Development of a Scalable Parallel Eigensolver for Large-scale Simulations and Data Analysis

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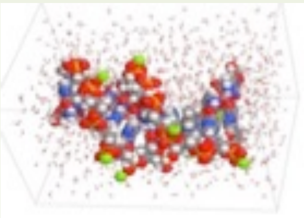
Eigenvalue Problems in Simulation and Data Analysis

Electronic State Analysis | Modeling | Eigenvalue Problem



Nano Materials

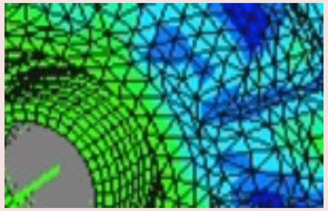
Basis Function Expansion

$$\psi_i(\boldsymbol{r}) = \sum_j \phi_j(\boldsymbol{r})$$

Interaction of Electrons

$$H\boldsymbol{x} = \lambda S\boldsymbol{x}$$

Structural Analysis



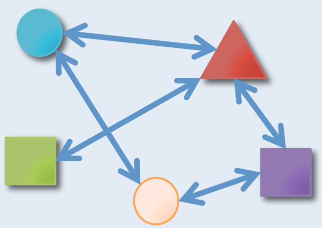
Car body design, etc.

Vibration Analysis

Interaction of Finite Elements

$$K\boldsymbol{x} = \lambda M\boldsymbol{x}$$

Data Analysis



Data

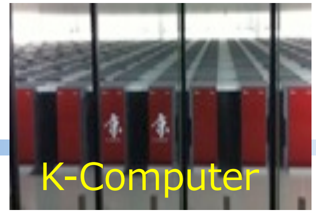
Similarity of data elements

$$d_i = \sum_j A_{i,j} \quad L = D - A$$

Interaction of Data Elements

$$L\boldsymbol{x} = \lambda D\boldsymbol{x}$$

Applications

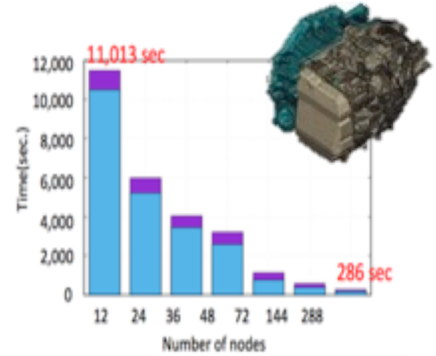


Simulation

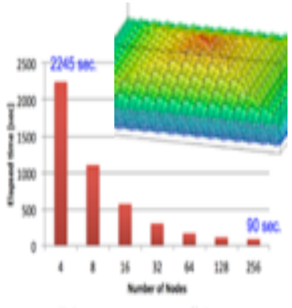
Structural Analysis

First-principles calculation

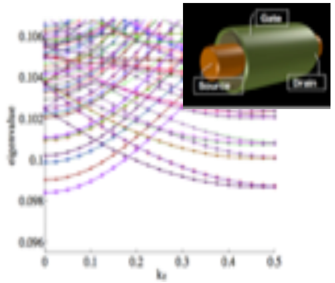
Elementary physics



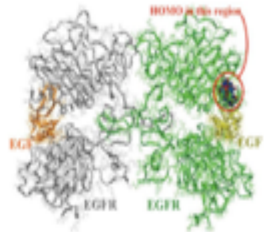
Vibration analysis



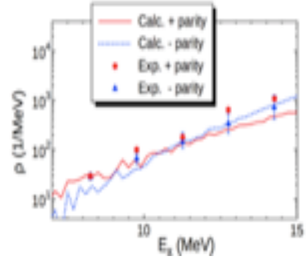
Quantum dots



Next generation silicon device

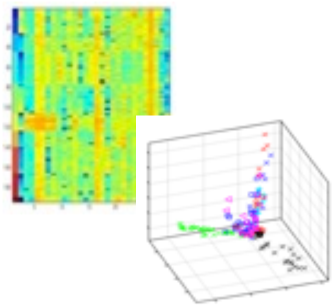


Molecular simulation

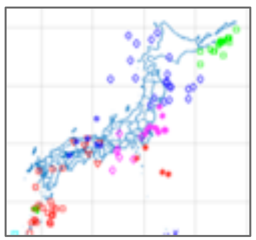


Lattice-QCD & Nuclei Physics

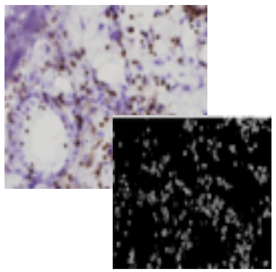
Data analysis, Deep learning



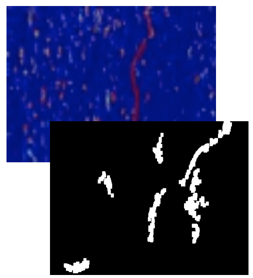
Gene data analysis



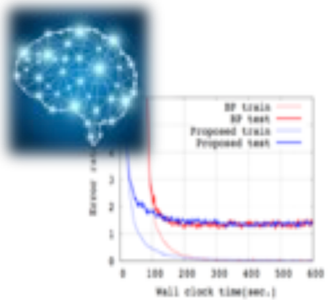
Earthquake risk evaluation



H&E image analysis



Anomaly detection of infrastructure

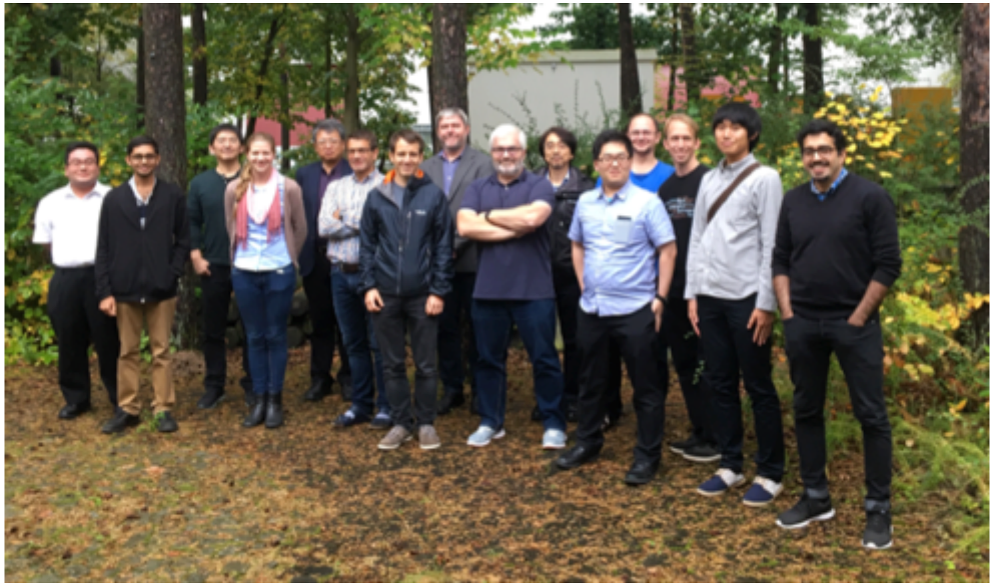


Neural network computation

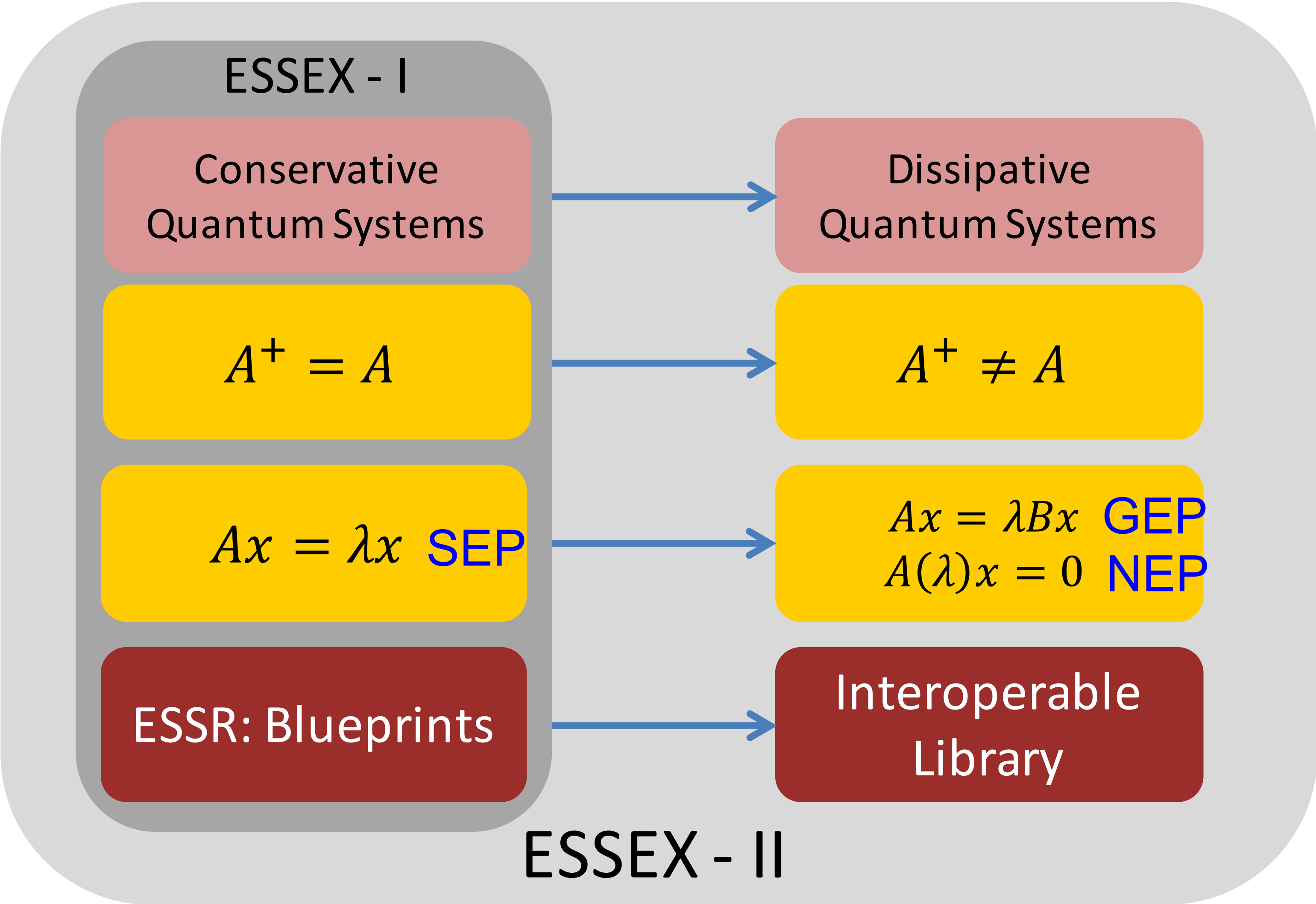
A Scalable Solver for Nonlinear Eigenvalue Problems

ESSEX II –
Equipping Sparse Solvers for Exascale

