A parallel solver for a linear system with symmetric sparse matrix by one-way dissection ordering

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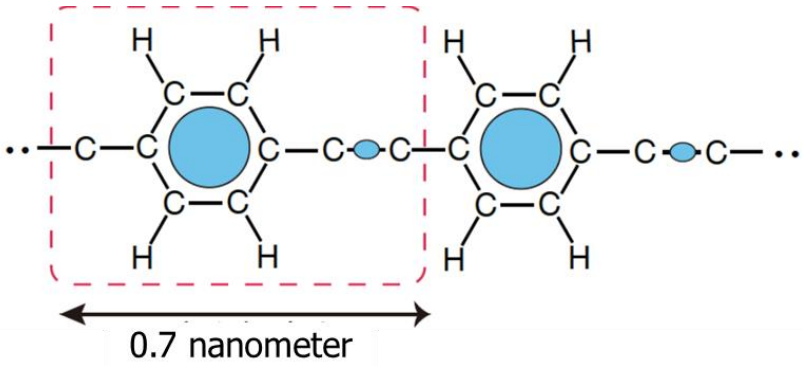
Motivation

- Organic polymer materials like poly-phenylene-ethynylene (PPE) are very attractive materials.



  - Electric current can flows on the materials.
  - Property of its easily processed is quite useful for manufacturing wearable devices.

- π electrons in benzene play an important role for electrons transfer along its long string-like polymer structure.

$\rightarrow$ Important to elucidate electron transport property

From http://main.spsj.or.jp/koho/24p/24p_9.pdf

Electron state calculation of polymers

- Time dependent Schrödinger equation $\frac{\partial \psi}{\partial t} = -iH\psi$

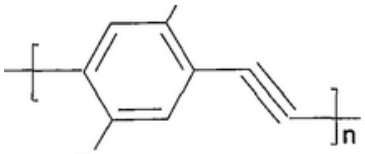
- Discretization in time by the Crank-Nicolson method

$$\frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} = -iH\frac{\psi(t+\Delta t) + \psi(t)}{2}$$

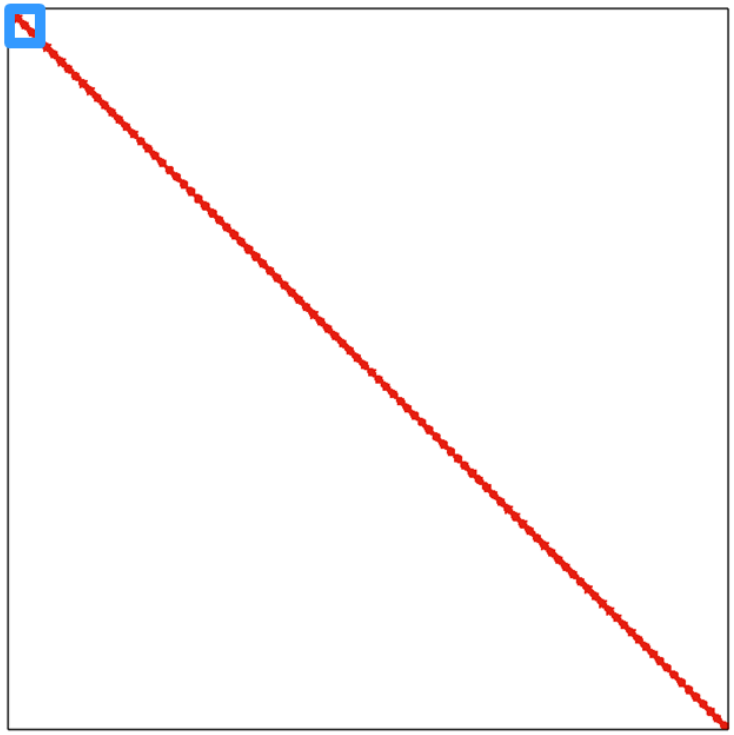
$$\Rightarrow \left(I + \frac{1}{2}i\Delta t H\right)\psi(t+\Delta t) = \left(I - \frac{1}{2}i\Delta t H\right)\psi(t)$$

- $\left(I + \frac{1}{2}i\Delta t H\right)^{-1}$ should be calculated.

