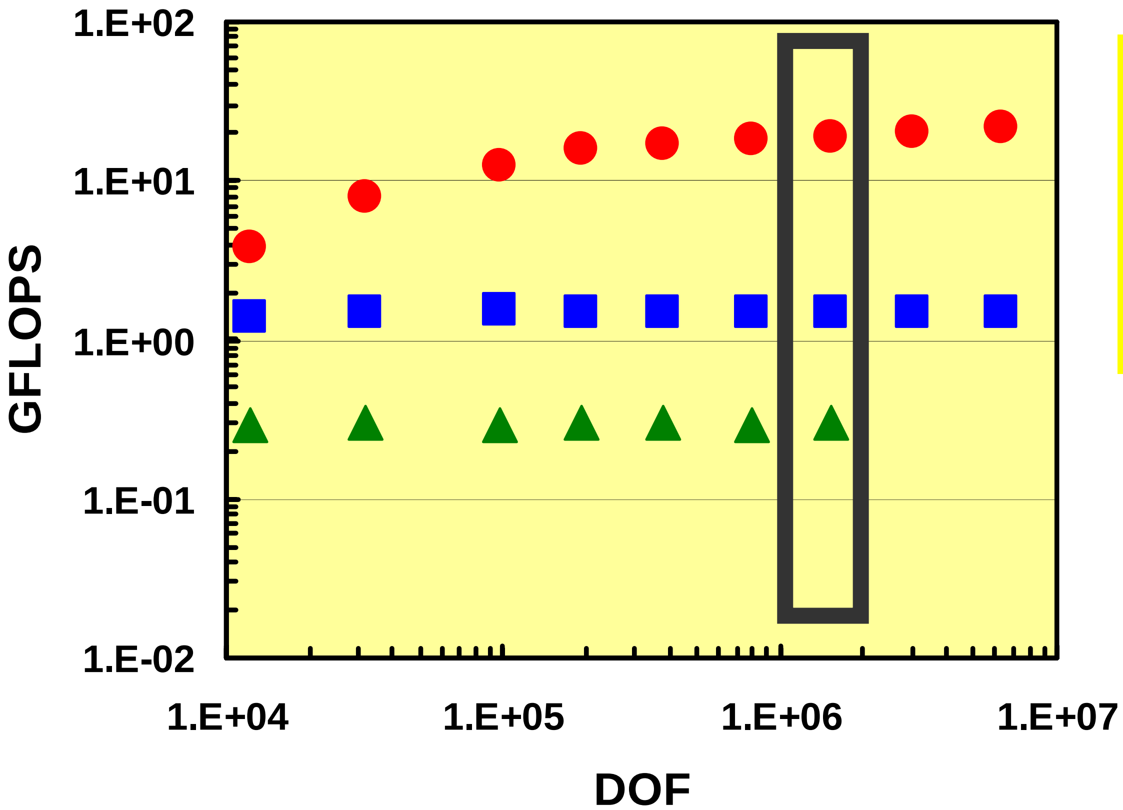
Color #: 99 (fixed)

Re-Ordering is REALLY required !!!





80x80x80 case (1.5M DOF)

● 212 iter's, 11.2 sec.
■ 212 iter's, 143.6 sec.
▲ 203 iter's, 674.2 sec.

Ideal Performance: 48.6% of Peak

Ideal performance of the following MVP process for 3×3 block operation on the Earth Simulator (peak performance: 8 GFLOPS/PE, peak memory bandwidth: 32 GB/sec/PE) is estimated as 48.6% of the peak performance (3.89 GFLOPS).

```
do j= 1, m
   do i= 1, N
      k=(j-1)*N + i
      kk= index(k)
      Y(3*i-2)= Y(3*i-2)  + A(9*k-8)*X(3*kk-2) &
                          + A(9*k-7)*X(3*kk-1) &
                          + A(9*k-6)*X(3*kk  )
      Y(3*i-1)= Y(3*i-1)  + A(9*k-5)*X(3*kk-2) &
                          + A(9*k-4)*X(3*kk-1) &
                          + A(9*k-3)*X(3*kk  )
      Y(3*i  )= Y(3*i  )  + A(9*k-2)*X(3*kk-2) &
                          + A(9*k-1)*X(3*kk-1) &
                          + A(9*k  )*X(3*kk  )
   enddo
enddo
```

SMP node # > 10
up to 176 nodes (1408 PEs)

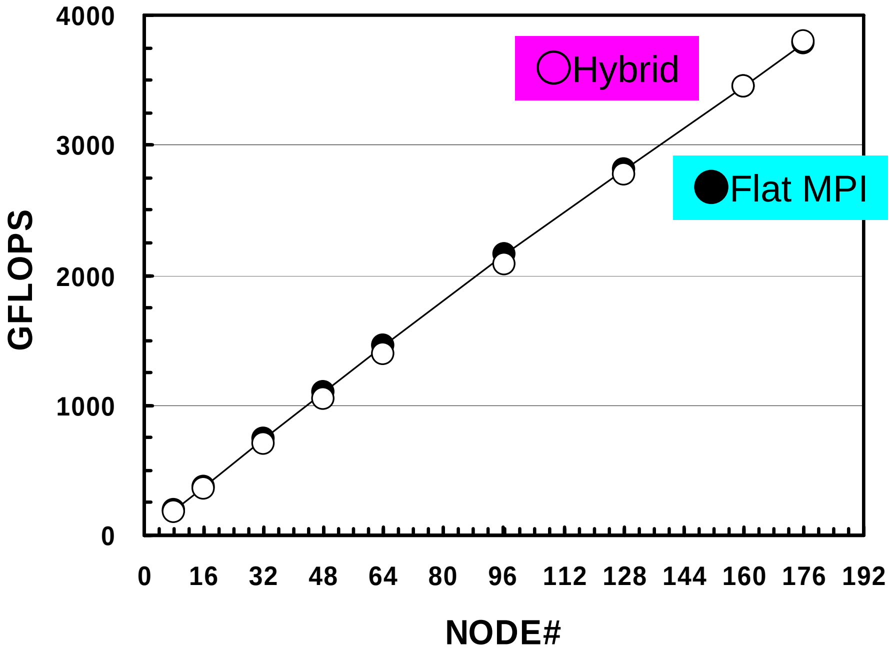
Problem size for each SMP node is fixed.

PDJDS-CMC/RCM, Color #: 99

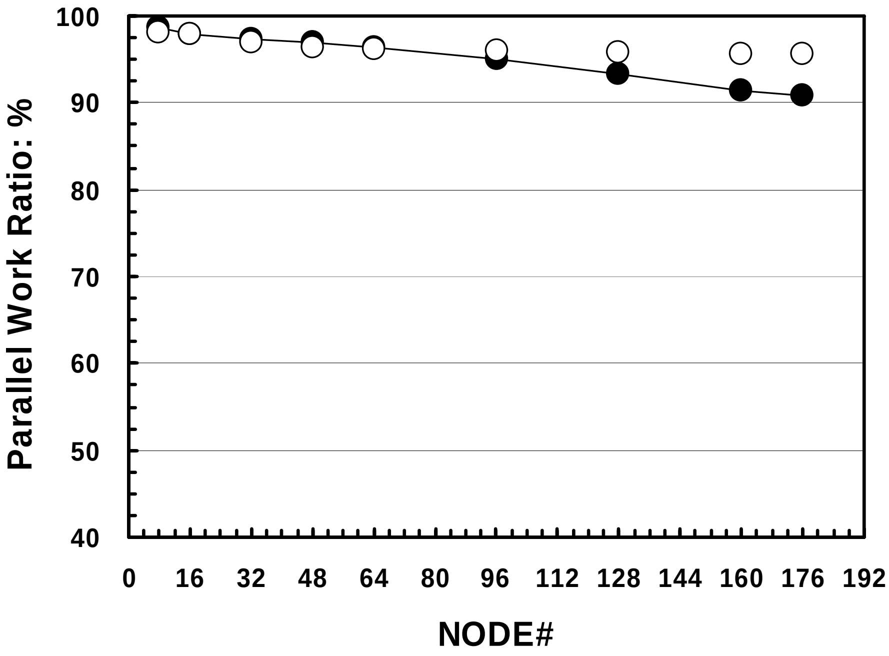
3D Elastic Model (Large Case)

256x128x128/SMP node, up to 2,214,592,512 DOF

GFLOPS rate



Parallel Work Ratio



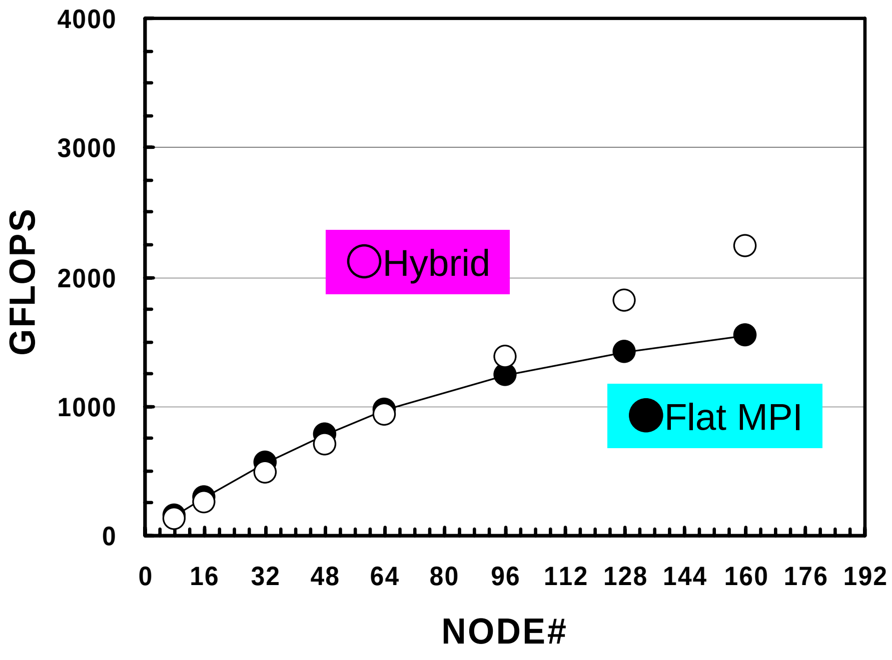
3.8TFLOPS for 2.2G DOF

176 nodes (33.8% of peak)

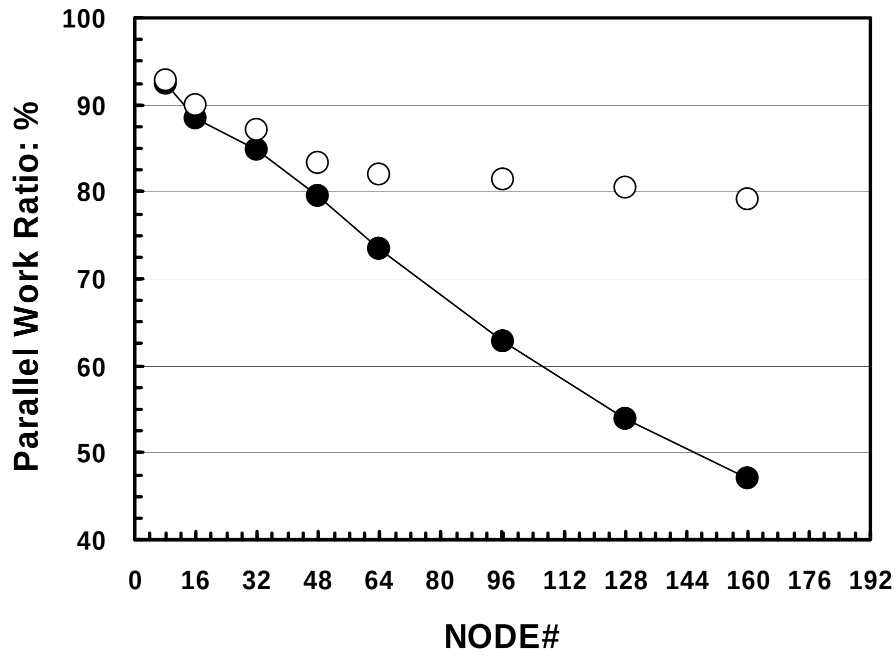
3D Elastic Model (Small Case)

64x64x64/SMP node, up to 125,829,120 DOF

GFLOPS rate



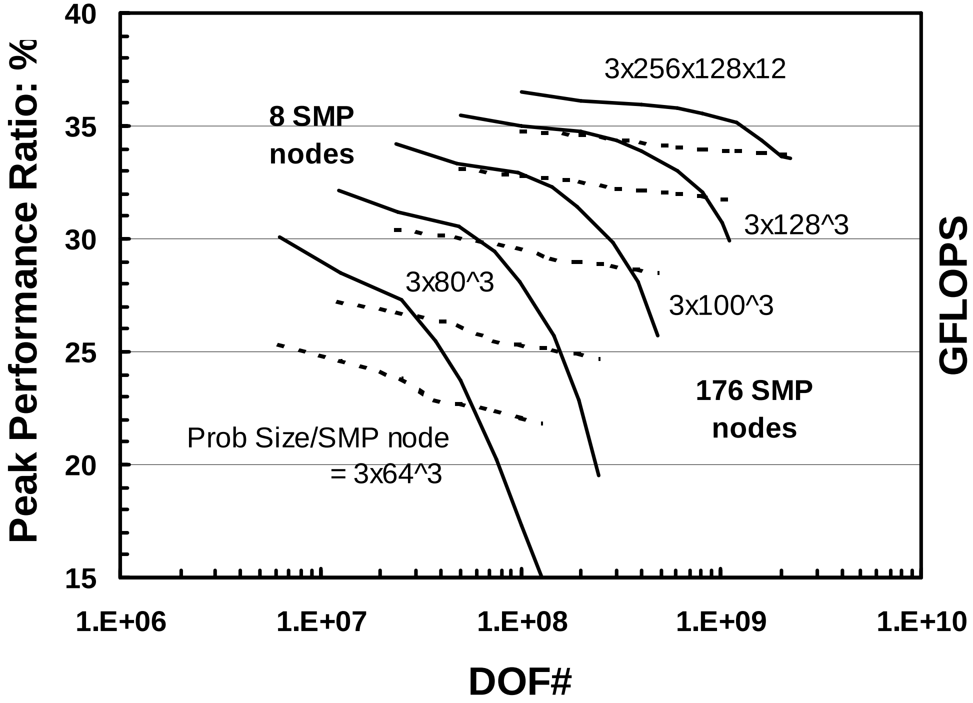
Parallel Work Ratio

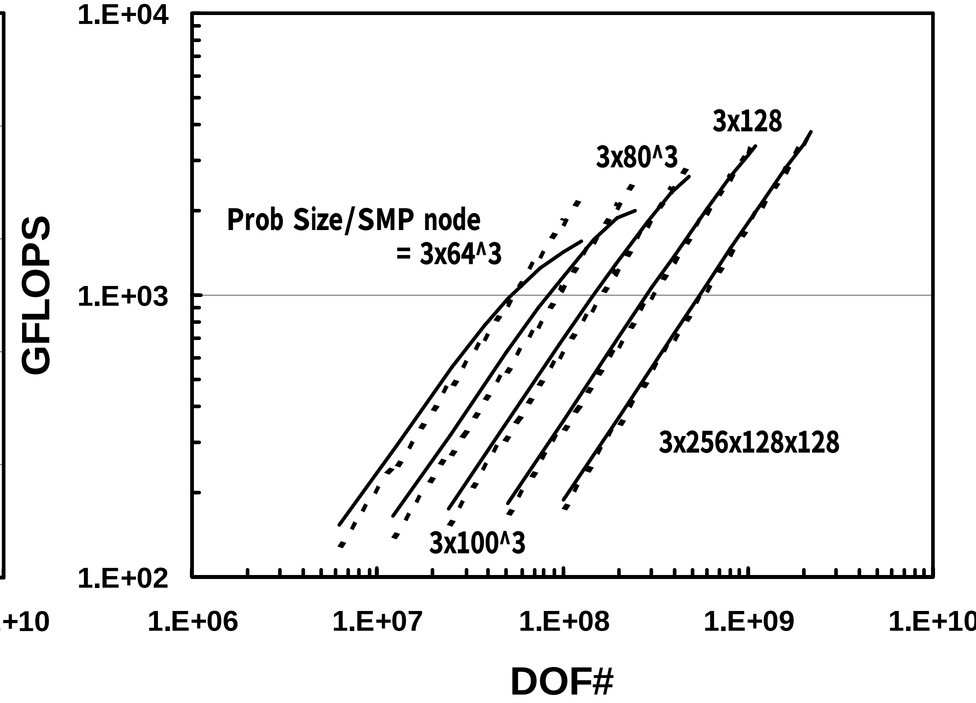


●：Flat MPI, ○：Hybrid

3D Elastic Model

Problem Size and Parallel Performance
8-176 SMP nodes of the Earth Simulator



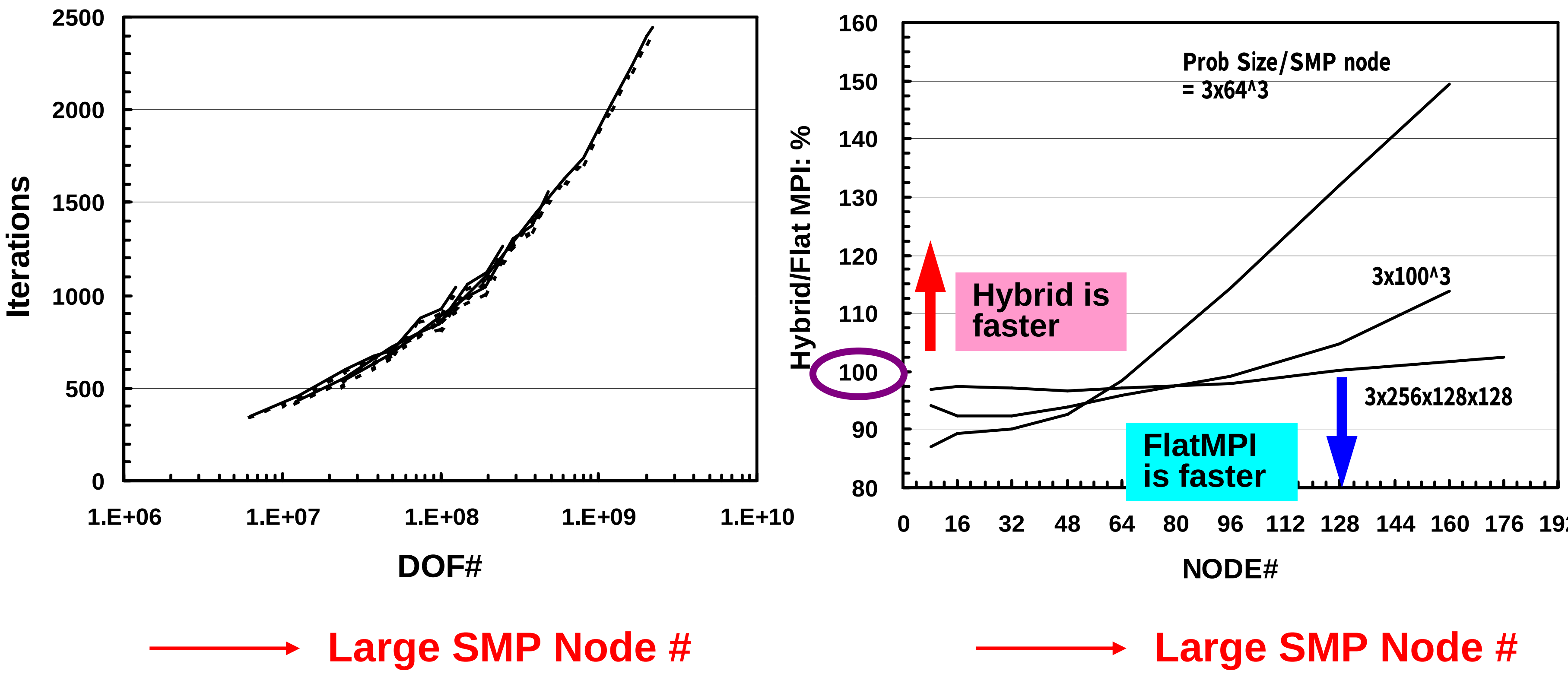


→ **Large SMP Node #** → **Large SMP Node #**

— : Flat MPI, --- : Hybrid

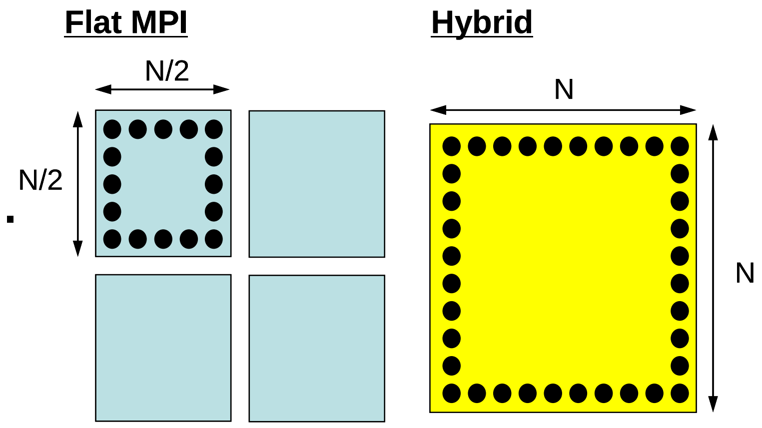
3D Elastic Model

Problem Size and Parallel Performance
8-176 SMP nodes of the Earth Simulator



— : Flat MPI, --- : Hybrid

Hybrid outperforms Flat-MPI



- when ...
  - number of SMP node (PE) is large.
  - problem size/node is small.
- because flat-MPI has ...
  - as 8 times as many communication processes
  - as TWICE as large communication/computation ratio
- Effect of communication becomes significant if number of SMP node (or PE) is large.
- Performance Estimation by D.Kerbyson (LANL)
  - LA-UR-02-5222
  - relatively larger communication latency of ES

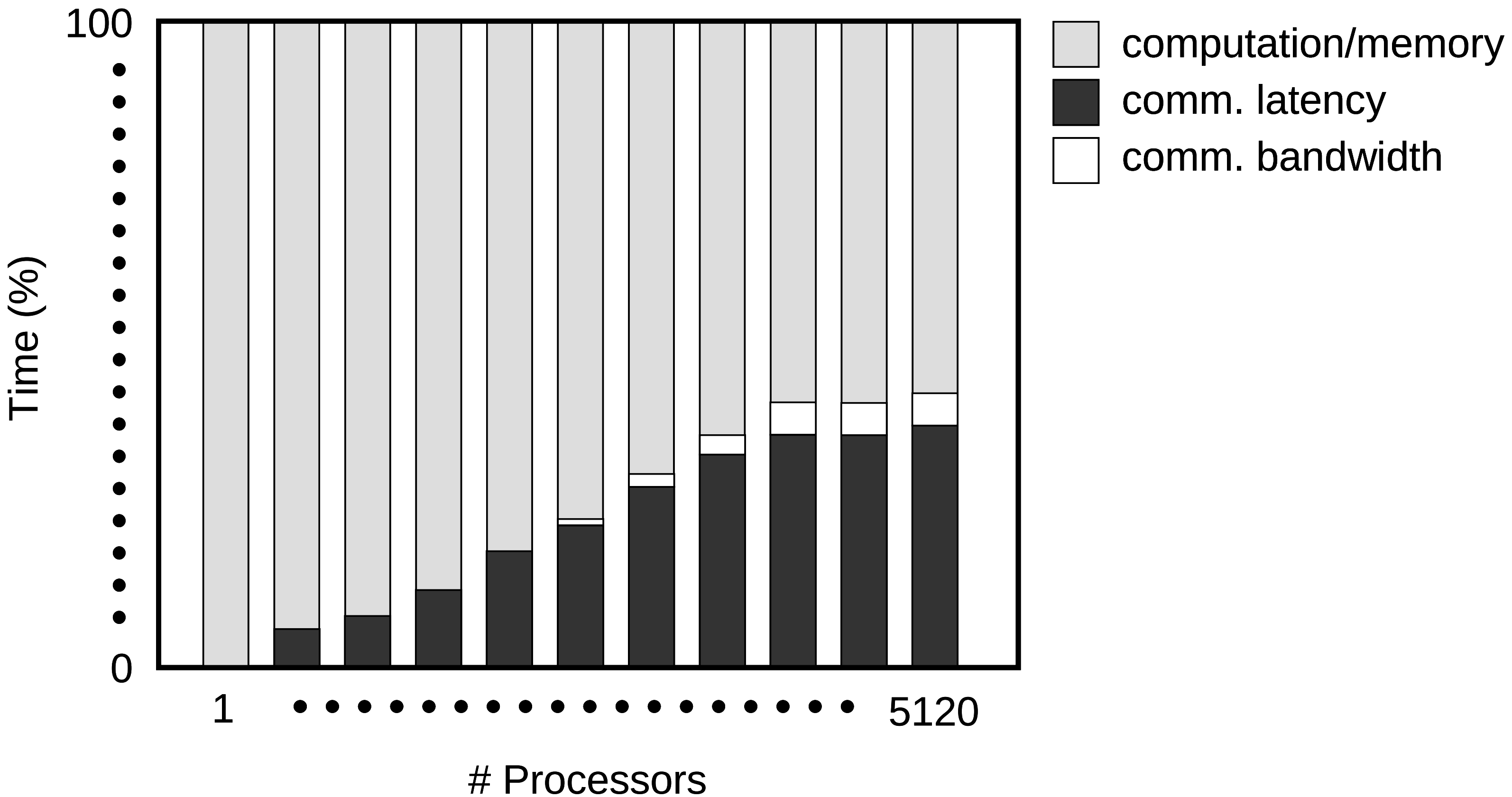
Comm. latency is relatively large in ES

D.J.Kerbyson et al. LA-UR-02-5222

	ES	ASCI-Q HP ES45
Proc. Speed	500 MHz	1.25 GHz
SMP nodes	8 x 640= 5,120	4 x 3,072=12,288
Peak Speed	8 x 5,120 = 40 TFLOPS	2.5 x 12,288 = 30 TFLOPS
Memory	2 x 5,120= 10 TB	4 x 12,288= 48 TB
Peak Memory BWTH	32 GB/s	2 GB/s L1/L2 20/30 GB/s
Inter-Node MPI Comm.	**Latency: 5.6 μsec** BWTH : 11.8 GB/s	**Latency: 5 μsec** BWTH : 300 MB/s

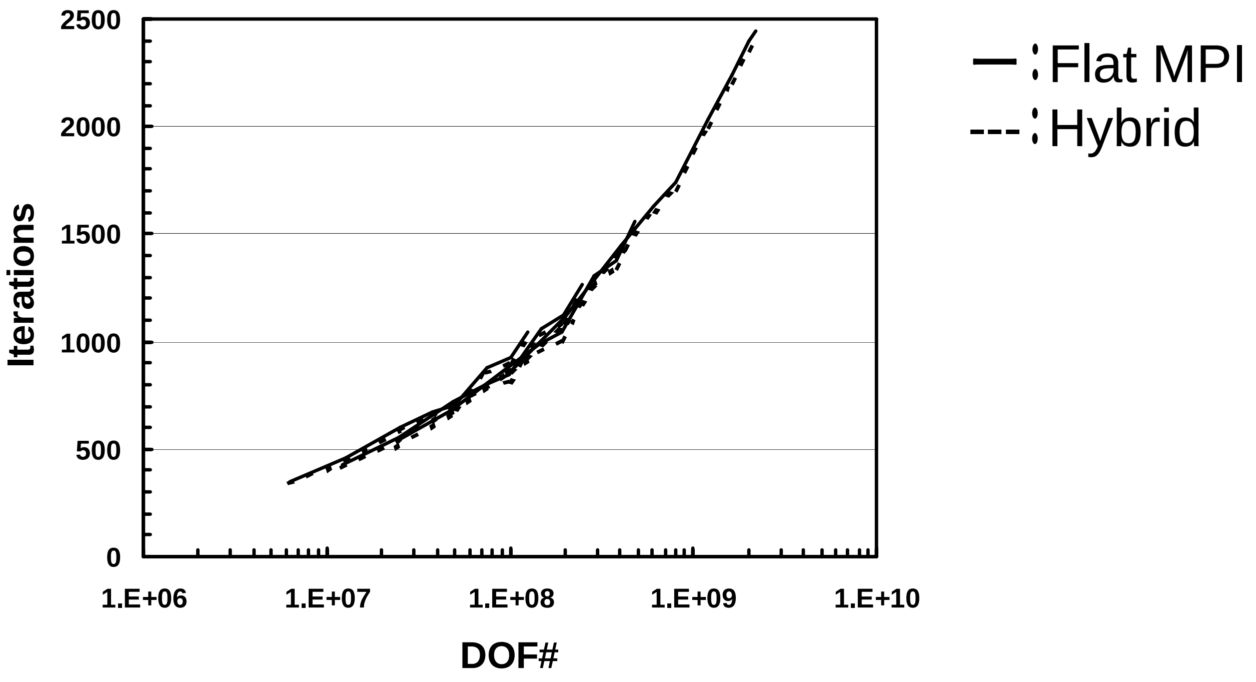
Performance Estimation for Finite-Element Type Application on ES

using performance model (not real computations)
D.J.Kerbyson et al. LA-UR-02-5222 (LANL)



Hybrid outperforms Flat-MPI (cont.)

- Difference between Hybrid & Flat MPI of iteration number for convergence is not so significant … due to additive Schwartz domain decomposition.



Large SMP Node #

Various Platforms

- Earth Simulator (ES)
  - Earth Simulator Center, JAMSTEC.
  - Vector Processors
- Hitachi SR8000
  - The University of Tokyo
  - Power-PC based Architecture
  - Pseudo-Vector Capability with Preload/Prefetch
- IBM SP-3
  - NERSC/Lawrence Berkeley National Laboratory: Seaborg
  - Power3
  - 8MB L2-cache for each PE

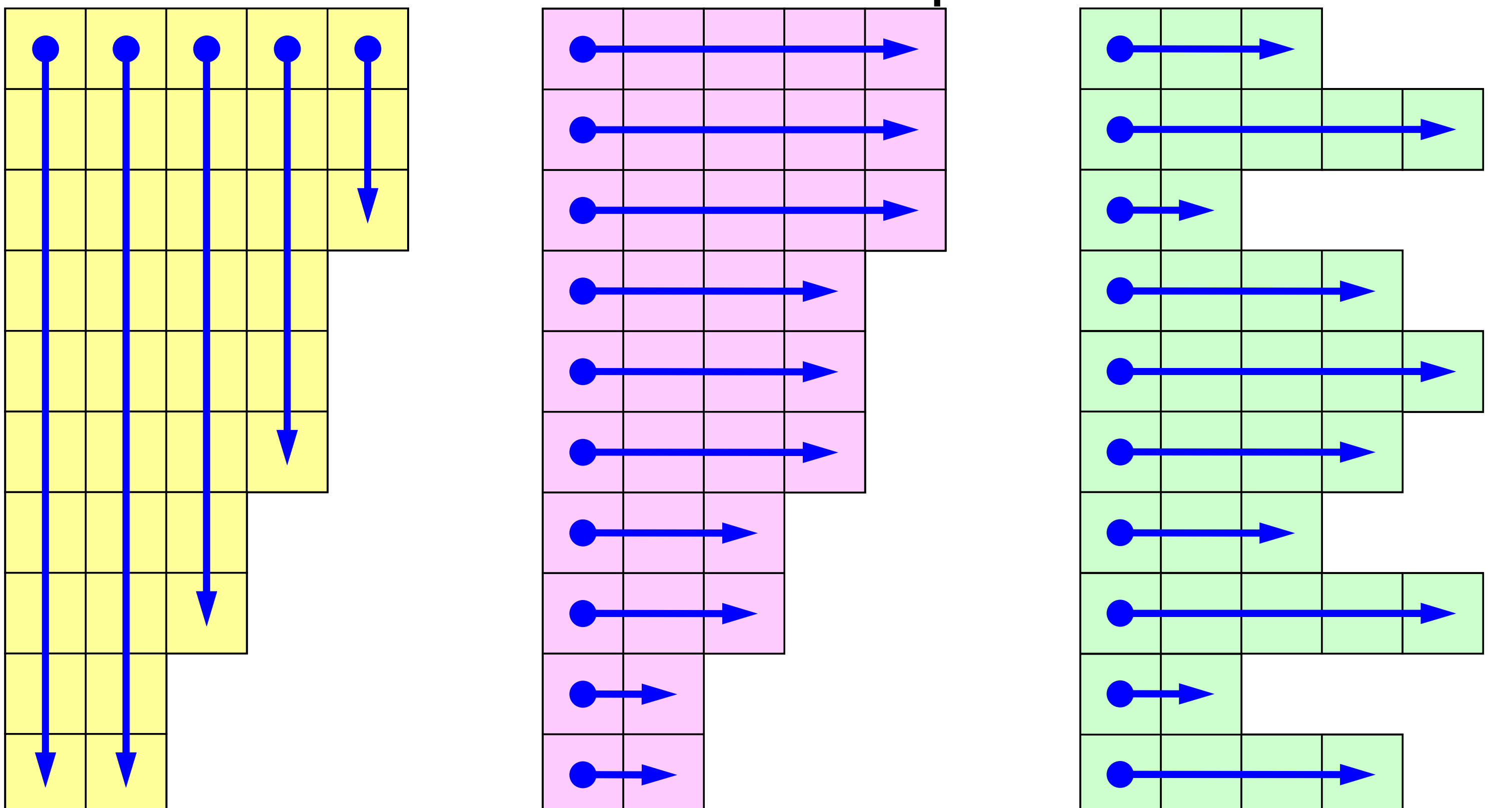
Platforms

	ES	SP3	SR8k
PE#/node	8	16	8
Peak GF/PE	8.0	1.5	1.8
Mem.BW GB/s/node	256	16	32
MPI lat. μsec	5.6	16.3*	6-20**
Network BW GB/s/Node	12.3	1.00	1.60

*) Oliker et al.
**) HLRS

Reordering for the Earth Simulator Matrix Storage for ILU Factorization

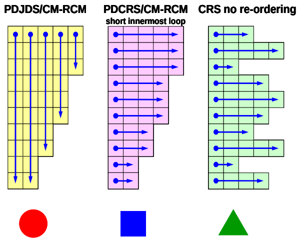
Long Loops Continuous Access	Short Loops Continuous Access	Short Loops Irregular Access
PDJDS/CM-RCM	**PDCRS/CM-RCM** **short innermost loop**	**CRS no re-ordering**