Gerhard Wellein	Computer Science, University Erlangen
Bruno Lang	Applied Computer Science, University Wuppertal
Achim Basermann	Simulation & SW Technology, German Aerospace
Holger Fehske	Institute for Physics, University Greifswald
Georg Hager	Erlangen Regional Computing Center
Tetsuya Sakurai	Applied Mathematics, University of Tsukuba
Kengo Nakajima	Computer Science, University of Tokyo



ESSEX-II


ESSEX - I
Conservative Quantum Systems
$A^+ = A$
$Ax = \lambda x$ SEP
ESSR: Blueprints
Dissipative Quantum Systems
$A^+ \neq A$
$Ax = \lambda Bx$ GEP
$A(\lambda)x = 0$ NEP
Interoperable Library
ESSEX - II

Nonlinear eigenvalue problems

Eigenvalue problem:

$$P(\lambda)\boldsymbol{x} = \boldsymbol{0} \qquad P(\lambda) \in \mathbb{C} \to \mathbb{C}^{n\times n} \quad \boldsymbol{x} \in \mathbb{C}^n \backslash \{\boldsymbol{0}\}$$

Quadratic eigenvalue problem:

$$P(\lambda) = \lambda^2 A_2 + \lambda A_1 + A_0$$

Polynomial eigenvalue problem:

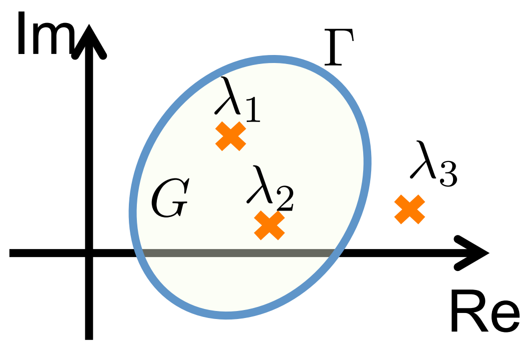
$$P(\lambda) = \lambda^k A_k + \lambda^{k-1} A_{k-1} + \cdots + A_0$$

General nonlinear:

$$P(\lambda) = \sqrt{\lambda} A + e^{-\lambda} B$$

Scalable Parallel Eigensolver

Quadrature-type Eigensolver:
Sakurai-Sugiura method (SSM) computes all the eigenvalues inside a given Jordan curve.



- For generalized eigenvalue problems (GEPs)
  - SS-Hankel (Sakurai and Sugiura, 2003)
  - SS-RR (Sakurai and Tadano, 2007)
  - SS-Arnoldi (Imakura, Du and Sakurai, 2013)

- For nonlinear eigenvalue problems (NEPs)
  - SS-Hankel (Asakura, Sakurai, et al. 2009)
  - SS-RR (Yokota and Sakurai, 2013)

NEP in Complex Band Structure Calculation

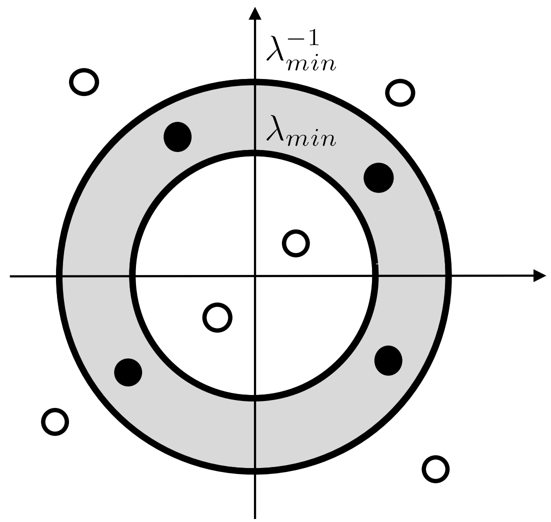
A nonlinear eigenvalue problem (NEP)

$$P(\lambda)\boldsymbol{x} = \boldsymbol{0} \qquad (\lambda \in \mathbb{C}, P(\lambda) \in \mathbb{C}^{n \times n}, \boldsymbol{x} \in \mathbb{C}^n \backslash \{\boldsymbol{0}\})$$