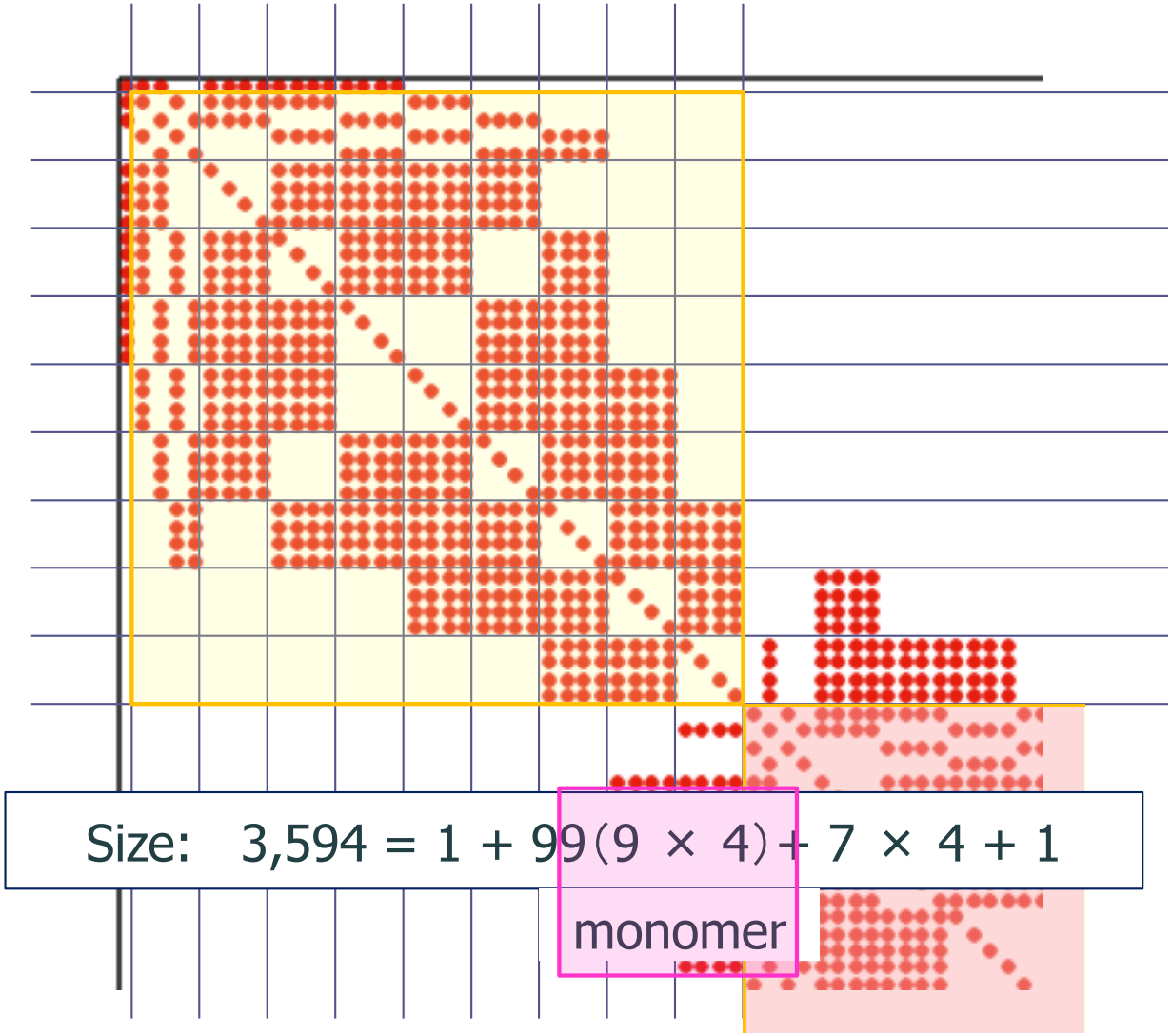
Shape of the matrix H

- Size: 3,594 × 3,594（  100）
- Number of non-zero elements: 41,781 (0.33%)
- Bandwidth: 29

$H =$



First 53 × 53 elements shape of matrix H



Trend of HPC system

- The linear system for this problem has been solved using iterative methods on the K computer.
  - Cf. H. Imachi, et al., (2016), DOI: http://dx.doi.org/10.1063/1.4968636

- Multi-core system → Many-core system

- Conventional method should be re-considered.
  - Direct method solving a linear system might be faster.

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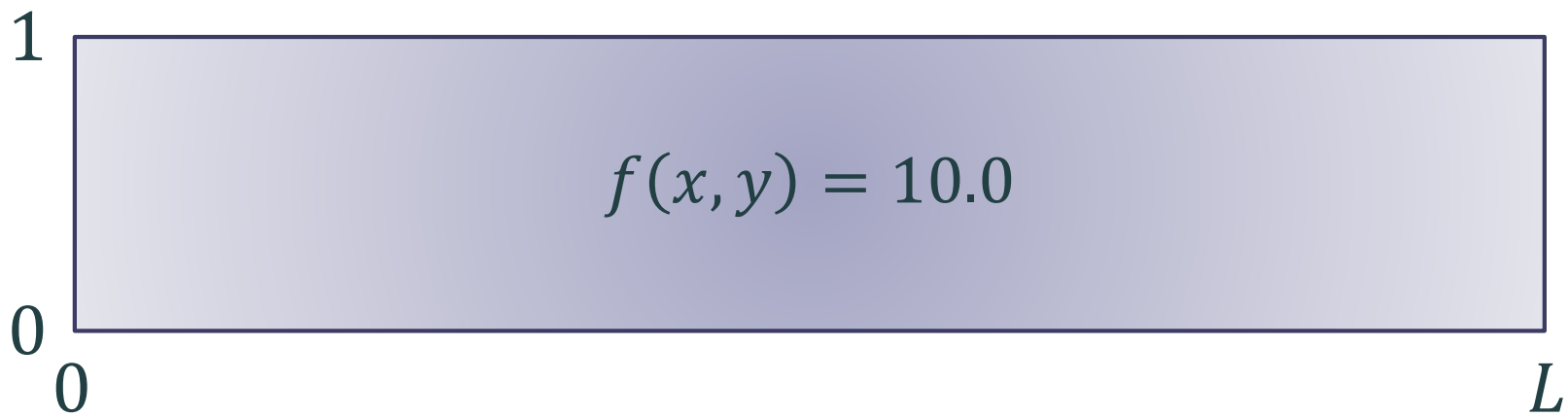
- $\left(I + \frac{1}{2}i\Delta t H\right)^{-1}$ should be calculated. ⇒ Direct method?