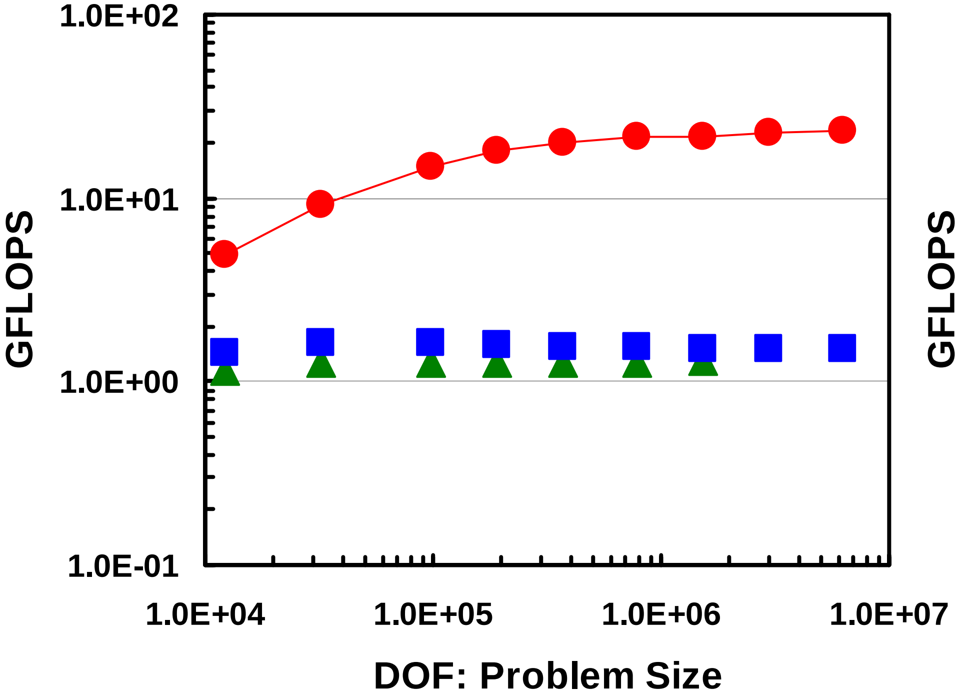


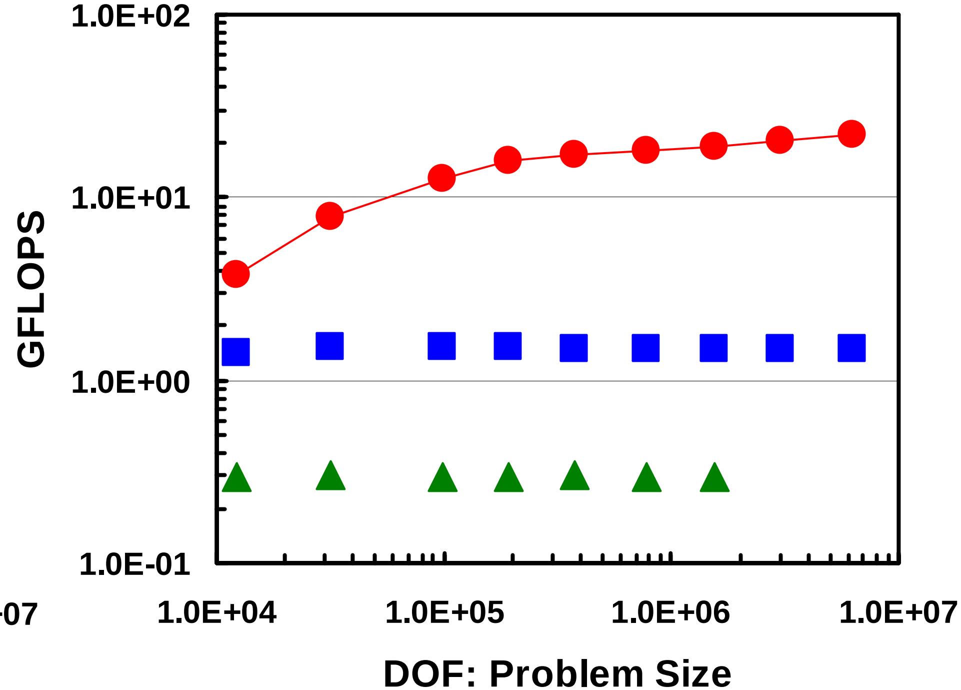
3D Elastic Simulation
Problem Size~GFLOPS

Earth Simulator

1 SMP node (8 PE's)







Flat-MPI

23.4 GFLOPS, 36.6 % of Peak

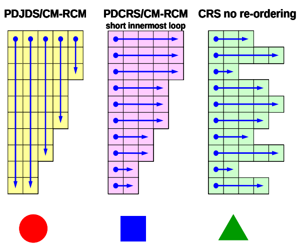
OpenMP

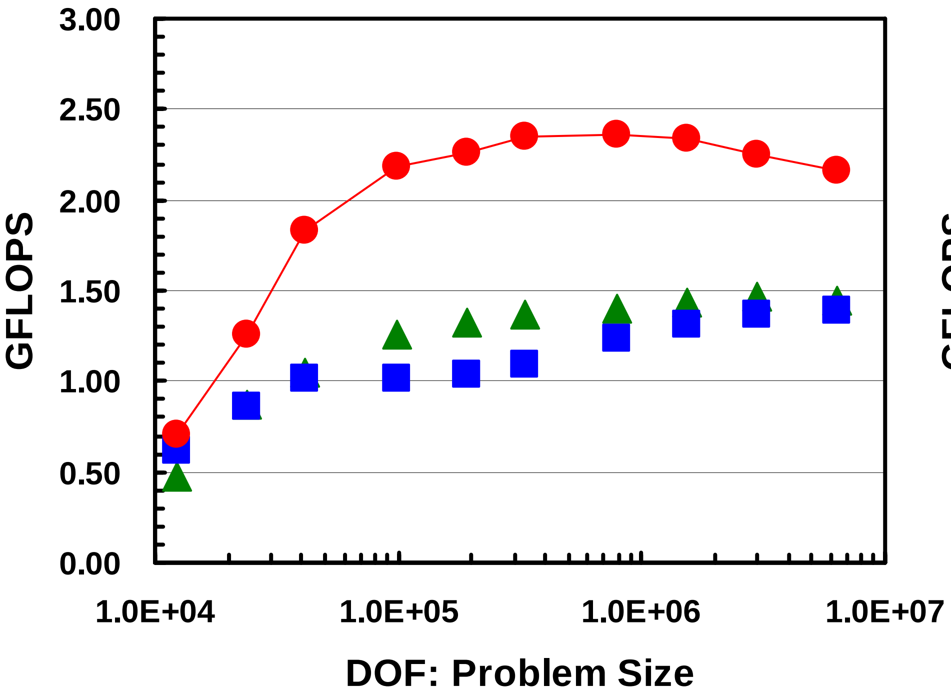
21.9 GFLOPS, 34.3 % of Peak

3D Elastic Simulation Problem Size~GFLOPS

Hitachi-SR8000-MPP with Pseudo Vectorization

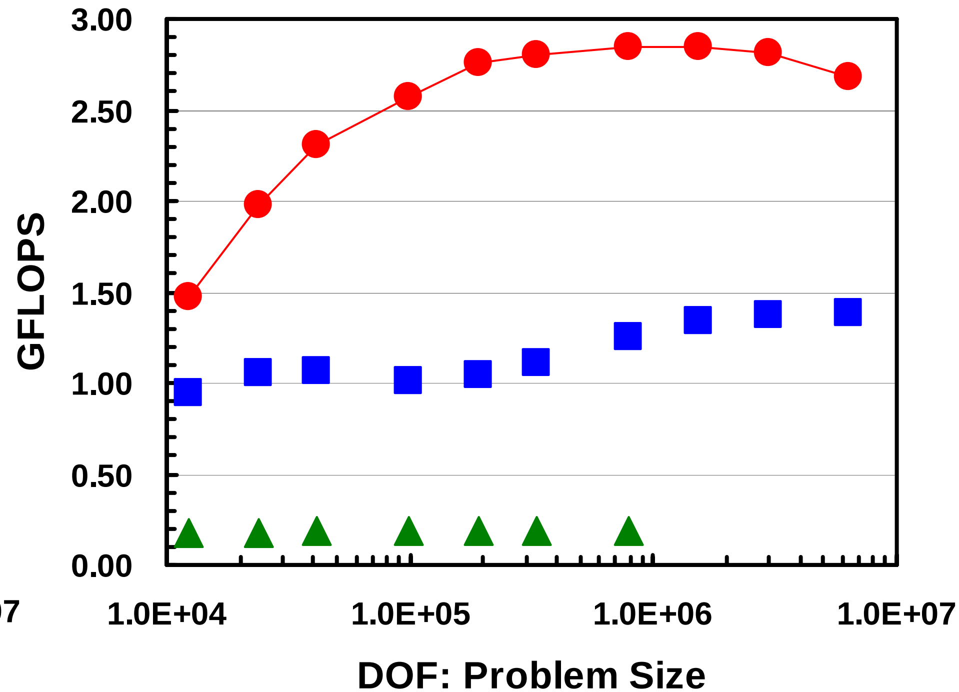
1 SMP node (8 PE's)





Flat-MPI

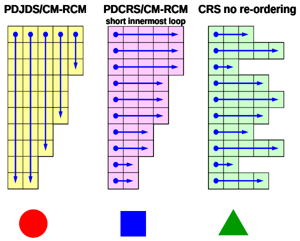
2.17 GFLOPS, 15.0 % of Peak



OpenMP

2.68 GFLOPS, 18.6 % of Peak

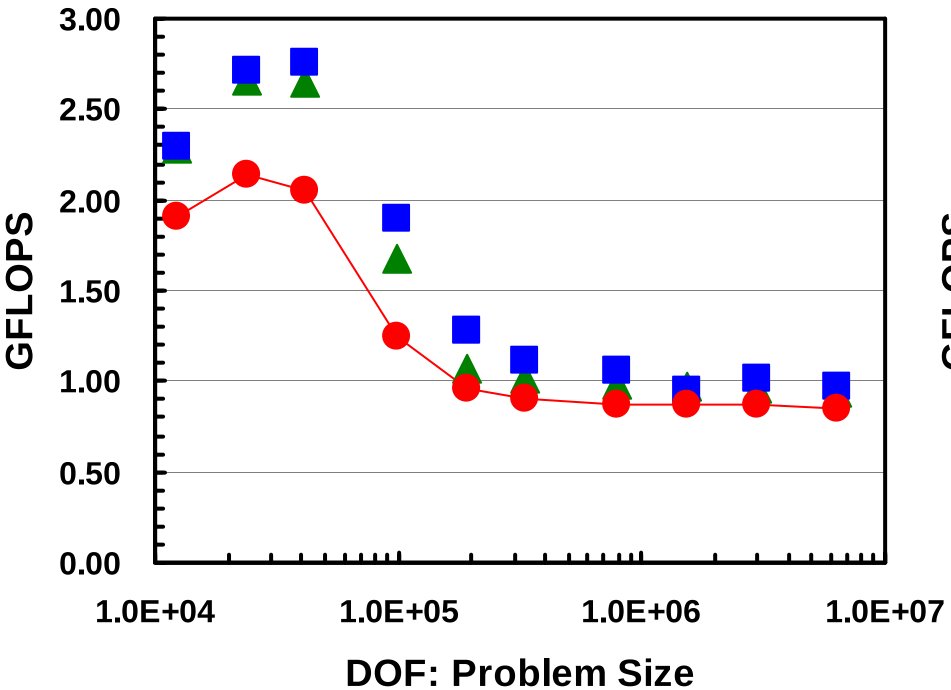
3D Elastic Simulation
Problem Size~GFLOPS

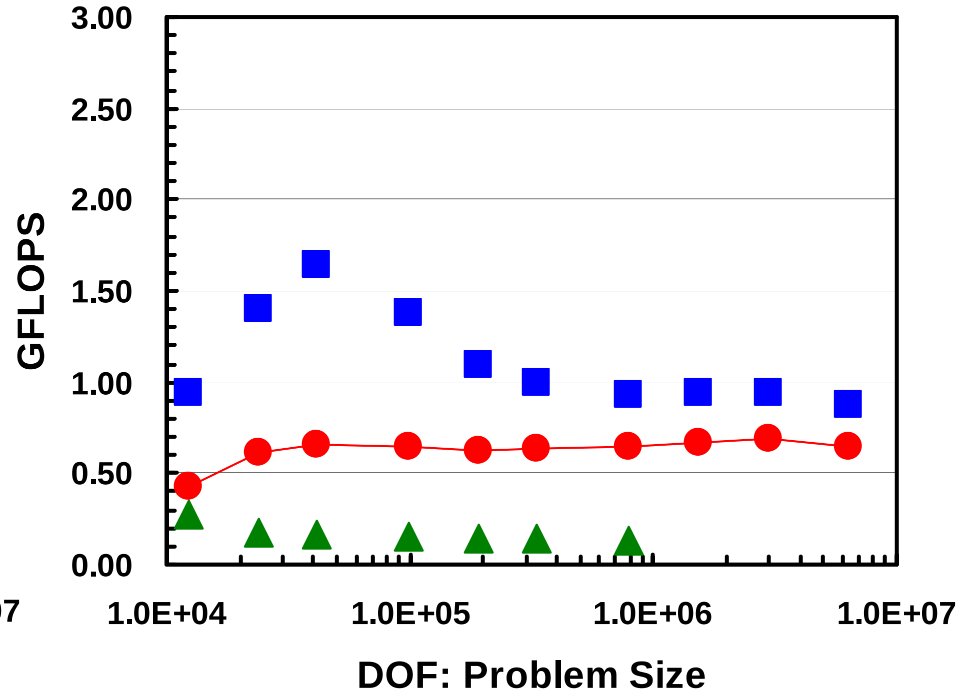


IBM-SP3 (NERSC)

1 SMP node (8 PE's)

Cache is well-utilized in Flat-MPI.

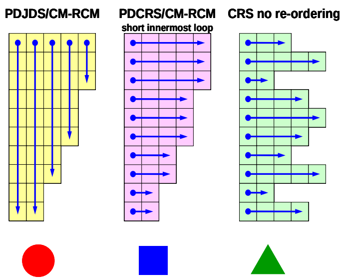




Flat-MPI **OpenMP**

3D Elastic Simulation
Single PE Performance

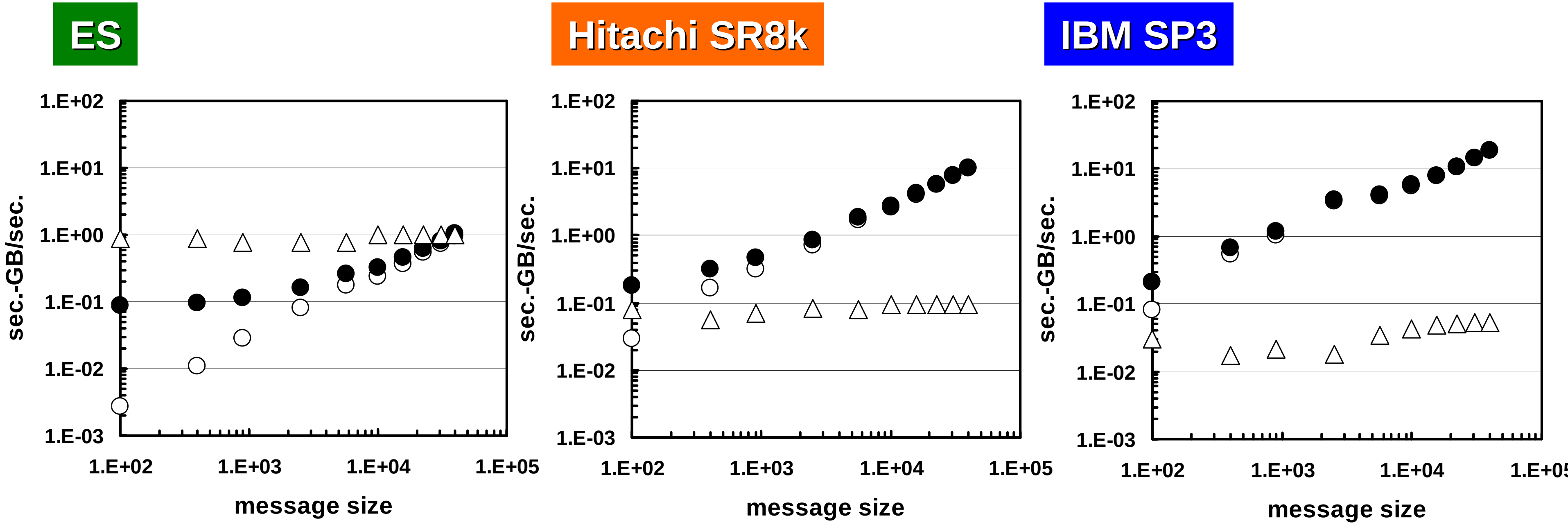
GFLOPS, 104 colors



		98,304 DOF (=3×32³)		331,776 DOF (=3×48³)		786,432 DOF (=3×64³)	
		DJDS ●	CRS ■	DJDS ●	CRS ■	DJDS ●	CRS ■
Earth Simulator	Hybrid	1.67	-	2.06	-	3.01	-
	FlatMPI	2.75	-	3.02	-	3.19	-
Hitachi SR8000	Hybrid	**0.404**	0.127	**0.437**	0.140	**0.423**	0.146
	FlatMPI	**0.366**	0.128	**0.343**	0.138	**0.322**	0.146
IBM SP3	Hybrid	0.145	0.167	0.142	0.165	0.137	0.145
	FlatMPI	0.138	0.165	0.135	0.159	0.126	0.141

Performance of Intra-Node MPI

8 PE's: Measurement using SEND/RECV subroutines in GeoFEM



- ● Elapsed time for 1,000 iterations (sec.)
- ○ Elapsed time for 1,000 iterations without estimated latency(sec.)
- △ Estimated communication bandwidth (GB/sec)

Performance of Intra-Node MPI

8 PE's: Measurement using inter-domain SEND/RECV subroutines in ***GeoFEM***

	ES	**SR8k**	**SP3**
PE#/node	8	8	16
Peak GF/PE	8.0	1.8	1.5
Mem.BW GB/s/node	256	32	16
MPI lat. μsec	5.6	6-20**	16.3*
Network BW GB/s/Node	12.3	1.60	1.00
Intra-node MPI lat. μsec	5.29	**9.17**	8.32
Intra-node MPI BW MB/s/PE	1018.	95.8	52.5

Intra-node communication performance seems reasonable according to memory BW, inter-node communication performance.

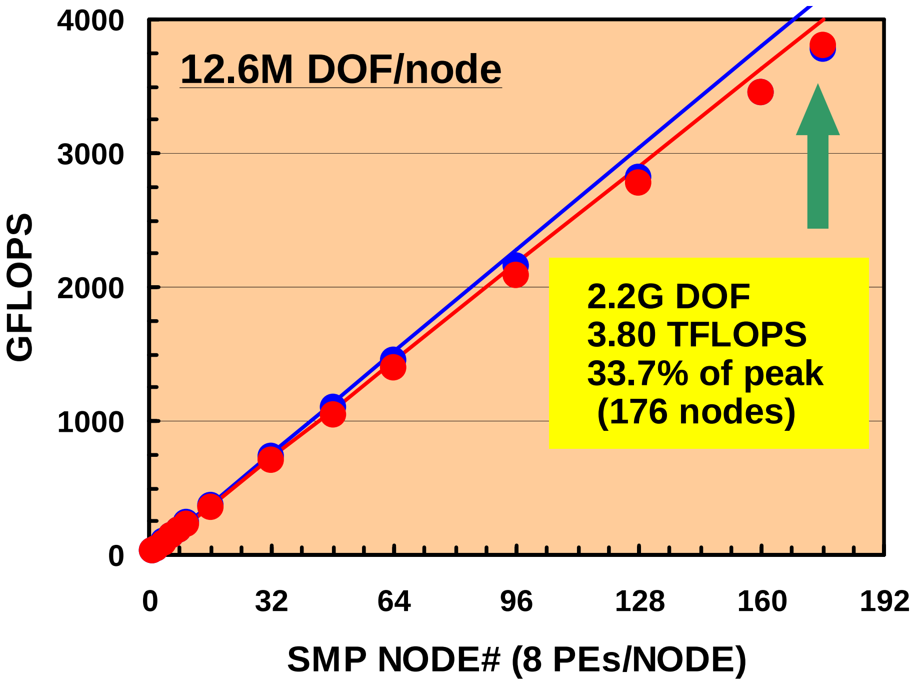
Summary: Single Node Performance Flat MPI vs. Hybrid

- Earth Simulator (ES)
  - Flat MPI is slightly better.
- Hitachi SR8000
  - Similar feature with that of ES
  - Hybrid is better for PDJDS/CM-RCM ordering.
  - Difference of single PE performance between Hybrid and Flat MPI for PDJDS/CM-RCM is significant.
    - compiler ?
- IBM SP-3
  - Effect of cache (8MB/PE) is significant.
  - Cache is well-utilized in Flat MPI
  - Performance in larger problems is similar

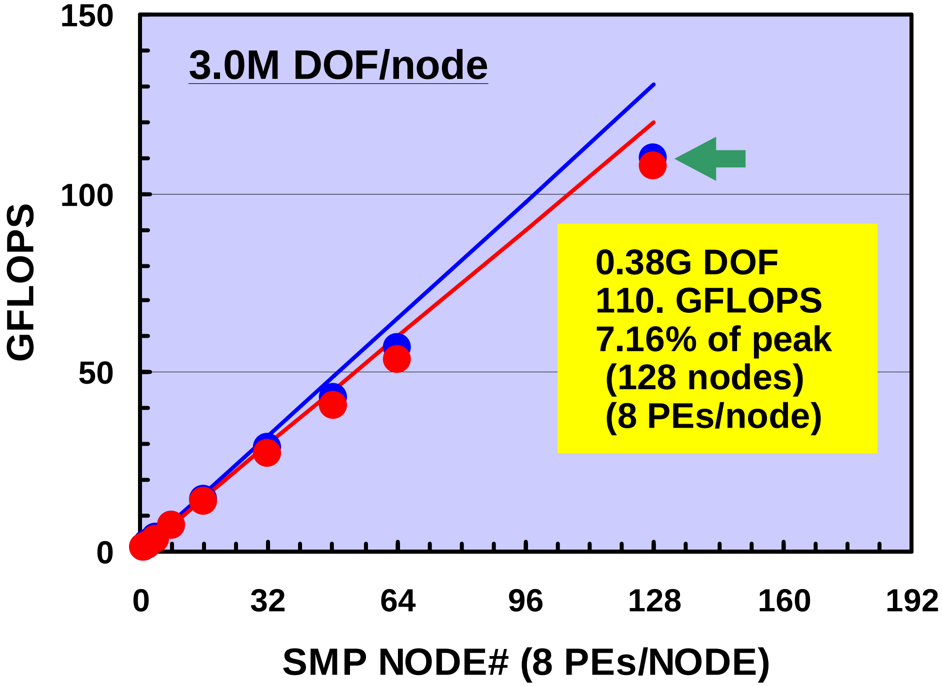
Speed-Up for Fixed Problem Size/PE

● Hybrid, ● Flat MPI (Lines: Ideal speed-up extrapolated from 1-node performance)

Earth Simulator



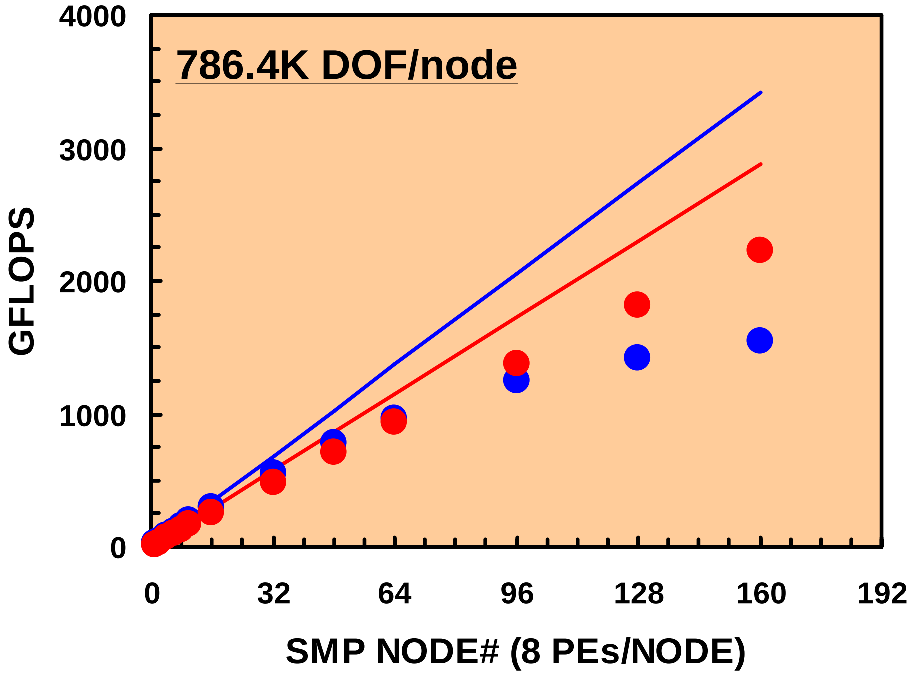
IBM SP-3 (Seaborg at NERSC)



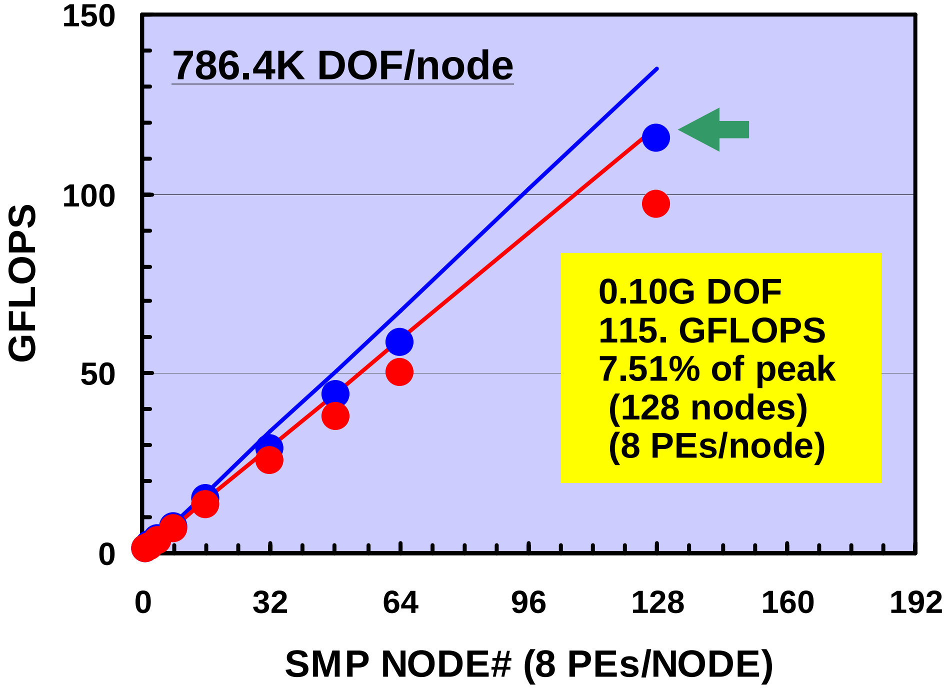
Speed-Up for Fixed Problem Size/PE

● Hybrid, ● Flat MPI (Lines: Ideal speed-up extrapolated from 1-node performance)

Earth Simulator



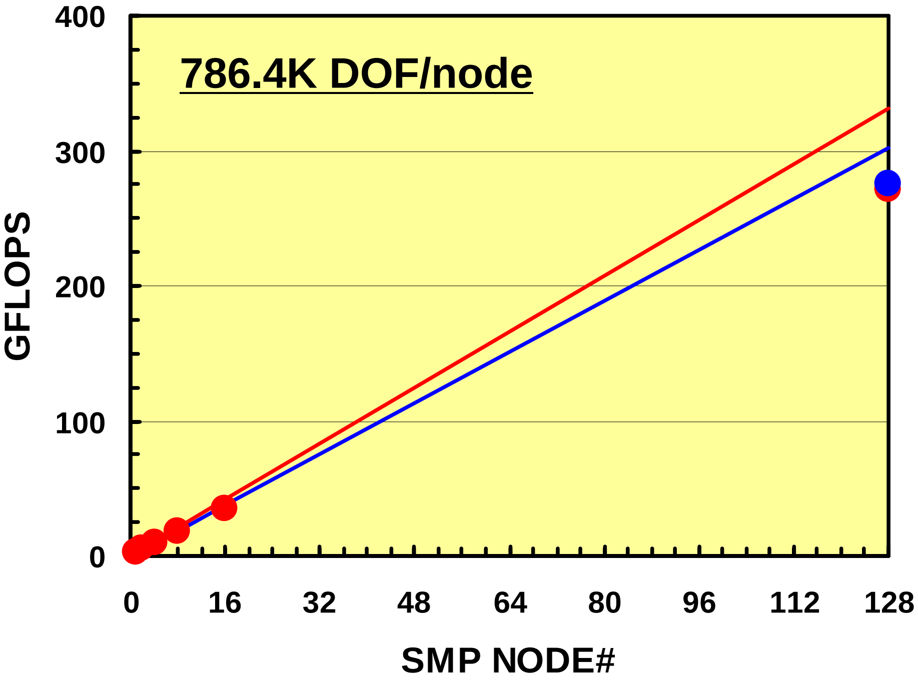
IBM SP-3 (Seaborg at NERSC)

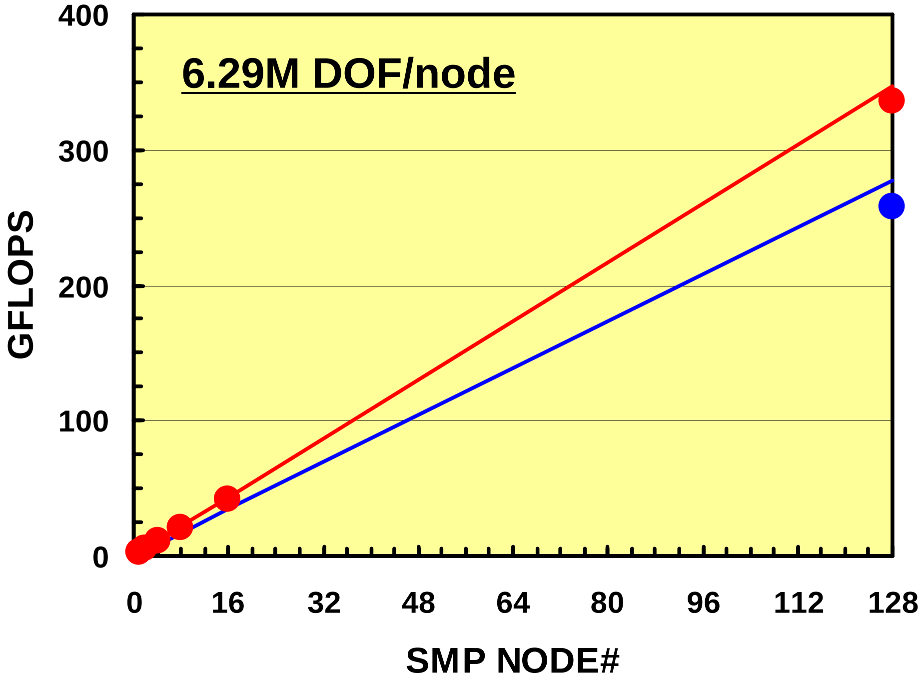


Speed-Up for Fixed Problem Size/PE

● Hybrid, ● Flat MPI (Lines: Ideal speed-up extrapolated from 1-node performance)

Hitachi SR8000





0.10G DOF, 128 nodes
- ● **271 GFLOPS, 14.7% of peak**
- ● **276 GFLOPS, 15.0%**

8.05G DOF, 128 nodes
- ● **335 GFLOPS, 18.2% of peak**
- ● **257 GFLOPS, 14.7%**

Platforms

	ES	SP3	SR8k	
PE#/node	8	16	8	
Peak GF/PE	8.0	1.5	1.8	
Mem.BW GB/s/node	256	16	32	
MPI lat. μsec	5.6	16.3*	6-20**	2.9 : 1 : 1.2-2.7
Network BW GB/s/Node	12.3	1.00	1.60	12 : 1 : 1.6

Summary: Performance for Many Nodes, Flat MPI vs. Hybrid

- Earth Simulator (ES)
  - Effect of MPI latency is significant for:
    - Flat MPI
    - Many node #
    - small problem size/node
- Hitachi SR8000
- IBM SP-3
  - Effect of MPI latency is hidden by their relatively low communication bandwidth.
  - Performance with 128 SMP nodes are identical with extrapolation of single node performance, especially if problem size/node is sufficiently large.

- Background
  - GeoFEM Project & Earth Simulator
  - Preconditioned Iterative Linear Solvers
- Optimization Strategy on the Earth Simulator
  - BIC(0)-CG for Simple 3D Linear Elastic Applications
- **Effect of reordering on various types of architectures**
  - **PGA (Pin-Grid Array)**
  - **Contact Problems**
  - **Multigrid**
- Summary & Future Works

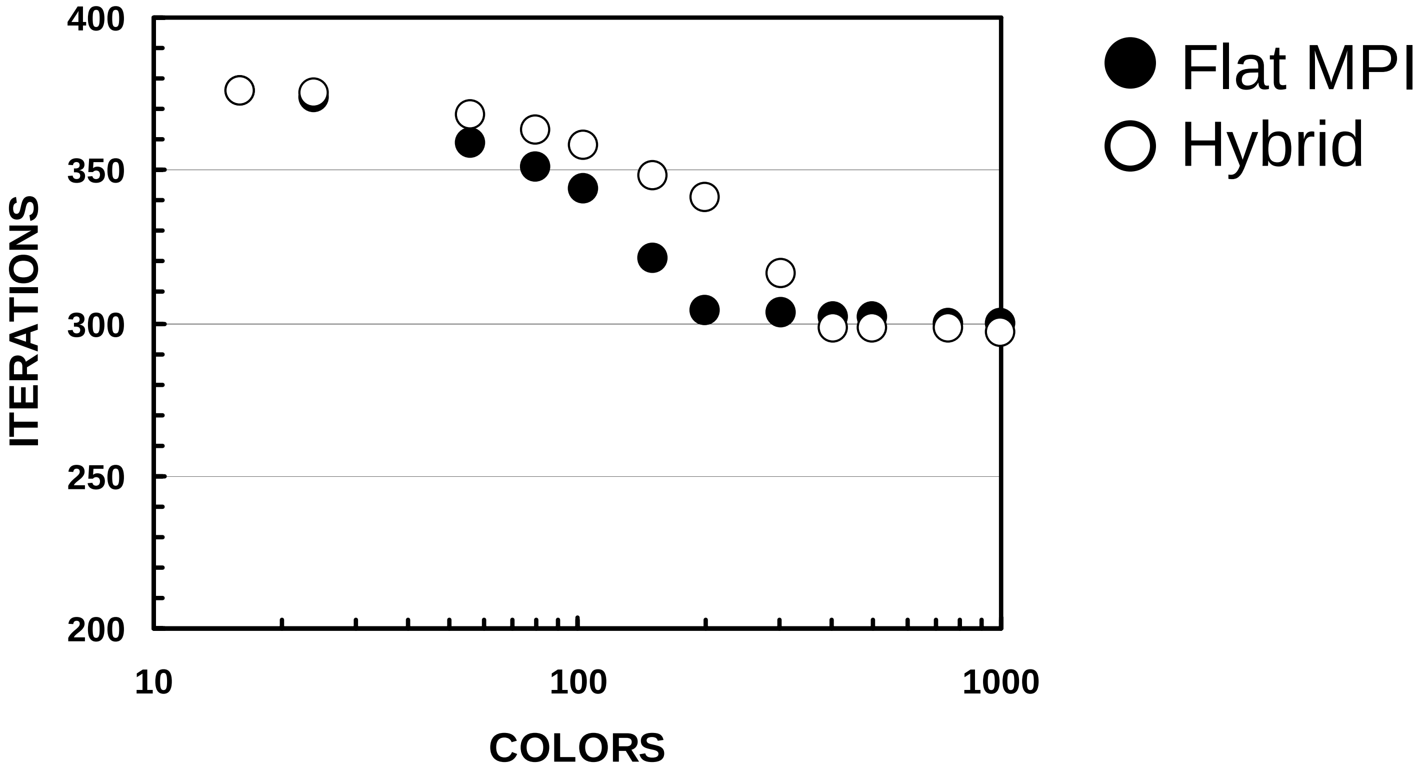
Elastic Problems with Cubic Model

Effect of Loop Length (Color#)

100^3 nodes= 3×10^6 DOF

PDCRS/CM-RCM Re-Ordering

Iterations for Convergence

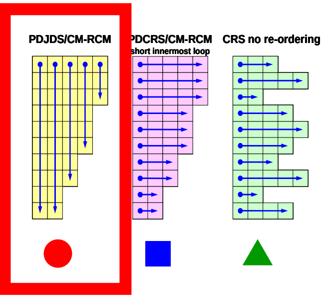


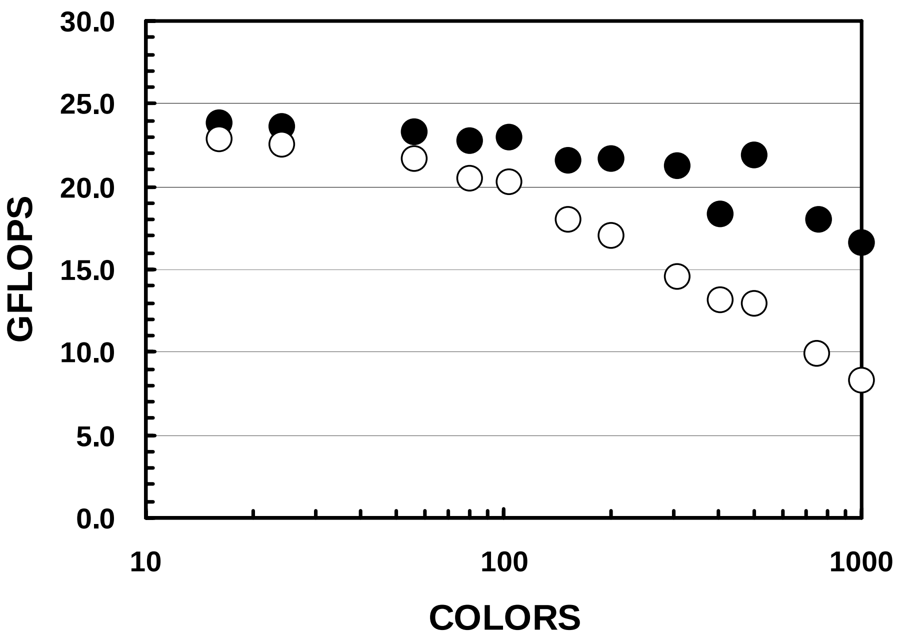
Effect of Loop Length (Color#)