appears in complex band structure (CBS) calculation where

$$P(\lambda) = -\lambda^{-1} H_{i-1,i} + (E - H_{i,i}) - \lambda H_{i,i+1}$$

Eigenvalues in a ring region are required

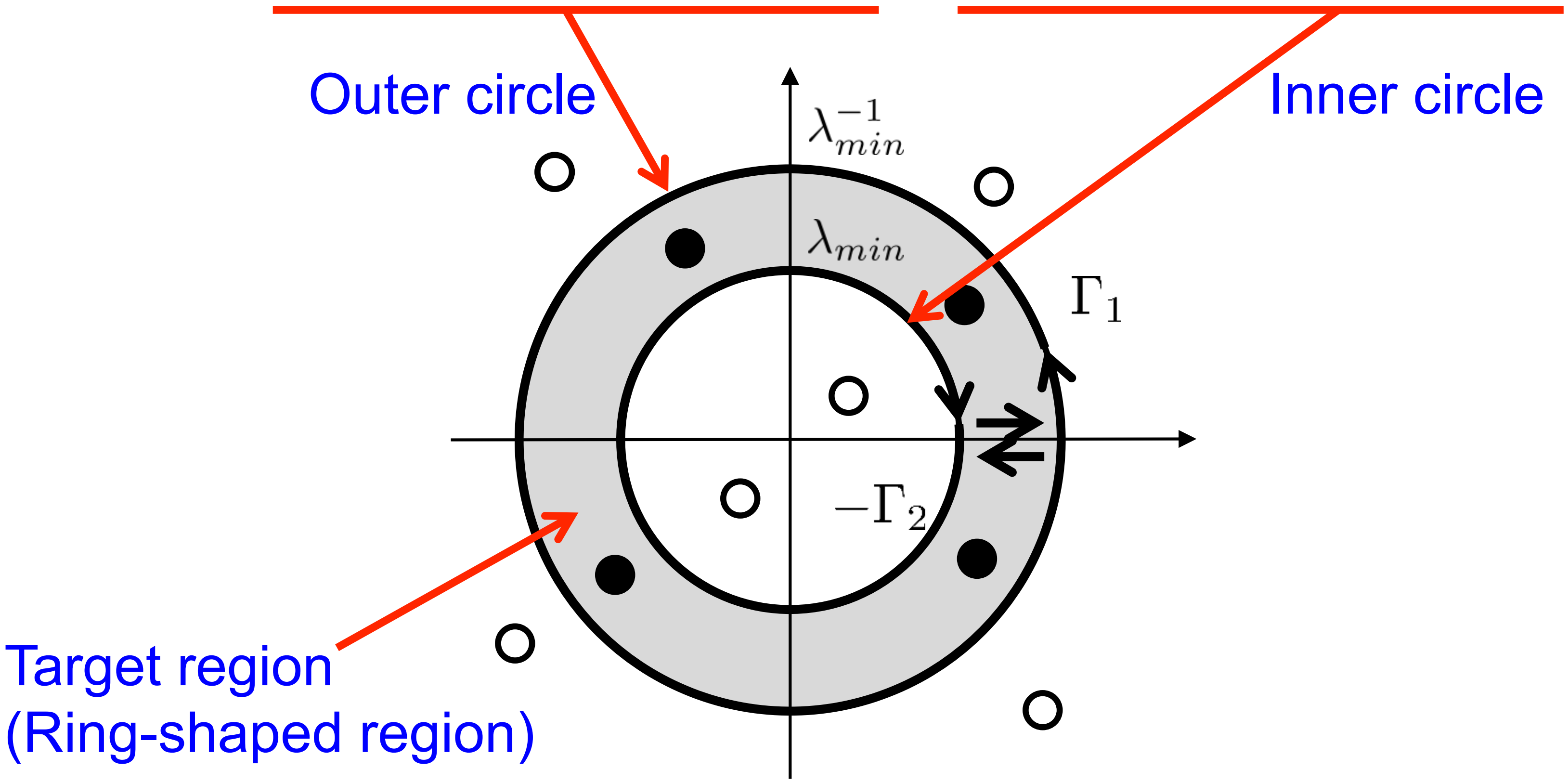


S. Iwase, Y. Futamura, A. Imakura, T. Sakurai, T. Ono, Efficient and Scalable Calculation of Complex Band Structure using Sakurai-Sugiura Method, Proc. SC17 (accepted).

Computing Eigenvalues in a Ring-shaped Region

Using SSM, we can compute the target eigenvalues by setting two circles (clockwise and anti-clockwise)

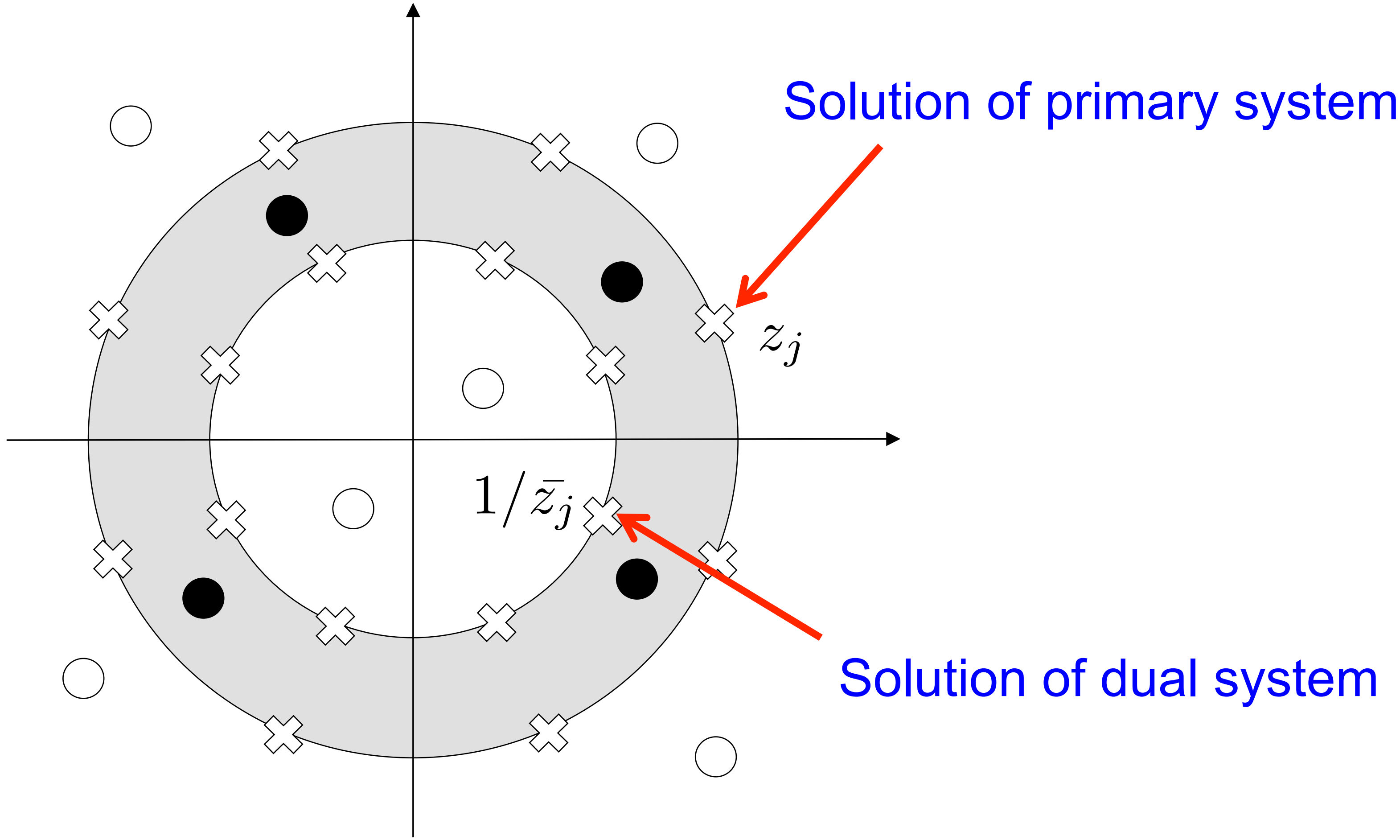
$$S_k := \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma_1} z^k P(z)^{-1} V \mathrm{d}z - \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma_2} z^k P(z)^{-1} V \mathrm{d}z$$



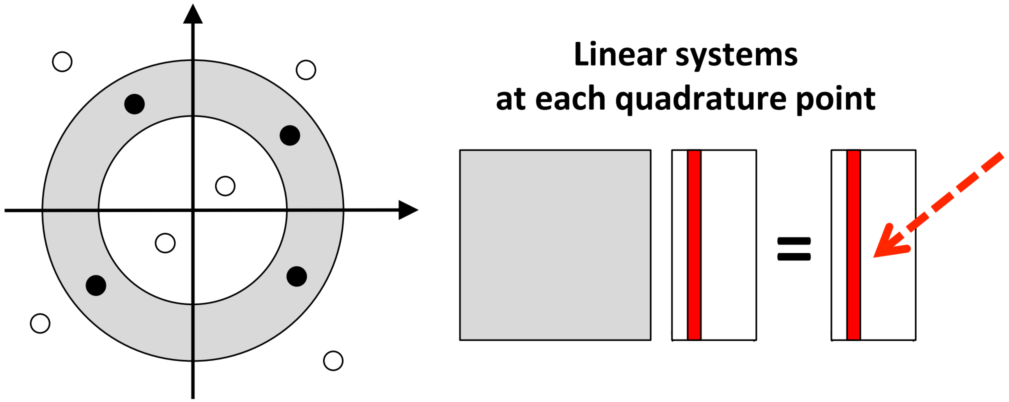
Utilization of BiCG

- BiCG method solves two linear systems:
  Primary system and Dual system

We can obtain solutions at z_j and $1/\bar{z}_j$ from one BiCG.

