ppOpen-SOL
Robust ILU Precondtioner for Exascal

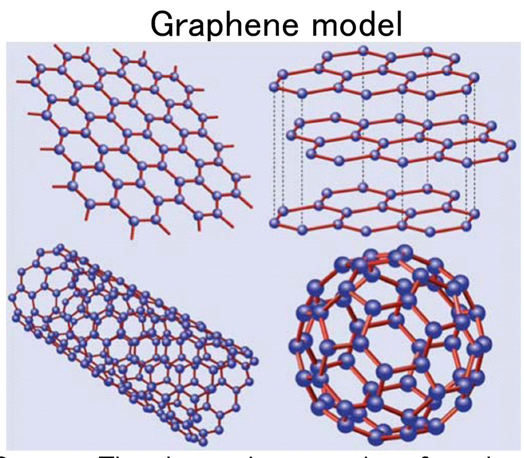
M. Kawai*1, A. Ida*2 and G. Wellein*3

*1 R-CCS Riken, *2 ITC The University of Tokyo, *3 Friedrich-Alexander-Universitat

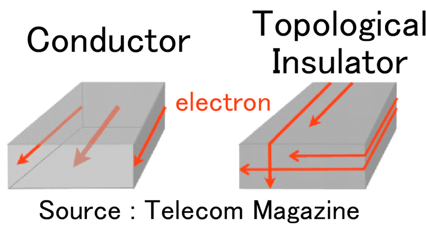
K computer
Computer simulations create the future

Solving generalized eigenvalue problems derived from quantum systems with exascale systems

Modeling special materials



Source : The electronic properties of graphene



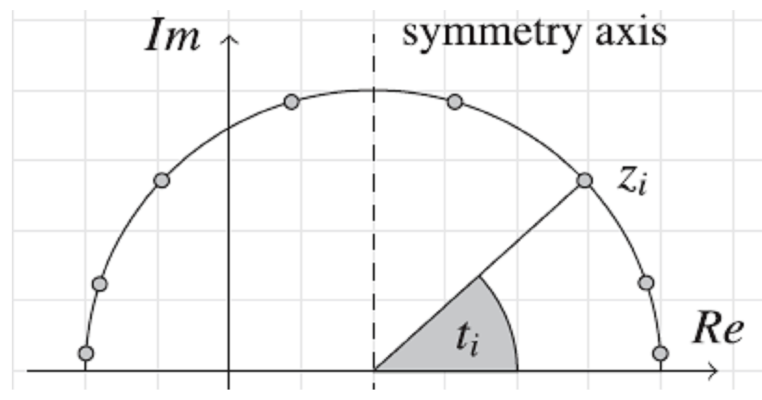
Source : Telecom Magazine

Sample of the topological insulator (SmB6)


Source : Nature
Hopes surface for exotic insulator

$$A\tilde{x} = \lambda B\tilde{x}$$

Applying Sakurai-Sugiura or FEAST to generalized eigenvalue problems



Derived systems of linear equations

$$(zB - A)x = b \rightarrow A_Z x = b$$

Properties of coefficient matrix
- Sparse
- Small diagonal entries
- Ill-conditioned

Objective : Developing an iterative solver for the ill-conditioned equations
Target of this study : ILU preconditioned Krylov subspace method with robustness and massive parallelism

For robustness

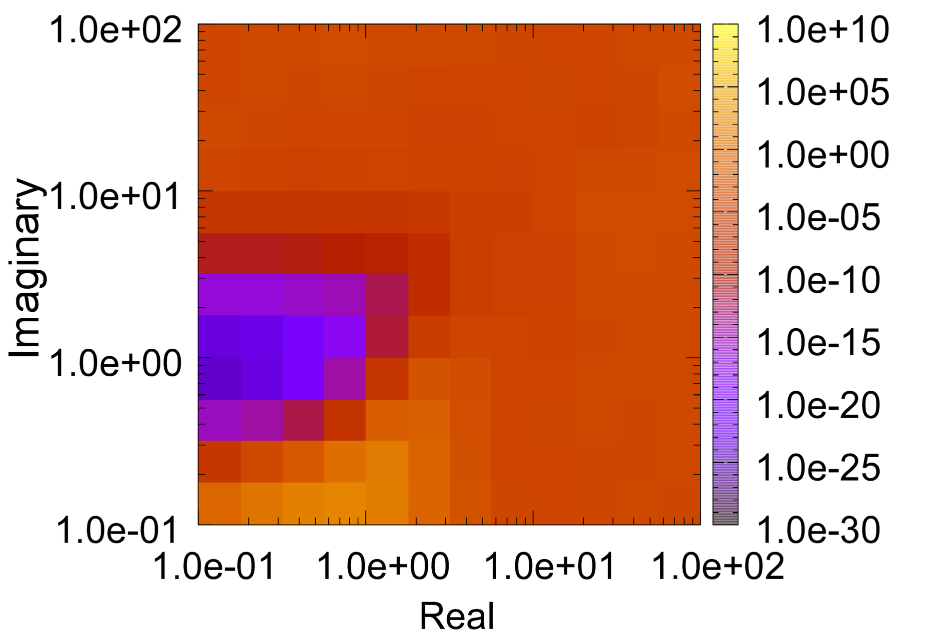
Preferred diagonal dominant coefficient matrices
→ Regularizations