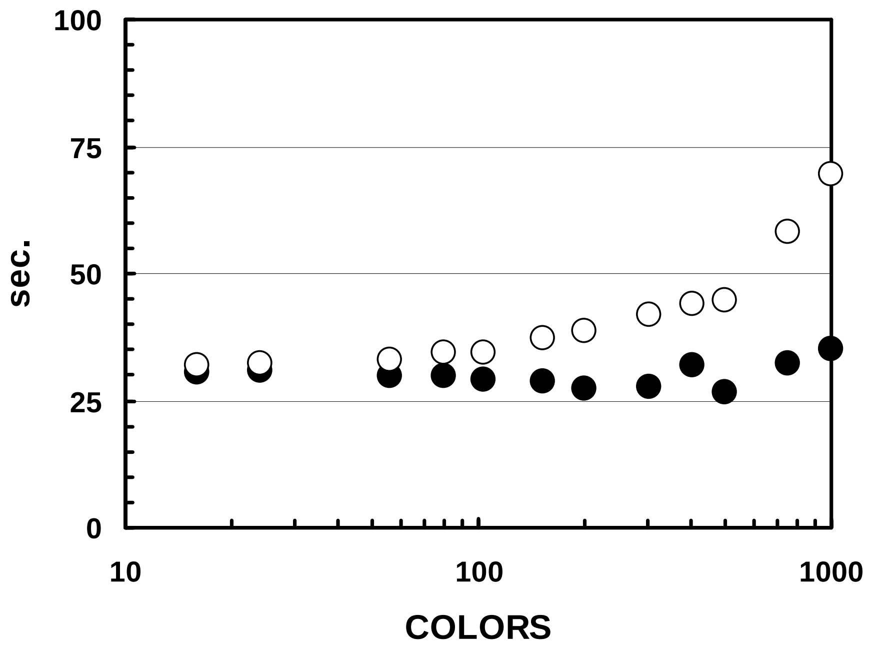
100^3 nodes= $3x10^6$ DOF

PDJDS/CM-RCM Re-Ordering

Earth Simulator (single node)





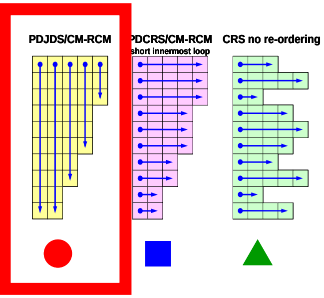


Effect of Loop Length (Color#)

100^3 nodes= $3x10^6$ DOF

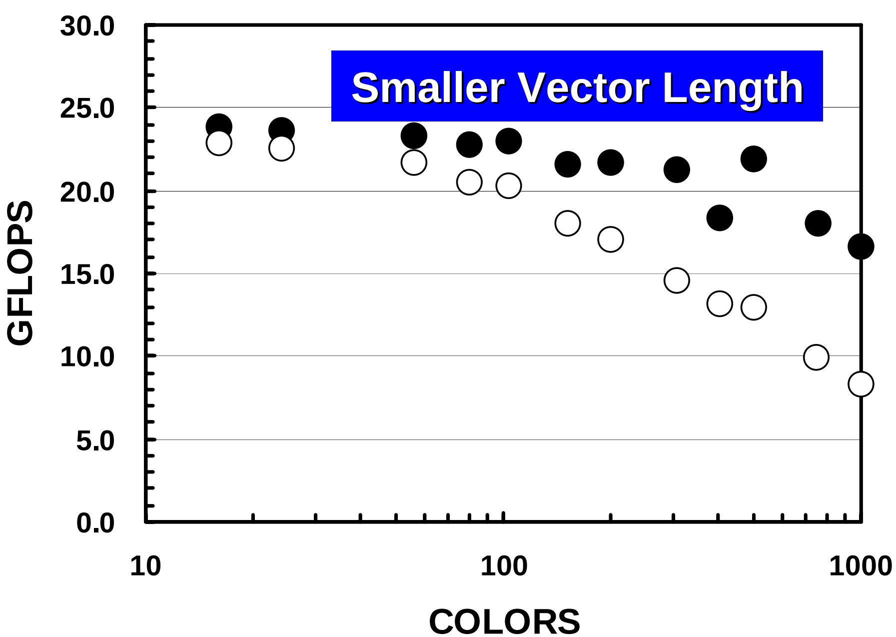
PDJDS/CM-RCM Re-Ordering

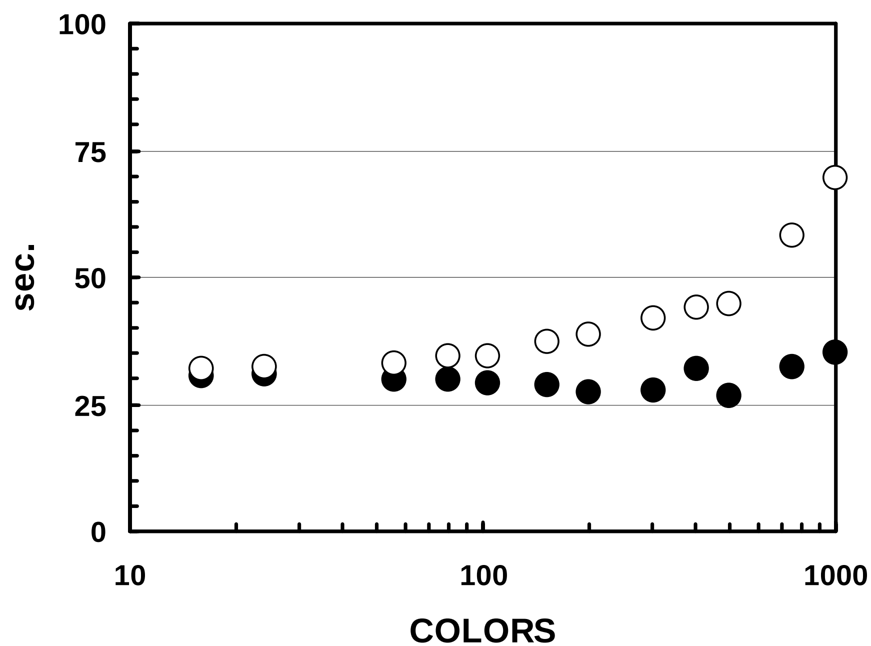
Earth Simulator (single node)



● Flat MPI

○ Hybrid



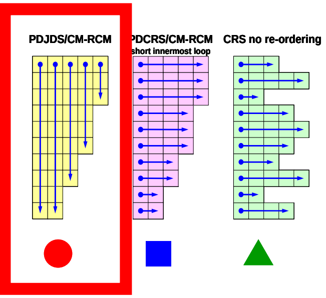


Effect of Loop Length (Color#)

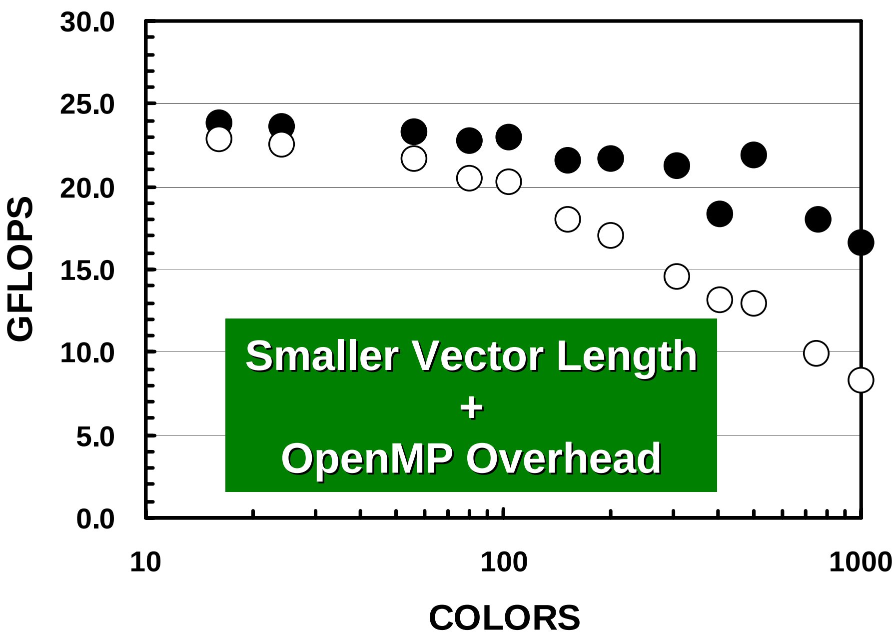
100^3 nodes= $3x10^6$ DOF

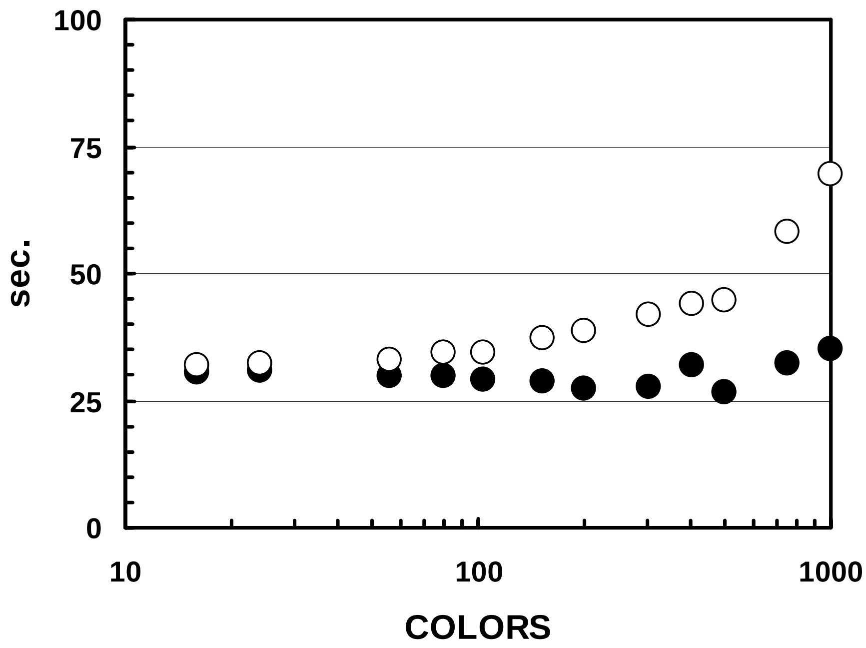
PDJDS/CM-RCM Re-Ordering

Earth Simulator (single node)



● Flat MPI
○ Hybrid





Many Colors ... Trade-Off

- Fast convergence according to iteration number
  - S.Doi et al.
- Smaller vector length
  - FLOPS rate decreases.

- Hybrid is much more sensitive to color number
  - Especially on the Earth Simulator

Hybrid is much more sensitive to color numbers !

```
      do iv= 1, NCOLORS
!$omp parallel do private (iv0,j,iS,iE,i,k,kk etc.)
        do ip= 1, PEsmpTOT
          iv0= STACKmc(PEsmpTOT*(iv-1)+ip- 1)
          do j= 1, NLhyp(iv)
            iS= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip-1)
            iE= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip  )
!CDIR NODEP
            do i= iv0+1, iv0+iE-iS
              k= i+iS - iv0
              kk= IAL(k)
              (Important Computations)
            enddo
          enddo
        enddo
      enddo
```

SMP parallel (outer `do ip` loop)

Vectorized (inner `do i` loop)

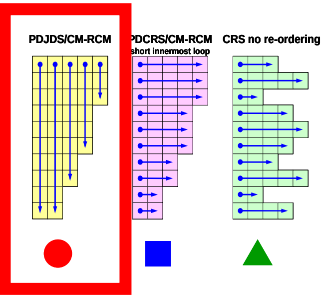
y(i)= y(i) + A(k)*X(kk)

Effect of Loop Length (Color#)

100^3 nodes= $3x10^6$ DOF

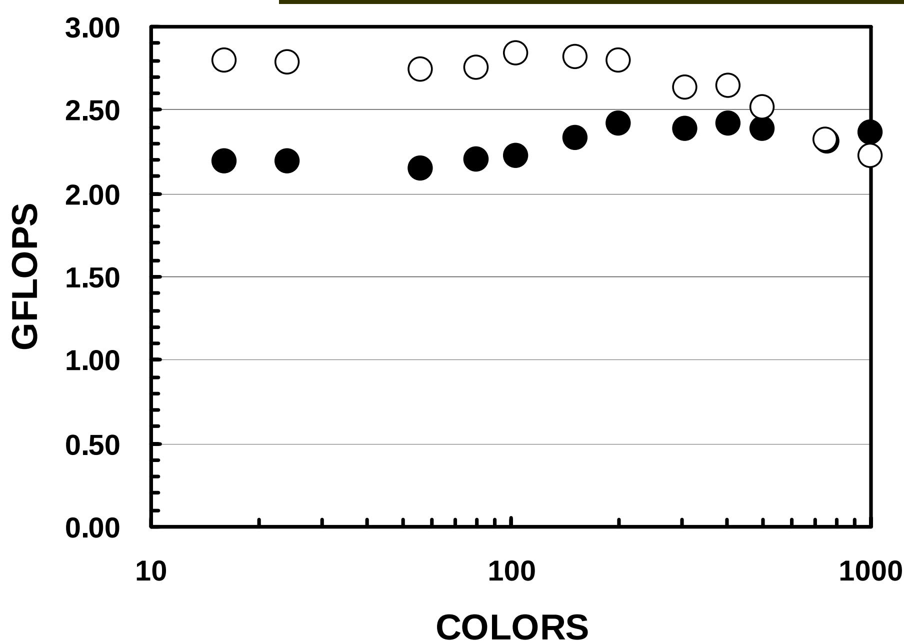
PDJDS/CM-RCM Re-Ordering

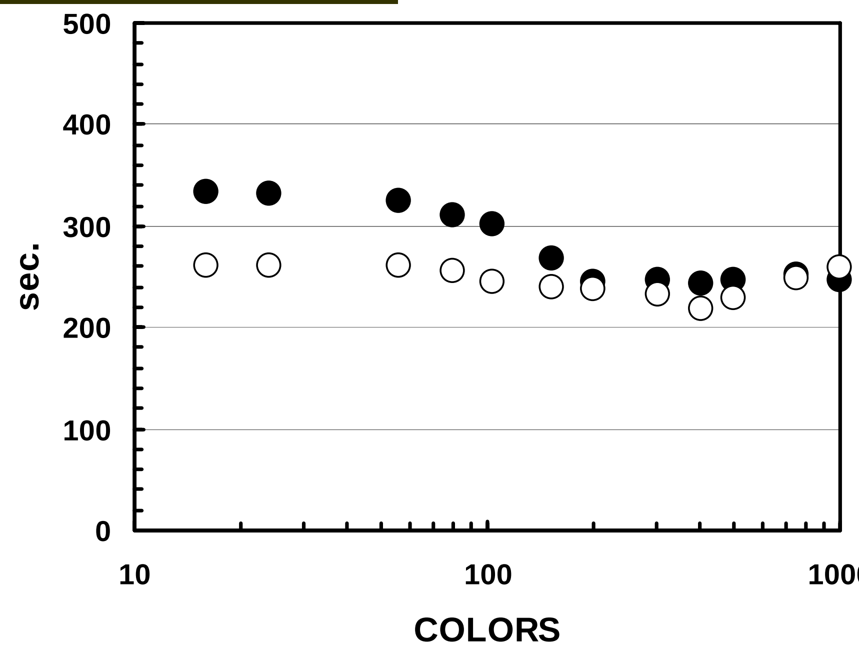
Hitachi SR8k (single node)



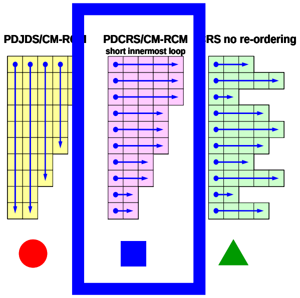
Performance is not so sensitive to color# as the Earth Simulator.
In Flat-MPI, performance is rather improved.

● Flat MPI
○ Hybrid





Effect of Loop Length (Color#)



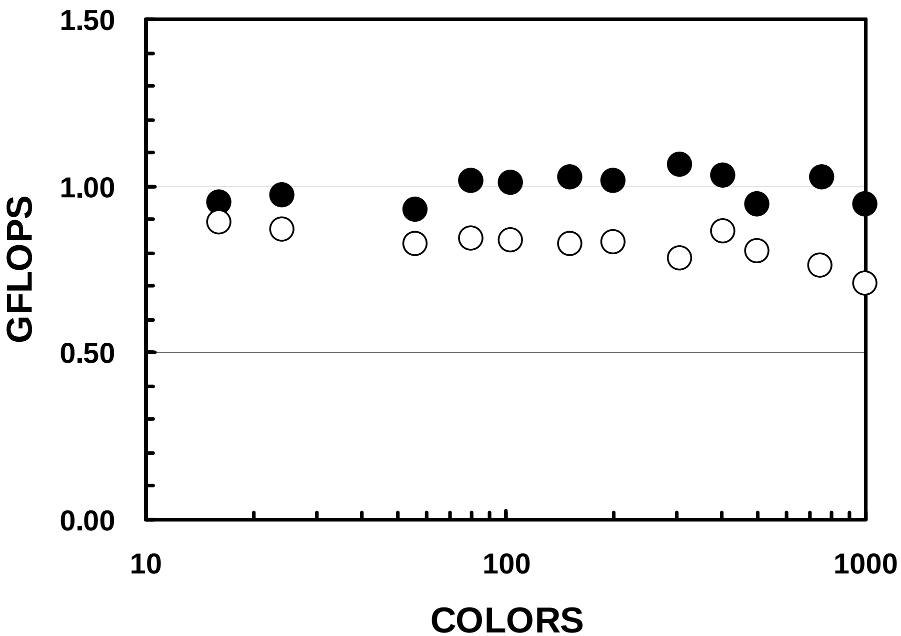
100^3 nodes= $3x10^6$ DOF

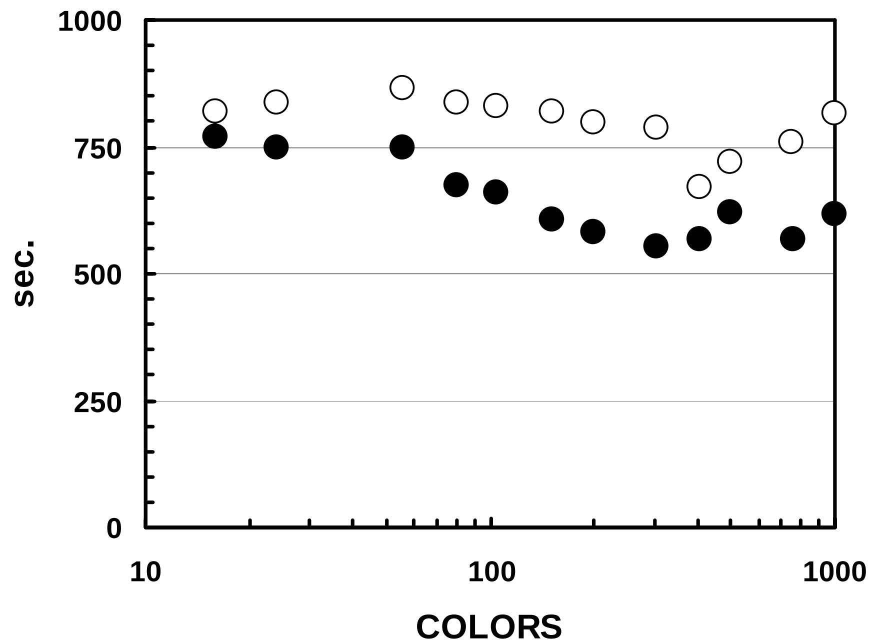
PDCRS/CM-RCM Re-Ordering

IBM SP3 (single node, 8PE's)

● Flat MPI
○ Hybrid

Performance is not so sensitive to color# as the Earth Simulator.



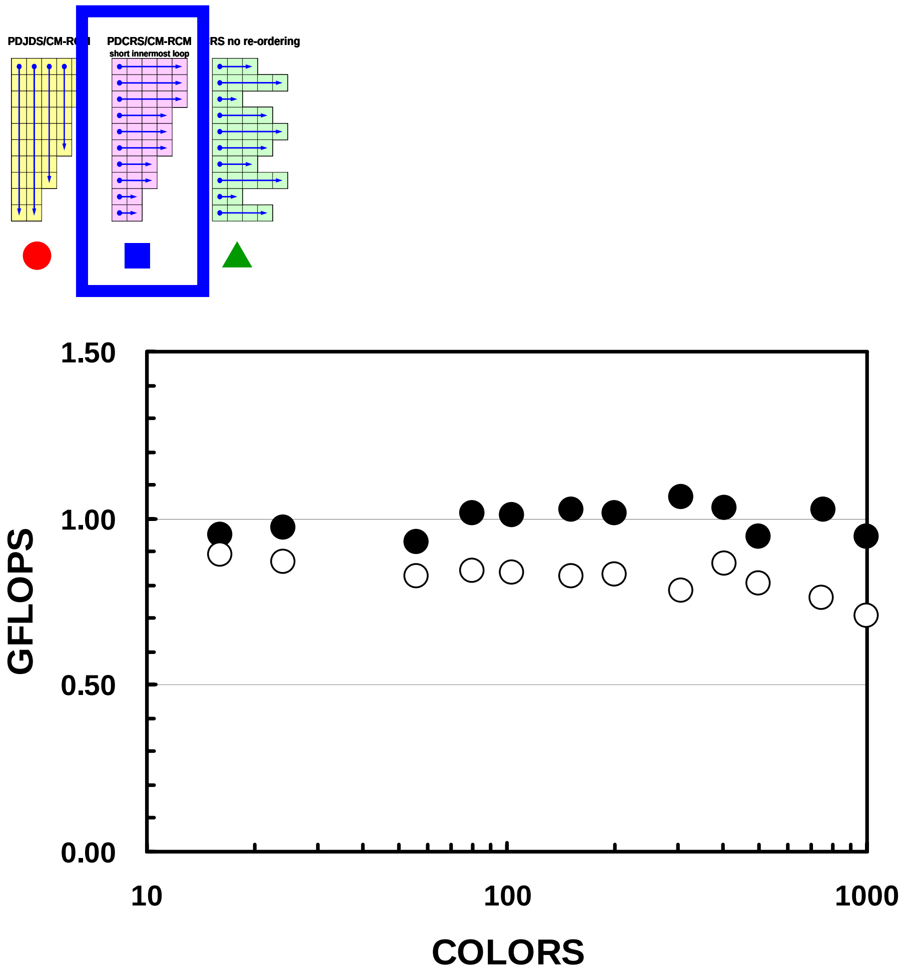


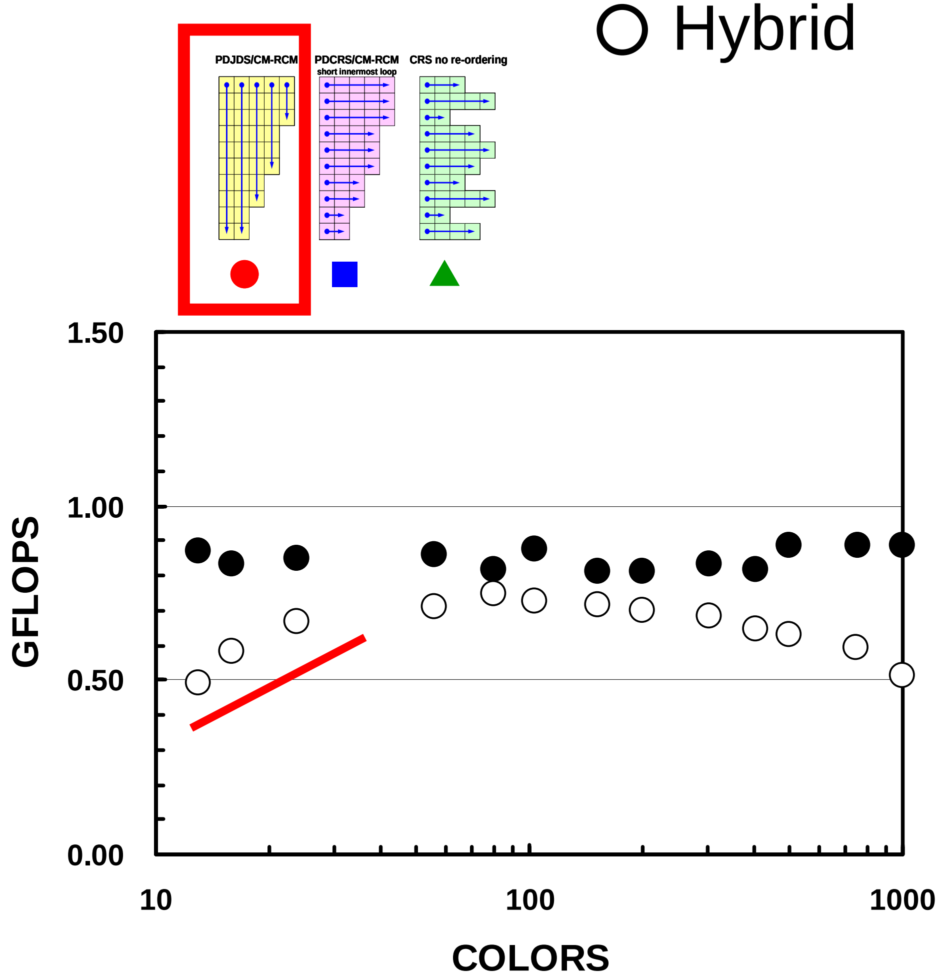
Effect of Loop Length (Color#)

100^3 nodes= 3×10^6 DOF

IBM SP3 (single node, 8PE's)

● Flat MPI
○ Hybrid

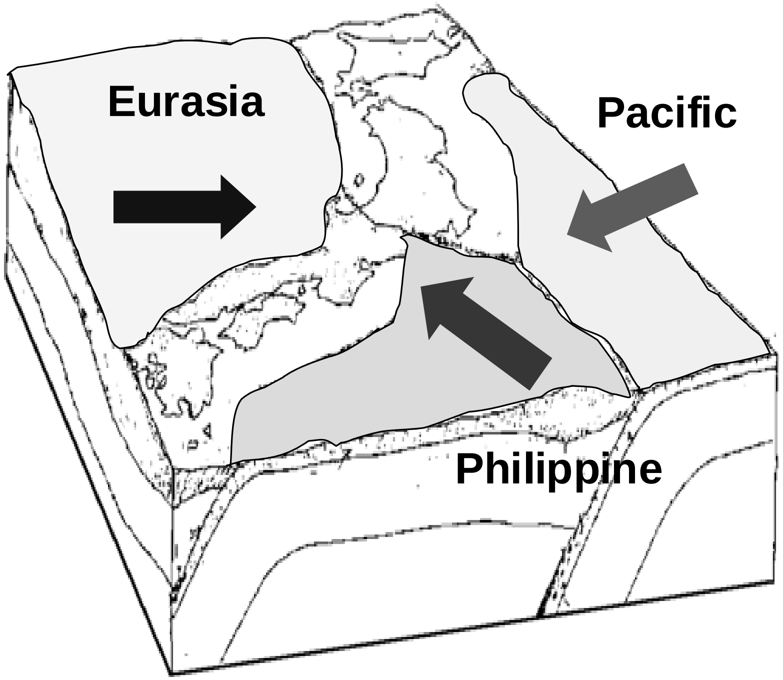


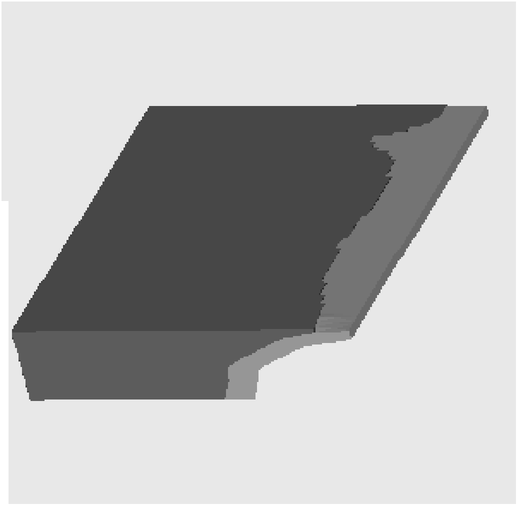


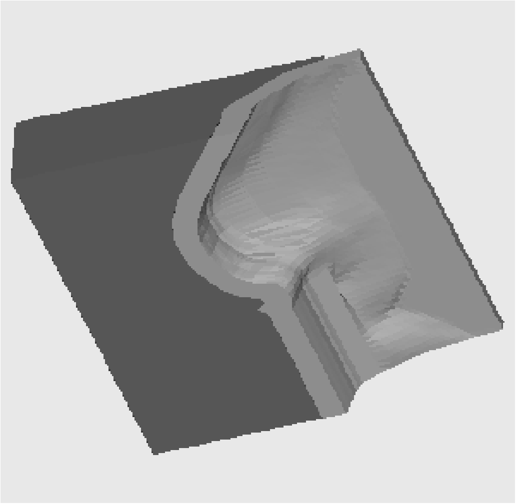
South-West Japan Model
Contact Problems

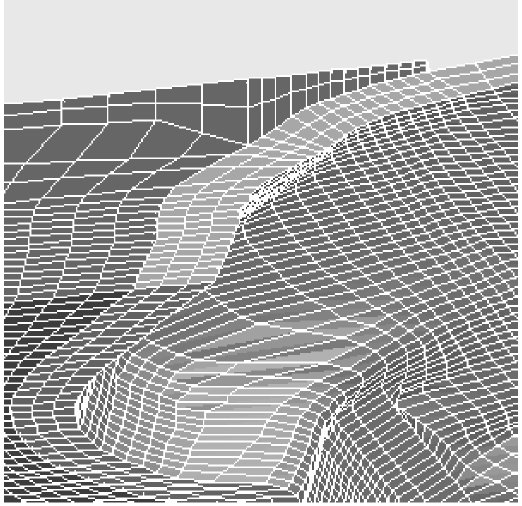
Selective Blocking Preconditioning

South-West Japan





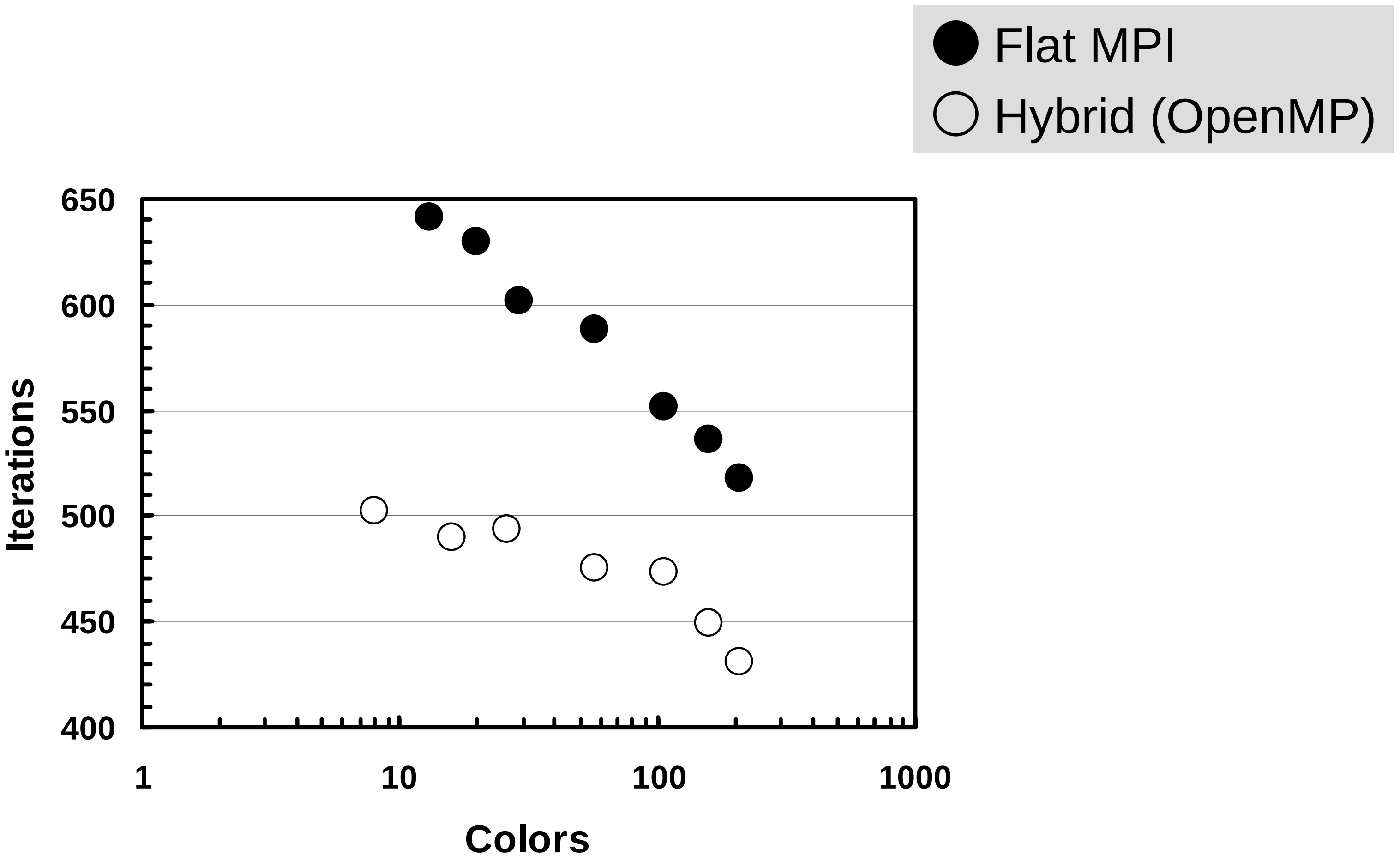




South-West Japan Model

800K nodes, 2.4M DOF

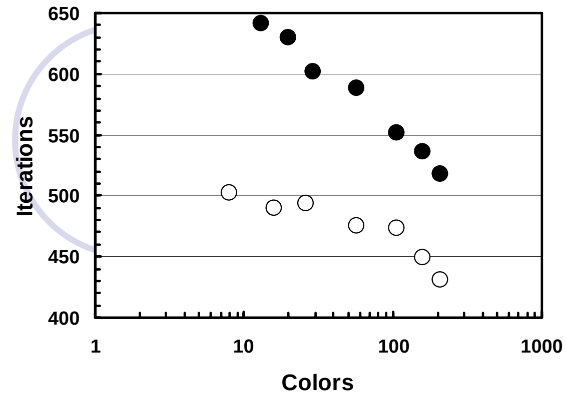
1-SMP nodes (8 PE's)