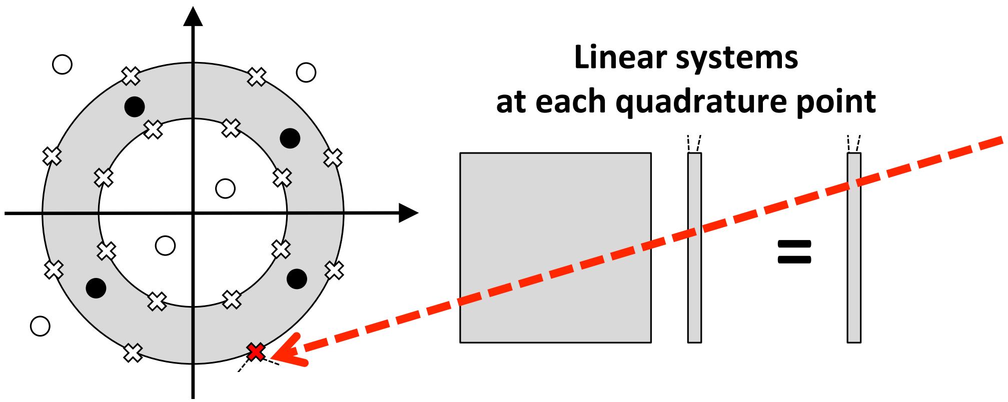


Three level parallelism of SSM in CBS calculation



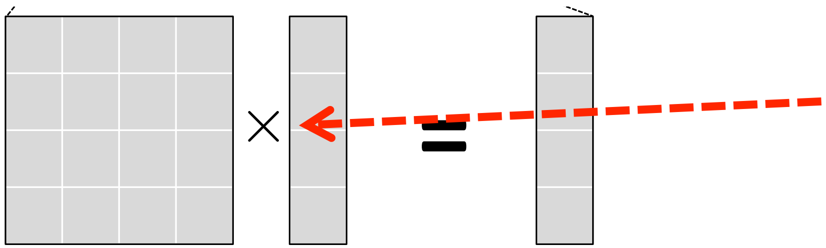
Top level:

Linear system for each right-hand side vector



Middle level:

Linear system for each quadrature point



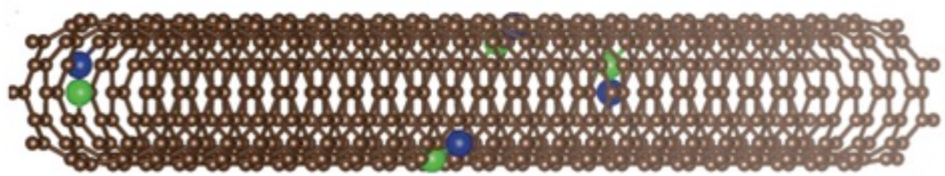
Bottom level:

Sparse matrix-vector product

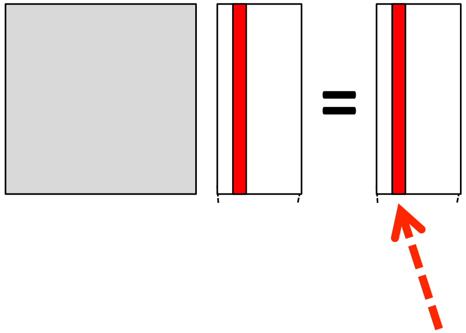
Performance Evaluation

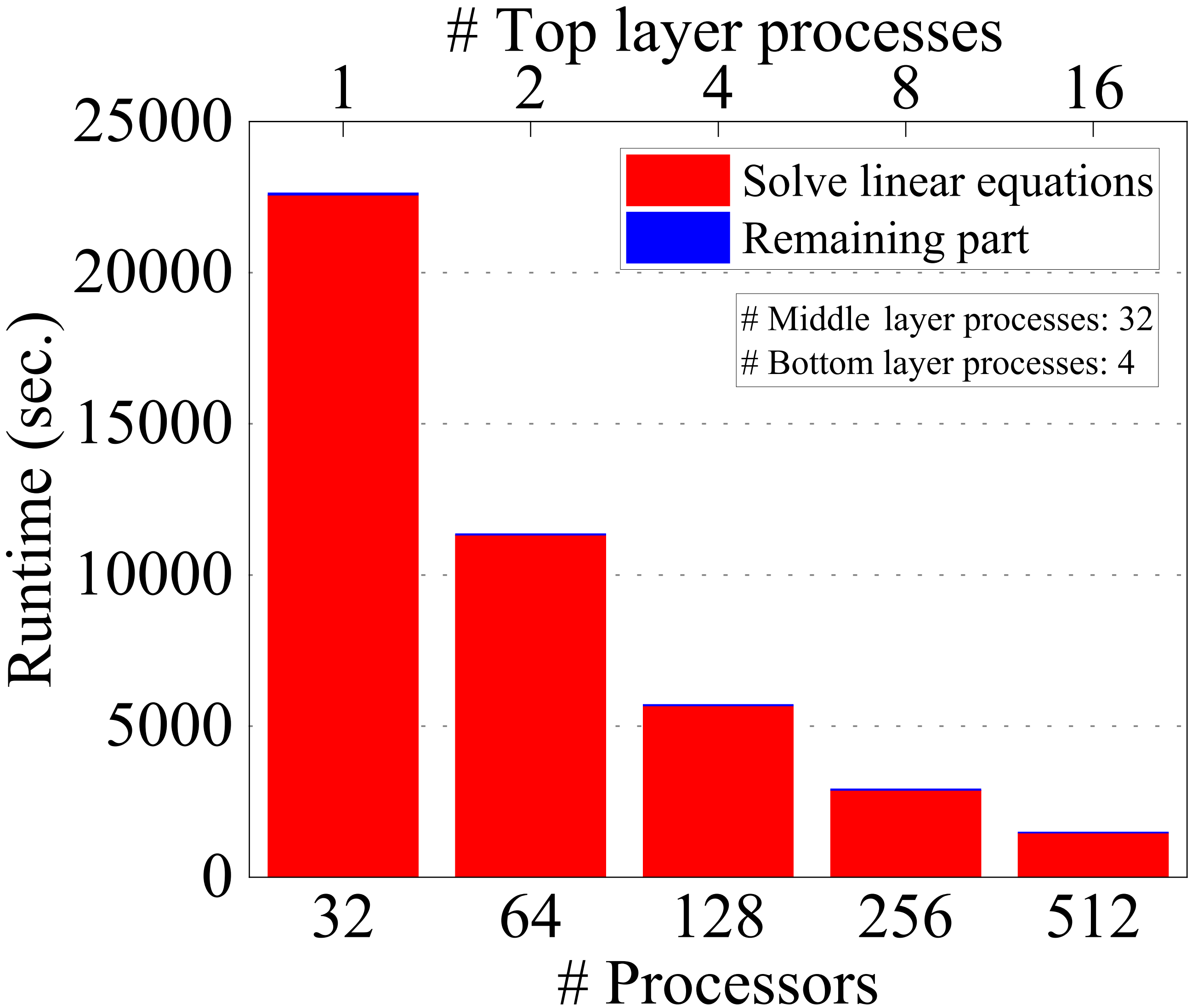
Performance evaluation

- BN-CNT with 1,024 atoms
  - # of grid points = 72x72x640 = 3,317,760 (matrix size)
  - # of eigenvalues = 22, λ_{min} = 0.5
- Parameters for SSM and BiCG
  - N=32, M=8, L=16
  - Stopping criterion for BiCG : Relative residual < 1e-10
- Computing environment: Oakforest-PACS
  - Parallelization setting
    - 17 threads/MPI
    - 4 MPI/node