Reference problem

- Poisson equation

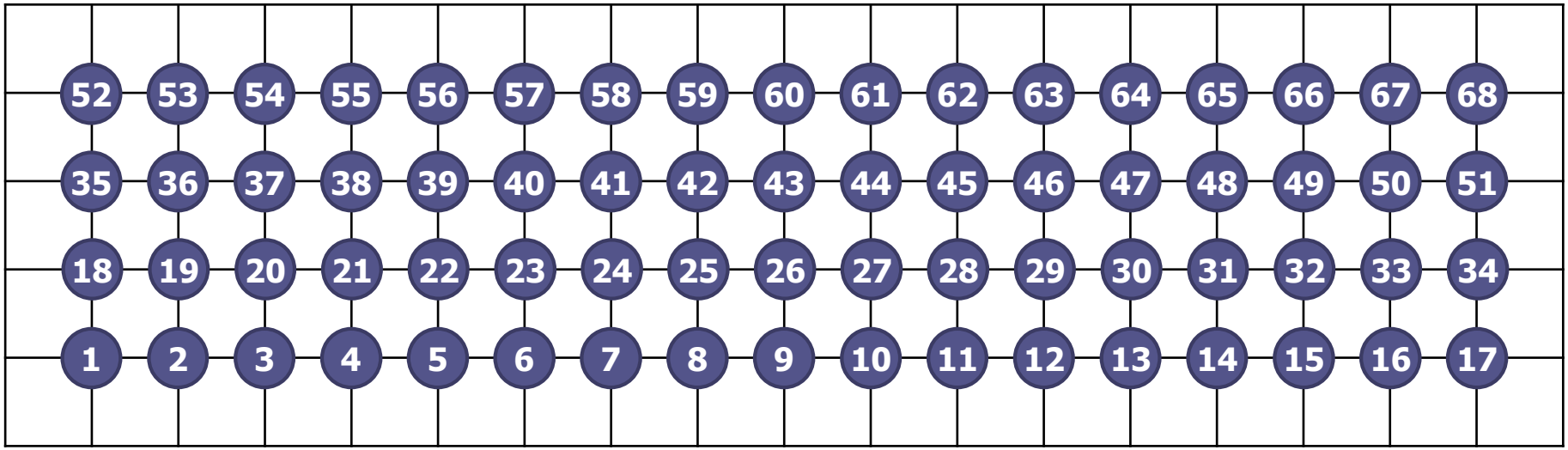
$$-\Delta u = f(x,y) \quad \text{in } \Omega = [0,L] \times [0,1]$$
$$u(x,y) = 0.0 \qquad \text{on } \partial\Omega$$



- Discretization by finite difference method $\rightarrow \quad \mathrm{A}\boldsymbol{x} = \boldsymbol{b}$

Natural ordering of variables (grid points)

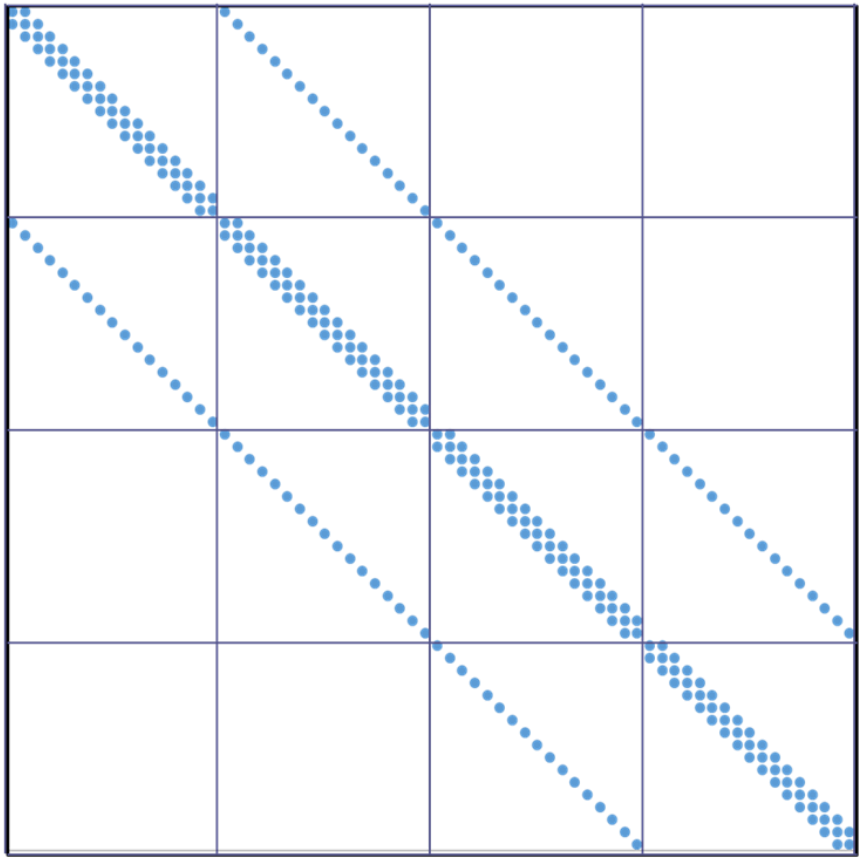
Example: 18 x 5 equi-divided regular grids



- Linear system $\mathrm{A}\boldsymbol{x} = \boldsymbol{b}$, where the size of matrix size is 68 x 68.

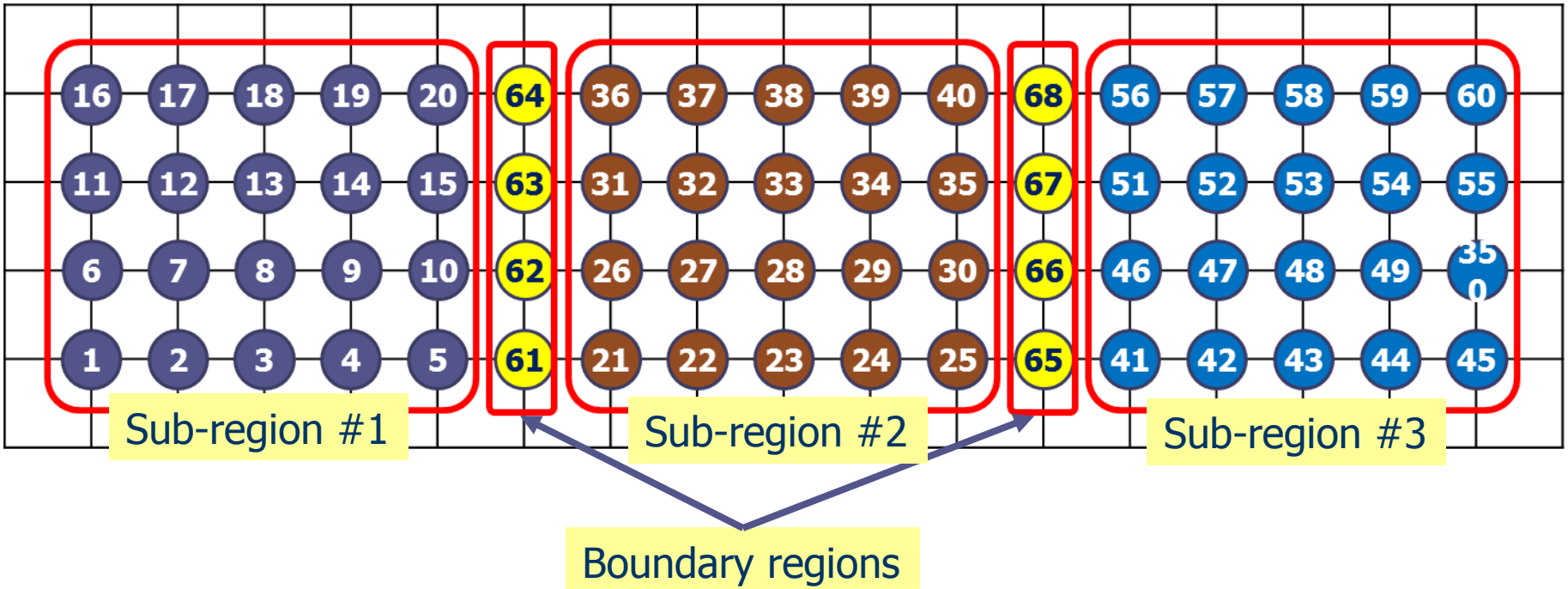
Non-zero elements of the matrix with natural ordering