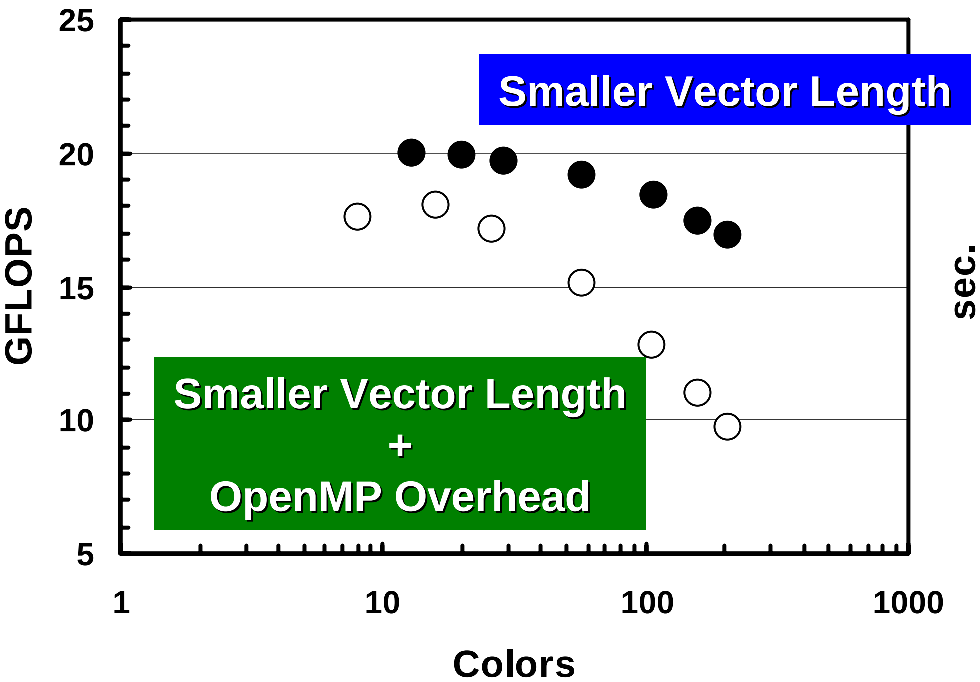
South-West Japan Model

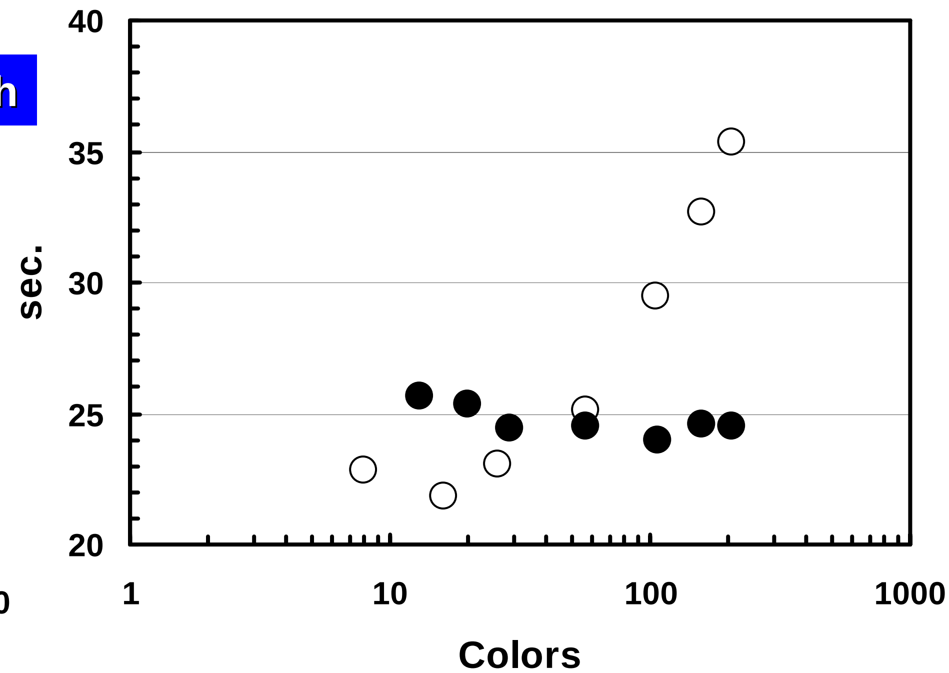
800K nodes, 2.4M DOF

ES, 1-SMP nodes (8 PE's)



● Flat MPI
○ Hybrid (OpenMP)

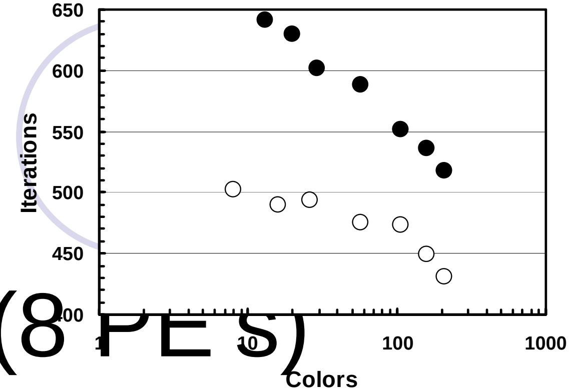




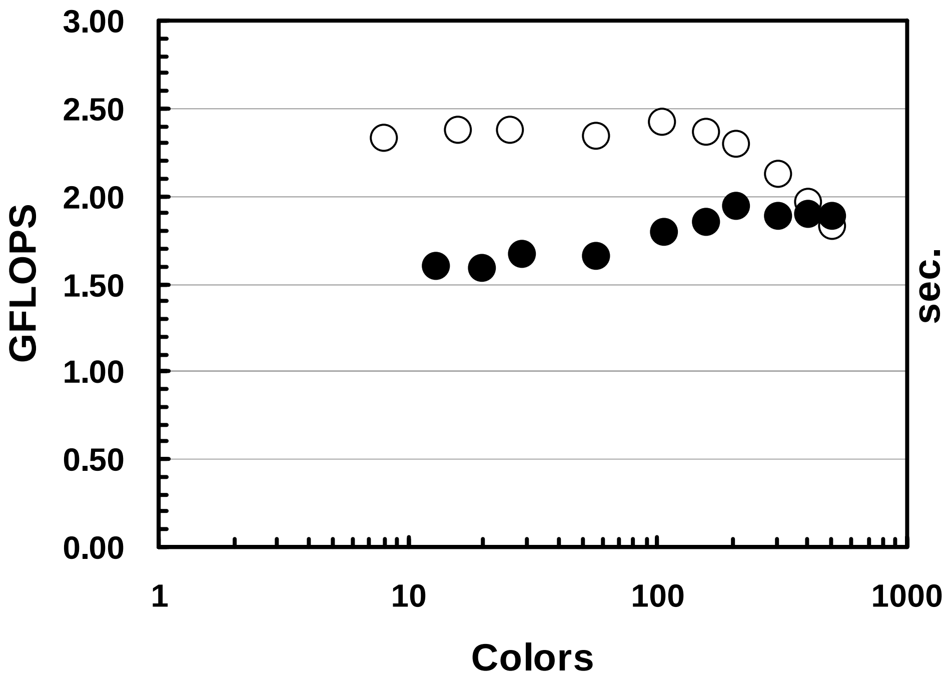
South-West Japan Model

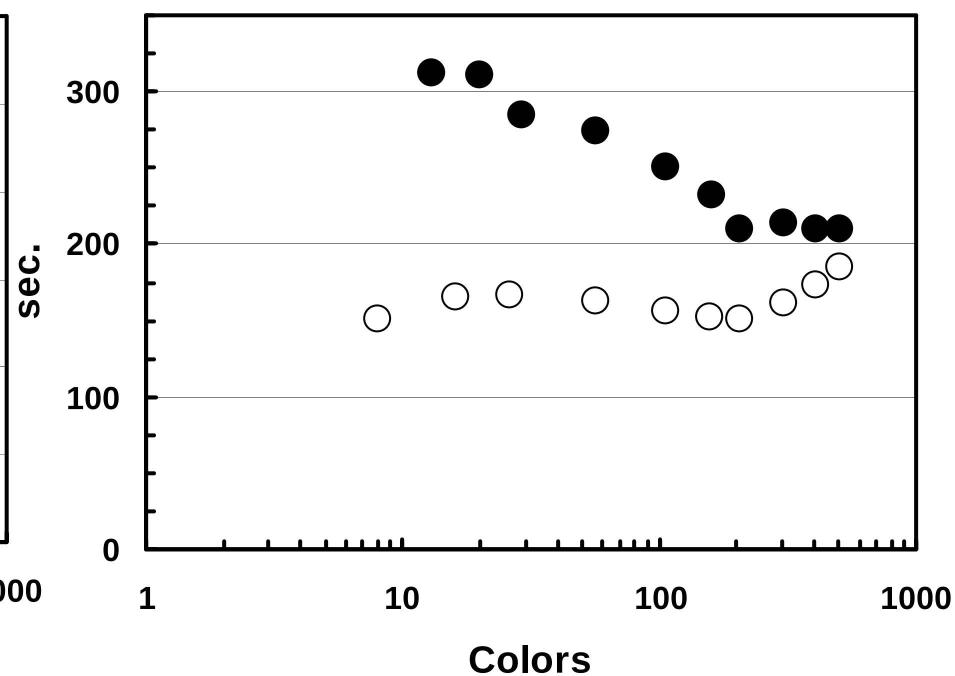
800K nodes, 2.4M DOF

Hitachi SR8000, 1-SMP nodes (8 PE's)



● Flat MPI
○ Hybrid (OpenMP)

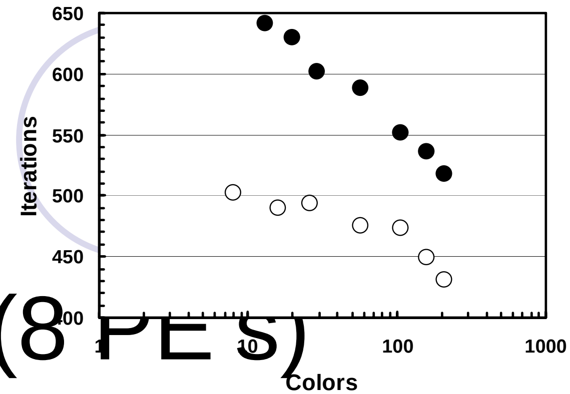




South-West Japan Model

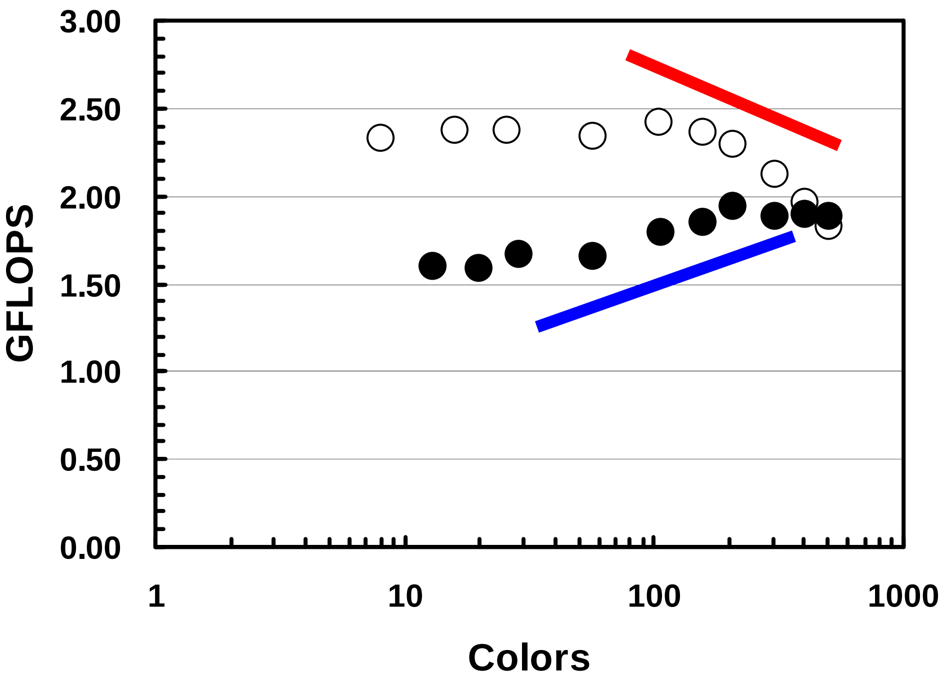
800K nodes, 2.4M DOF

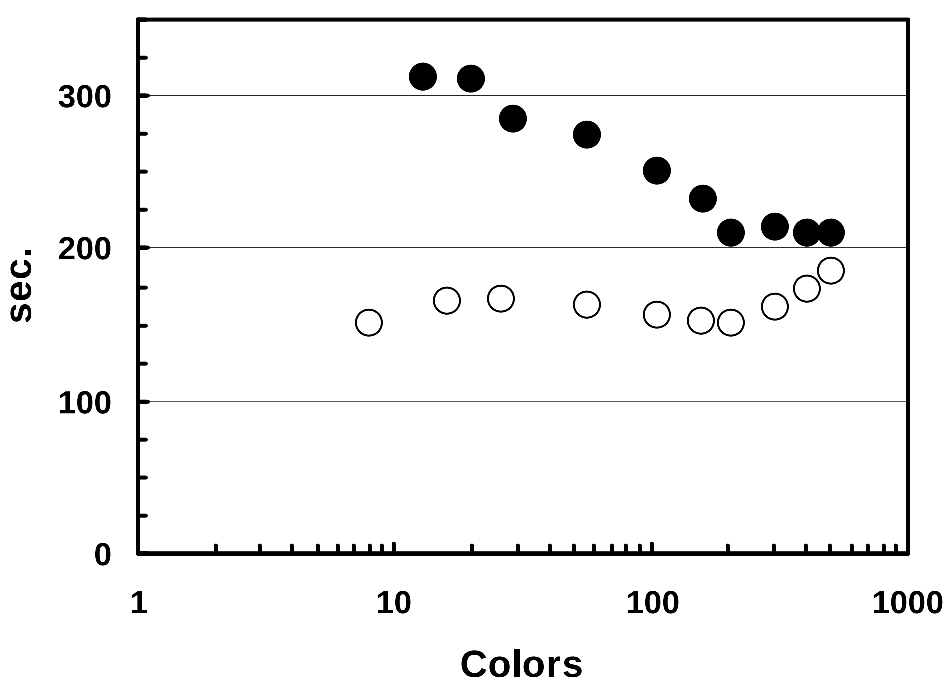
Hitachi SR8000, 1-SMP nodes (8 PE's)



● Flat MPI

○ Hybrid (OpenMP)

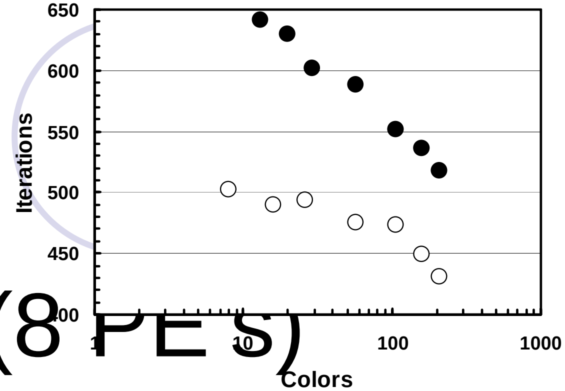




South-West Japan Model

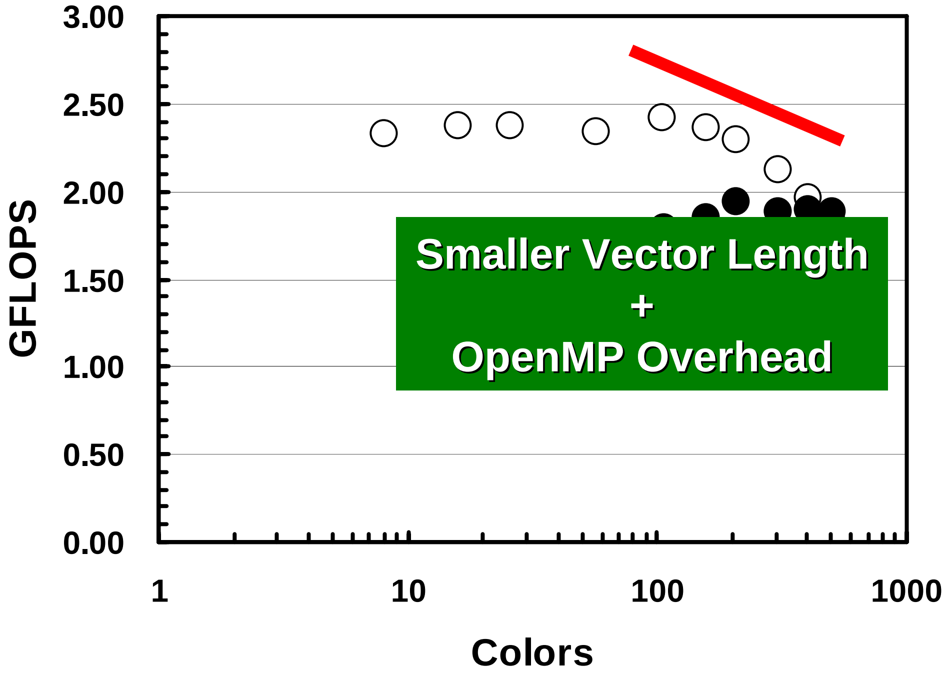
800K nodes, 2.4M DOF

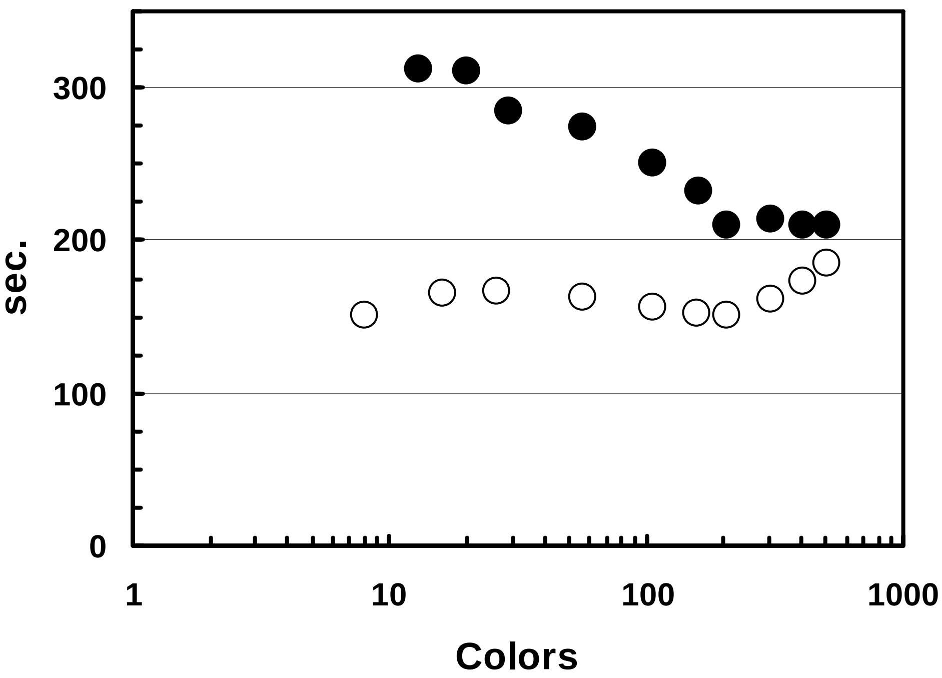
Hitachi SR8000, 1-SMP nodes (8 PE's)



● Flat MPI

○ Hybrid (OpenMP)

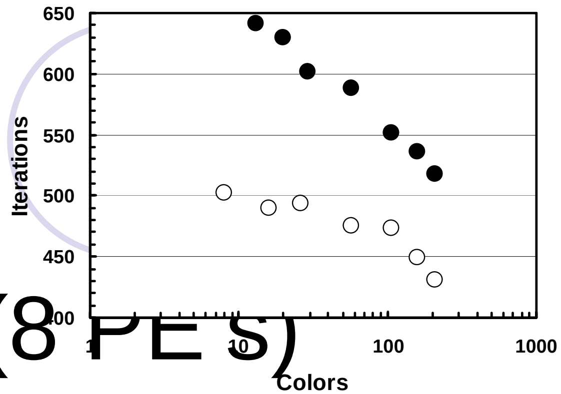




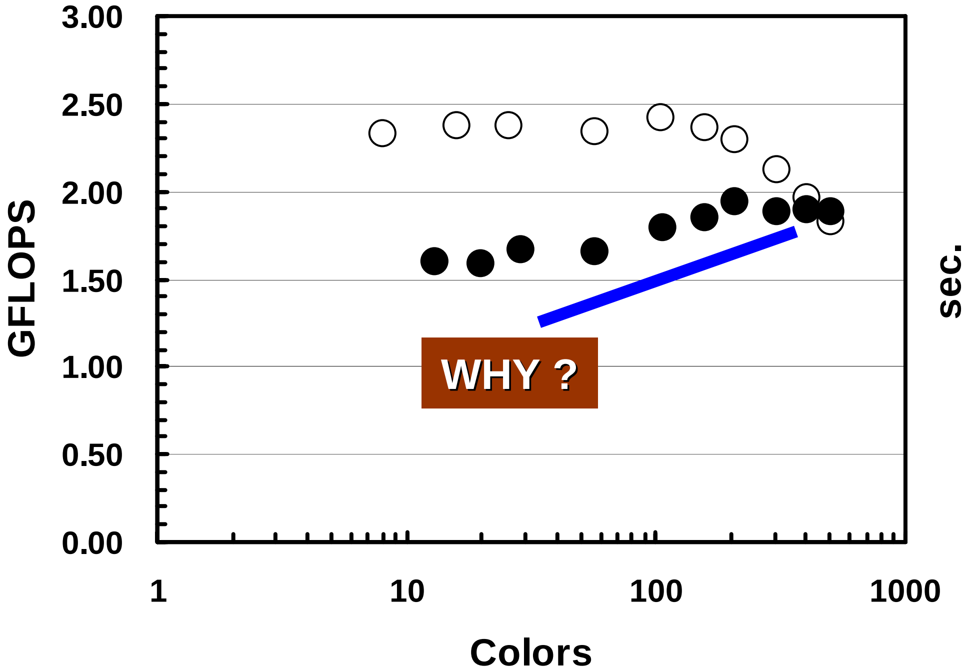
South-West Japan Model

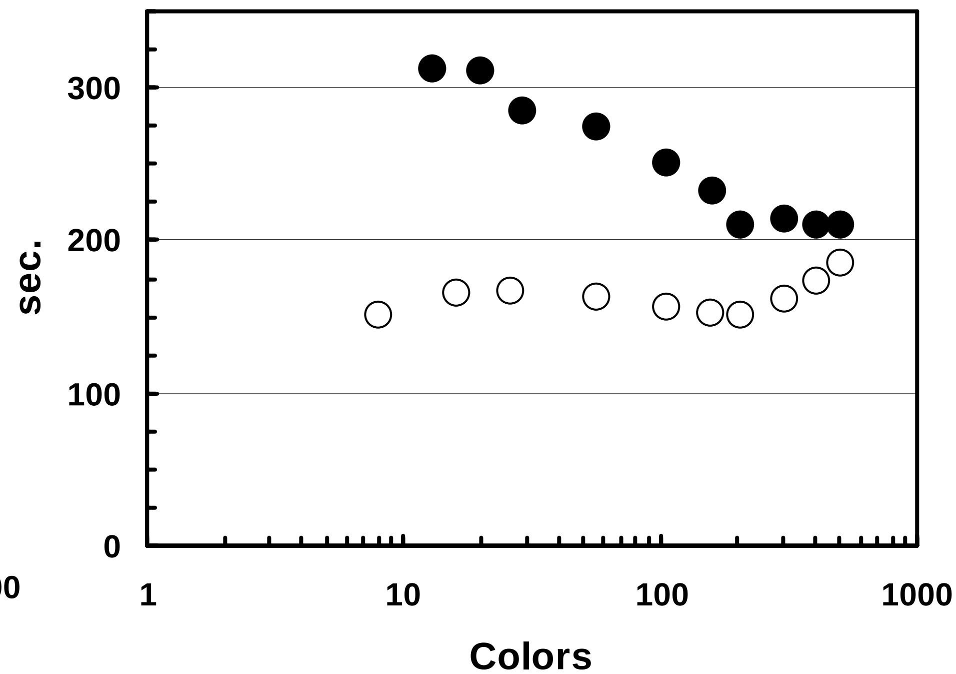
800K nodes, 2.4M DOF

Hitachi SR8000, 1-SMP nodes (8 PE's)



● Flat MPI
○ Hybrid (OpenMP)

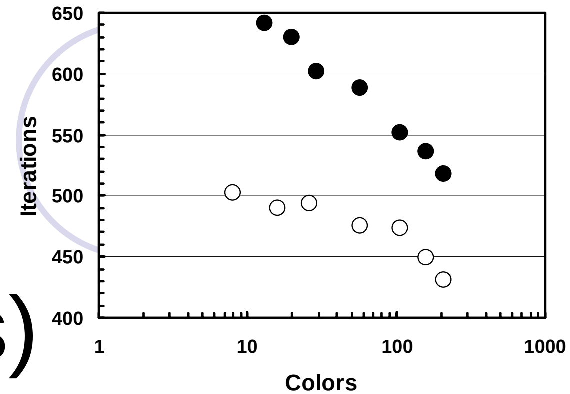




South-West Japan Model

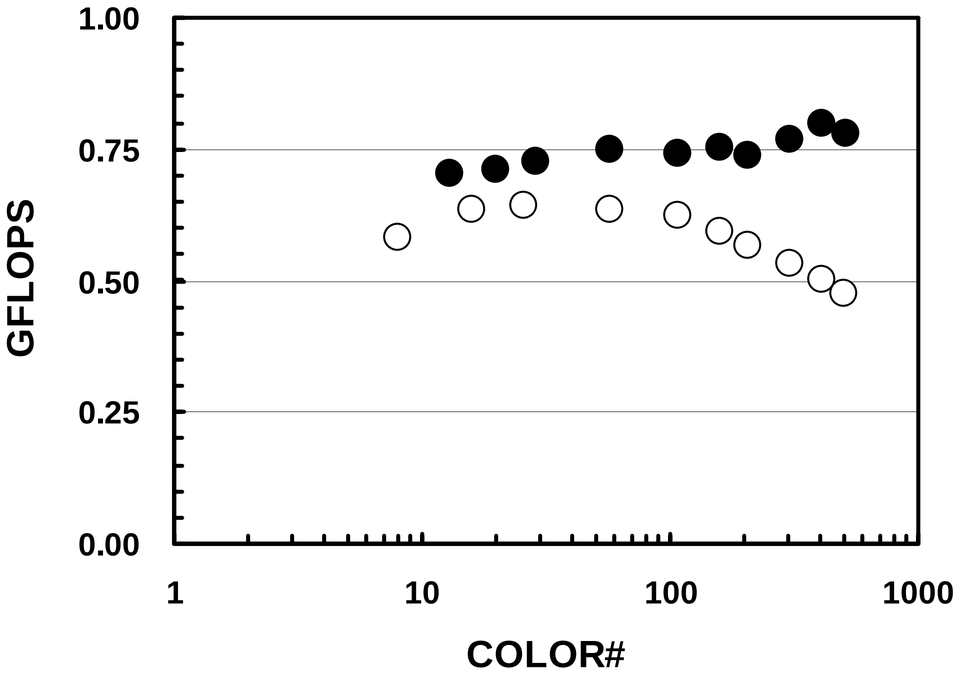
800K nodes, 2.4M DOF

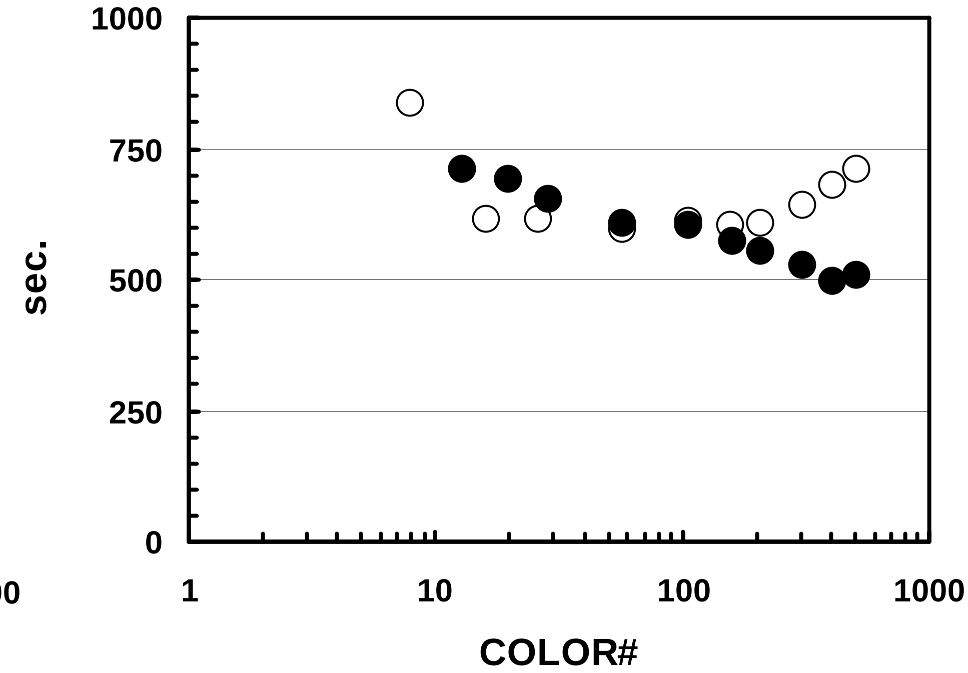
IBM SP3, 1-SMP nodes (8 PE's)



● Flat MPI

○ Hybrid (OpenMP)

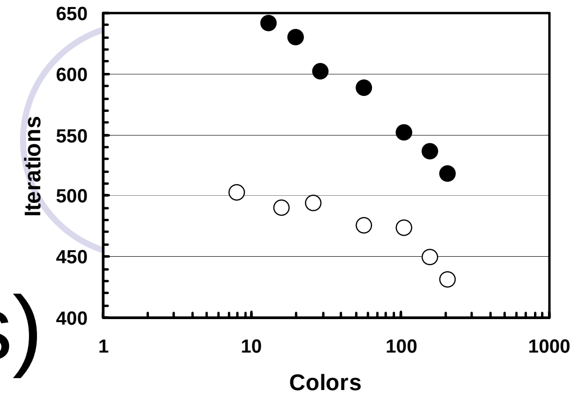




South-West Japan Model

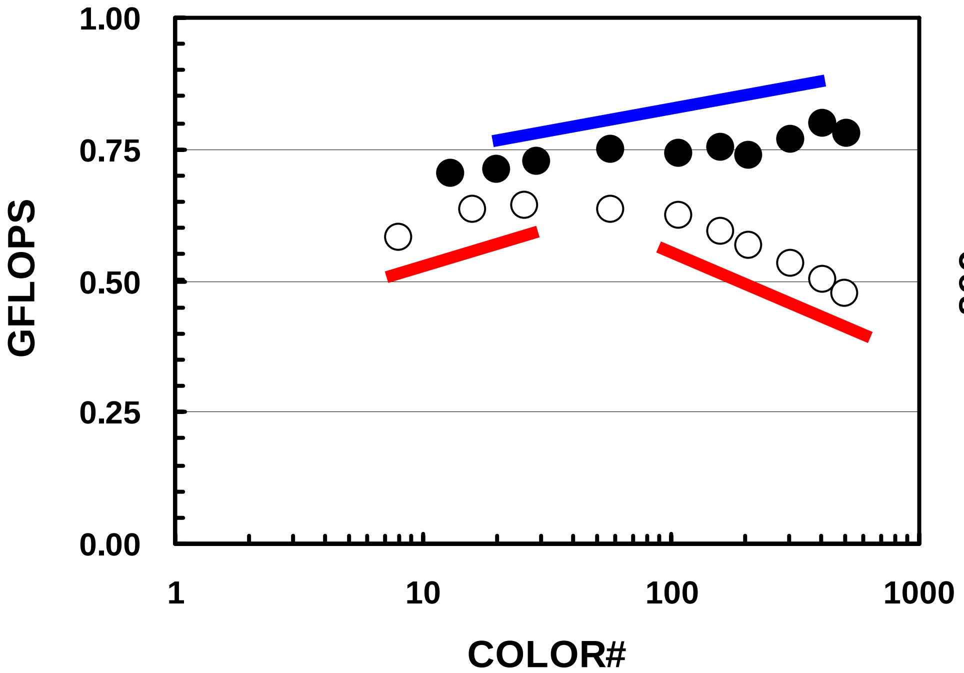
800K nodes, 2.4M DOF

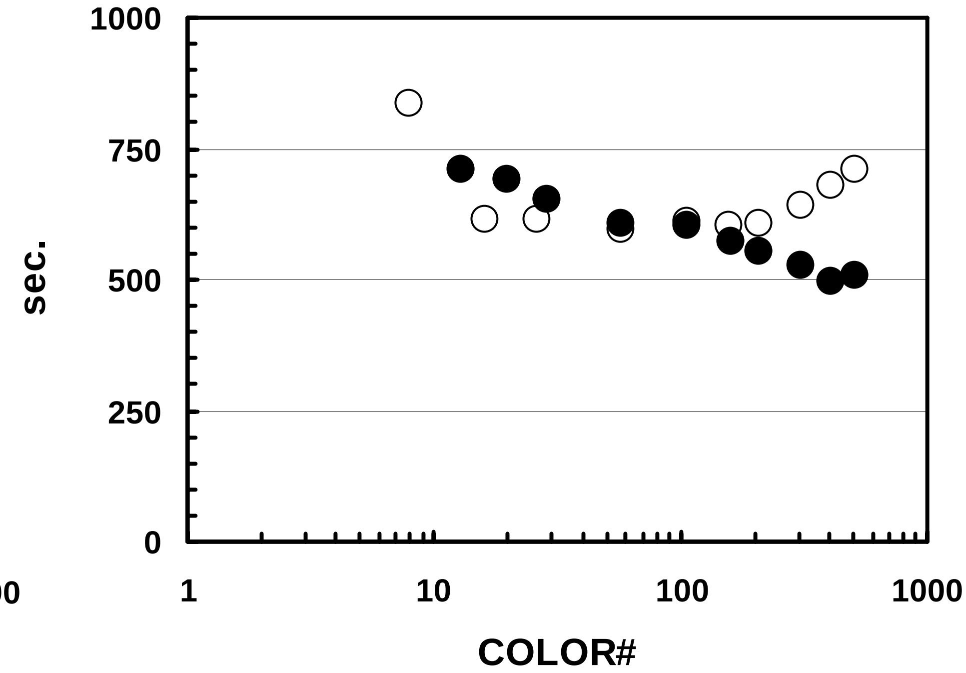
IBM SP3, 1-SMP nodes (8 PE's)



● Flat MPI

○ Hybrid (OpenMP)