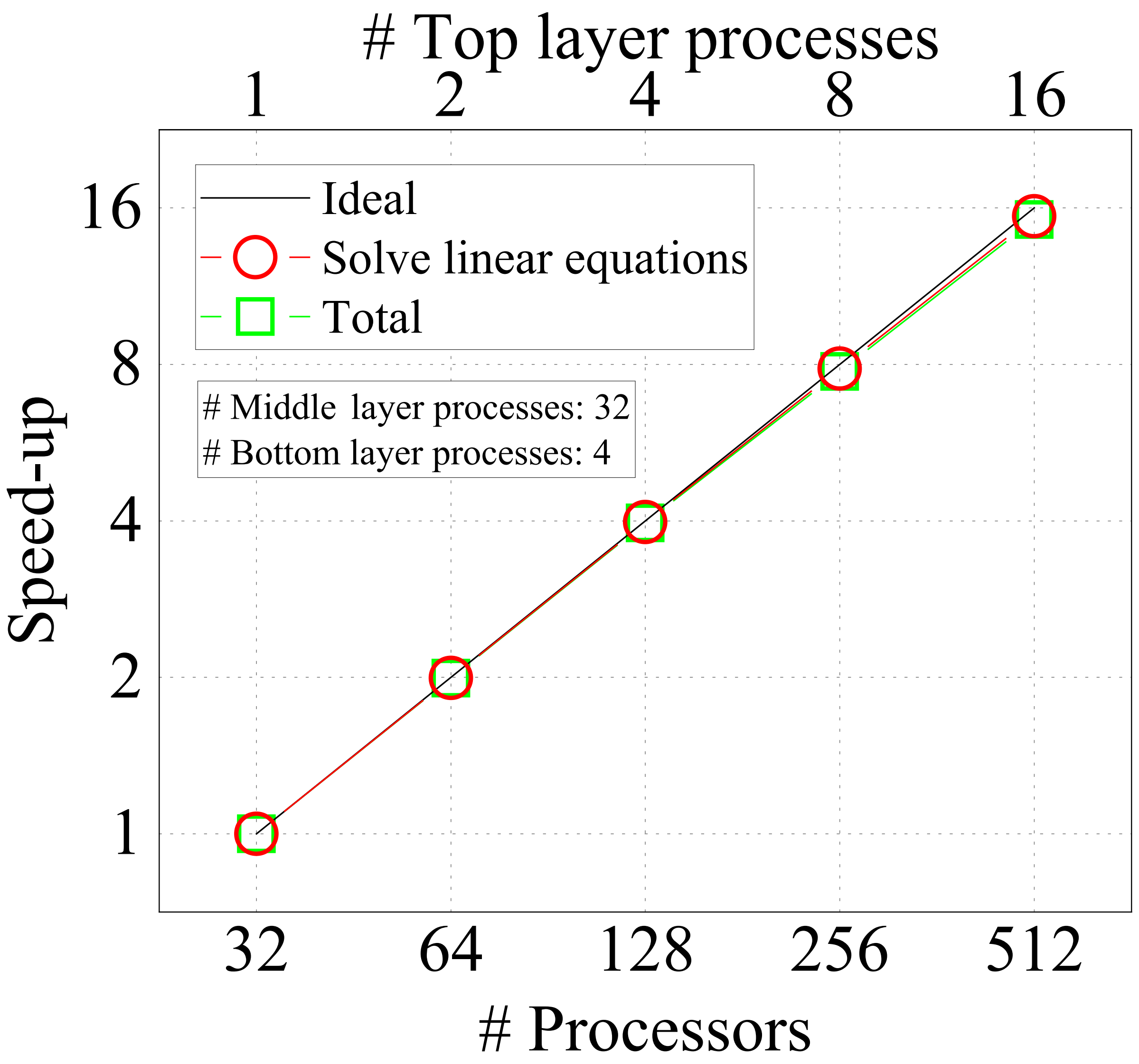
Top layer



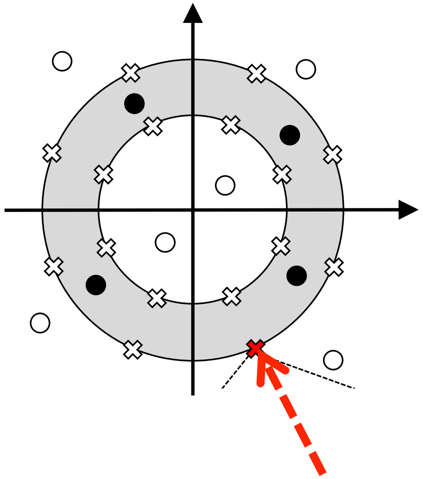


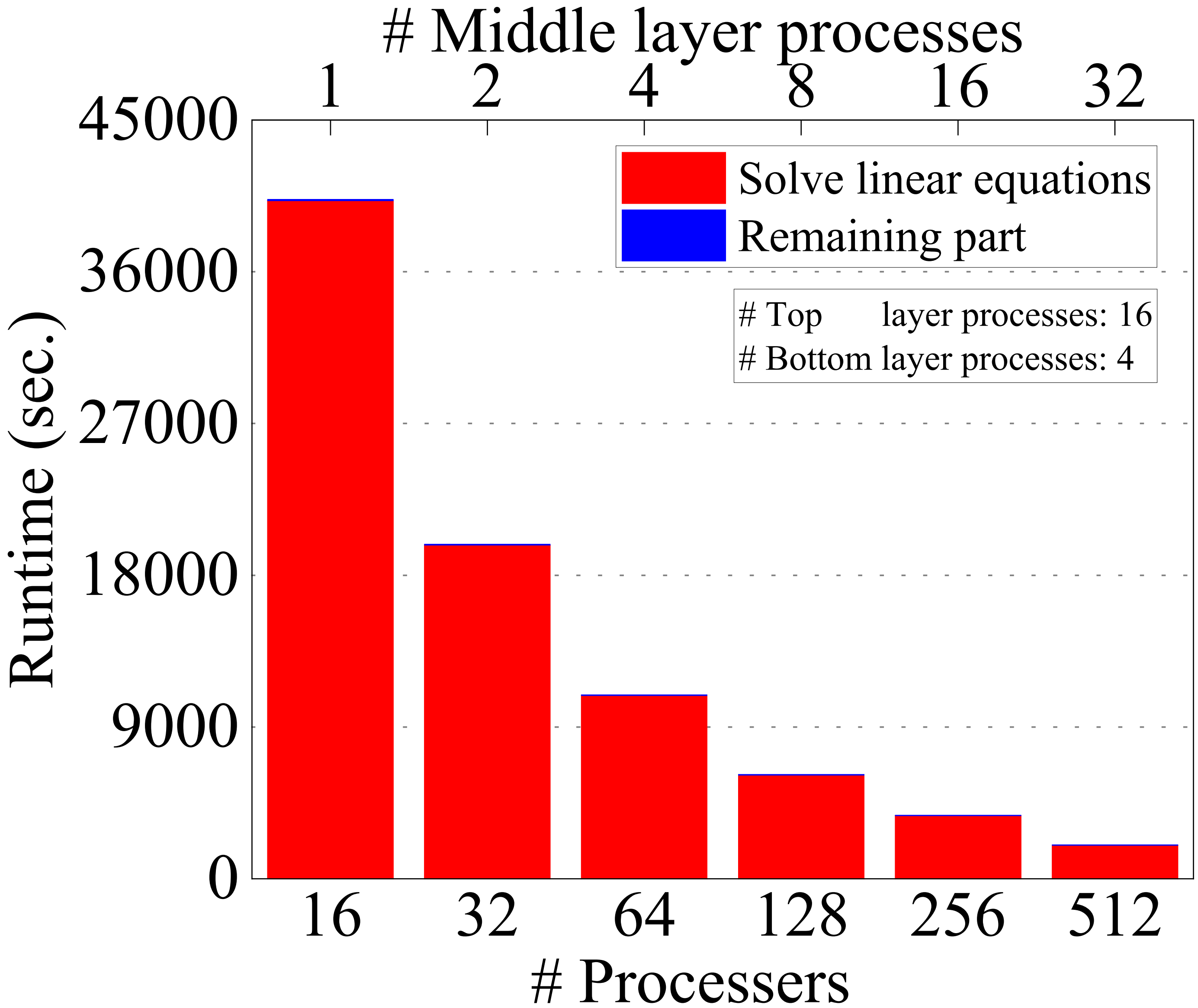
Top layer processes
1
2
4
8
16
25000
20000
15000
10000
5000
0
Runtime (sec.)
Solve linear equations
Remaining part
Middle layer processes: 32
Bottom layer processes: 4
32
64
128
256
512
Processors

Top layer (speedup ratio)