$A =$



Note) This matrix is symmetric matrix.

One-way dissection ordering



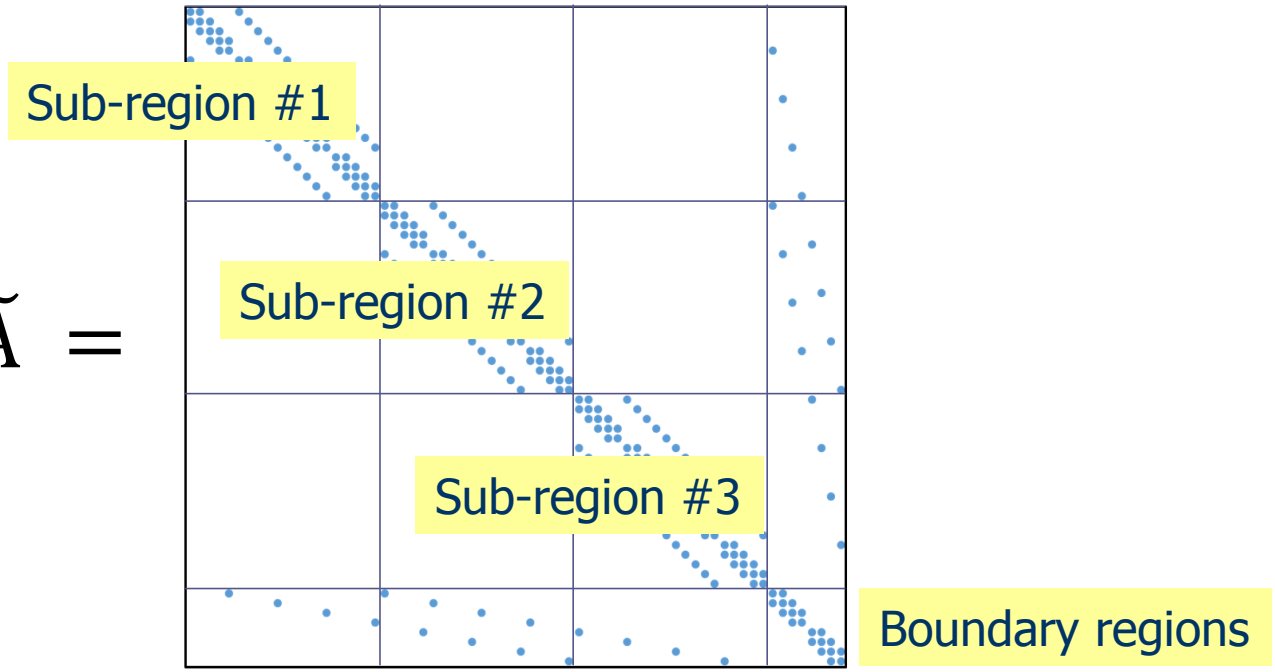
- Total number of grids $(\mathrm{N}_x \times n_y)$: 17×4
- Number of sub-regions (n_B): 3
- Number of grids in a sub-region $(n_x \times n_y)$: 5×4
- Number of grids in boundary regions: $(n_\mathrm{B} - 1) \times n_y = 8$

Non-zero elements by one-way dissection ordering

- Permutation Matrix P can change the ordering of variables.

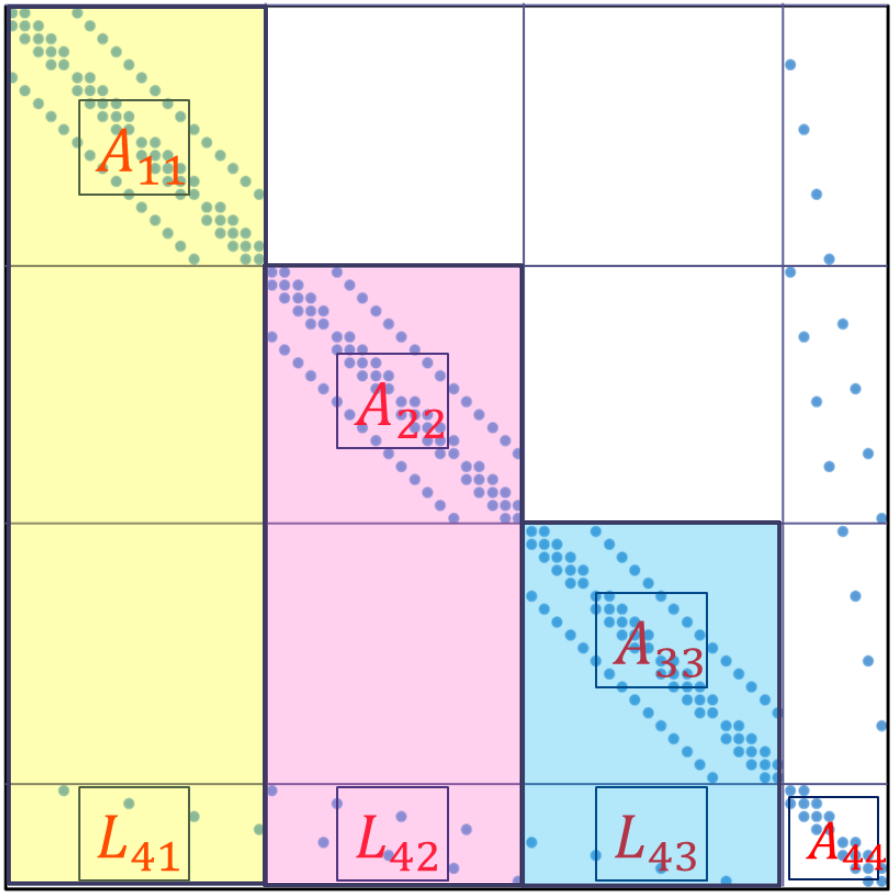
$$(\mathrm{PAP^t})(\mathrm{P}\boldsymbol{x}) = \mathrm{P}\boldsymbol{b} \quad \rightarrow \quad \tilde{\mathrm{A}}\,\tilde{\boldsymbol{x}} = \tilde{\boldsymbol{b}}$$