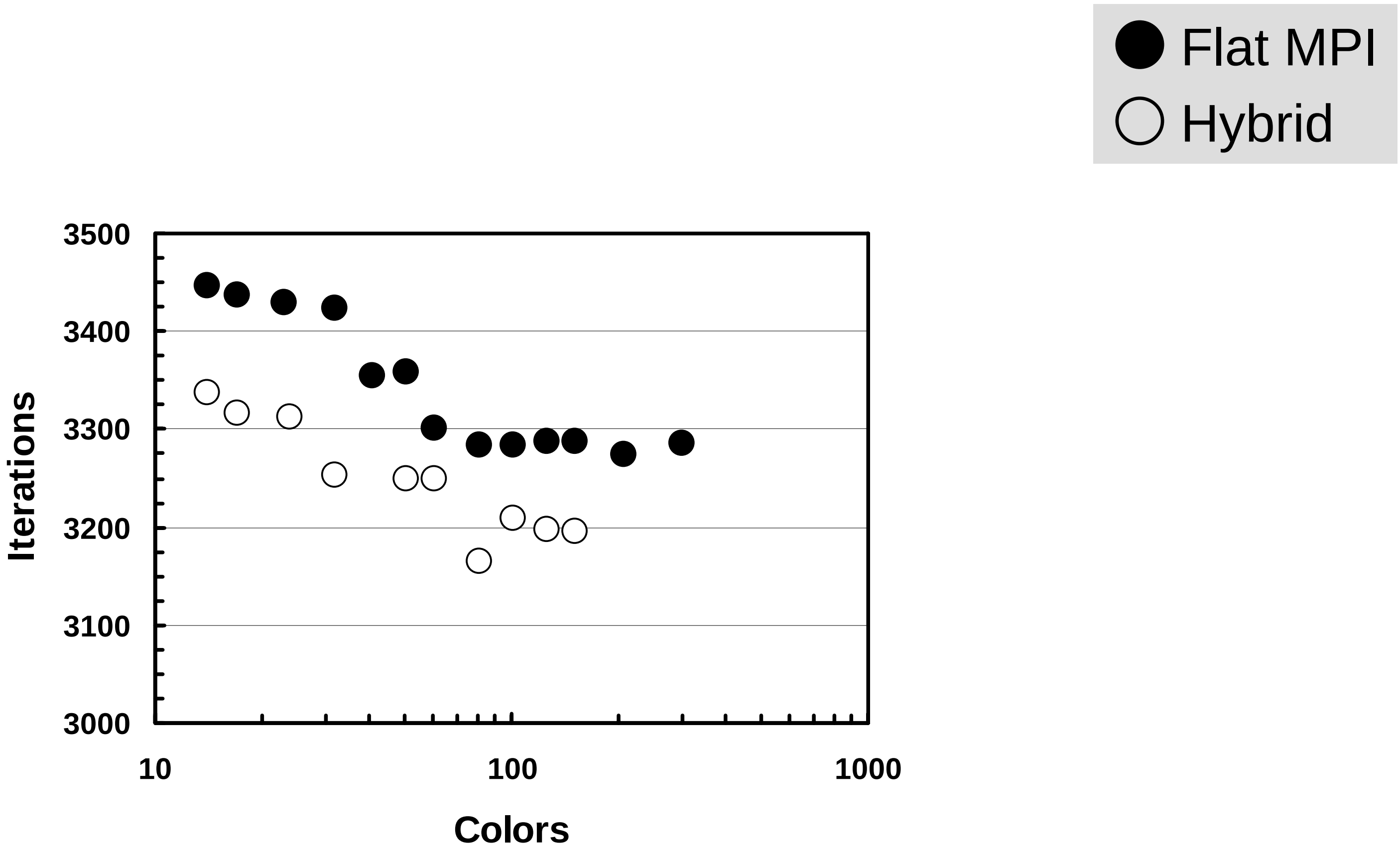




South-West Japan Model

7,767,002 nodes, 23,301,006 DOF

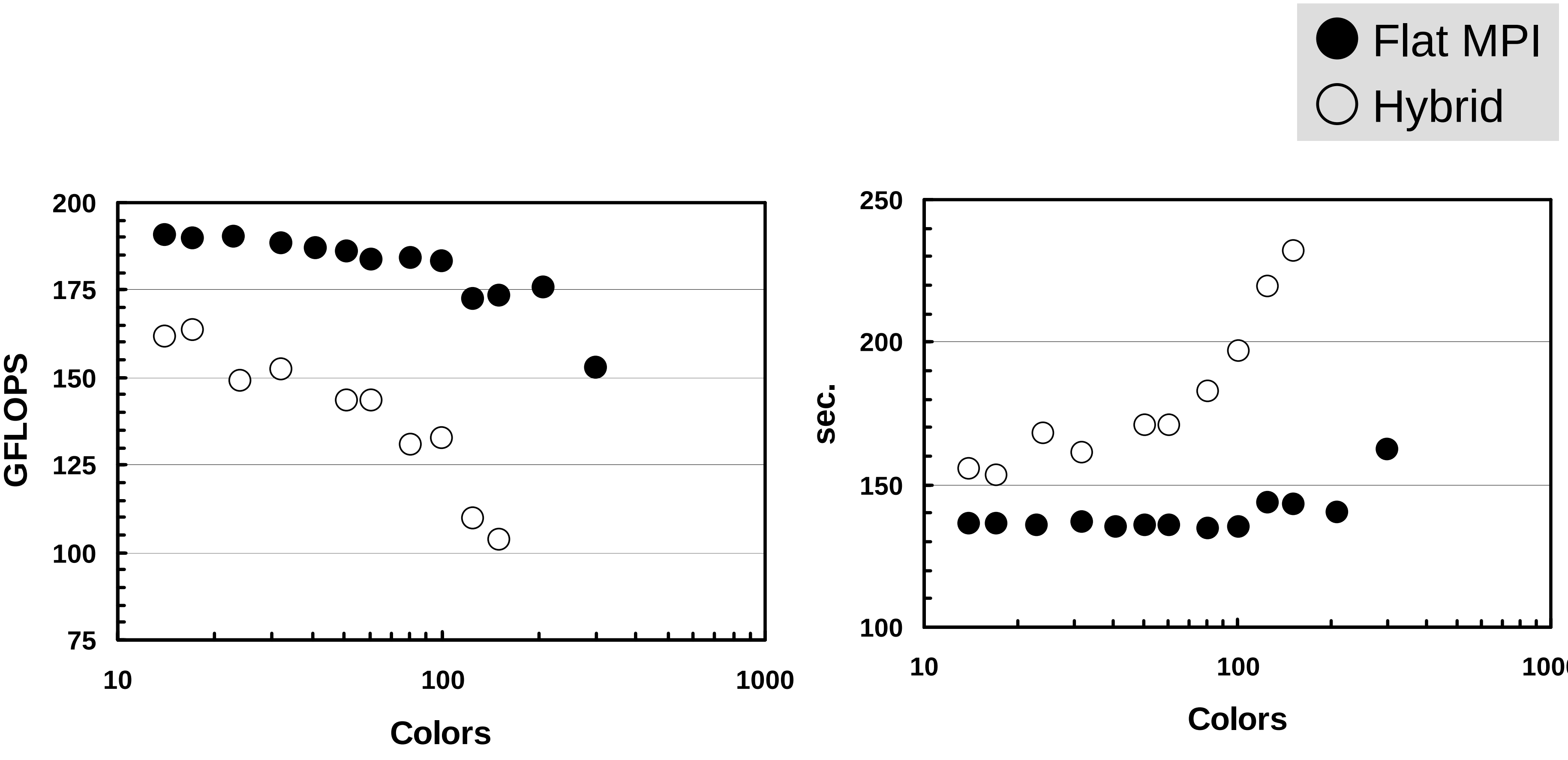
ES, 10 SMP nodes (Peak= 640 GFLOPS)



South-West Japan Model

7,767,002 nodes, 23,301,006 DOF

ES, 10 SMP nodes (Peak= 640 GFLOPS)

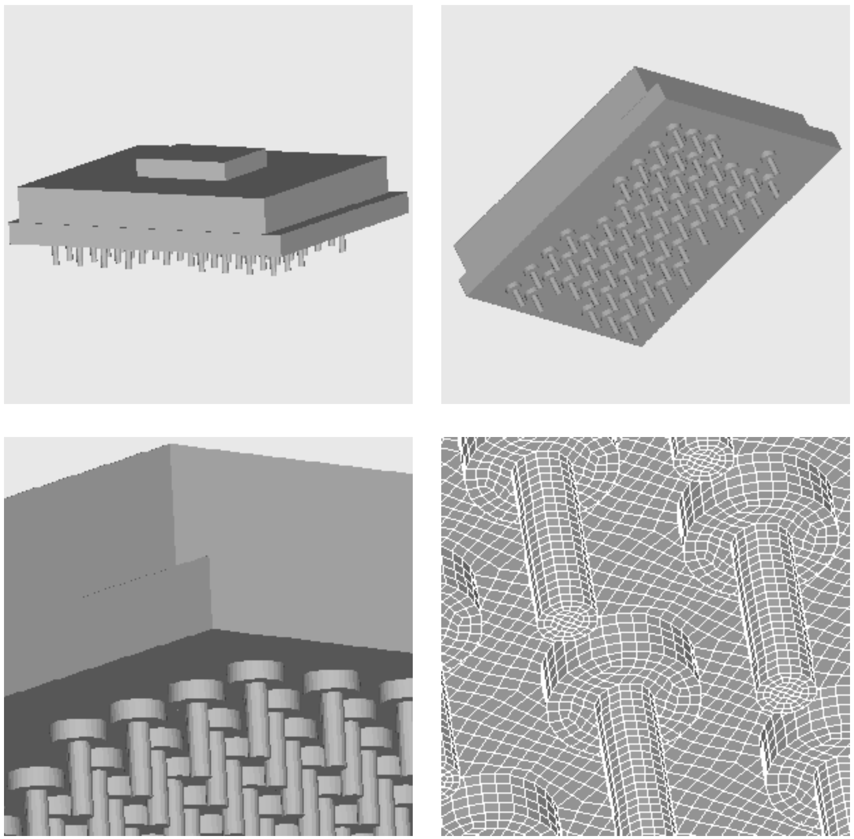


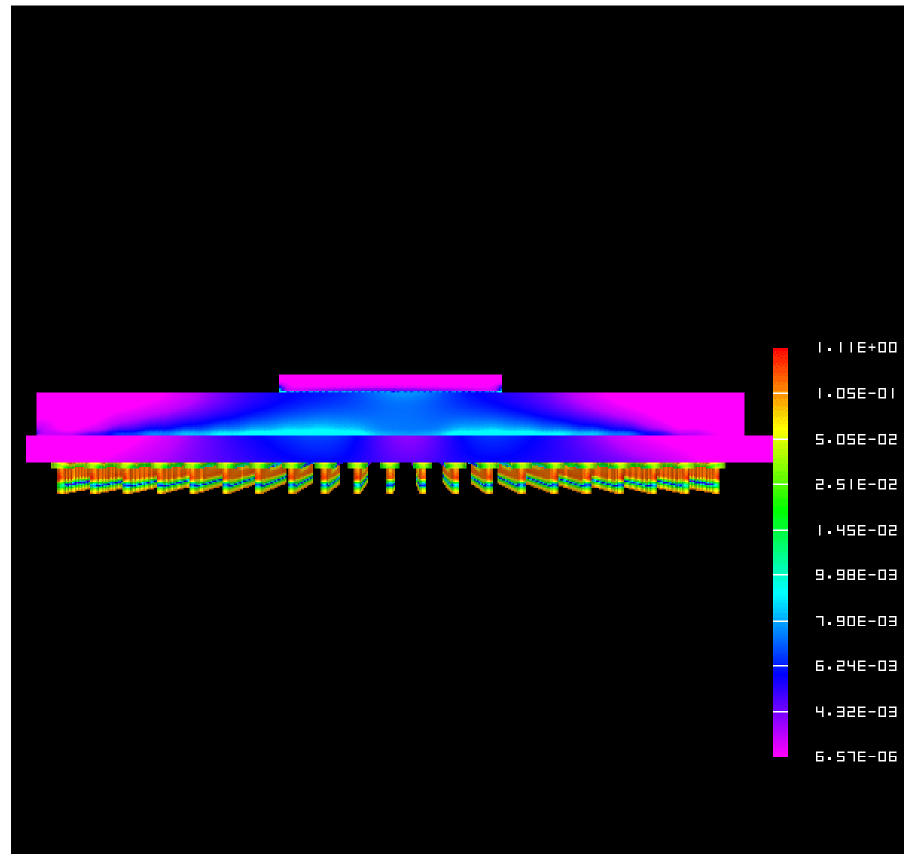
Complicated Geometries

PGA for Mobile Pentium III

PGA model

61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF)

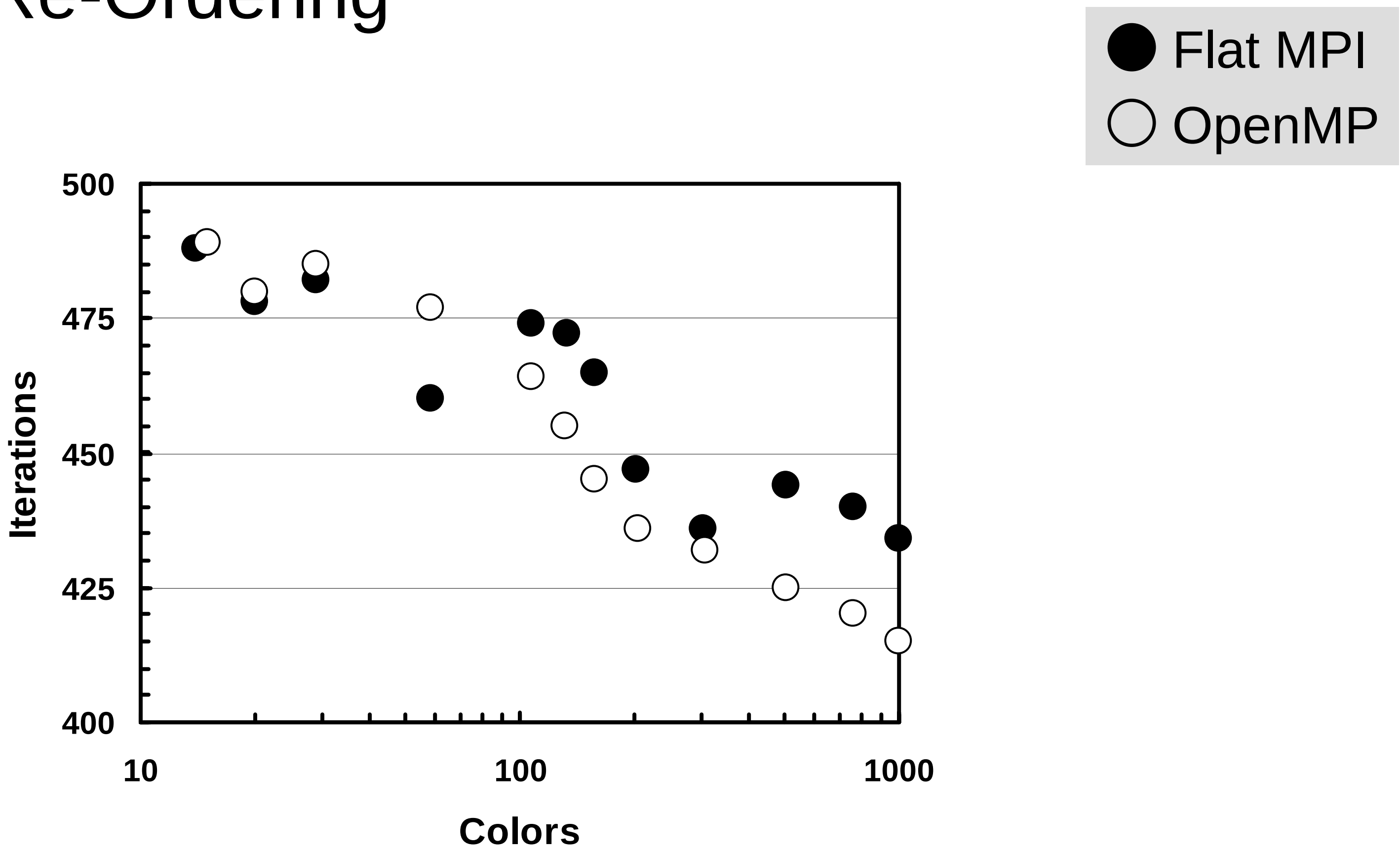




PGA model

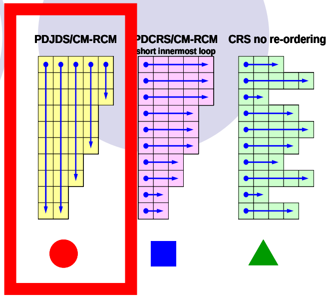
61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF) , **1 SMP node**

PDJDS/MC Re-Ordering

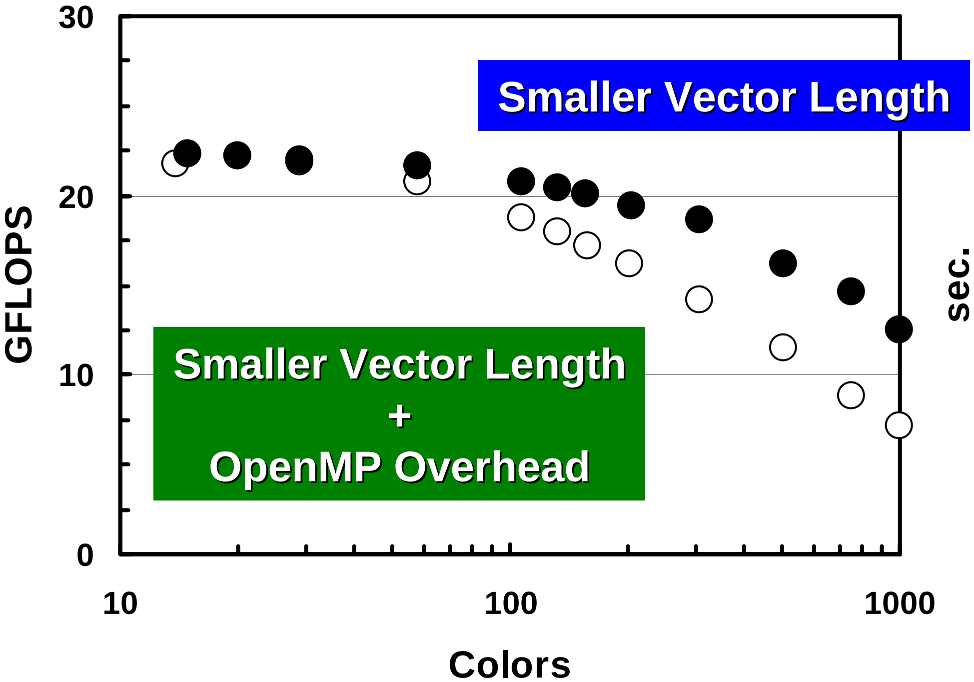


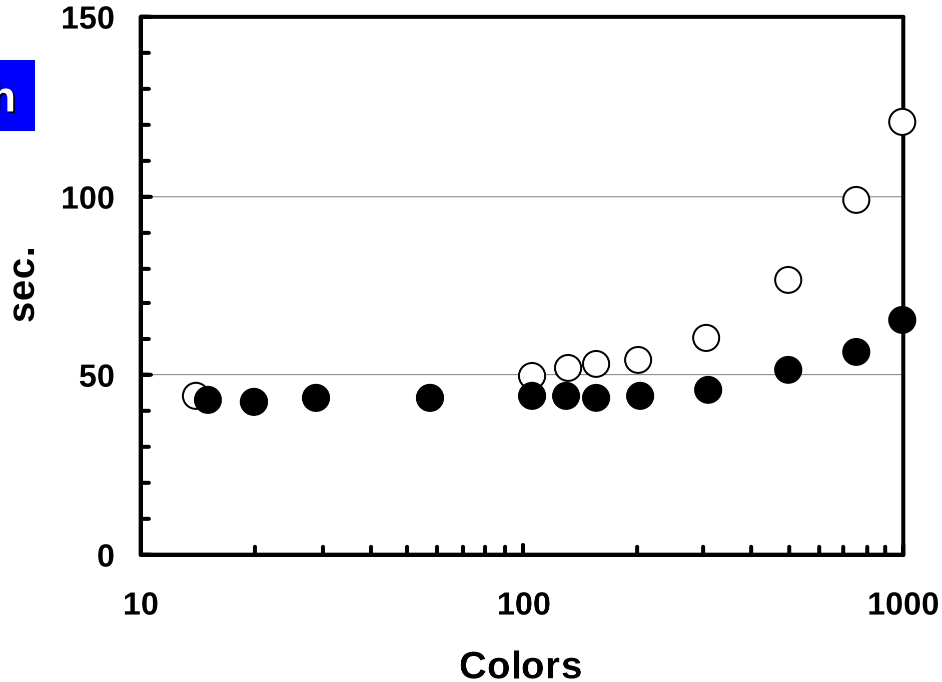
PGA model

61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node
PDJDS/MC Re-Ordering, **Earth Simulator**



● Flat MPI
○ OpenMP

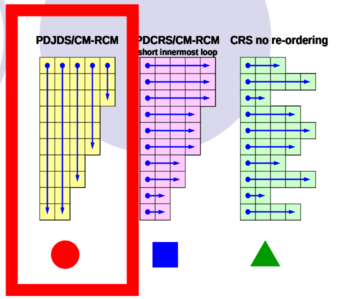


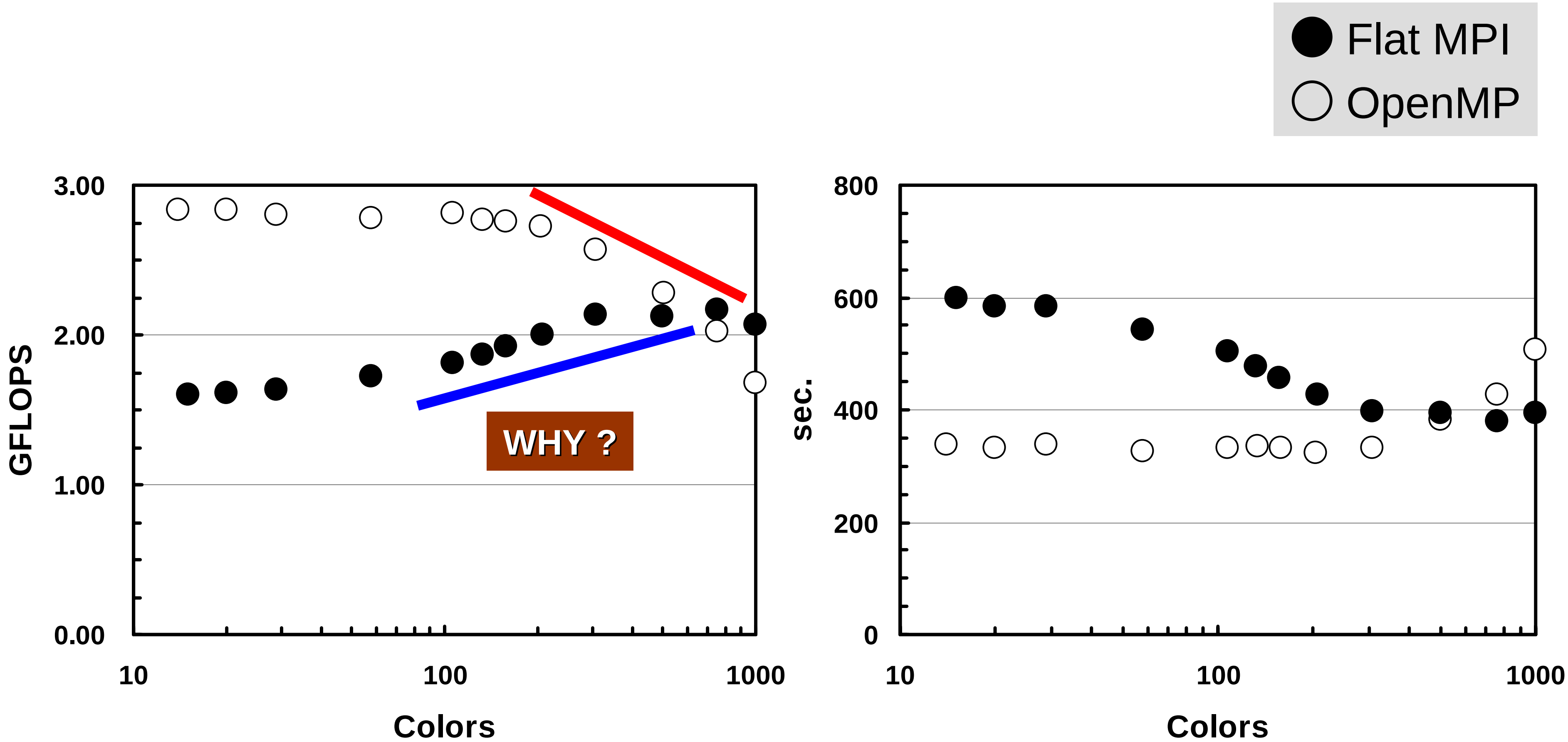


PGA model

61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF) , 1 SMP node

PDJDS/MC Re-Ordering, **<u>Hitachi SR8000</u>**

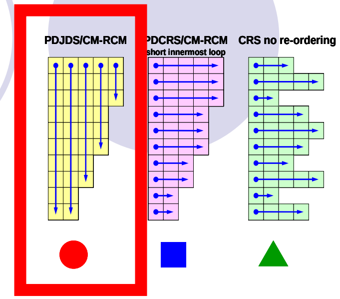


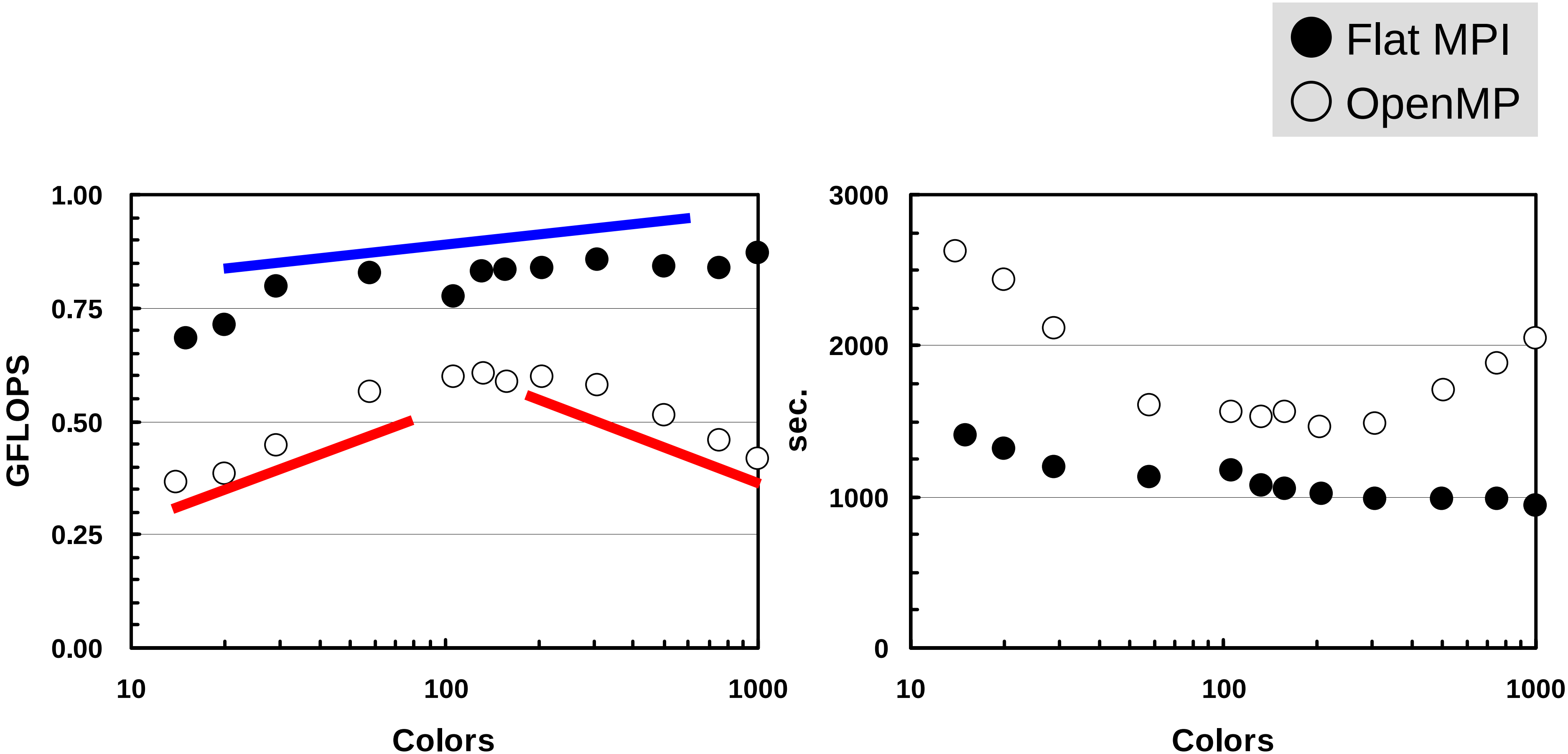


PGA model

61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node

PDJDS/MC Re-Ordering, **IBM-SP3**

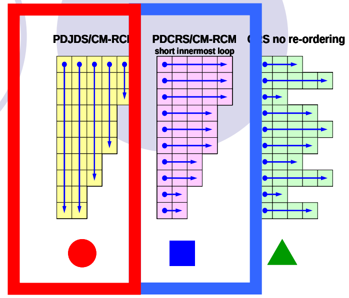




PGA model

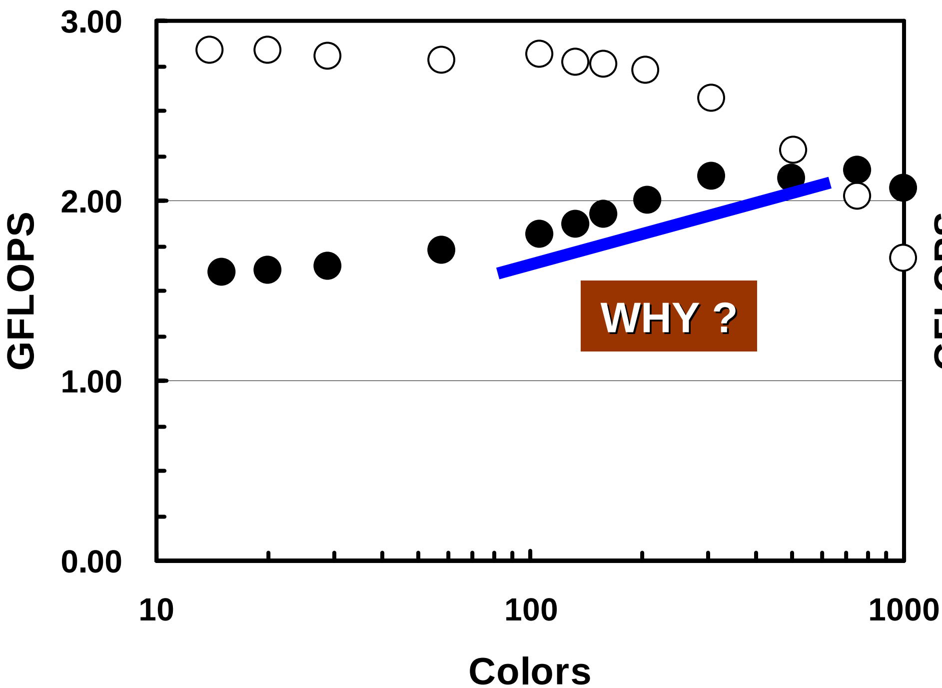
61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node

Hitachi SR8000

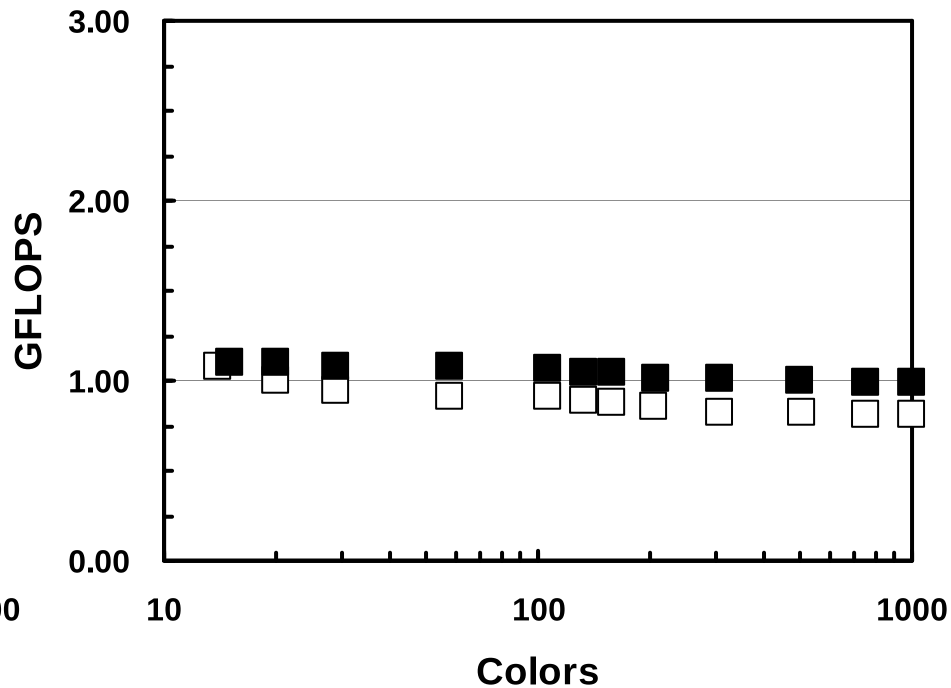


●■ Flat MPI
○□ OpenMP

PDJDS/MC



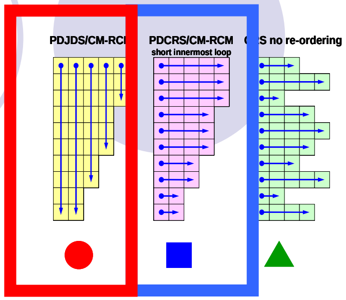
PDCRS/MC



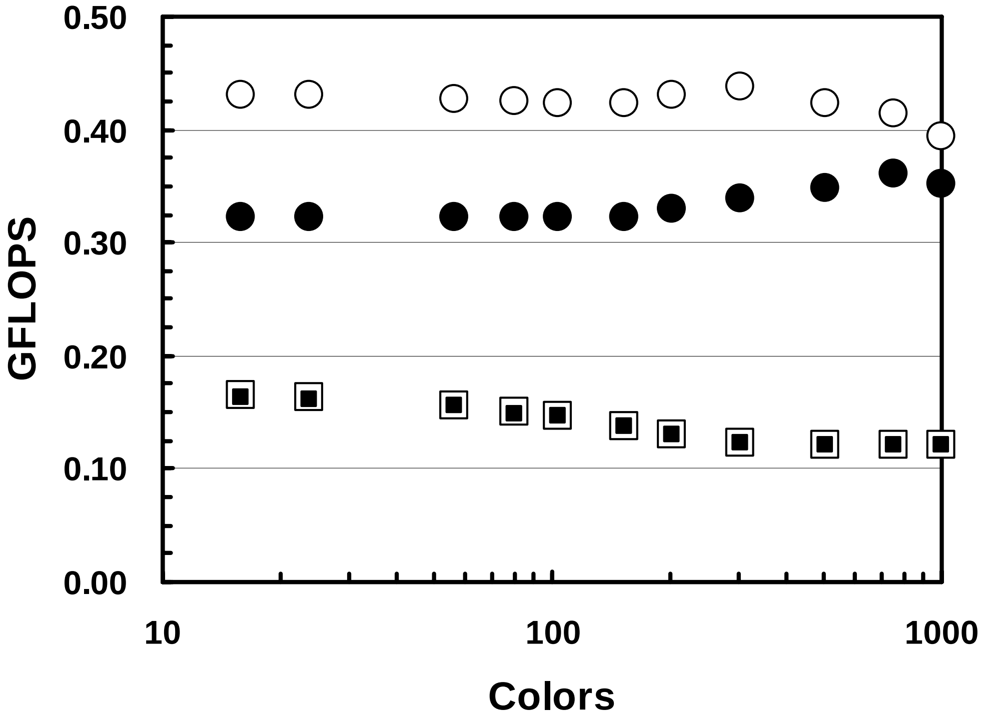
Single PE test for simple cubic model

786,432 DOF= 3×64^3 nodes

Hitachi SR8000



- ● Flat MPI (PDJDS)
- ■ Flat MPI (PDCRS)
- ○ OpenMP (PDJDS)
- □ OpenMP (PDCRS)



Behavior of Flat MPI with PDJDS seem like that of scalar processors, while OpenMP/PDJDS looks like vector processors.

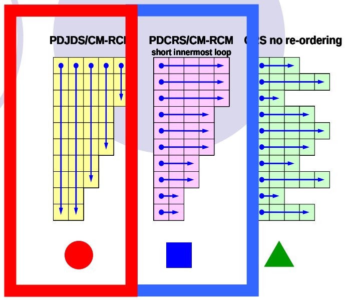
↓

Feature (or problem) of compiler ? Pseudo-Vector option does not work well in Flat MPI.