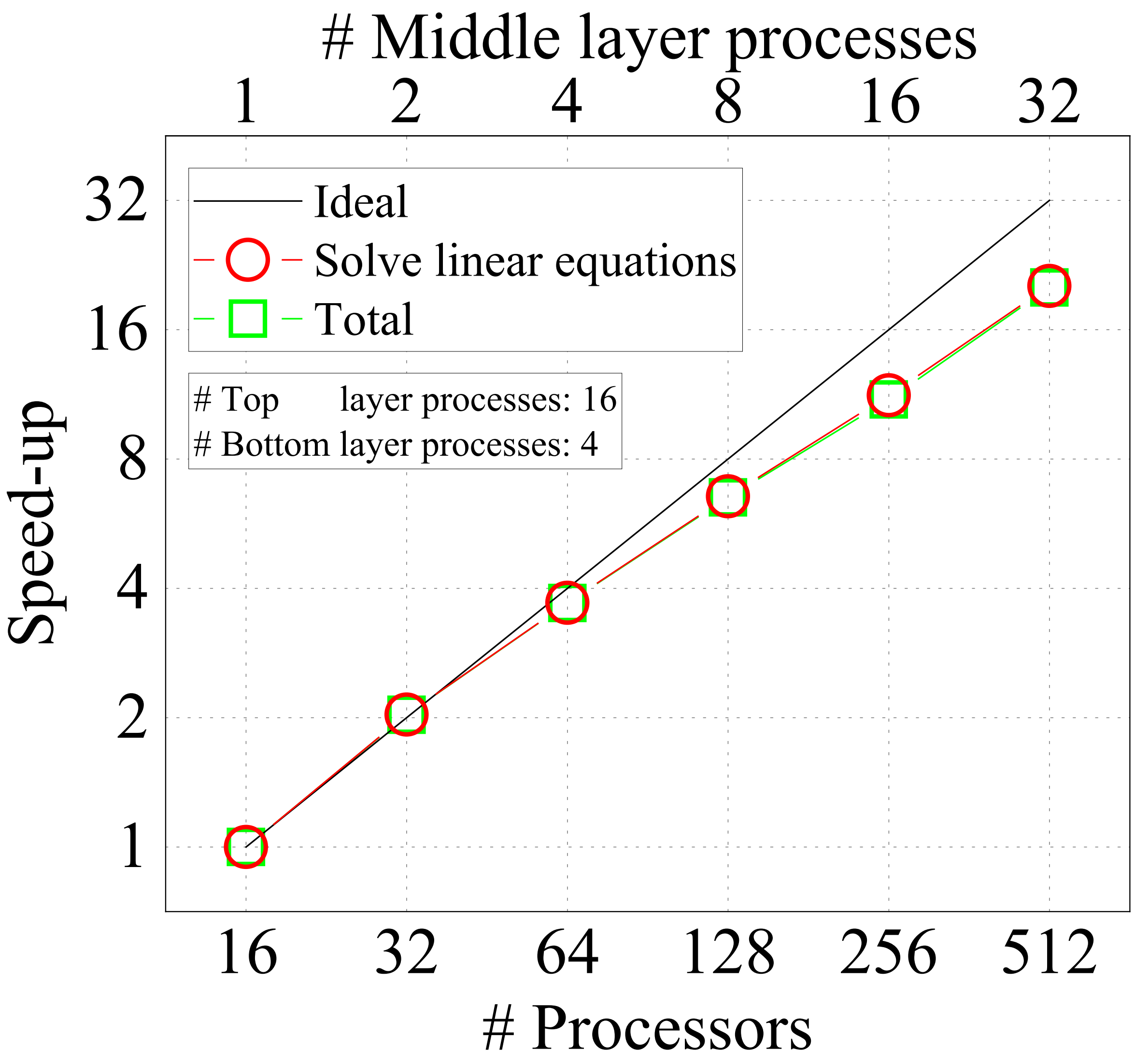


Middle layer

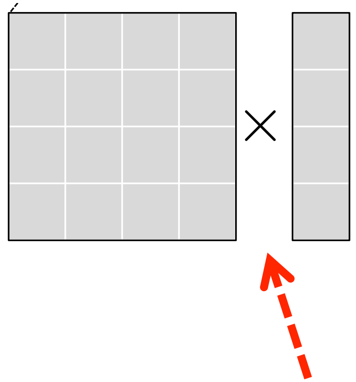


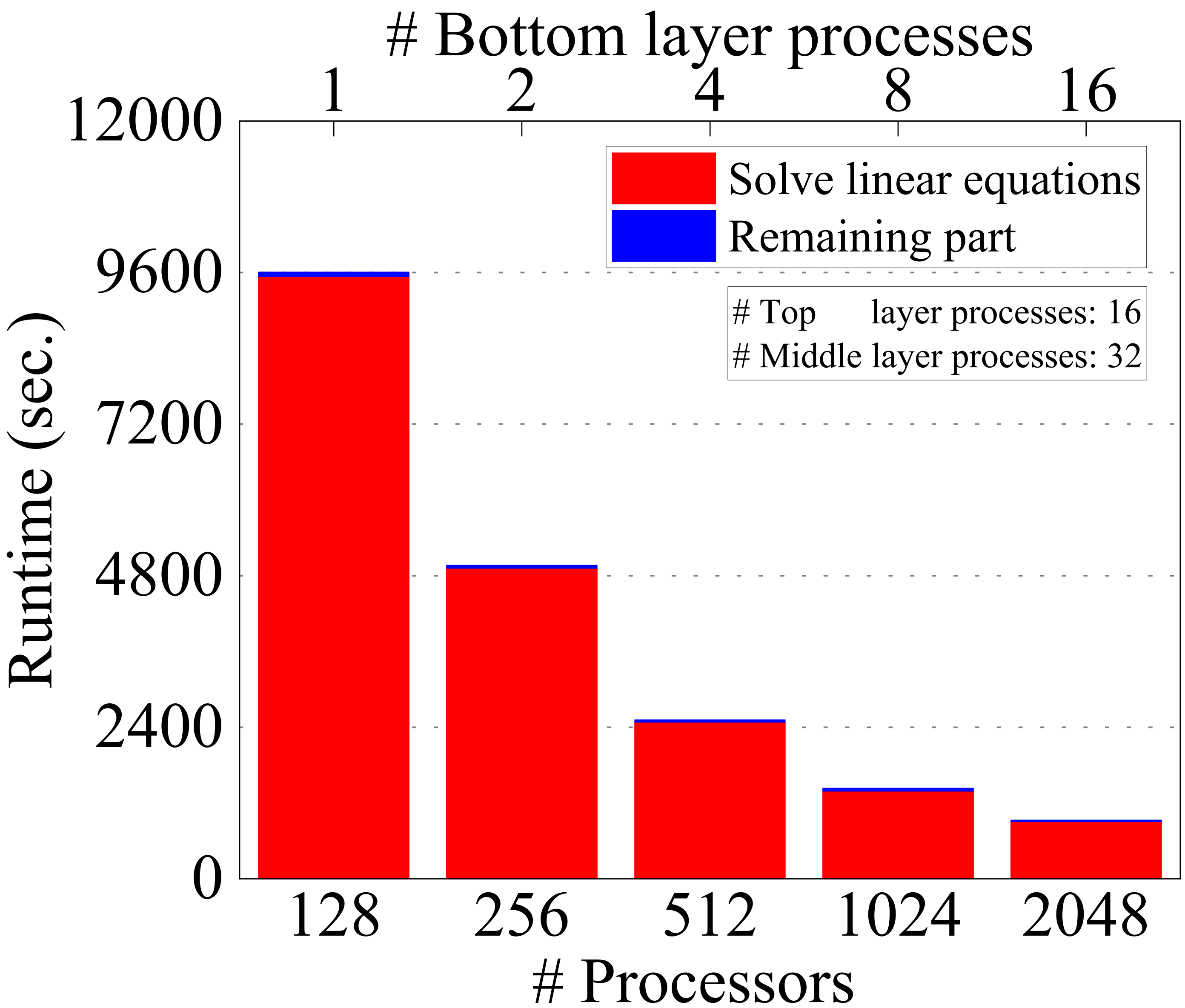


Middle layer (speedup ratio)

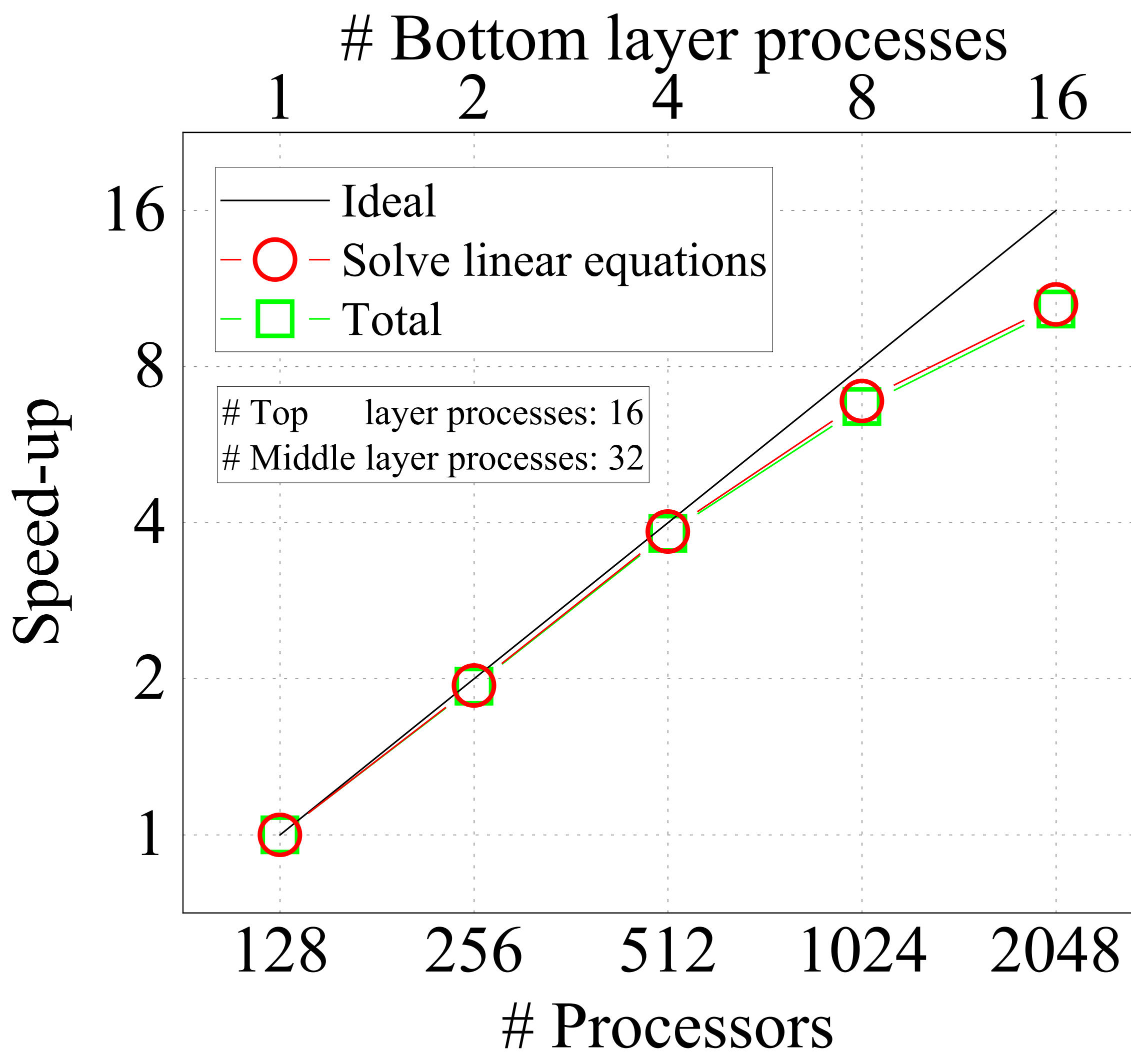


Bottom layer



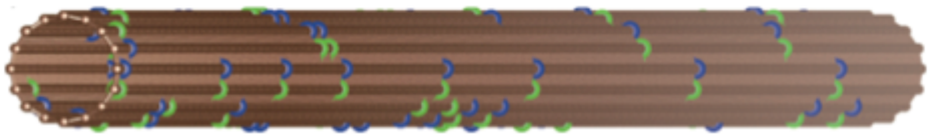


Bottom layer (speedup ratio)