1st regularization : Diagonal shifting
- Adding a constant value to the diagonals
- Direct method to make dominant diagonals

$$\tilde{A}_Z = A_Z + \alpha I$$

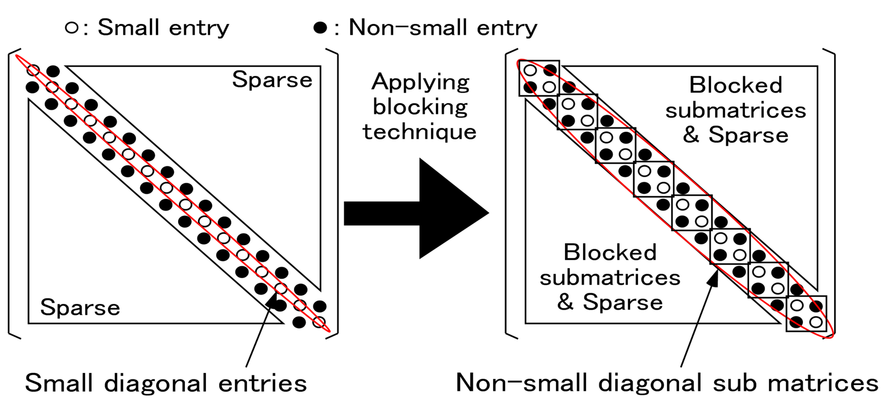
Applying ILU decomposition to $\tilde{A}_Z$