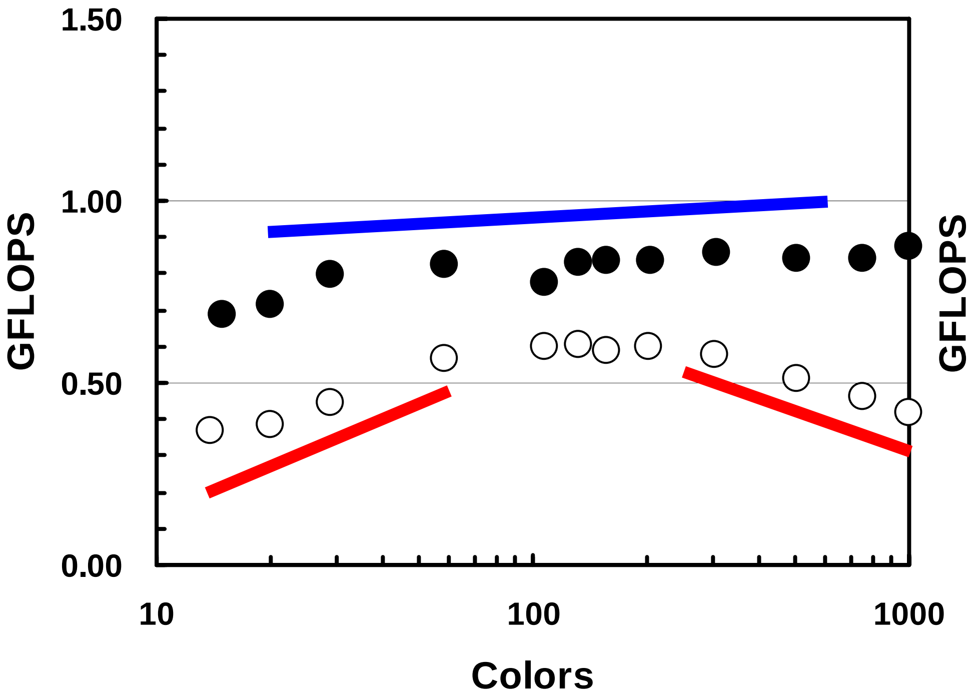
PGA model

61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node

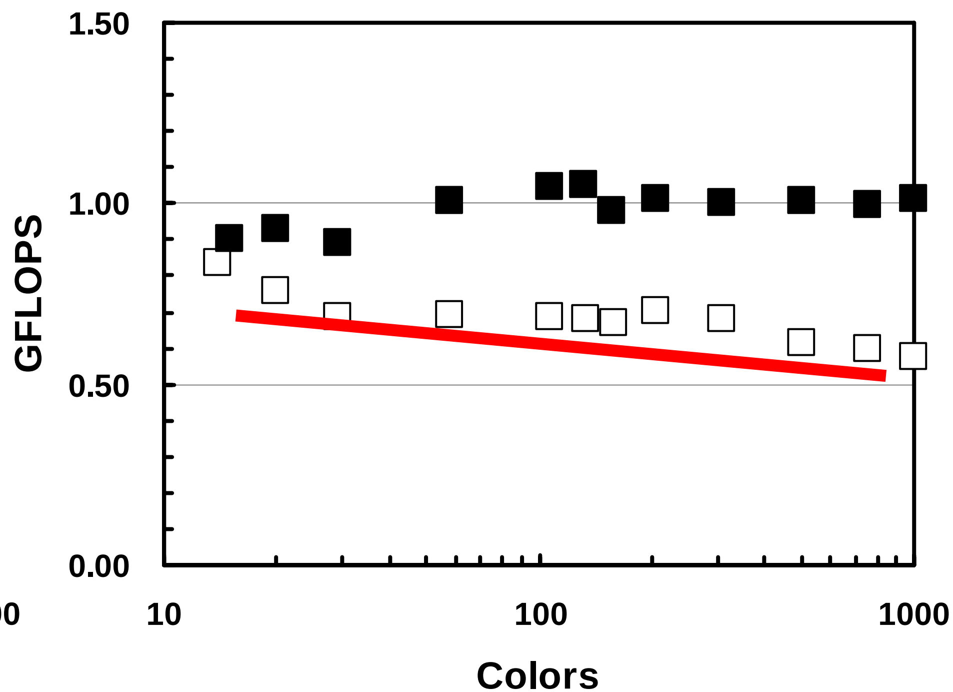
IBM-SP3



PDJDS/MC

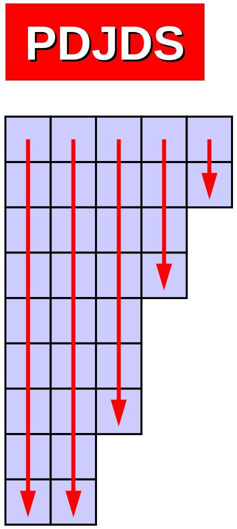


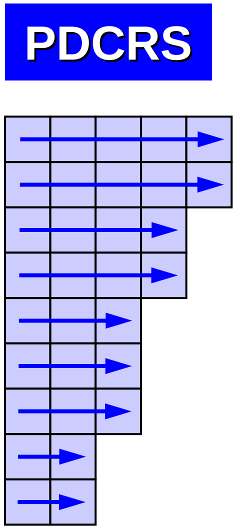
PDCRS/MC



PDCRS is more suitable for scalar processors

- Reduction type loop of CRS is more suitable for cache-based scalar processor because of its localized operation.
- PDJDS provides data locality if the color number increases.
  - On scalar processors, performance may be improved as color number increases.





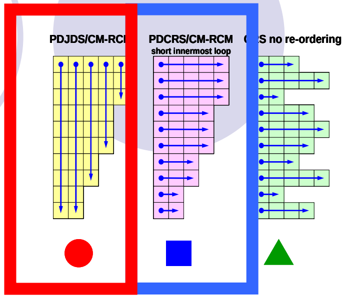

```
do j= 1, NCON
  do i= 1, NN(j)
    k = index(j-1) + i
    kk= item (k)
    Y(i)= Y(i)+A(k)*x(k)
  enddo
enddo
```

```
do i= 1, N
  k1= index(i-1)+1
  k2= index(i)
  do k= k1, k2
    kk= item(k)
    Y(i)= Y(i)+A(k)*x(k)
  enddo
enddo
```

PGA model

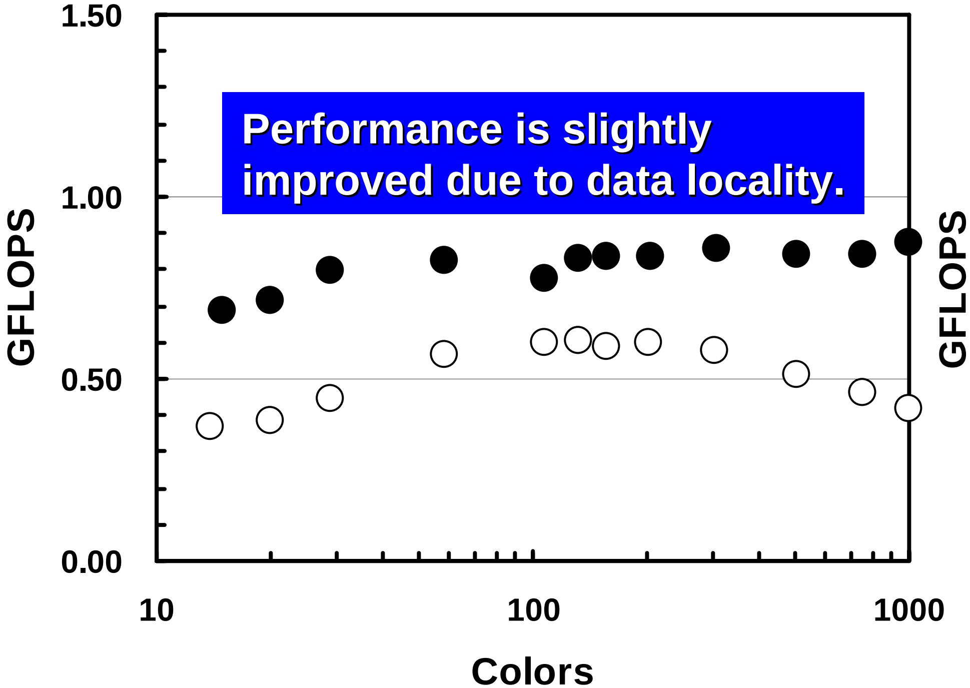
61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF) , 1 SMP node

IBM-SP3

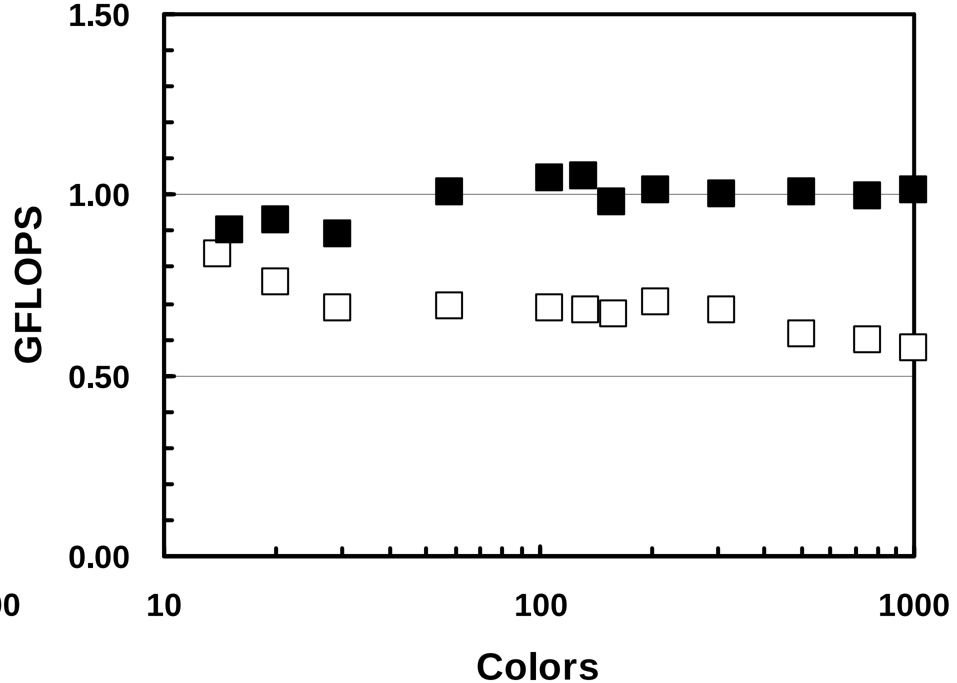


●■ Flat MPI
○□ OpenMP

PDJDS/MC



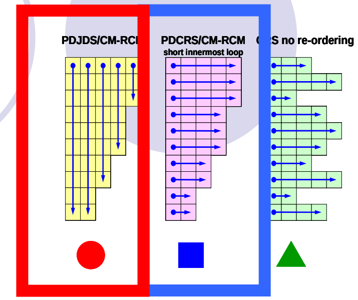
PDCRS/MC

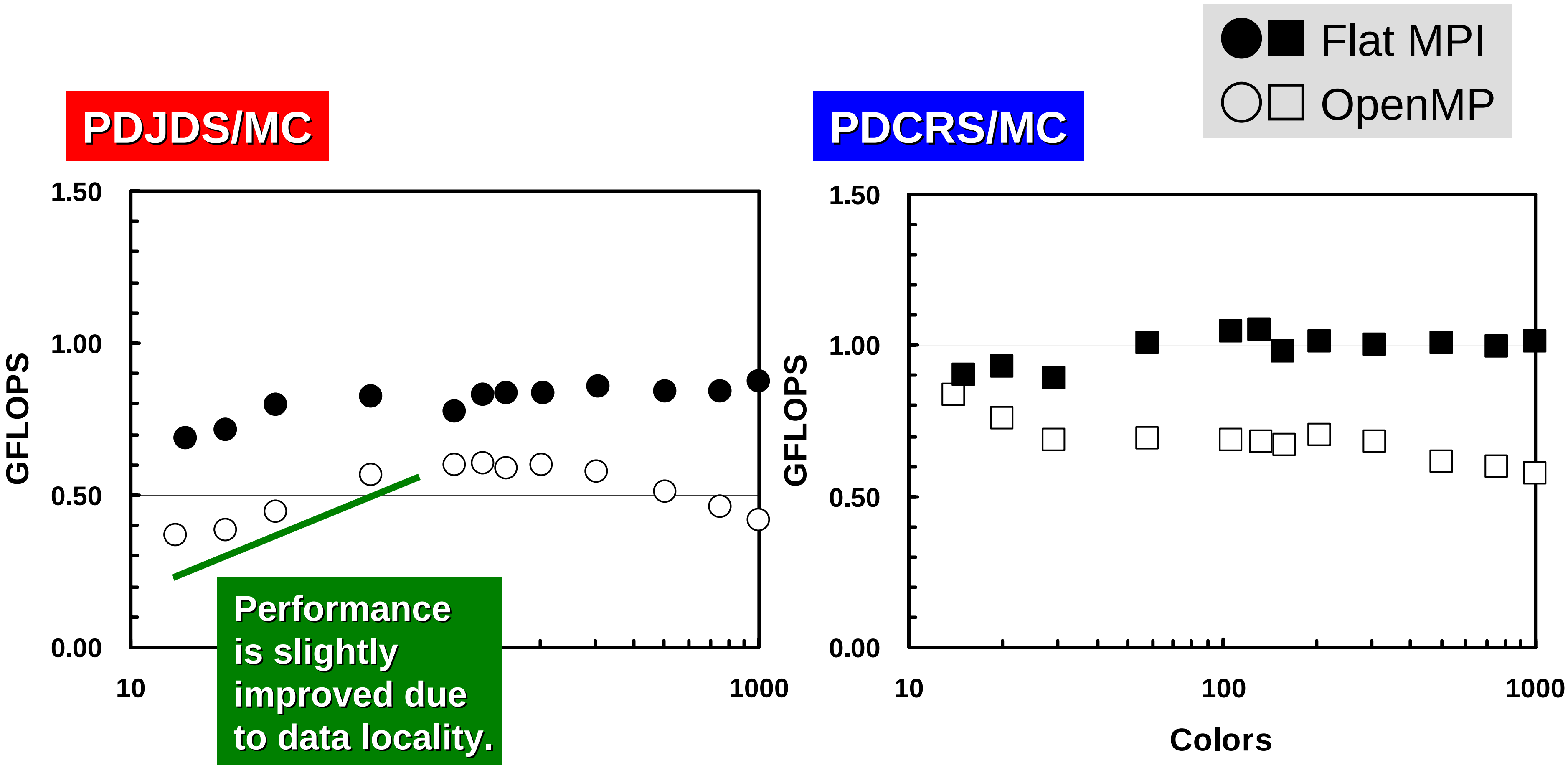


PGA model

61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node

IBM-SP3

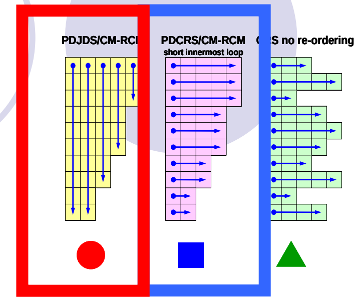


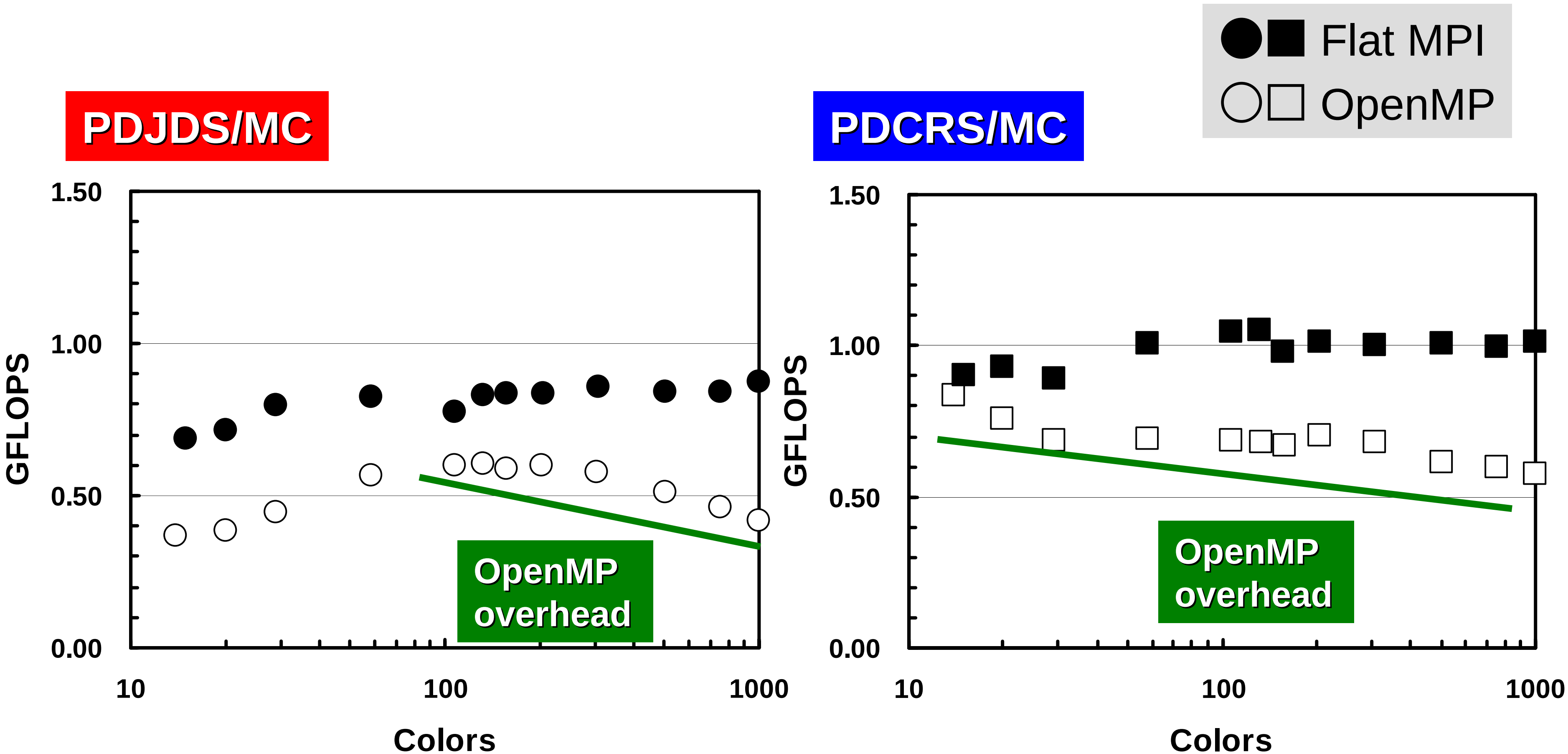


PGA model

61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF) , 1 SMP node

IBM-SP3

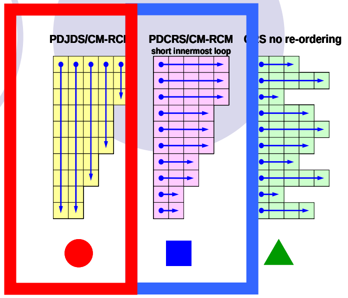




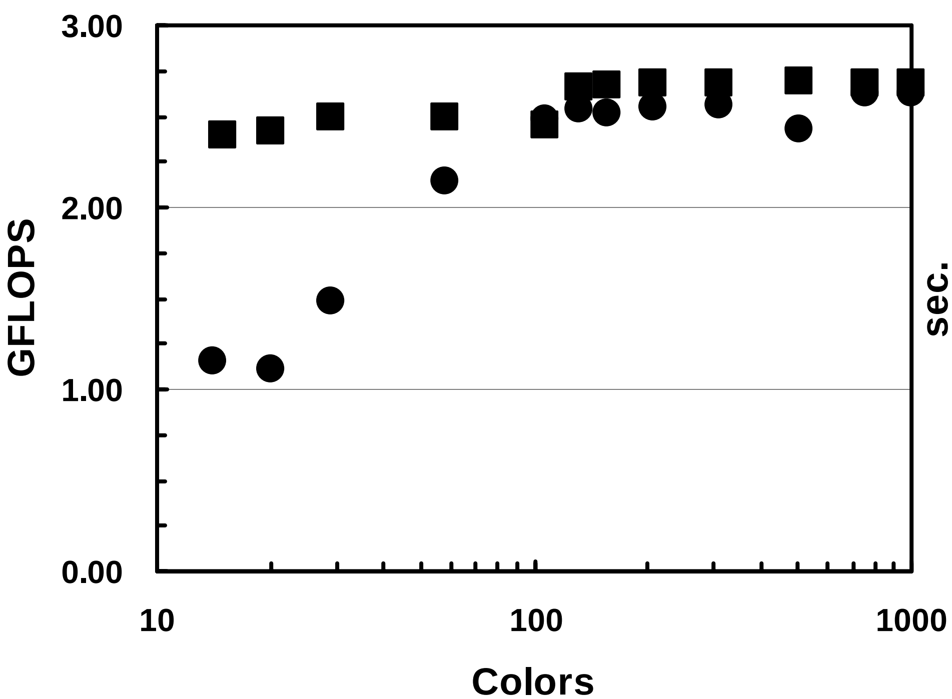
PGA model

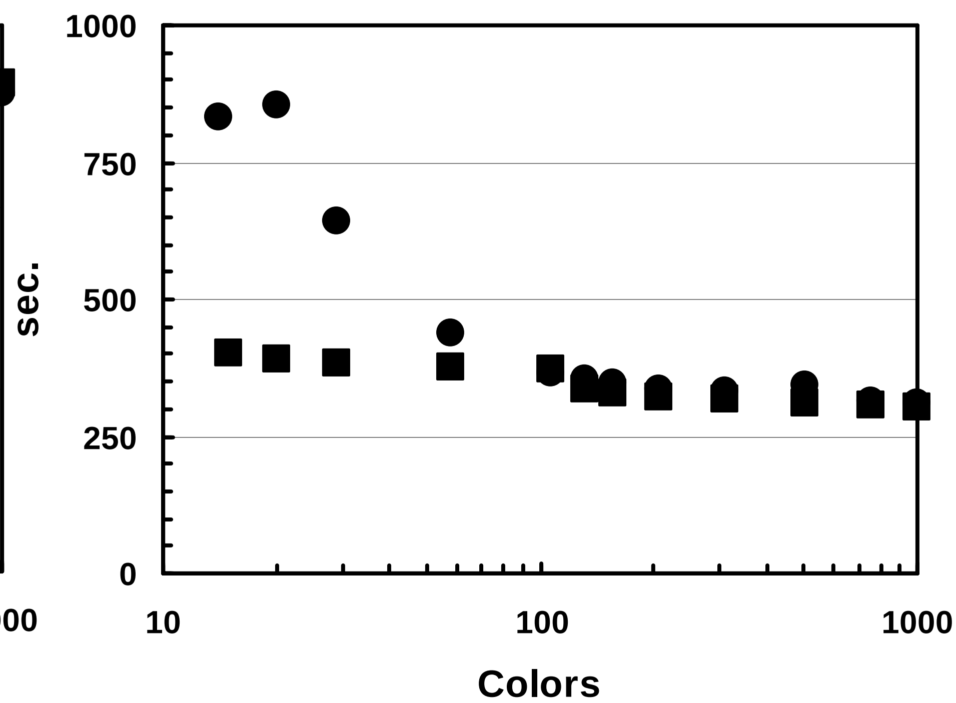
61 pins, 956,128 elem, 1,012,354 nodes
(3,037,062 DOF) , 1 SMP node

Itanium II (SGI/Altix) (8 PE's)



● Flat MPI (PDJDS)
■ Flat MPI (PDCRS)

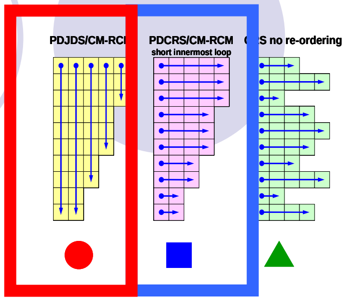




PGA model

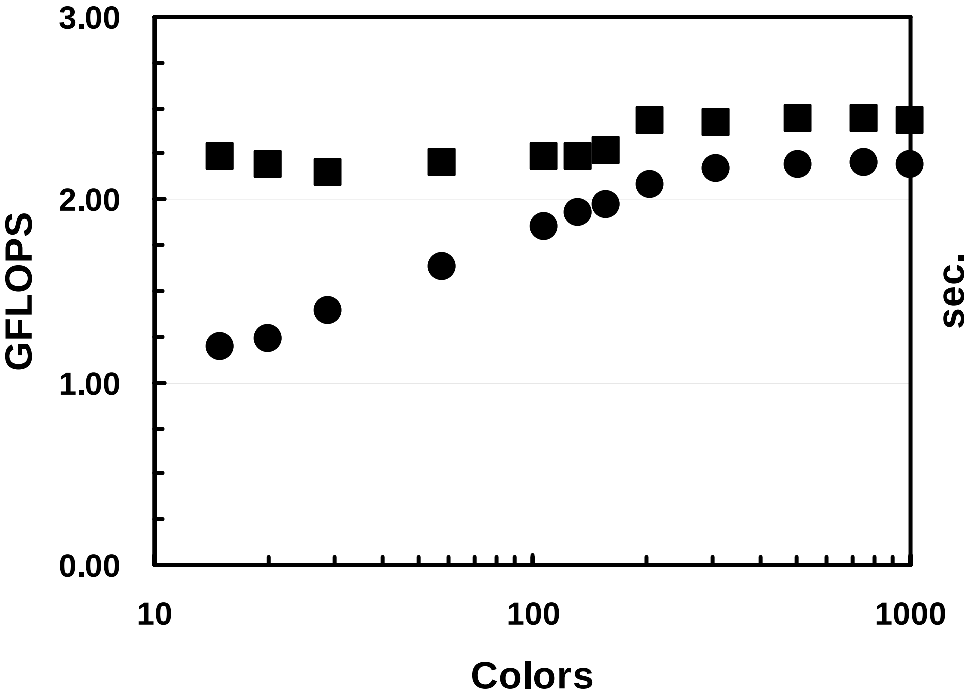
61 pins, 956,128 elem, 1,012,354 nodes (3,037,062 DOF) , 1 SMP node

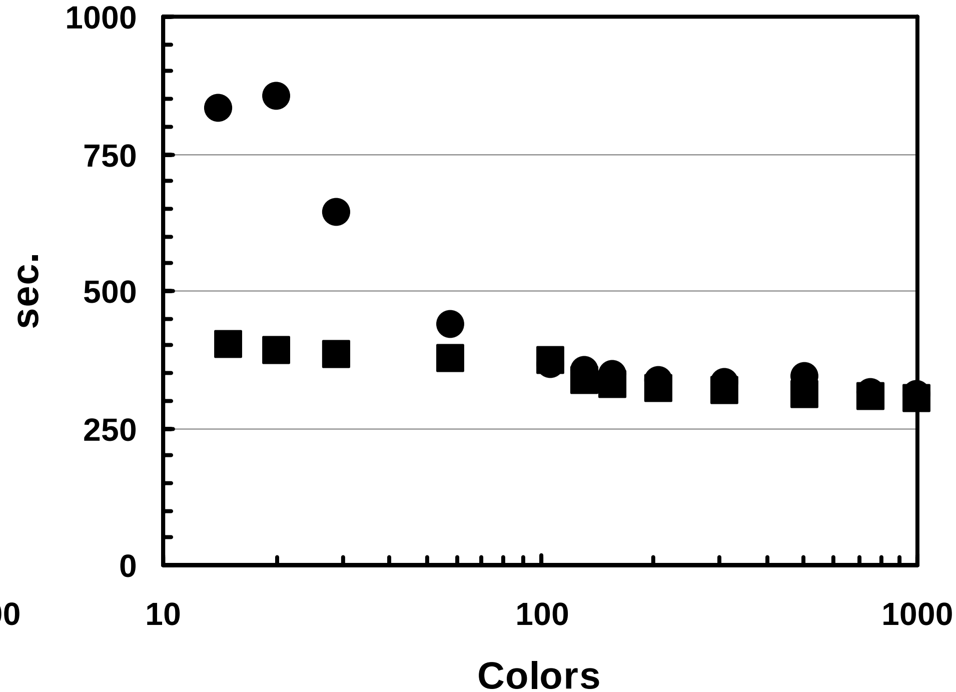
<u>**AMD Opteron (8 PE's)**</u>



● Flat MPI (PDJDS)

■ Flat MPI (PDCRS)

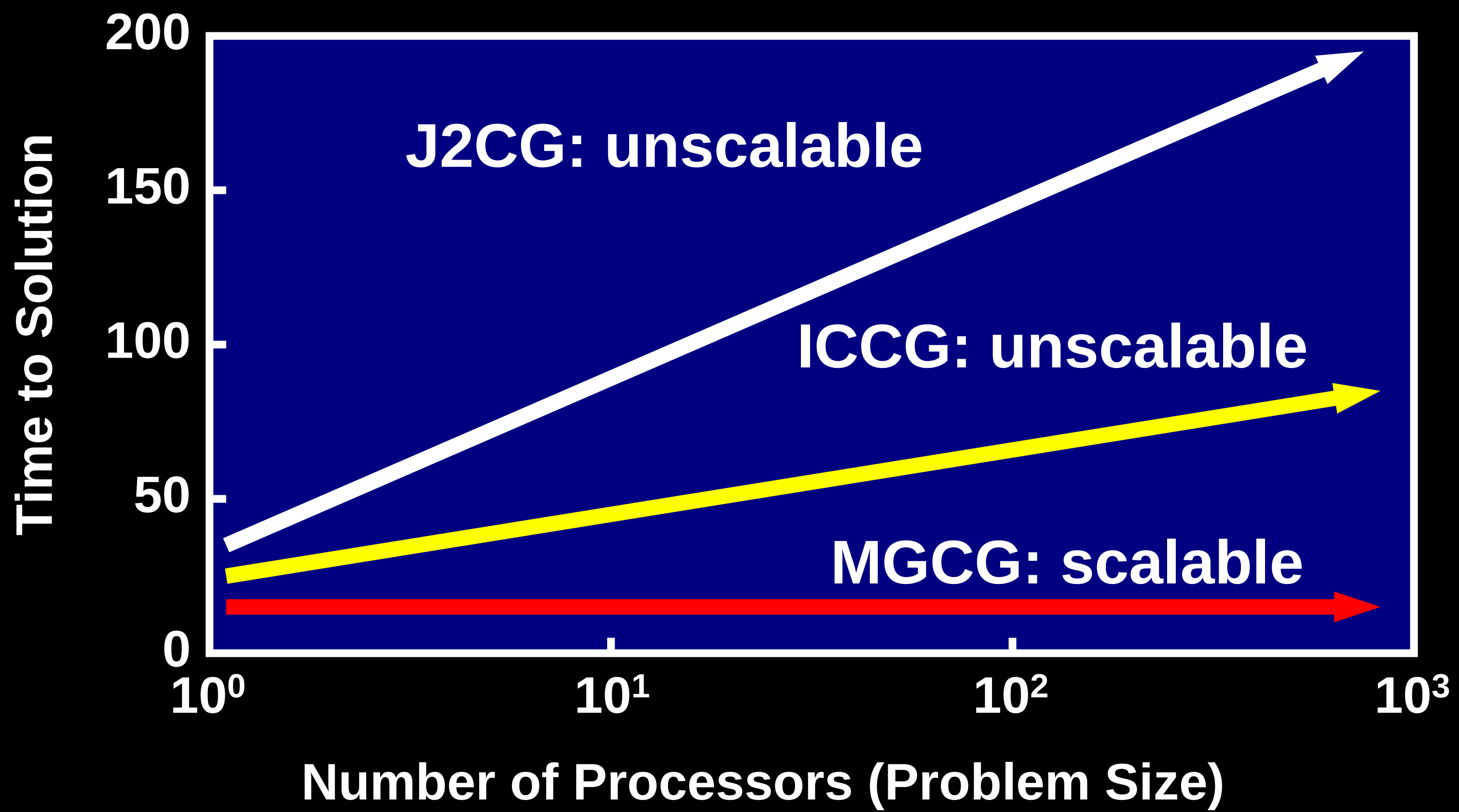




Multigrids

Multigrid

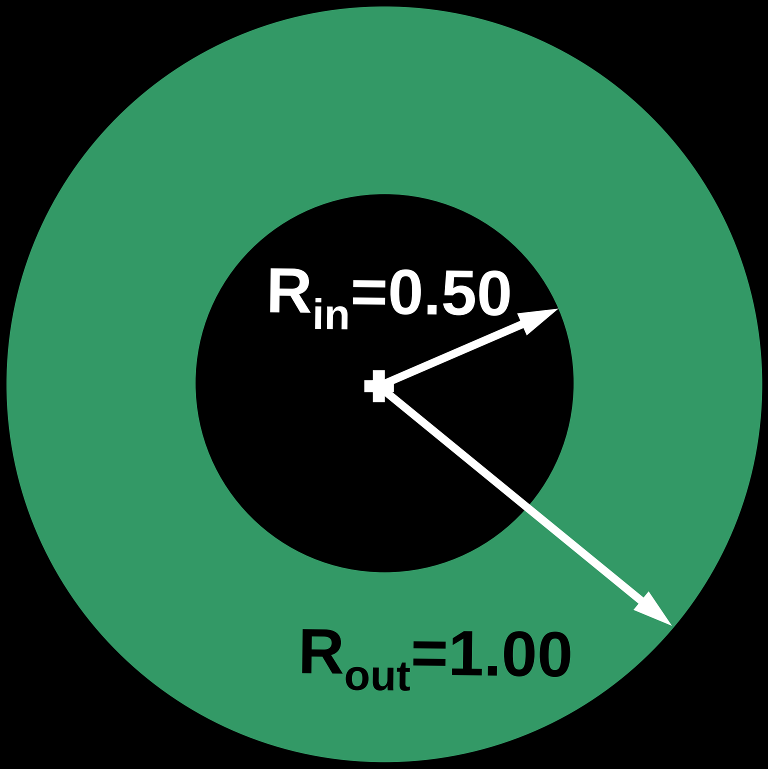
Multigrid is scalable !!!