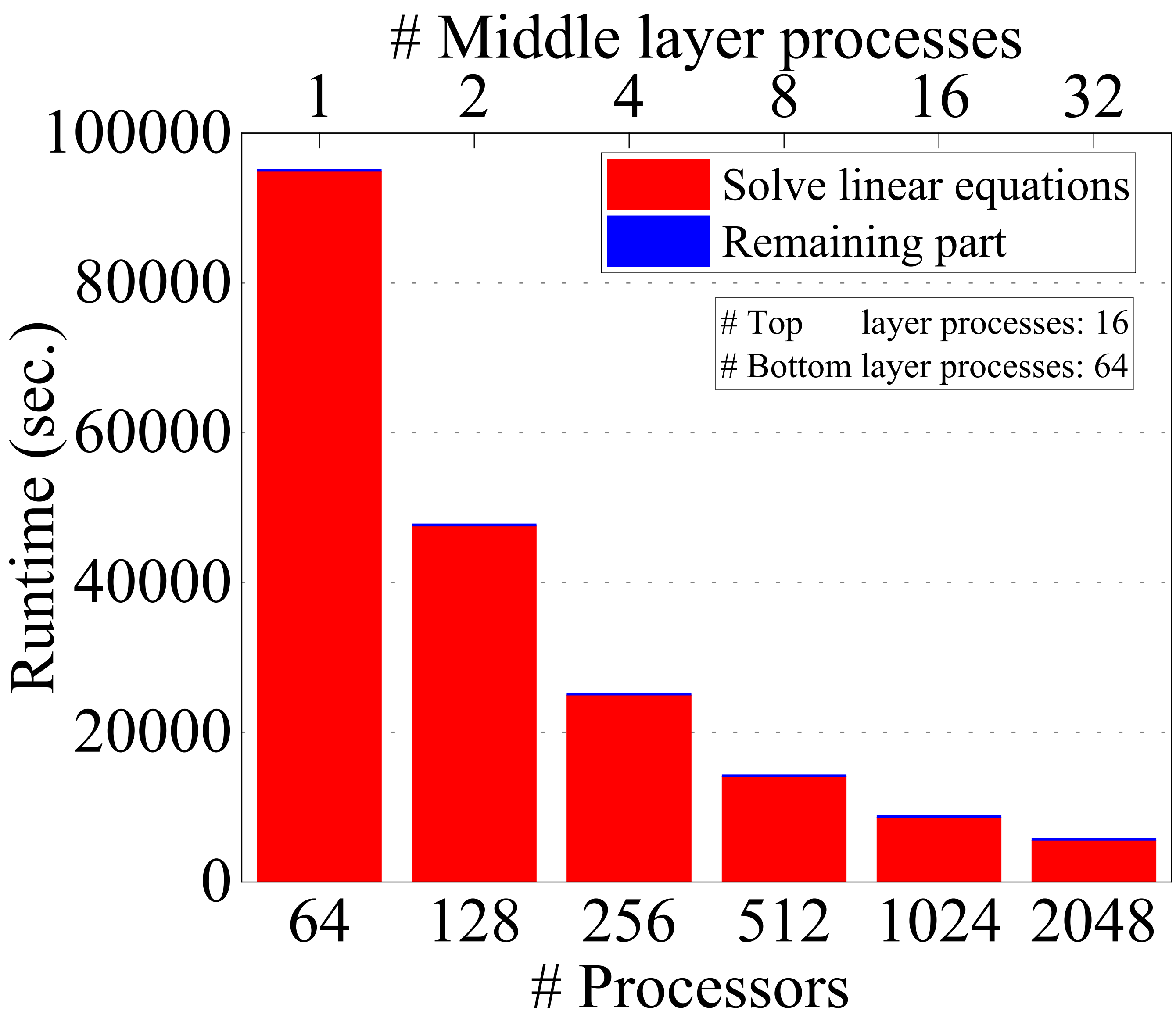


Performance evaluation

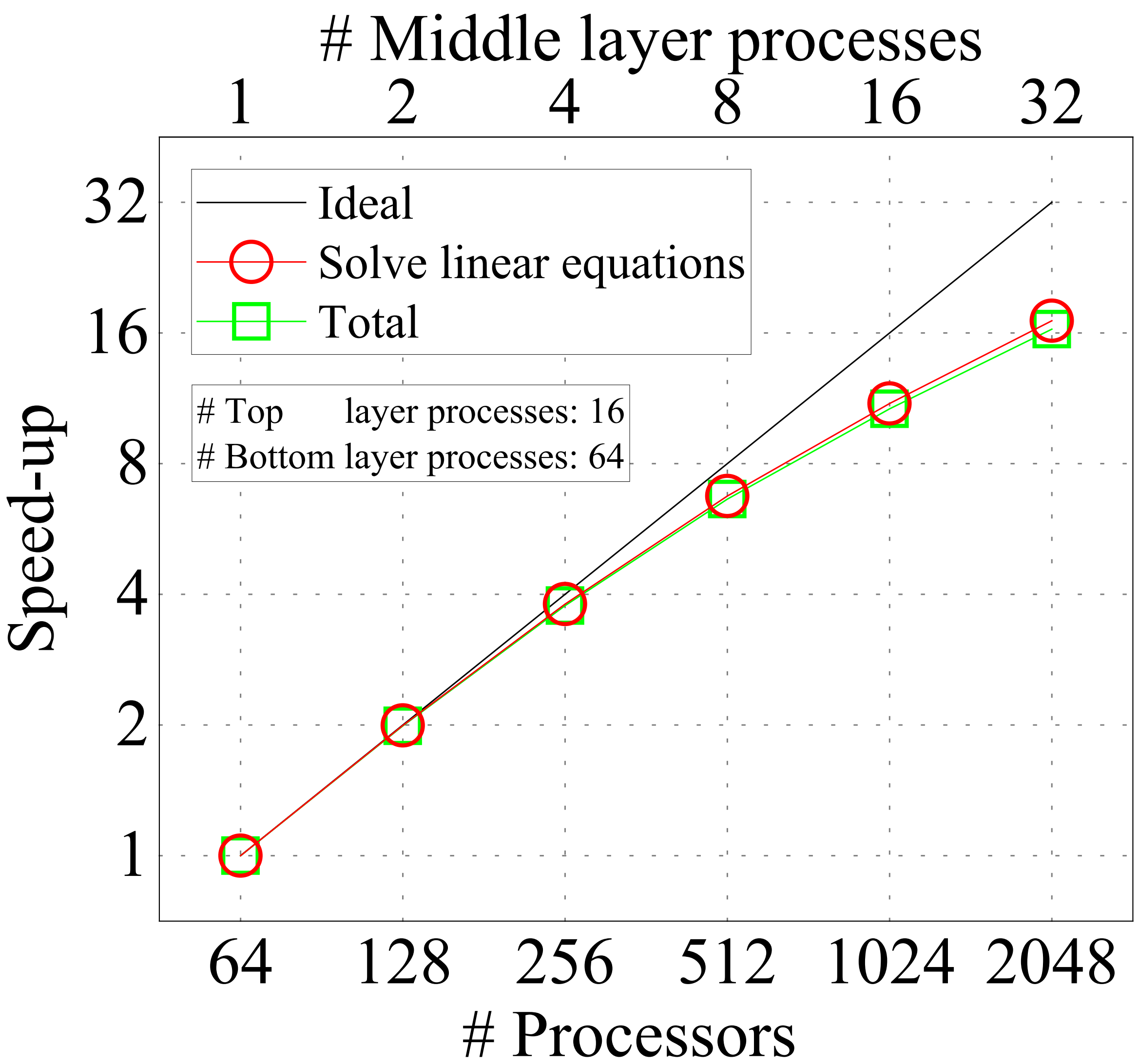
- BN-CNT with 10,240 atoms
  - # of grid points = 72x72x6400 = 33,177,600 (matrix size)
  - # of eigenvalues = 34, λ_{min} = 0.5
- Parameters for SSM and BiCG
  - N=32, M=8, L=16
  - Stopping criterion for BiCG : Relative residual < 1e-10
- Computing environment: Oakforest-PACS
  - Parallelization setting
    - 4 threads/MPI
    - 16 MPI/node