$\tilde{\mathrm{A}} =$



- Cholesky decomposition is applied to obtain LL^t form.

Parallelization of Cholesky decomposition



① A_{11}, L_{41} : LL^t *decomp.*

② A_{22}, L_{42} : LL^t *decomp.*

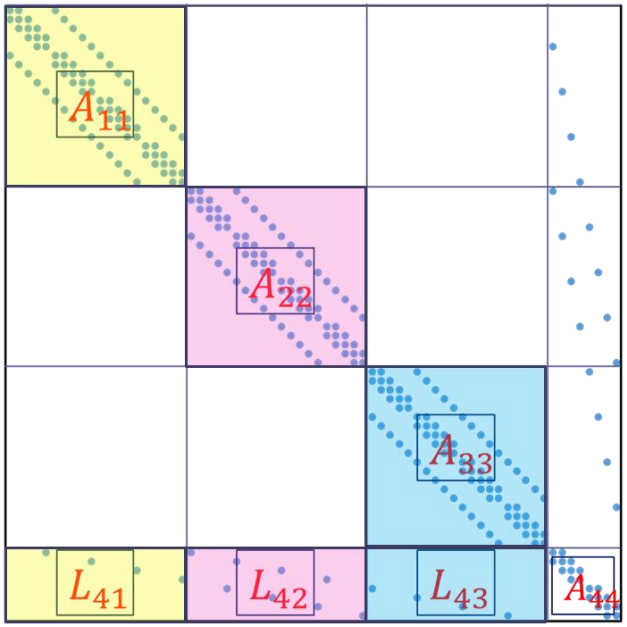
③ A_{33}, L_{43} : LL^t *decomp.*

④ $\widetilde{A_{44}} = A_{44} - \sum_{i=1}^{3} L_{4i} {L_{41}}^t$

⑤ $\widetilde{A_{44}}$: LDL^t *decomp.*

①, ②, and ③ can be calculated concurrently.

Algorithm for obtaining LL^{t} form



① A_{ii} $(\mathrm{i} = 1 \ldots\ldots n_{\mathrm{B}})$ are decomposed concurrently.

② $L_{n_{\mathrm{B}}\mathrm{i}}$ $(\mathrm{i} = 1 \ldots\ldots n_{\mathrm{B}})$ are decomposed concurrently.

③ Calculate $\widetilde{A_{n_{\mathrm{B}}n_{\mathrm{B}}}} = A_{n_{\mathrm{B}}n_{\mathrm{B}}} - \sum_{\mathrm{i}=1}^{n_{\mathrm{B}}} L_{n_{\mathrm{B}}\mathrm{i}}\, L_{n_{\mathrm{B}}\mathrm{i}}{}^{\mathrm{t}}$

Reduction

Matrix multiplication: Parallelizable

④ Finally, $\widetilde{A_{n_{\mathrm{B}}n_{\mathrm{B}}}}$ are decomposed.