Based on LLNL

Target Application

Thermal Convection between 2 Spherical Surfaces



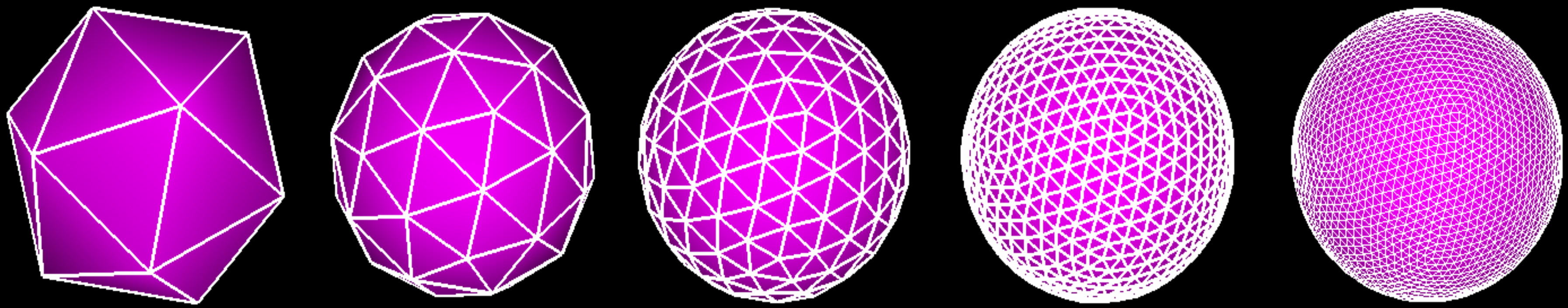
- Typical Geometry in Earth Science Simulations
  - Mantle, Core etc.
  - Also applicable to external flow
- Boundary Conditions
  - r= R_{in}
    - u=v=w=0, T=1
  - r= R_{out}
    - u=v=w=0, T=0
  - Heat Generation

Semi-Implicit Pressure Correction Scheme

- Governing equations
  - Momentum (Navier-Stoke)
  - Continuity
  - Energy
- Poisson equations for pressure correction derived from continuity constraint.
- Parallel MGCG iterative method for Poisson eqn's
  - V-cycle, Geometrical Multigrid
  - Gauss-Seidel Smoothing
  - Semi-coarsening
  - Multilevel communication table

Start from Icosahedron

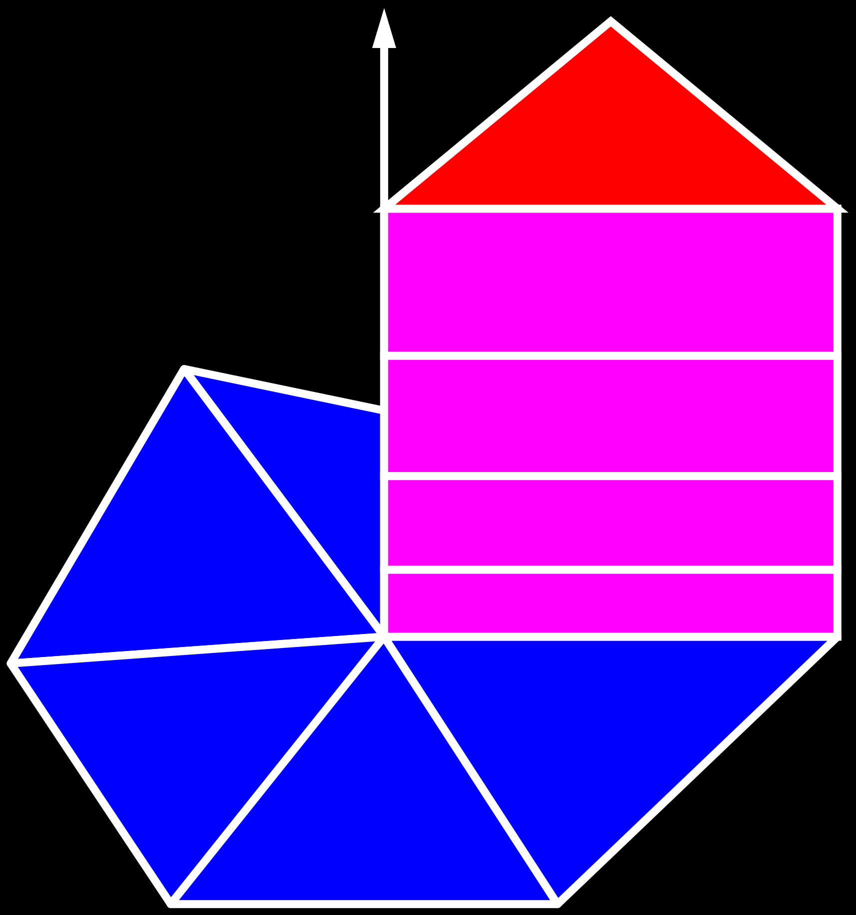
Surface Grid by Adaptive Mesh Refinement (AMR)



Level 0	Level 1	Level 2	Level 3	Level 4
12 nodes	42 nodes	162 nodes	642 nodes	2,562 nodes
20 tri's	80 tri's	320 tri's	1,280 tri's	5,120 tri's

Semi-Unstructured Prismatic Grids

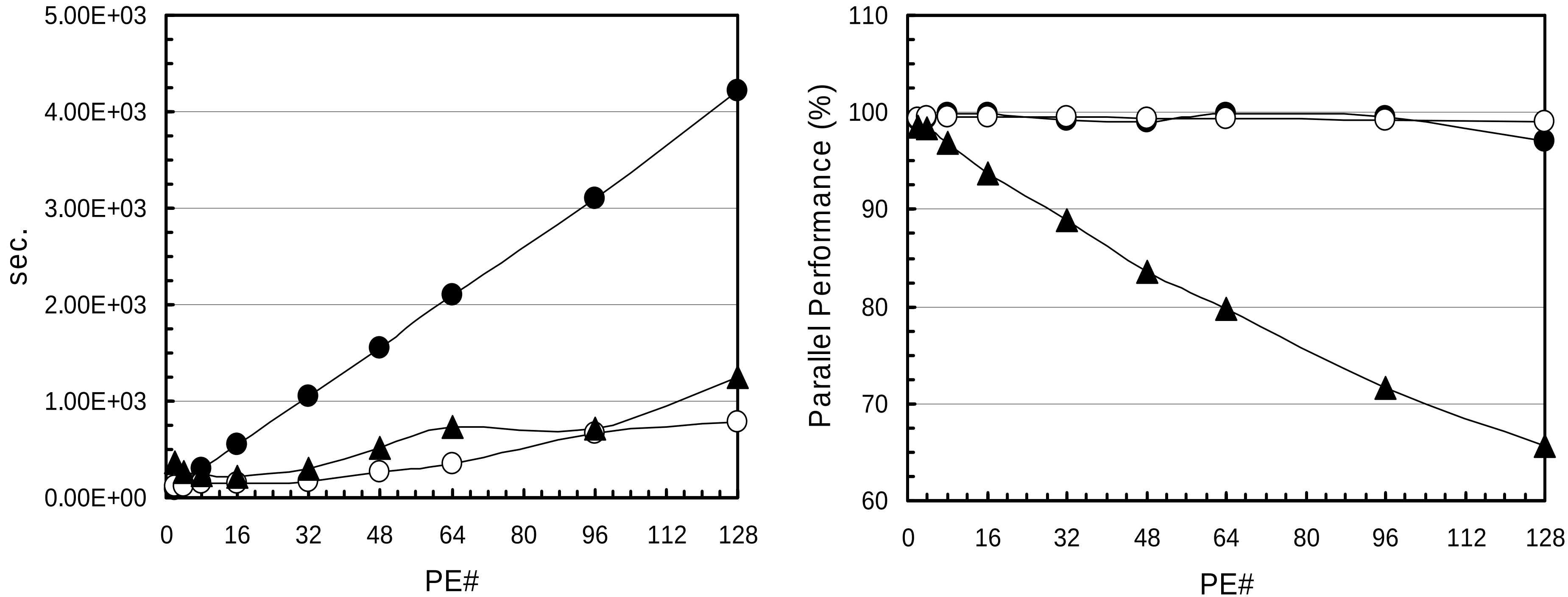
- generated from unstructured surface triangles
- structured in normal-to-surface direction
- flexible
- suitable for near-wall boundary layer computation



Results on Hitachi SR2201

320x900=288,000 cells/PE

up to 37M DOF on 128 PEs



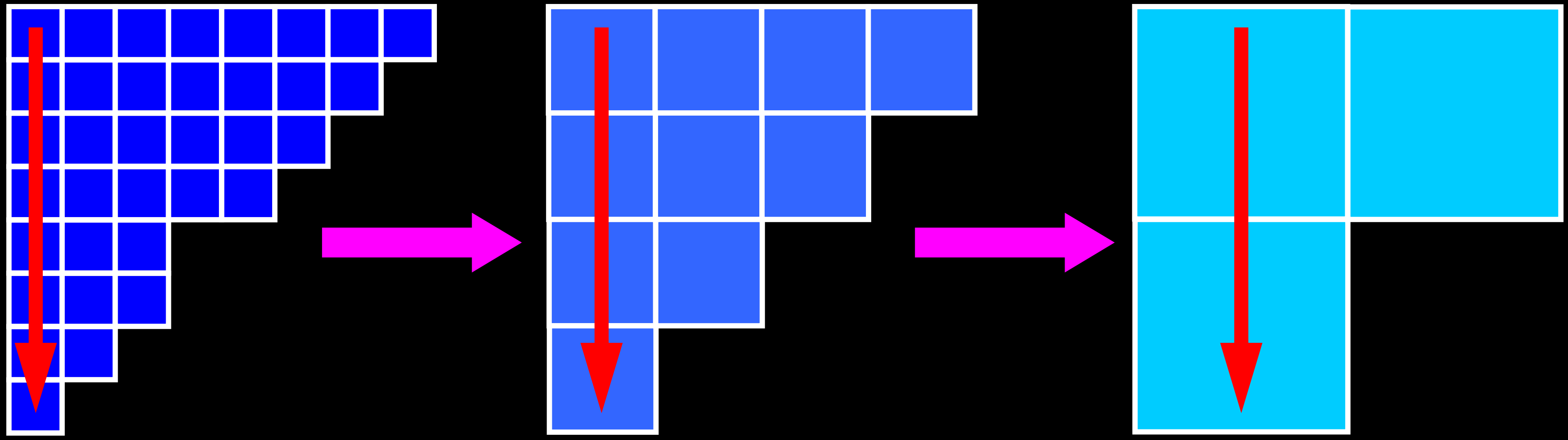
●ICCG ○MGCG/FGS ▲MGCG/ILUs

How about on ES ?

- 1 CPU
  - 768,000 elements (1280×600)
  - ICCG : 29 sec. (Xeon 2.8GHz) ⇒169 sec. (ES)
  - MGCG： 58 sec. (Xeon 2.8GHz) ⇒345 sec. (ES)
- Why ?
  - CRS: loop length is small
- Remedy
  - Reordering done in BILU(0)
    - Gauss-Seidel smoothing: dependency
  - Traditional Multicoloring

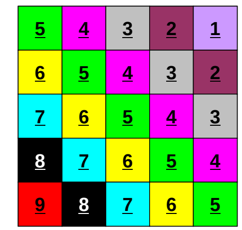
Critical Issue of Multigrid for Vector Computer

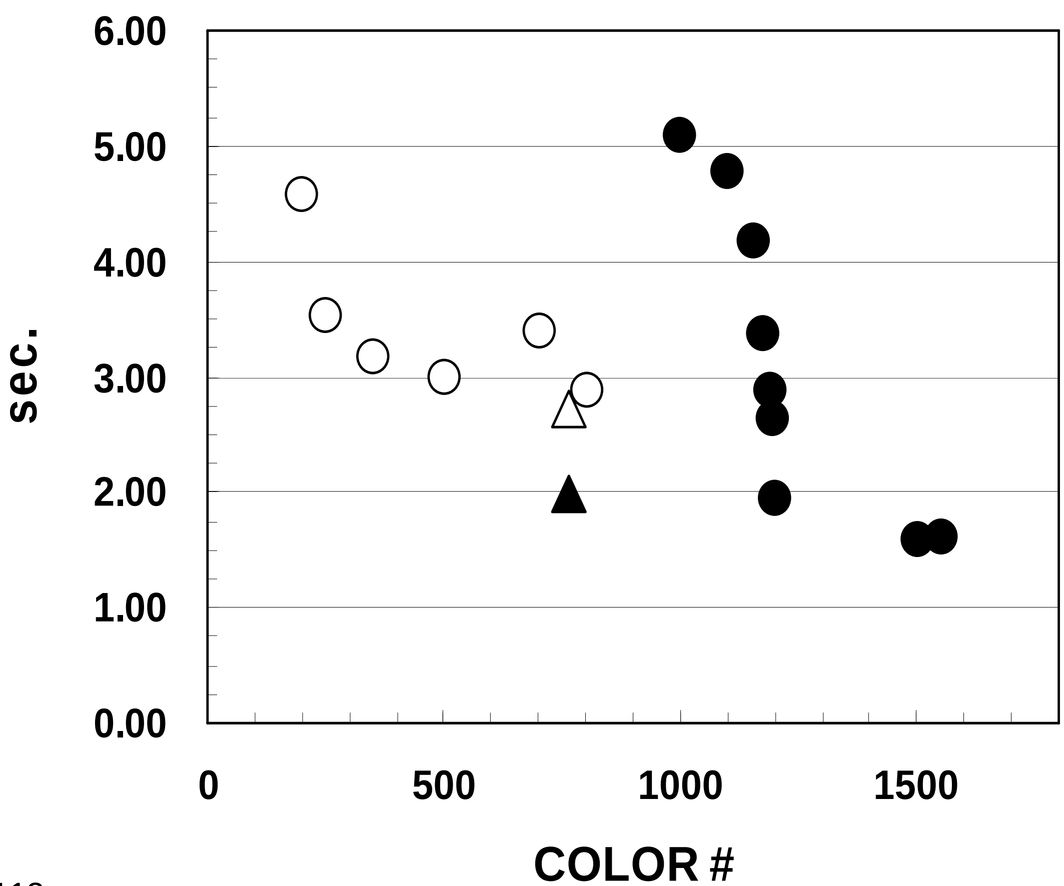
- Shorter Loop-Length for Coarse Grid Level.



Vectorization：Re-Ordering Earth Simulator

- RCM (Reverse Cuthil-Mckee) , Multicolor

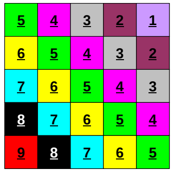




768,000 elem's
ES, 1 PE

○ MGCG (MC)
△ MGCG (RCM)
● ICCG (MC)
▲ ICCG (RCM)

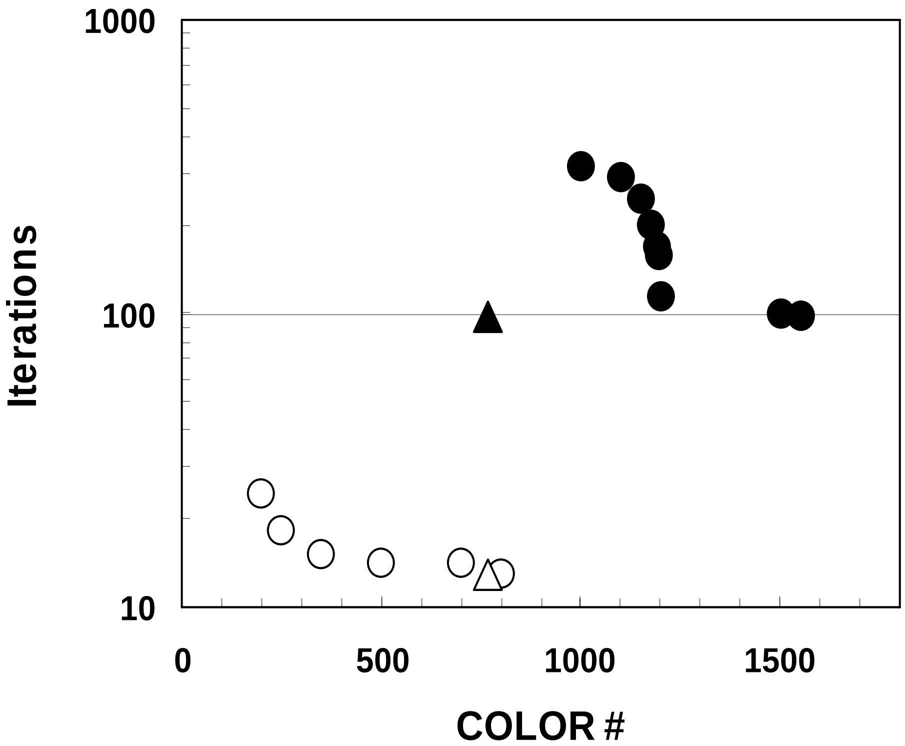
MGCG (original)：345 sec.
ICCG (original)：169 sec.

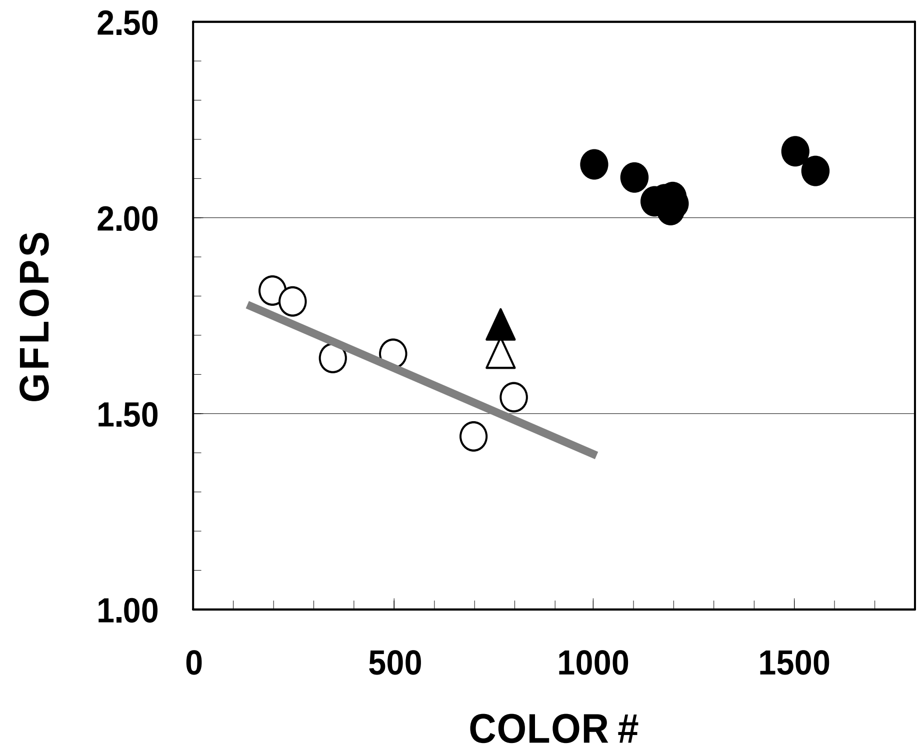


GFLOPS, Iterations

768,000 elem's, ES 1PE

○ MGCG (MC)
△ MGCG (RCM)
● ICCG (MC)
▲ ICCG (RCM)

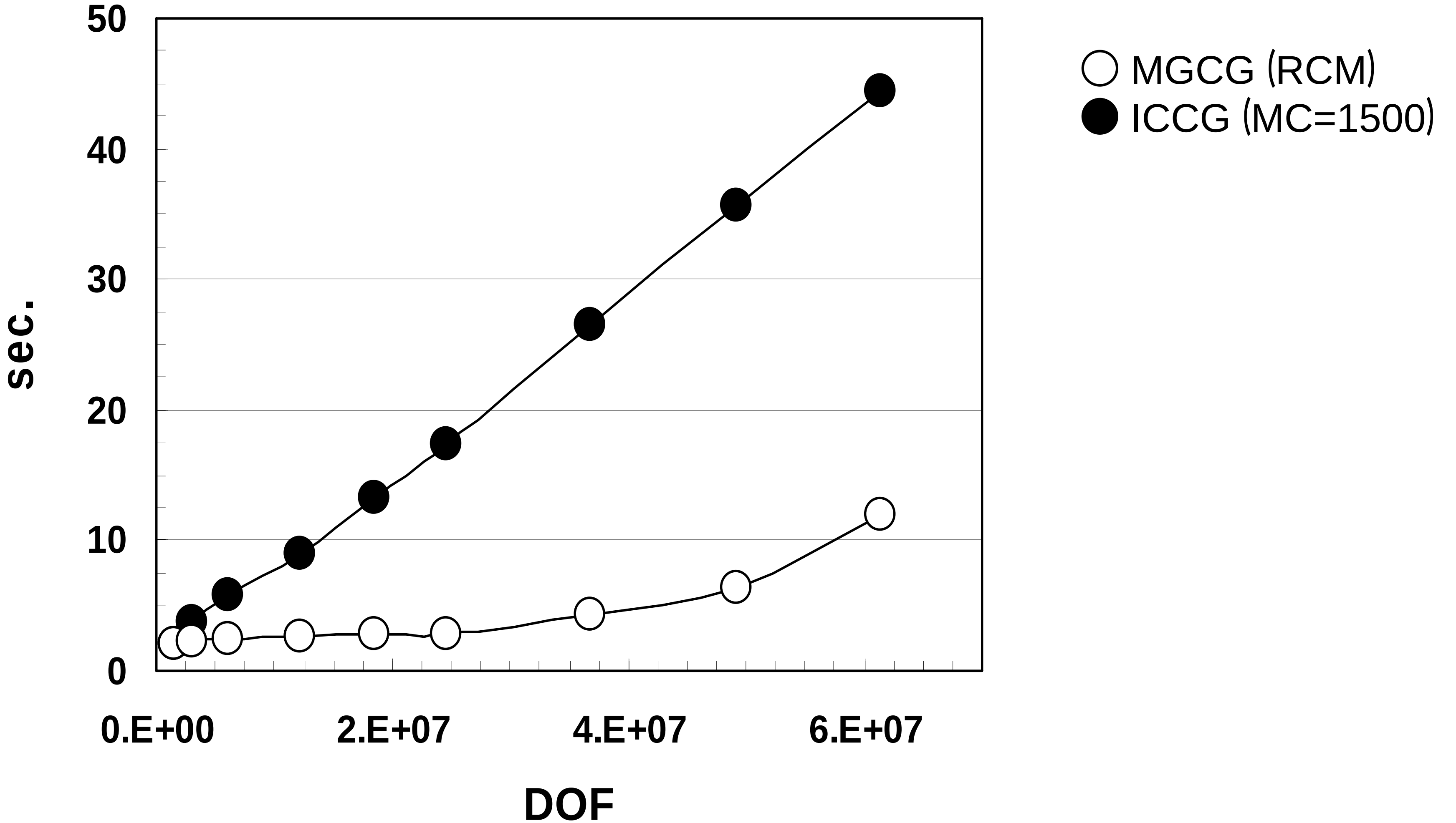




<u>Many colors...</u>

- **fewer iterations for convergence**
- **lower performance due to shorter loops (especially in MG)**

Scalability: Flat MPI
768,000 elem's/PE, up to 80 PE's



Next step: Hybrid

- Many colors are required for reasonably fast convergence.
- Overhead of OpenMP.

SMP parallel

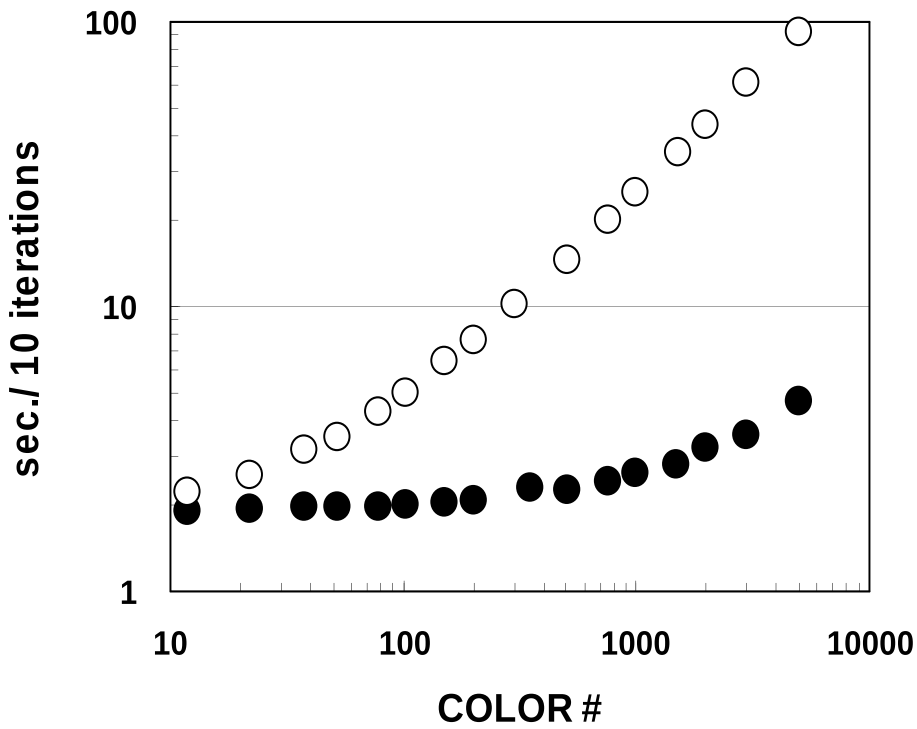
Vectorized

```
do iv= 1, NCOLORS
!$omp parallel do private (iv0,j,iS,iE,i,k,kk etc.)
do ip= 1, PEsmpTOT
  iv0= STACKmc(PEsmpTOT*(iv-1)+ip- 1)
  do j= 1, NLhyp(iv)
    iS= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip-1)
    iE= INL(npLX1*(iv-1)+PEsmpTOT*(j-1)+ip  )
!CDIR NODEP
    do i= iv0+1, iv0+iE-iS
      k= i+iS - iv0
      kk= IAL(k)
      (Important Computations)
    enddo
  enddo
enddo
enddo
```

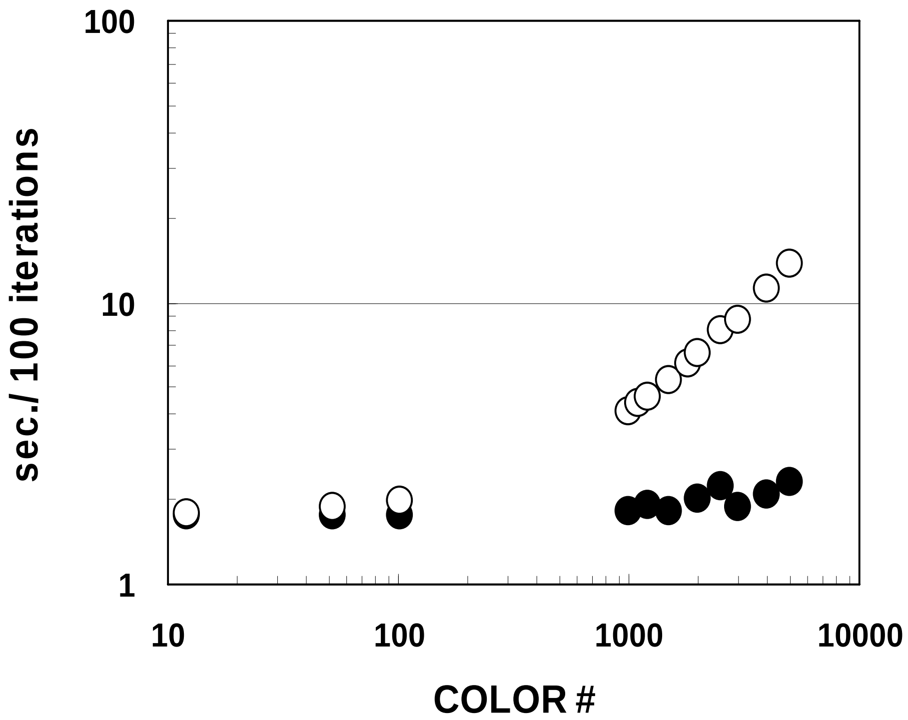
Hybrid vs. Flat MPI
8PEs on ES (1 SMP node)

○ Hybrid
● Flat MPI

MGCG (10 iterations)



ICCG (100 iterations)



MGCG on ES

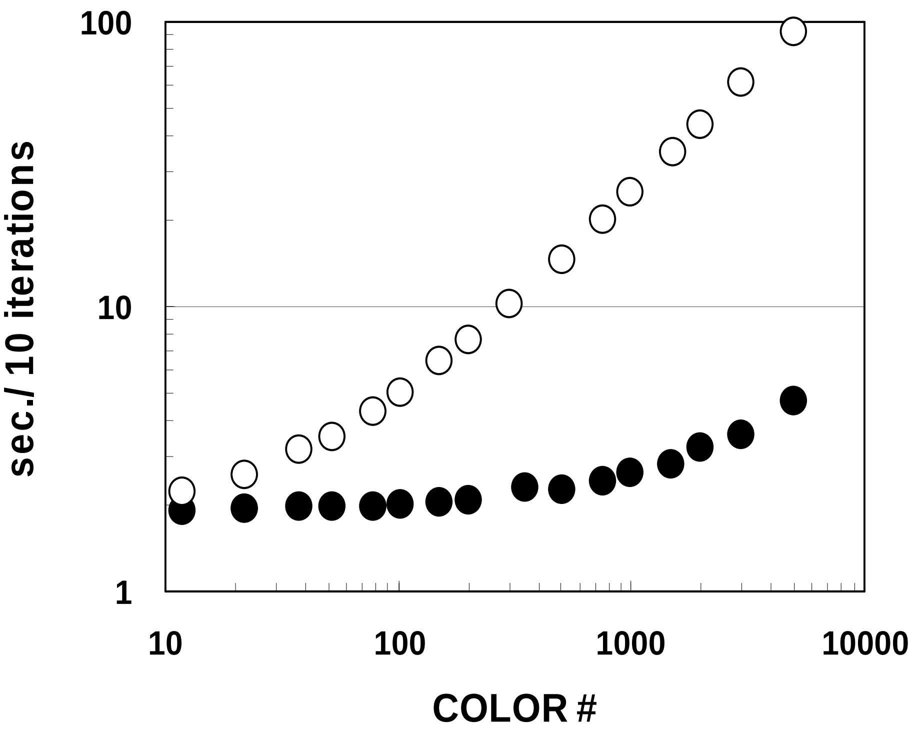
- Excellent performance by reordering
  - More than 20% of peak even in MGCG
    - Nice for Poisson solvers
    - 75% of ICCG
- Excellent scalability for flat-MPI
- Hybrid
  - Low performance for many colors
    - Significant for MGCG
  - But we need many colors for reasonably fast convergence
  - Not recommended

Hybrid vs. Flat MPI 8PE's on ES (1 SMP node)

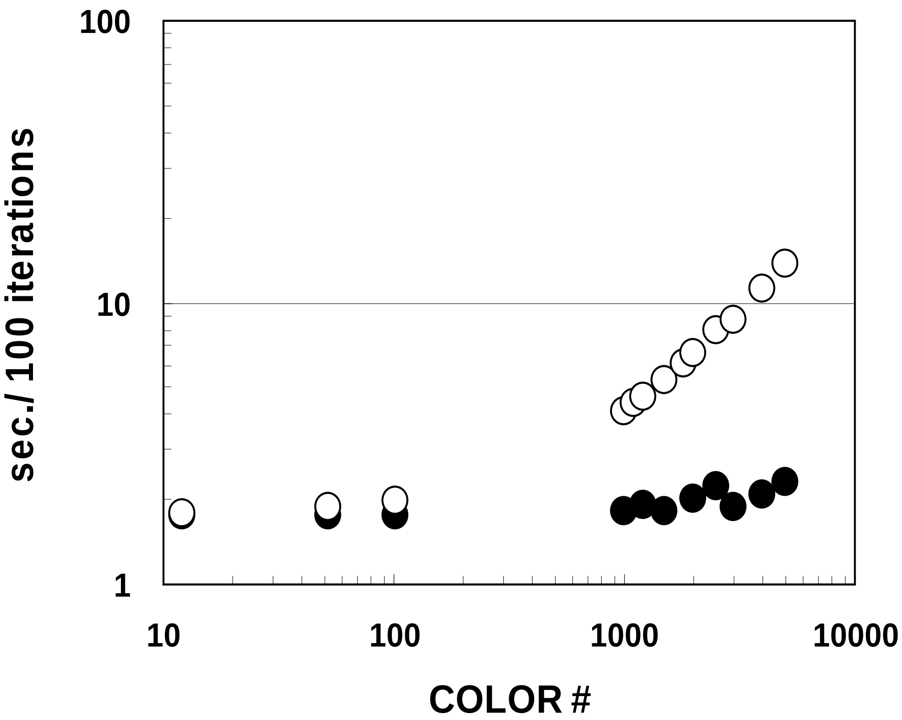
1280x600x8= 6,144,000 elements

○ Hybrid
● Flat MPI

MGCG (10 iterations)



ICCG (100 iterations)

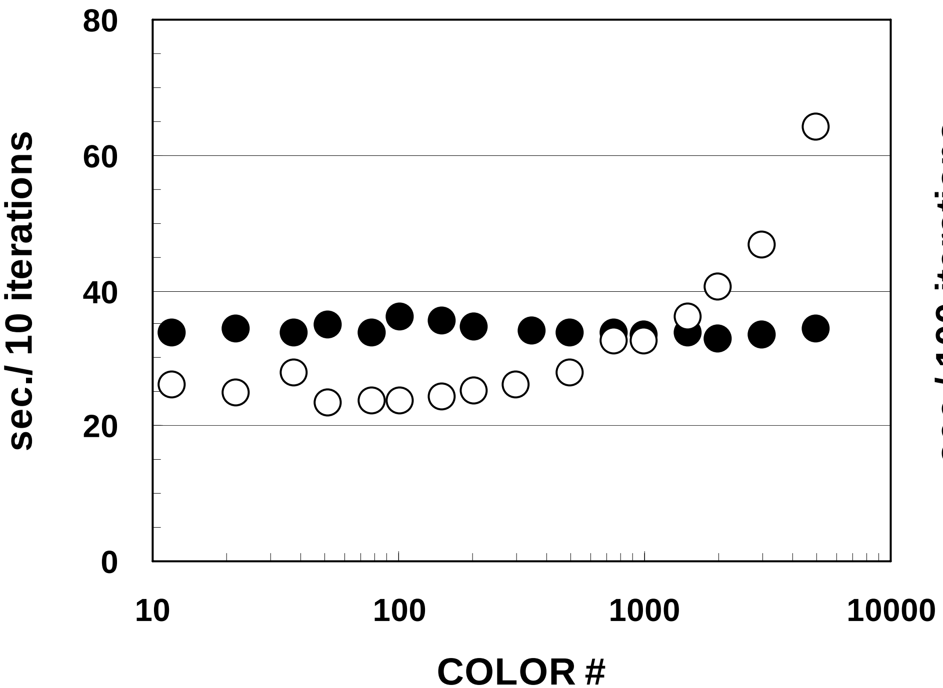


Hybrid vs. Flat MPI 8PE's on Hitachi SR8000 (1 SMP node)

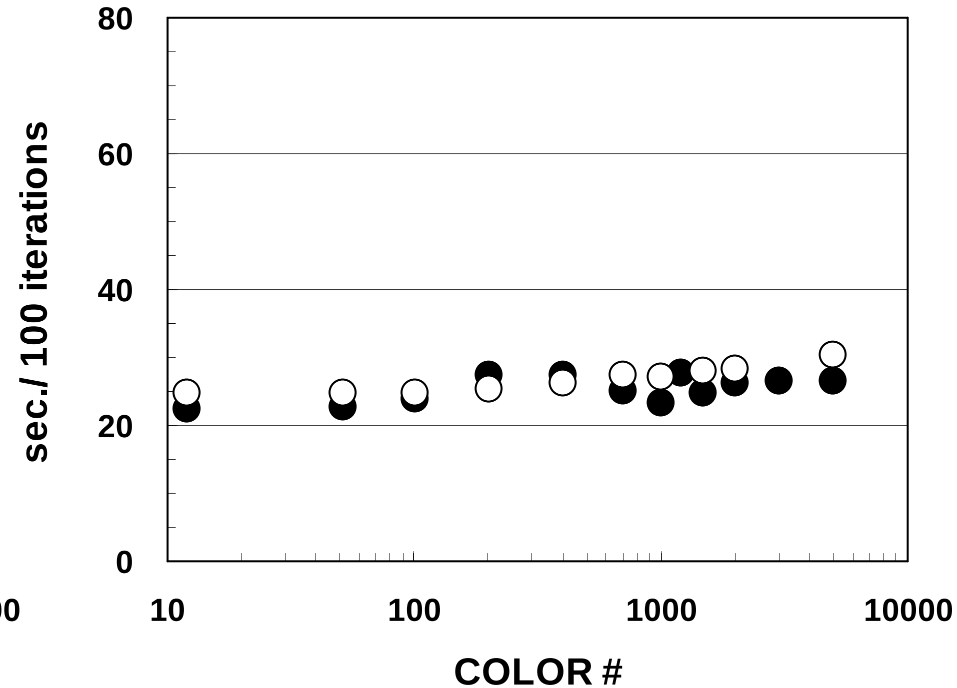
1280x600x8= 6,144,000 elements

○ Hybrid
● Flat MPI

MGCG (10 iterations)



ICCG (100 iterations)

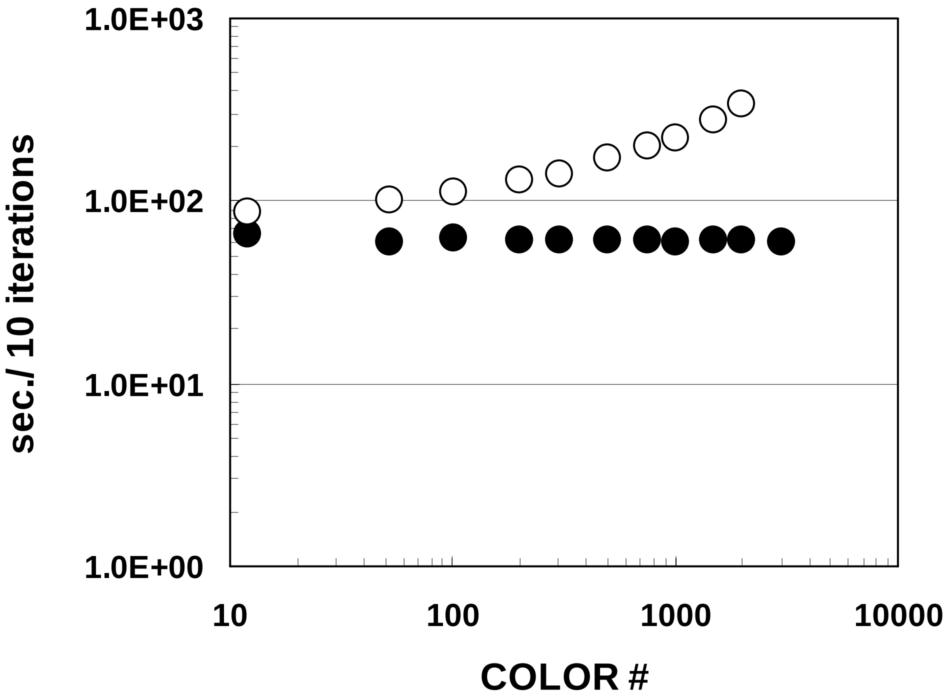


Hybrid vs. Flat MPI 8PE's on IBM-SP3 (1 SMP node)

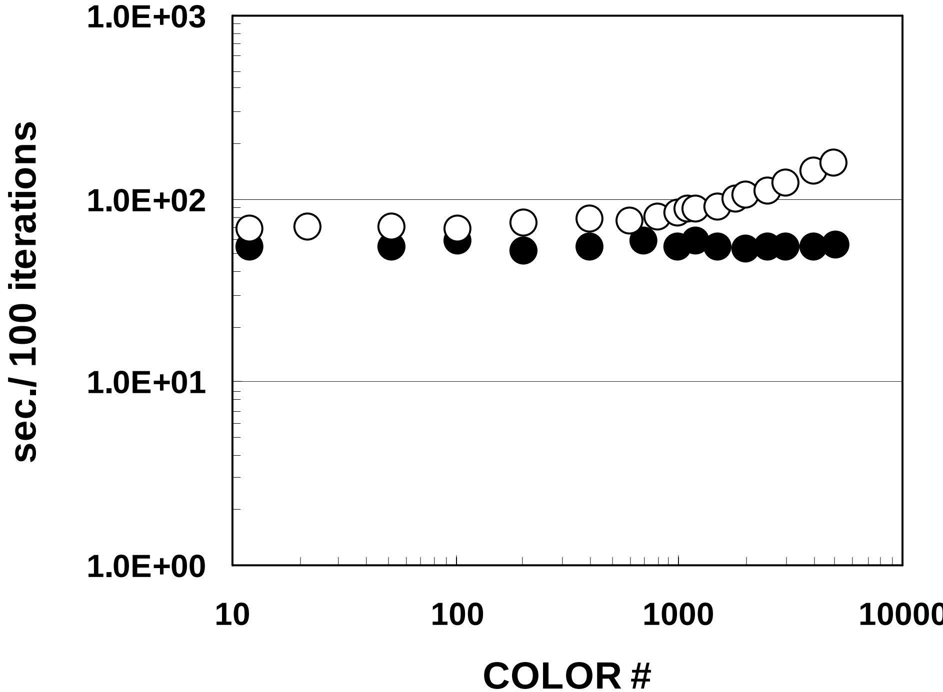
1280x600x8= 6,144,000 elements

○ Hybrid
● Flat MPI

MGCG (10 iterations)



ICCG (100 iterations)



- Background
  - GeoFEM Project & Earth Simulator
  - Preconditioned Iterative Linear Solvers
- Optimization Strategy on the Earth Simulator
  - BIC(0)-CG for Simple 3D Linear Elastic Applications
- Effect of reordering on various types of architectures
  - PGA (Pin-Grid Array)
  - Contact Problems
  - Multigrid
- **Summary & Future Works**

Summary (Earth Simulator)

- Hybrid Parallel Programming Model on SMP Cluster Architecture with Vector Processors for Unstructured Grids
  - Nice parallel performance for both inter/intra SMP node on ES, **3.8TFLOPS for 2.2G DOF on 176 nodes (33.8%)**
  - Re-Ordering is really required
  - Simple multicoloring is better for complicated geometries.