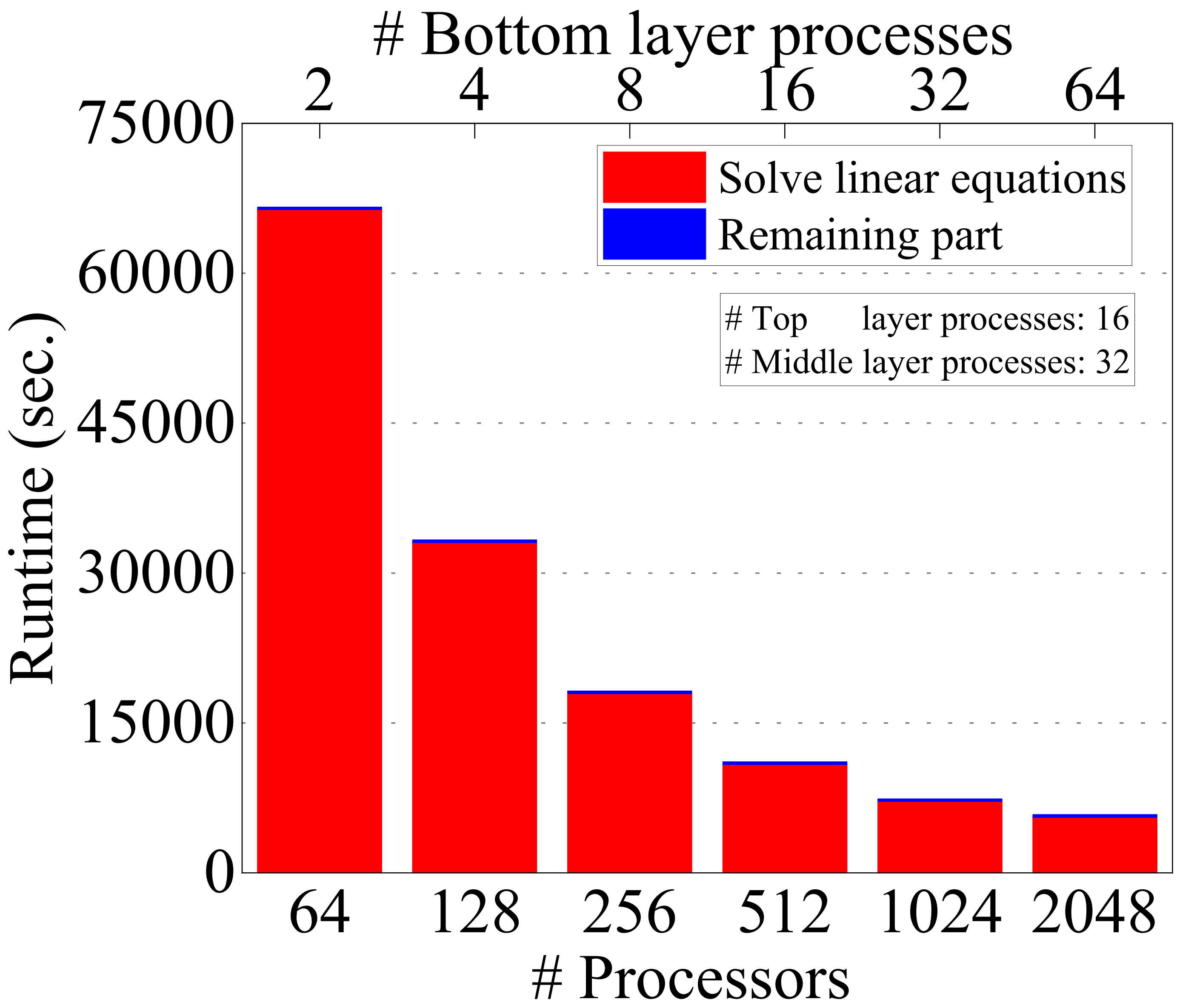
Middle layer



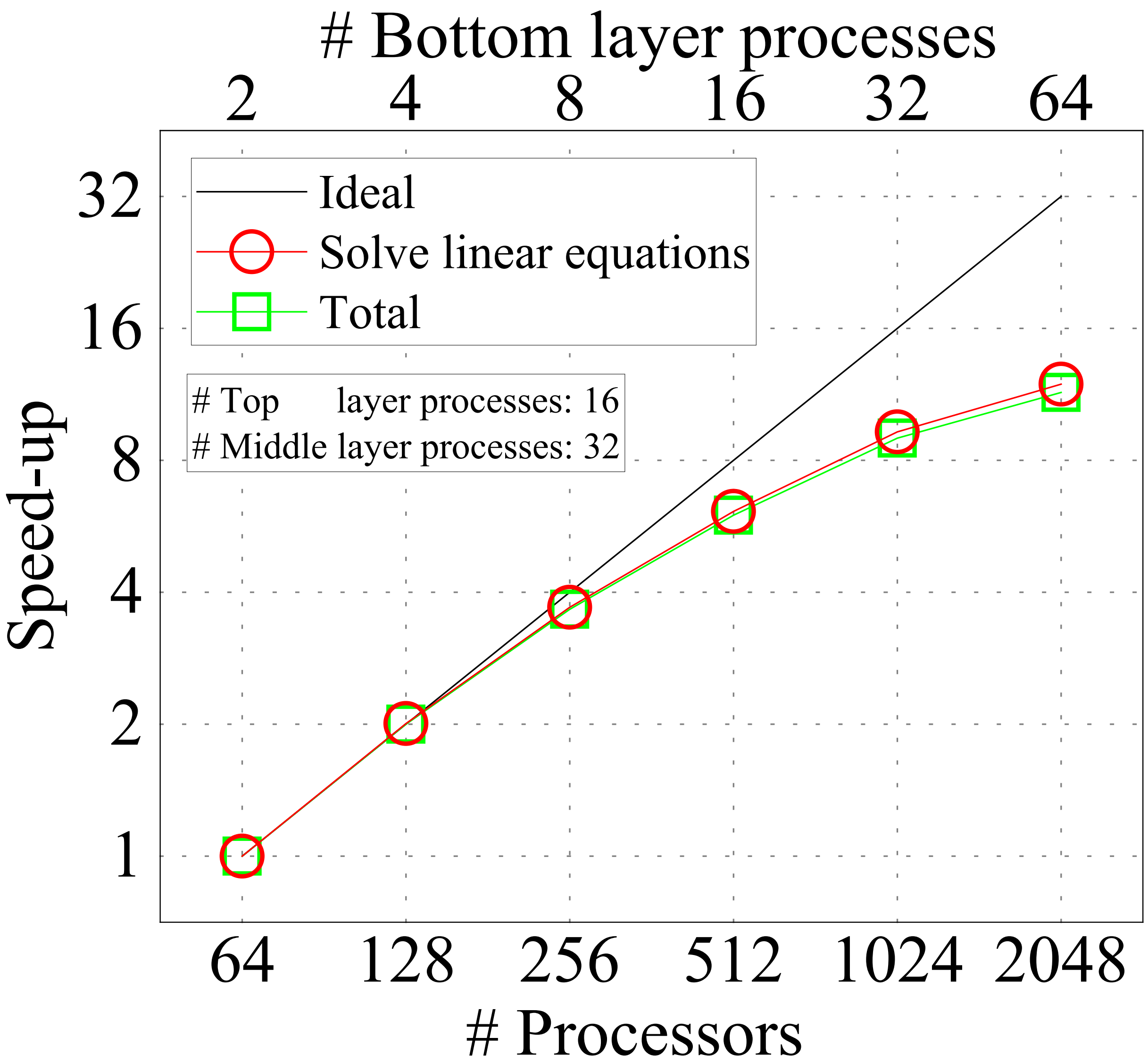
Middle layer (speedup ratio)



Bottom layer



Bottom layer (speedup ratio)



Conclusions

- Simulation and Data Analysis
  - Large-scale problems
  - High performance eigenvalue solver
  - Various applications

- Developing a scalable parallel eigensolver
  - Sakurai-Sugiura method (SSM)
    - Quadrature-type parallel eigensolver
    - Hierarchical parallel structure

- Nonlinear Sakurai-Sugiura method for ring-shaped region
  - Application for complex band structure calculation
    - Performance evaluation on Oakforest-PACS
    - BN-CNT with 10,240 atoms