Evaluation of parallel performance

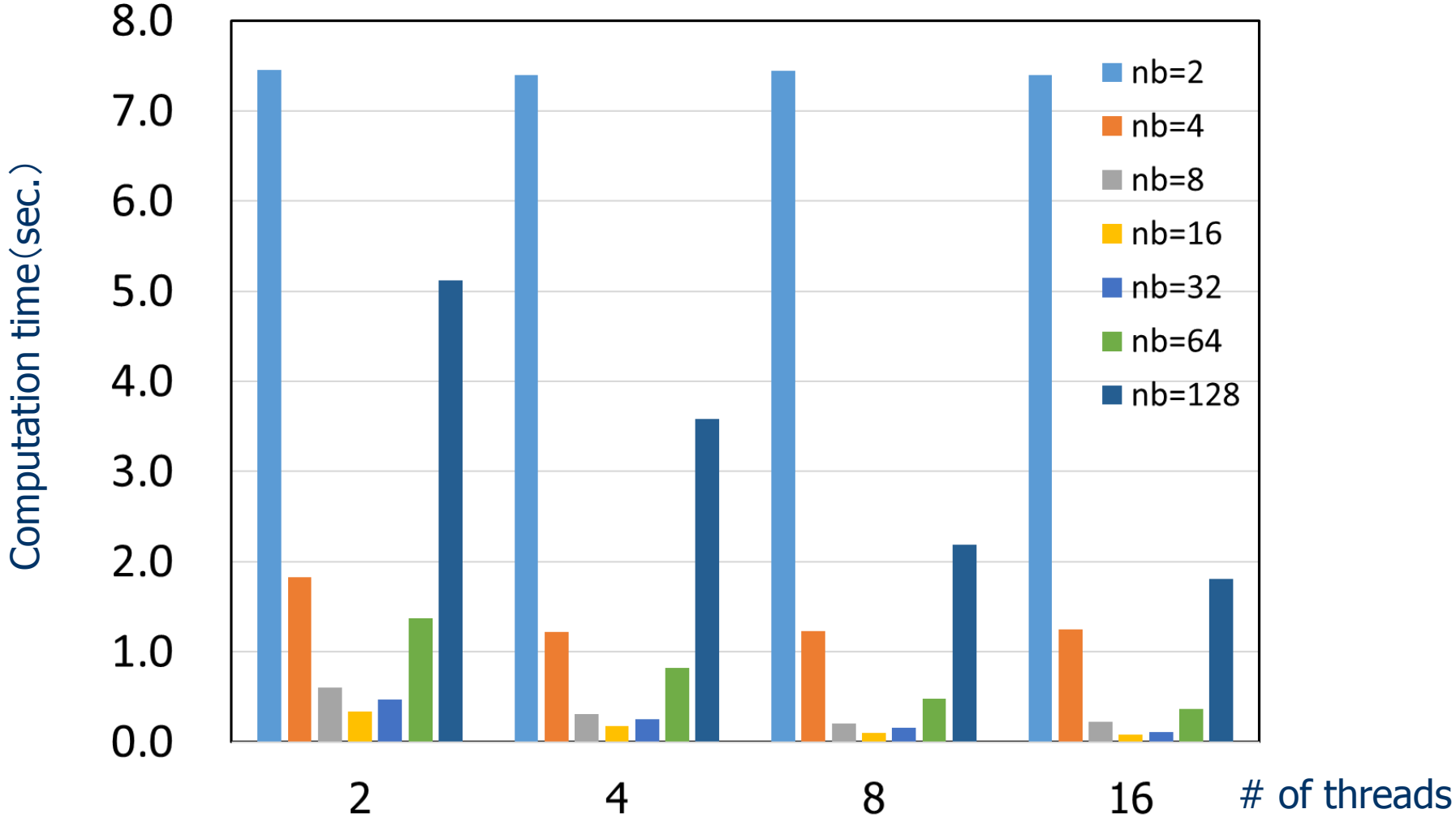
- Parameters

	Case 1	Case 2
Total number of grids ($\mathrm{N}_x \times \mathrm{N}_y$)	639 x 9	2047 x 49
Number of sub-regions (n_B)	2, 4, 8, 16, 32, 64, 128	16, 32, 64, 128

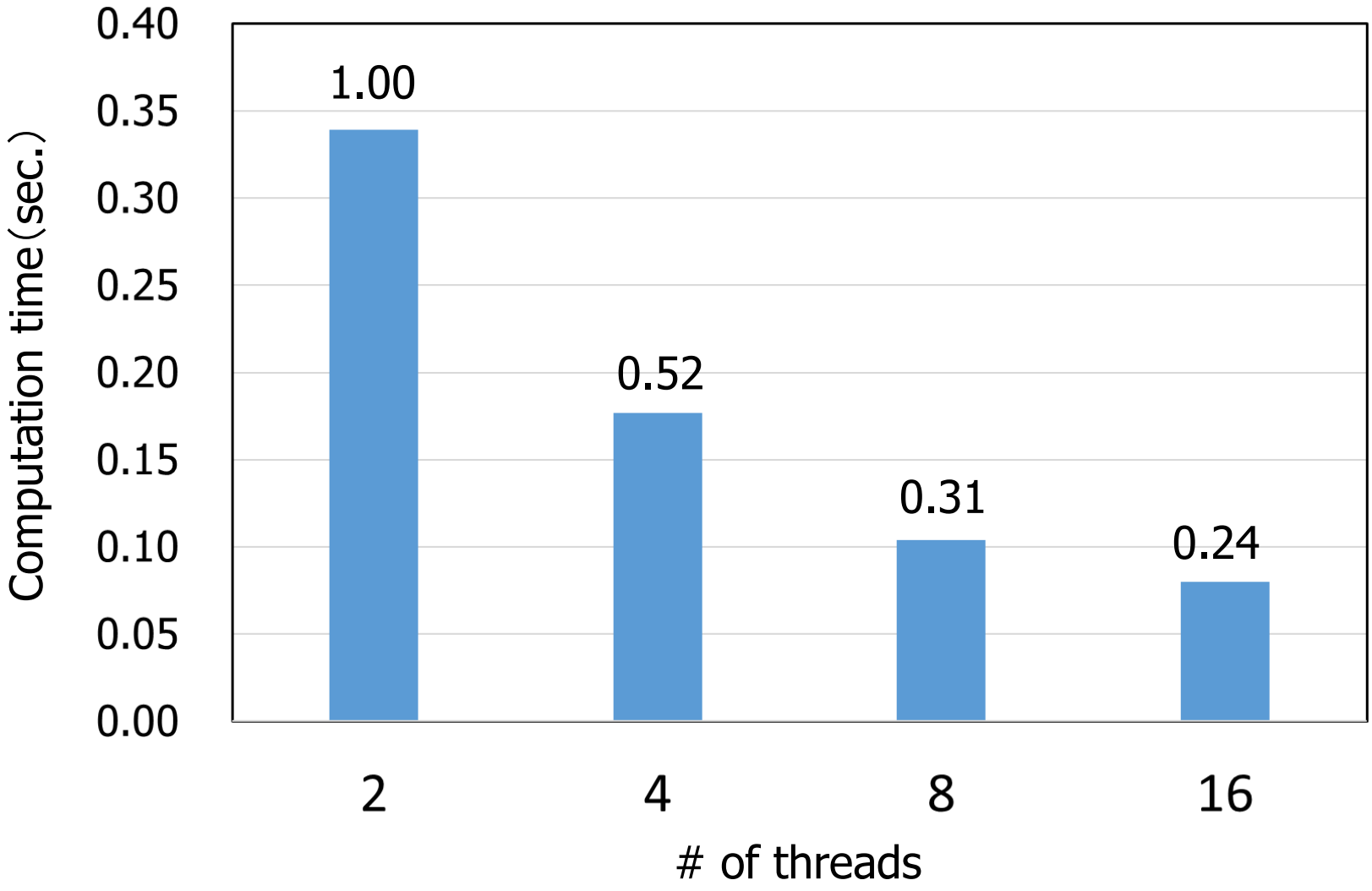
  - Number of thread(s): 1, 2, 4, 8, 16

- System used in evaluation
  - Fujitsu FX10 (SPARC64 IXfx, 16 cores in a socket)
  - Compiler (frtpx –Kfast,openmp)