Summary (cont.) (Earth Simulator)

- Hybrid vs. Flat MPI
  - Flat-MPI is better for small number of SMP nodes.
  - Hybrid is better for large number of SMP nodes: Especially when problem size is rather small.
  - **Flat MPI: Communication, Hybrid: Memory**
  - depends on application, problem size etc.
  - **Hybrid is much more sensitive to color numbers than flat MPI due to synchronization overhead of OpenMP, especially on the Earth Simulator.**
    - **This is not so significant in Hitachi SR8k & IBM SP3**

Summary (cont.) (General)

- Hybrid vs. Flat MPI
  - In IBM SP-3, difference between flat-MPI and hybrid is not so significant, although flat-MPI is slightly better.
  - In Hitachi SR8000, pseudo-vector works better for hybrid cases.
- Effect of Color
  - In scalar processors (especially for flat-MPI), performance is getting better as color number increases, due to efficient utilization of cache.

Hybrid vs. Flat MPI

- **Generally speaking, they are competitive.**
  - **Flat-MPI is better for multigrid type applications with multicolor ordering.**
  - **In ill-conditioned problems, Flat-MPI may require more iterations.**
  - **Depends on implementation of compiler**

Hybrid vs. Flat MPI (cont.)

- Earth Simulator
  - Flat MPI is better
  - Hybrid is better for large PE number with small problem size.
- IBM SP-3
  - Flat MPI is better for small problem size because cache is utilized more efficiently
- Hitachi SR8000
  - Hybrid is better (mainly because of feature of compiler)
- **Careful treatment on color number is required for Hybrid programming model.**

My current feeling is …

- Flat MPI is slightly better on the Earth Simulator in FEM-type applications with multicoloring.

Can Hybrid survive ?
SAI (Sparse Approximate Inverse) preconditioning

- Suitable for parallel & vector computation.
  - especially for Hybrid Parallel Programming Model
  - only Mat-Vec. product.
  - **reordering for avoiding dependency is not required.**
    - **corresponds to single-color**

- Preconditioning for contact problems.
  - J.Zhang, K.Nakajima et al. (2003) for scalar processors
  - K.Nakajima (2005) for ES at WOMPEI05

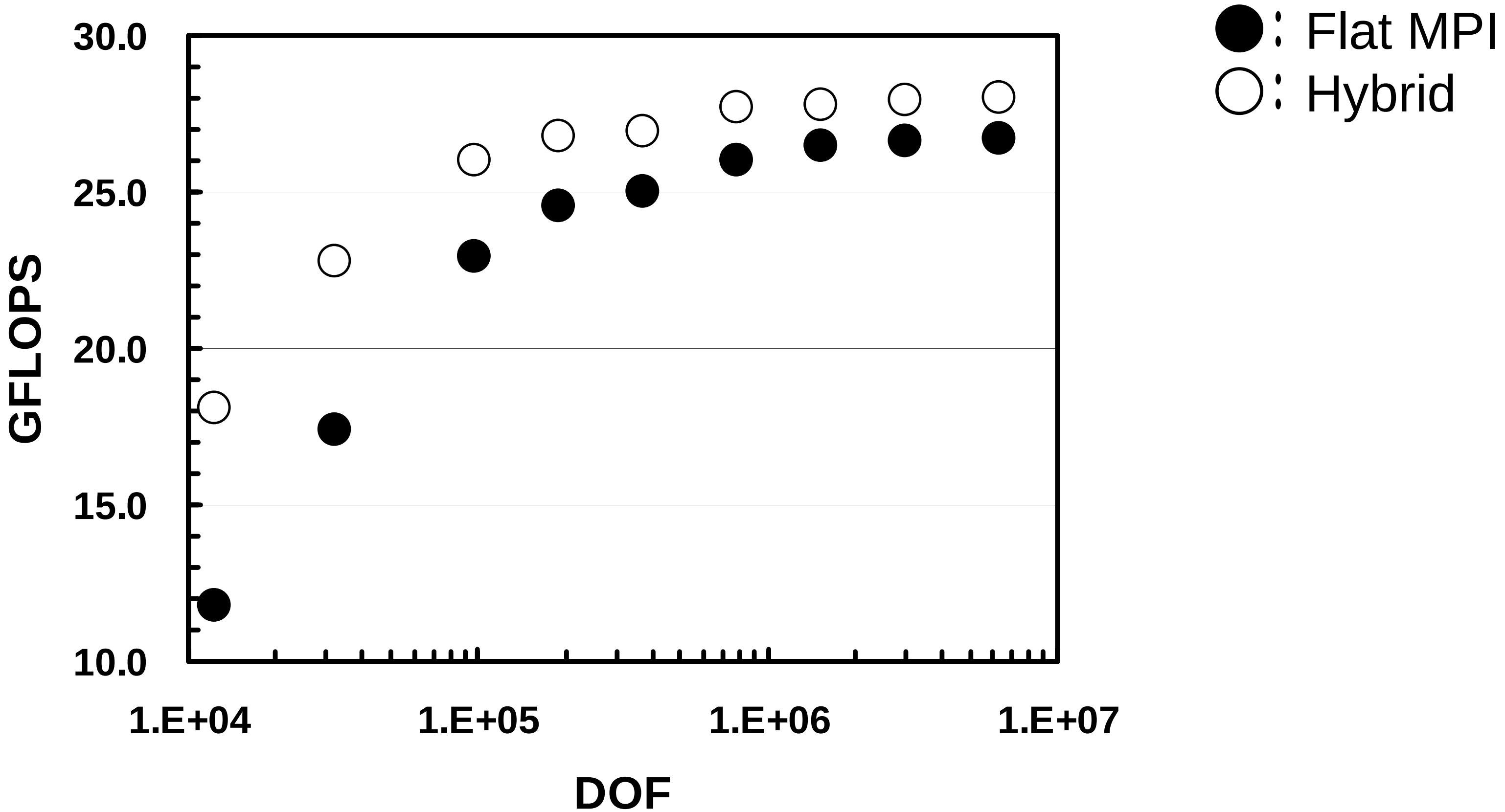
Matrix-Vector Product ONLY

```
!OMP PARALLEL DO
  do ip= 1, PEsmpTOT
    iv0= STACKmc(ip)
    do j= 1, NONdiagTOT
      iS= indexS(ip, j)
      iE= indexE(ip, j)
!CDIR NODEP
      do i= iv0+1, iv0+iE-iS
        (computations)
      enddo
    enddo
  enddo
!OMP END PARALLEL DO
```

Earth Simulator, Mat-Vec.

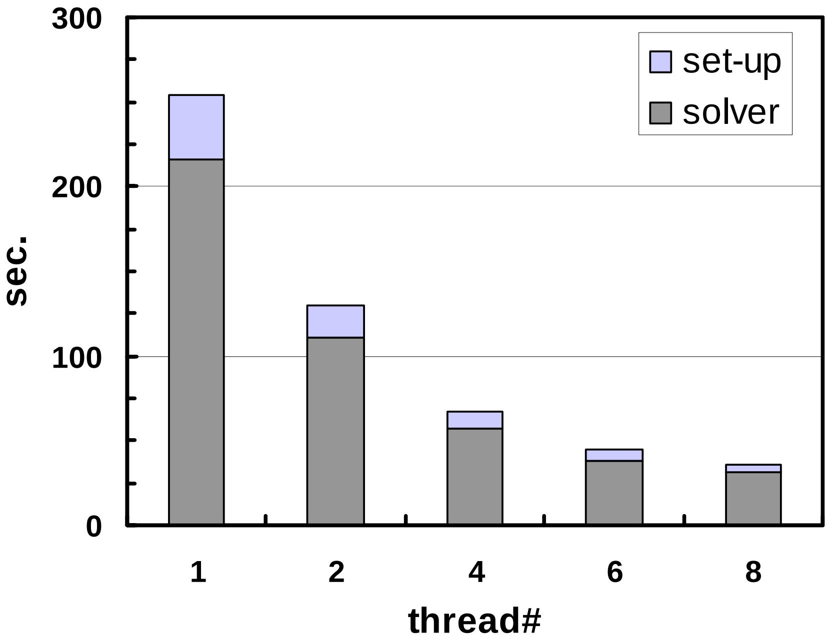
1 SMP node (64GFLOPS peak), 500 Iter's.

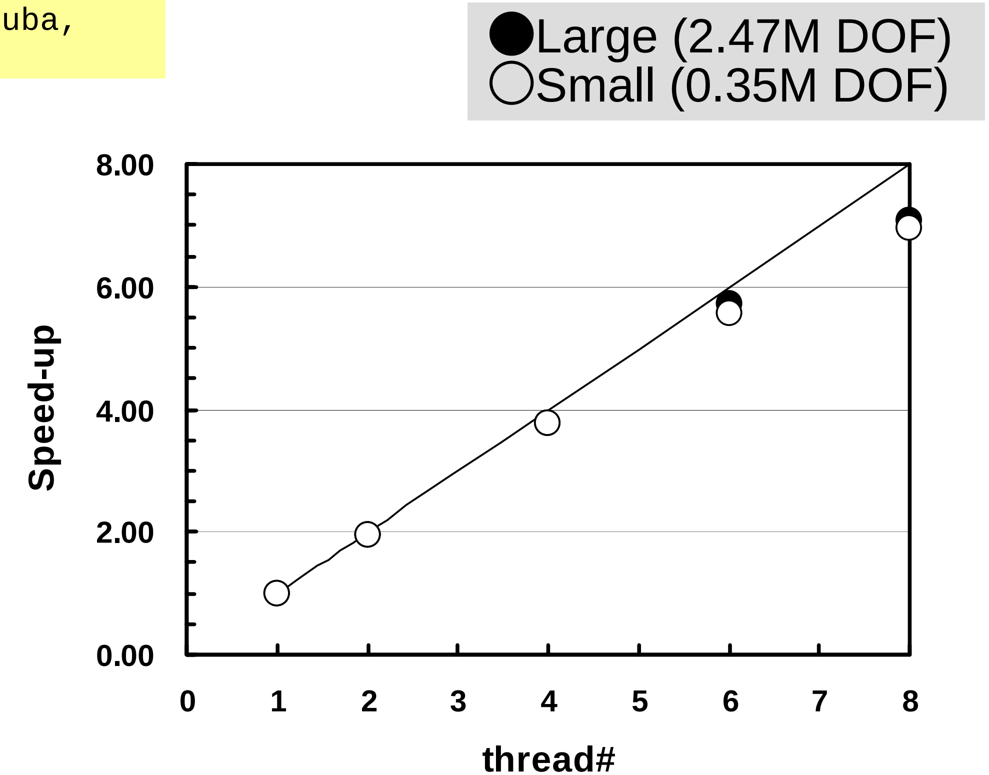
Hybrid is rather faster !!



Results: ES (1/2)

Nakajima, K. (2005), "Sparse Approximate Inverse Preconditioner for Contact Problems on the Earth Simulator using OpenMP", International Workshop on OpenMP: Experiences and Implementations (WOMPEI 2005), Tsukuba, Japan.





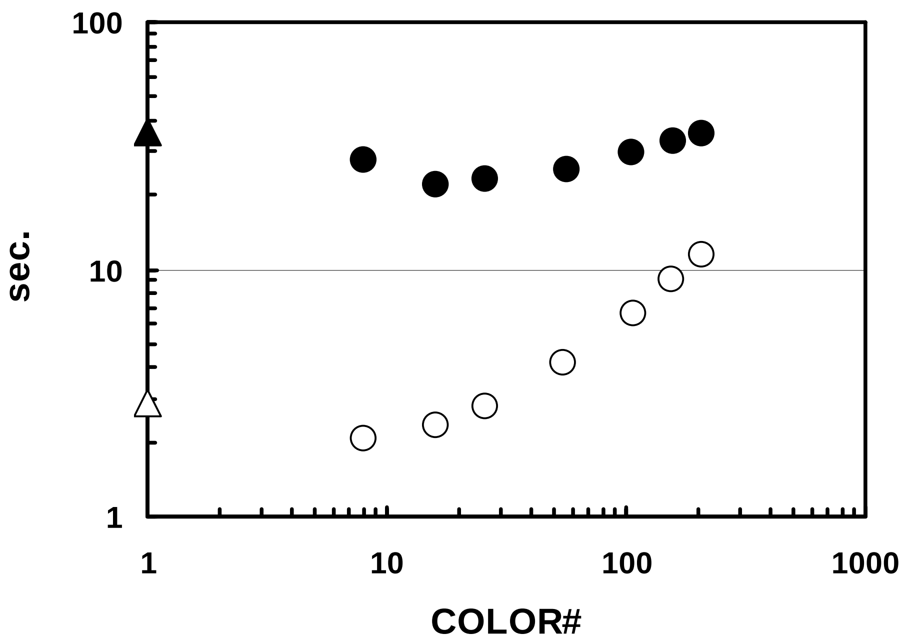
Large Problem

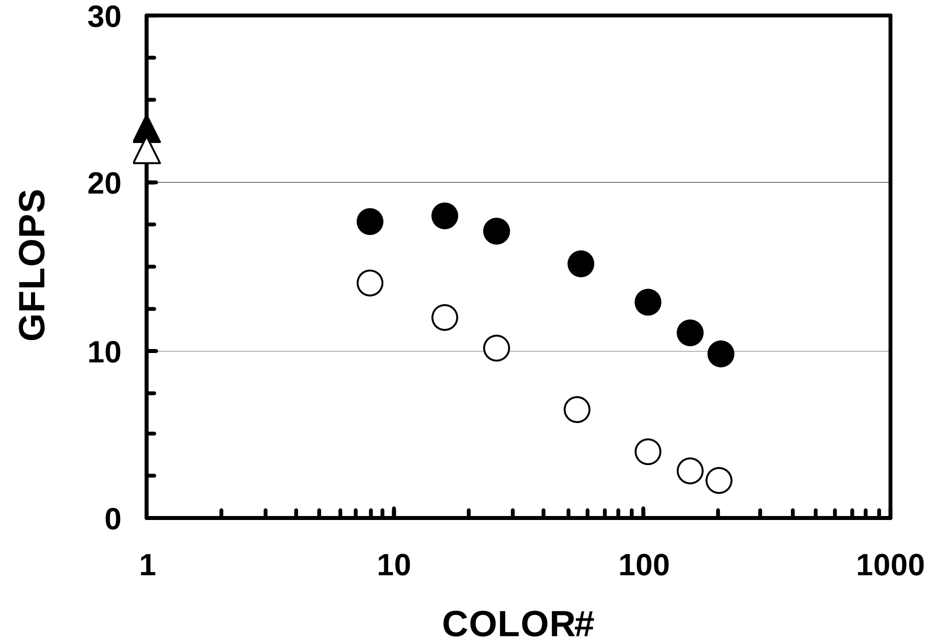
IWOMP, JUN05

Results: ES (2/2)

Nakajima, K. (2005), "Sparse Approximate Inverse Preconditioner for Contact Problems on the Earth Simulator using OpenMP", International Workshop on OpenMP: Experiences and Implementations (WOMPEI 2005), Tsukuba, Japan.

●: SB-BIC(0), ▲: SAI: Large
○: SB-BIC(0), △: SAI: Small
Large (2.47M DOF)
Small (0.35M DOF)





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Results: ES (2/2)

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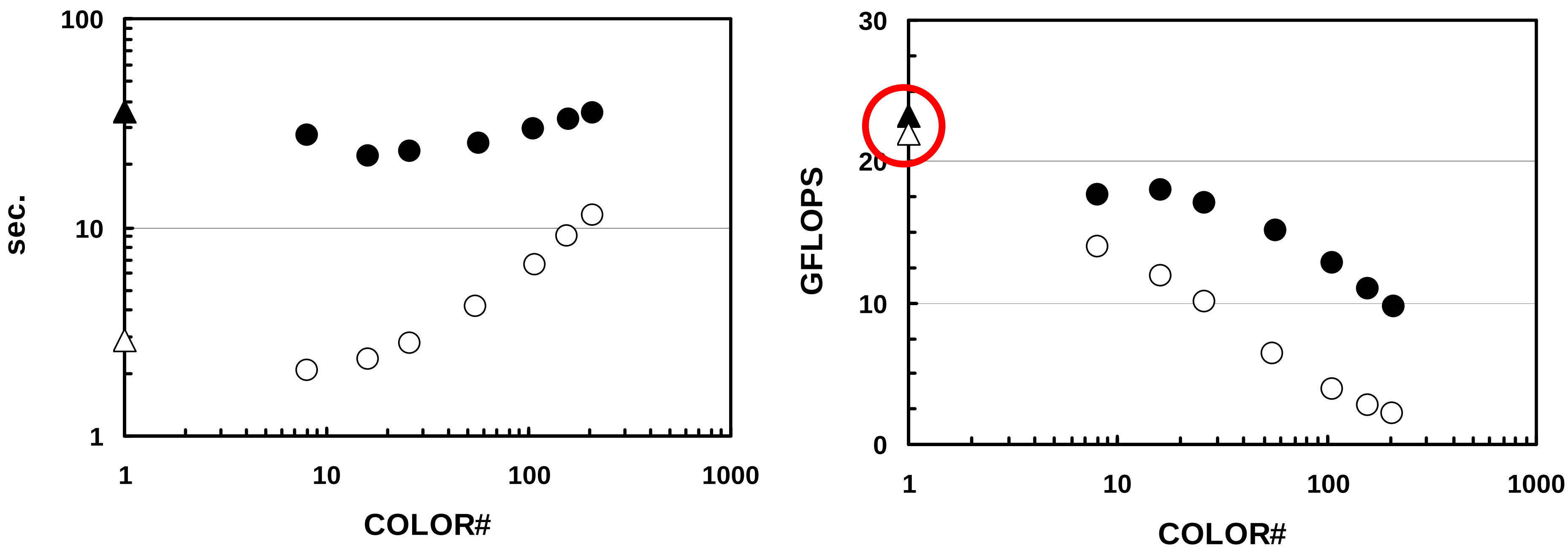

Results: Hitachi SR8000 (1/2)

Nakajima, K. (2005), "Sparse Approximate Inverse Preconditioner for Contact Problems on the Earth Simulator using OpenMP", International Workshop on OpenMP: Experiences and Implementations (WOMPEI 2005), Tsukuba, Japan.

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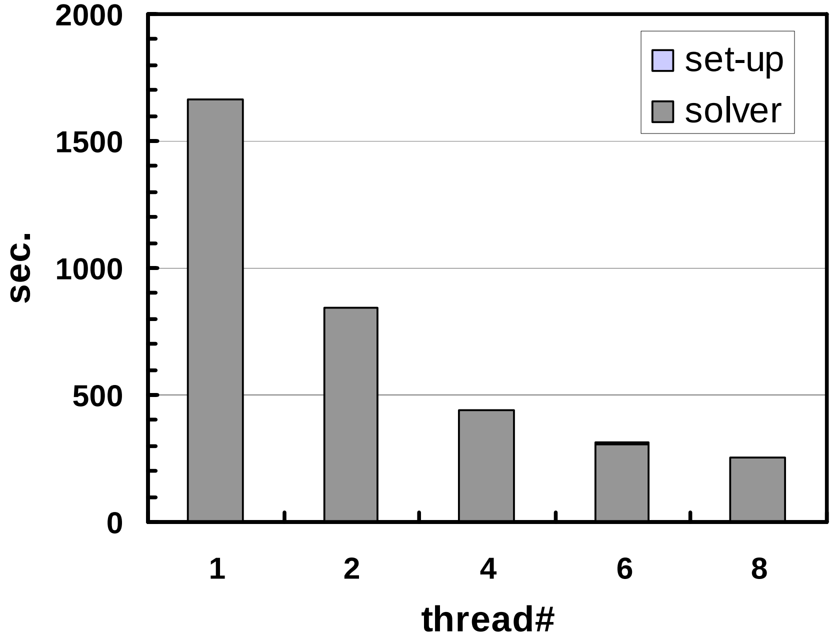
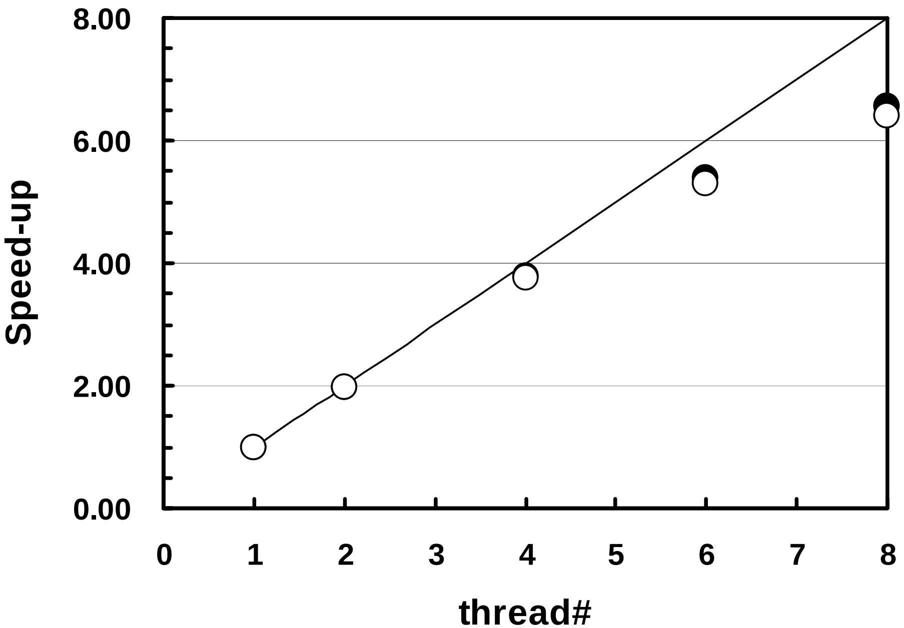
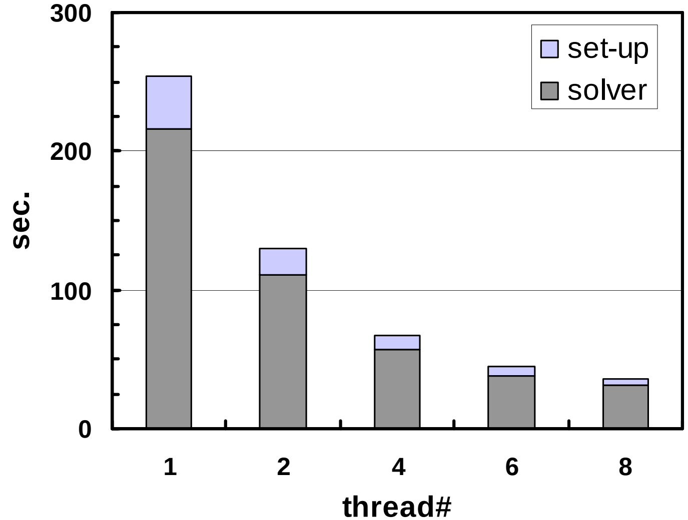


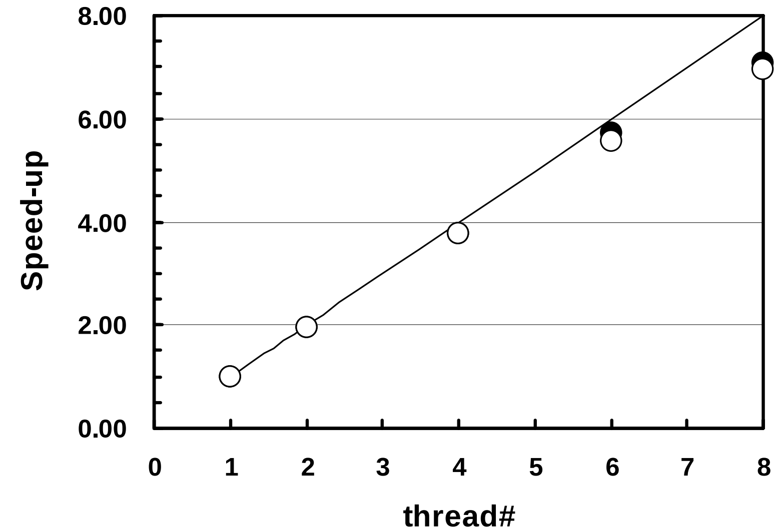


Large Problem

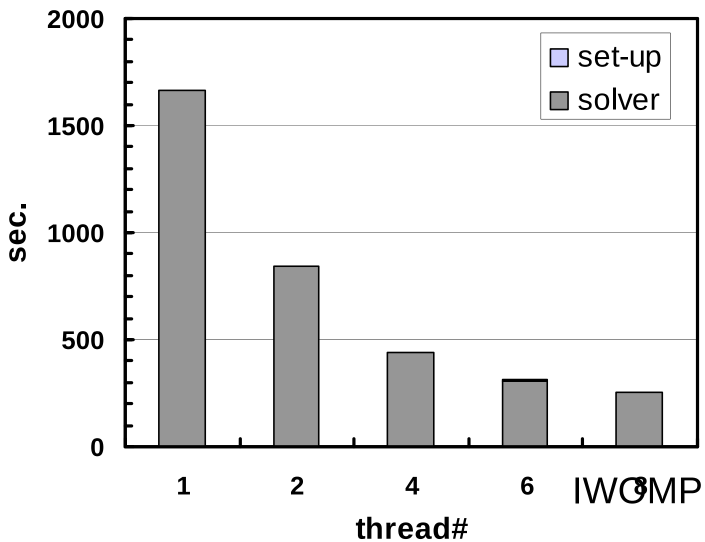
Comparison: ES vs. Hitachi SR8k

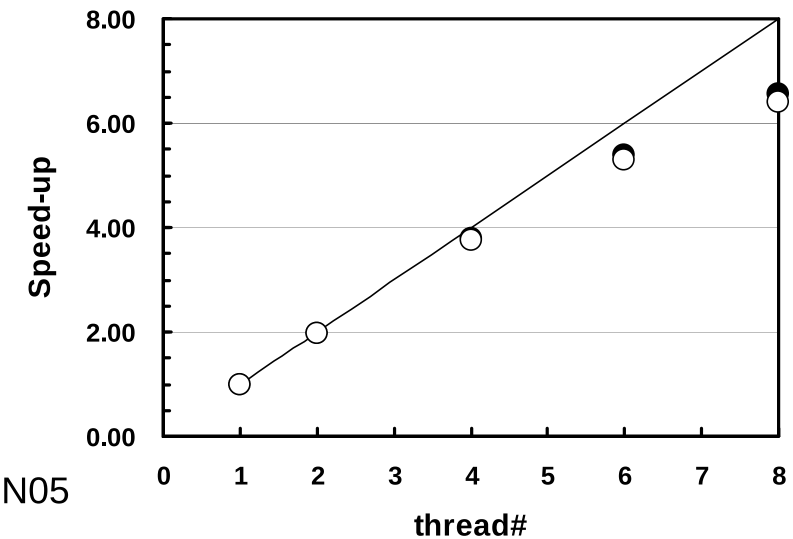
ES





SR8k





Results: Hitachi SR8000 (2/2)

Nakajima, K. (2005), "Sparse Approximate Inverse Preconditioner for Contact Problems on the Earth Simulator using OpenMP", International Workshop on OpenMP: Experiences and Implementations (WOMPEI 2005), Tsukuba, Japan.

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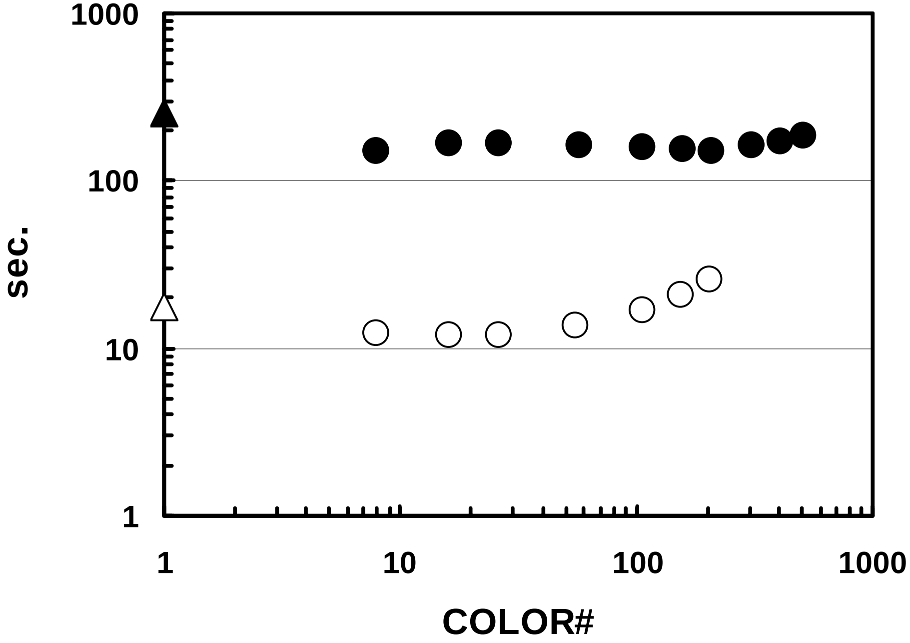

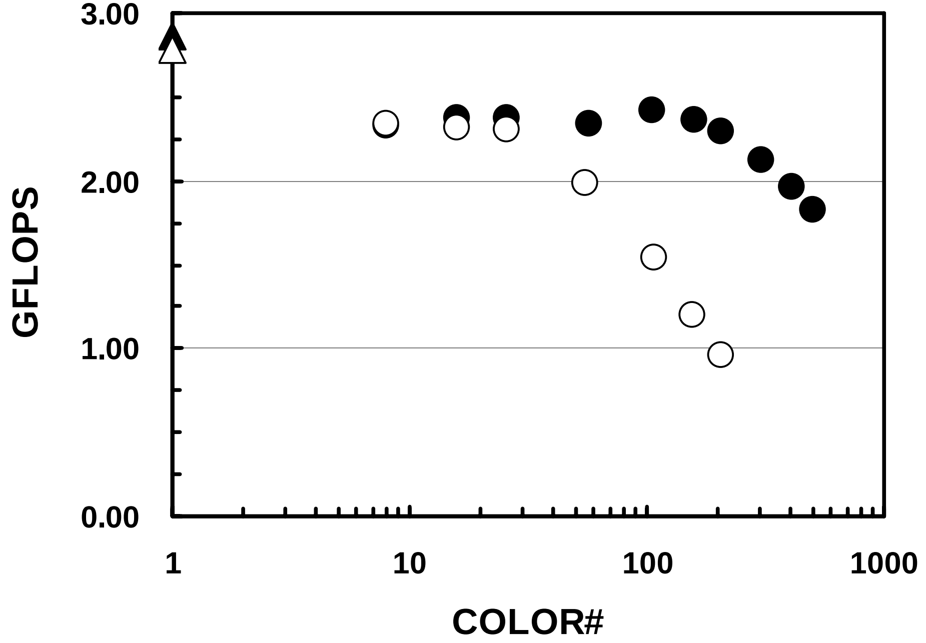

Results: IBM SP-3 (1/2)

Nakajima, K. (2005), "Sparse Approximate Inverse Preconditioner for Contact Problems on the Earth Simulator using OpenMP", International Workshop on OpenMP: Experiences and Implementations (WOMPEI 2005), Tsukuba, Japan.

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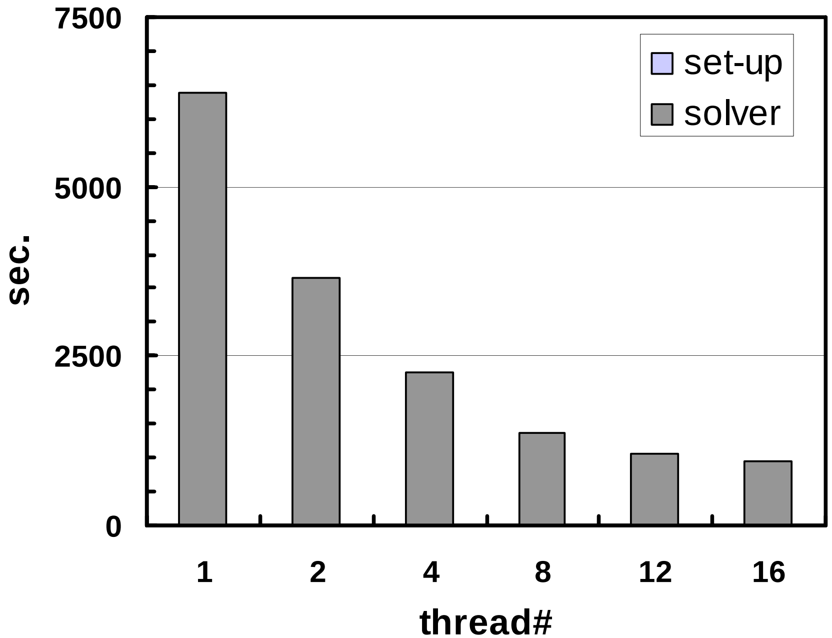
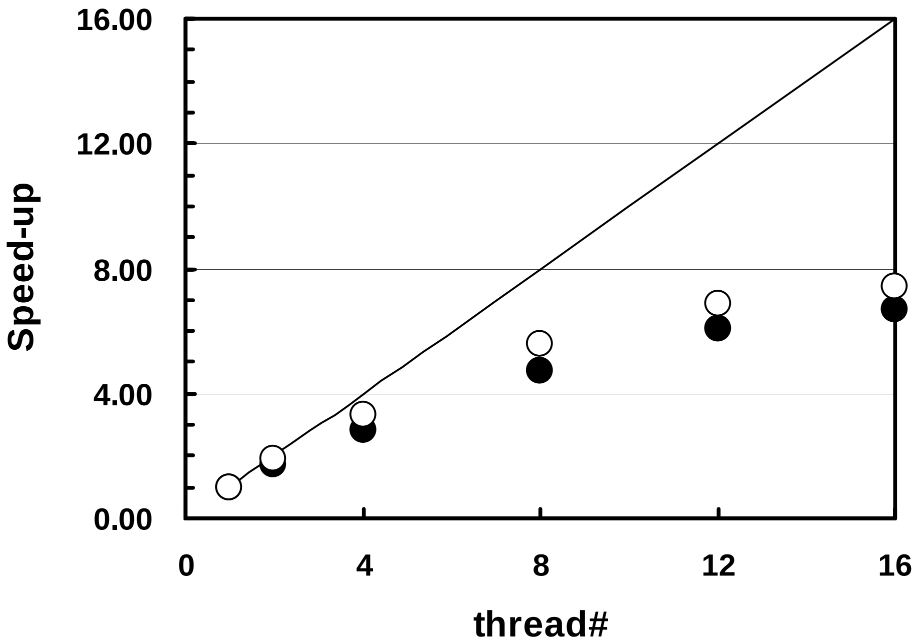
○Small (0.35M DOF)





Large Problem

IWOMP, JUN05

Acknowledgements

- Sponsor
  - MEXT, Japan.
- Computational Resources
  - Earth Simulator Center, Japan.
  - NERSC/Lawrence Berkeley National Laboratory, USA.
    - Dr. Horst D. Simon
    - Dr. Esmond G. Ng
  - Information Technology Center, The University of Tokyo, Japan.
- Colleagues ...
  - GeoFEM Project
- IWOMP Committee