The effect of diagonal shifting

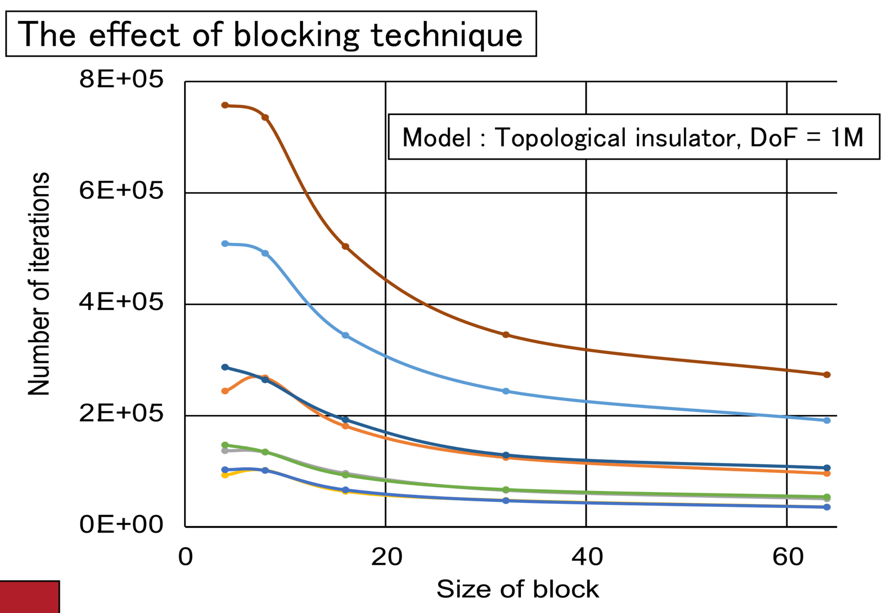


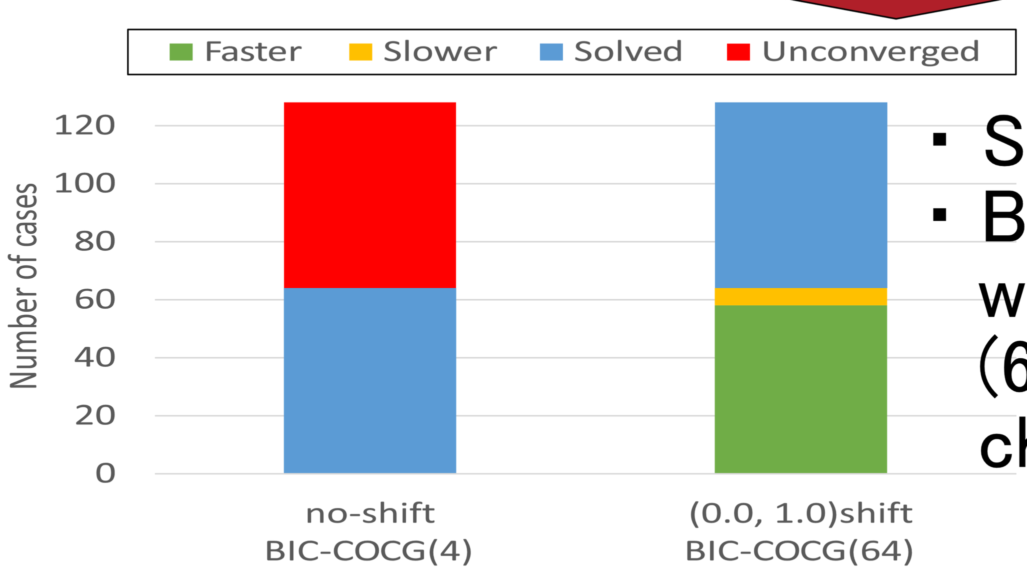
Model : Topological insulator, DoF = 100k

2nd regularization : Blocking
- Diagonal blocks including non-small entries.
- More fill-ins