[Case 1] # of threads vs. # of sub-regions n_{B}



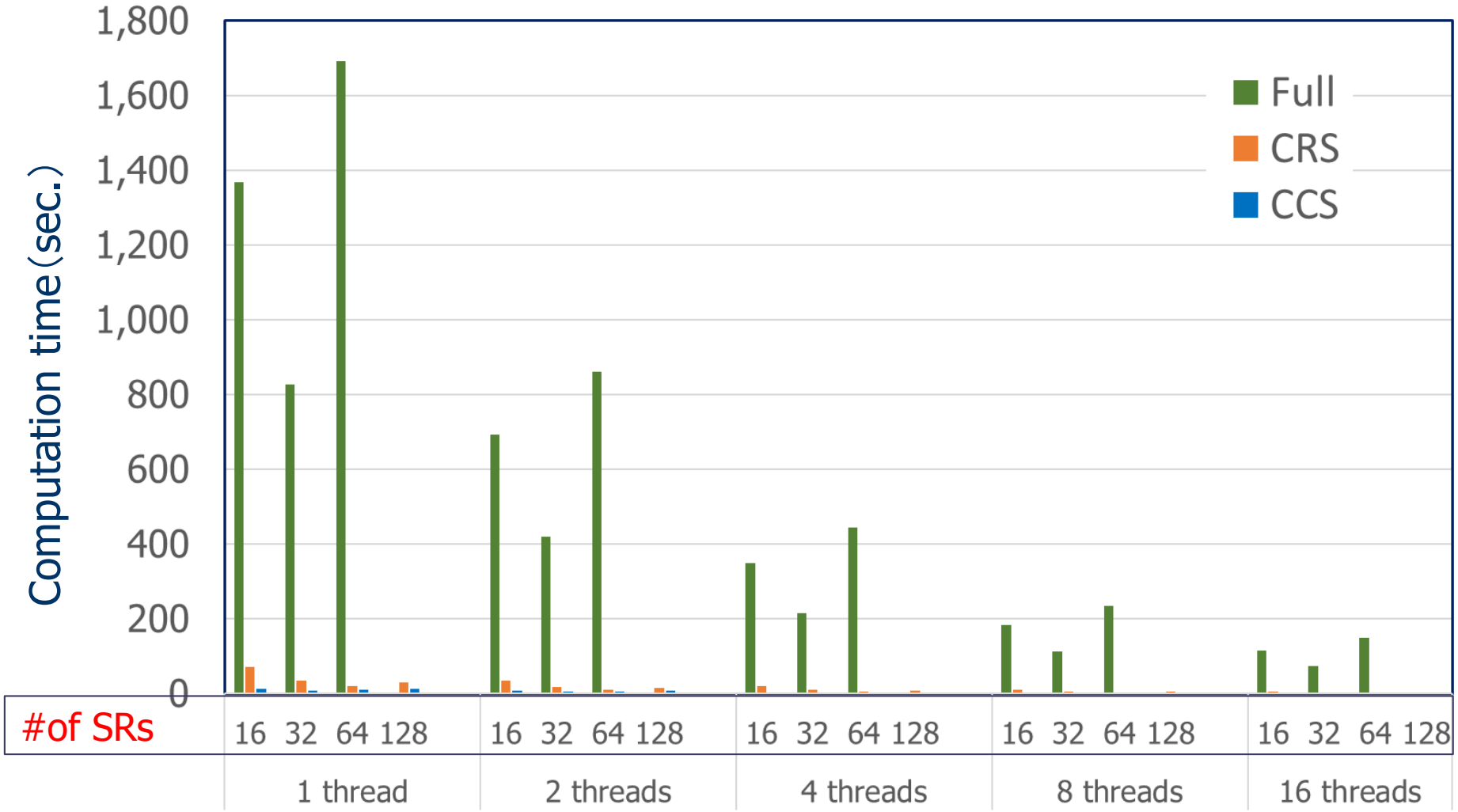
[Case 1] Scalability for the number of sub-regions $n_{\mathrm{B}} = 16$