The effect of blocking technique



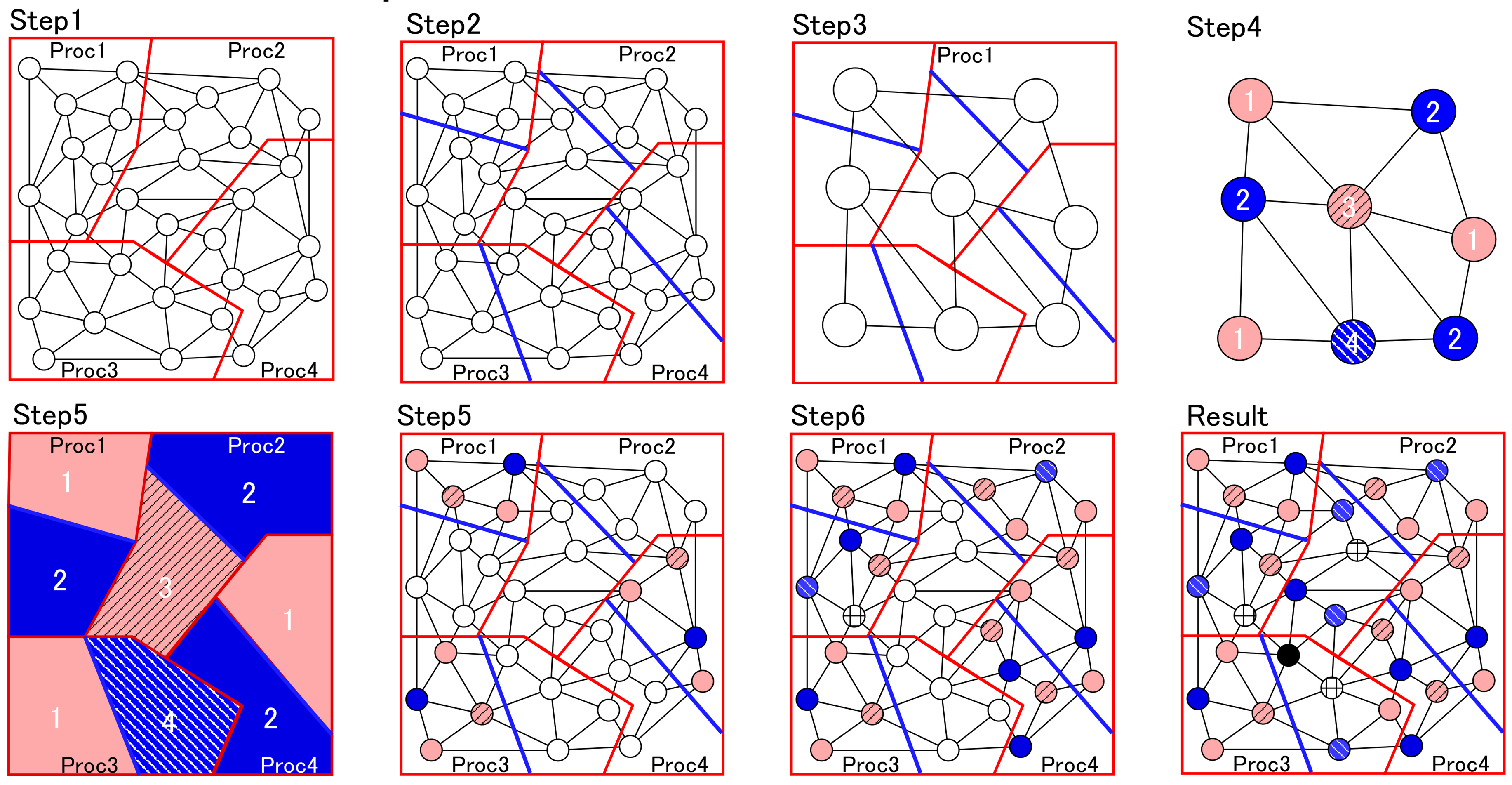


- Solving all data sets
- Better convergence with 58 data cases (63 data cases if we choose best block size)

For massively parallelism

Parallelize ILU preconditioner with multi-coloring (MC)
- Have to parallelize MC algorithm without changing properties

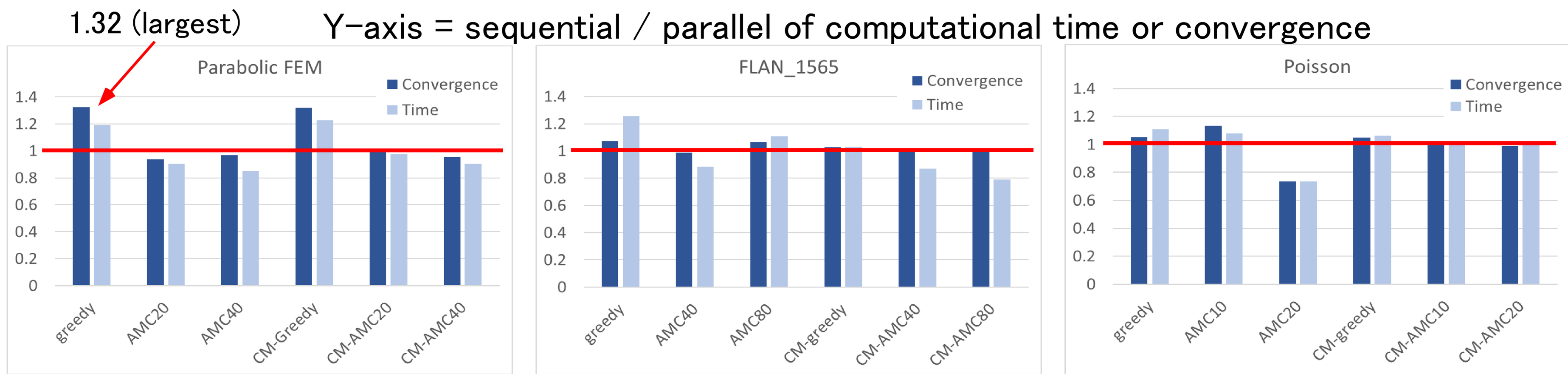
→ Hierarchical parallelization



Providing colored area
→ Parallelizing MC algorithms without changing convergence and performance

The effect of hierarchical parallelization

1.32 (largest) Y-axis = sequential / parallel of computational time or convergence



Figures show the result which MC algorithms are parallelized without changing properties.

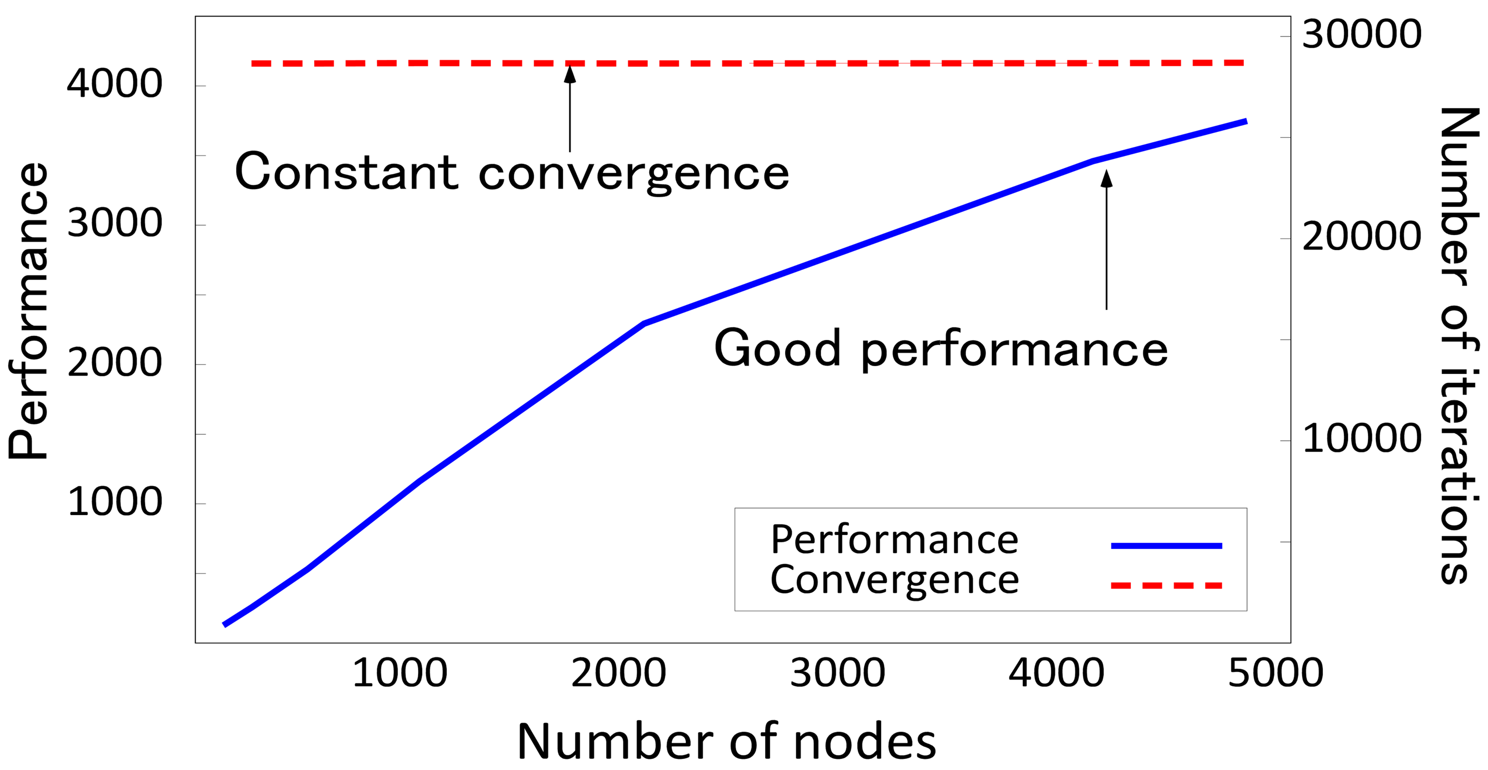
You can download from here

PHIST

a Pipelined Hybrid Parallel Iterative Solver Toolkit

ppOpen-SOL

A part of ppOpen-HPC
Supporting Fortran interface



Good convergence and performance on a large graphene

System : Oakleaf-FX (ITC The university of Tokyo)
SPARC64™ IXfx
128〜4800 nodes
DoF : 500M
Threshold of iteration : Residual norm < 10^{-7}
Iterative method : ICCG
Coloring method : 10 colors algebraic multi-coloring*1
Parameter : Block size = 4, Diagonal shifting = 1.0

Future works
- Double double precision
- Applying low-rank approximations

Collaboration with

CREST
戦略的創造研究推進事業
Core Research for Evolutionary Science and Technology

ppOpen-HPC

&

SPPEXA

ESSEX-II

Conclusion

■Developing an ILU precoinditioner with highly robustness and massive parallelism
- ●For highly robustness : Applying two regularizations (Blocking and diagonal shifting)
- ●For massive parallelism : Proposing the hierarchical parallelization of MC algorithms

→ Solved a graphene problem (500M Do) with 4800 nodes (76,800 cores)

RIKEN Center for Computational Science