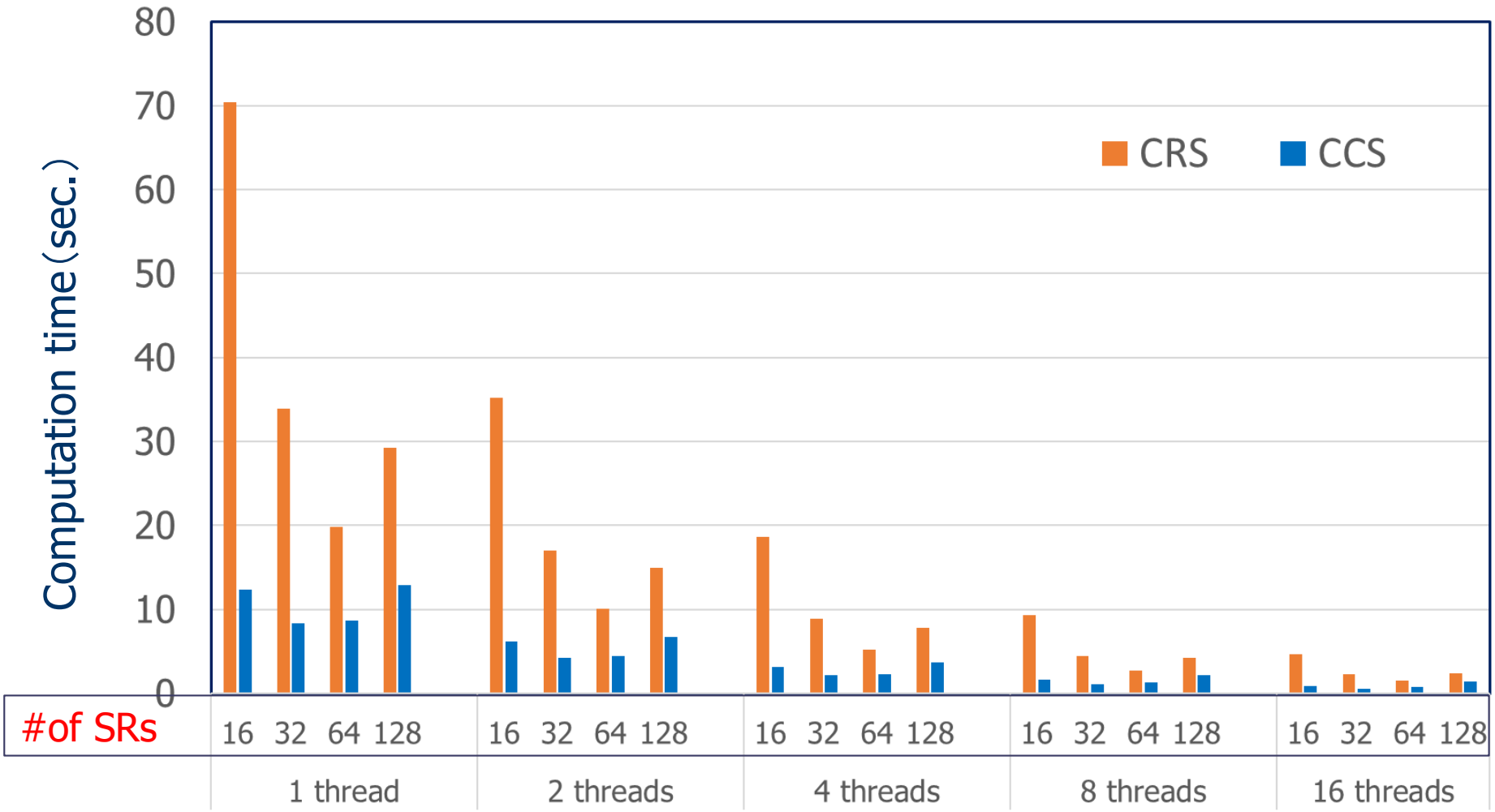
Application of CRS and CCS representations to the algorithm

- CRS (Compressed Row Storage) and CCS (Compressed Column Storage) were considered in the implementation
- We expected computation time was drastically decreased.

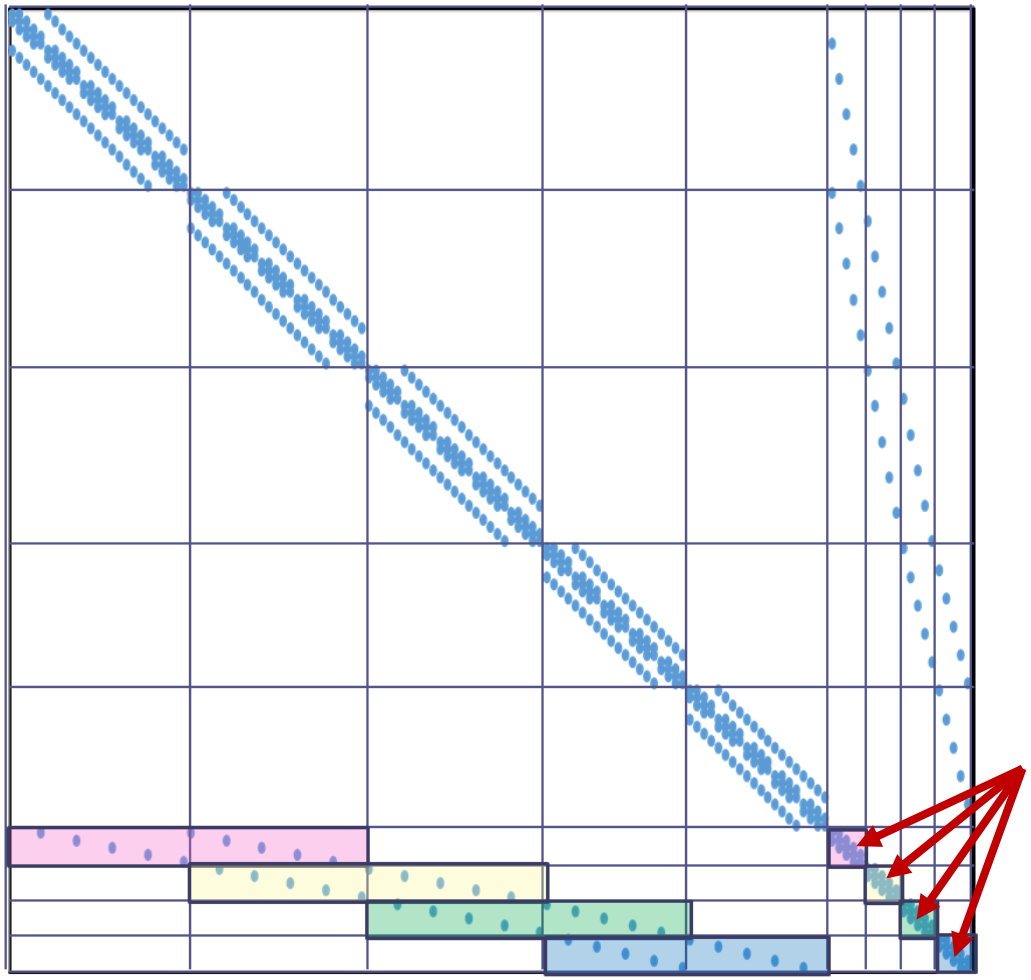
[Case 2] Time for three implementations



[Case 2] Comparison between CRS versus CCS



Parallelization of decomposition at the last part



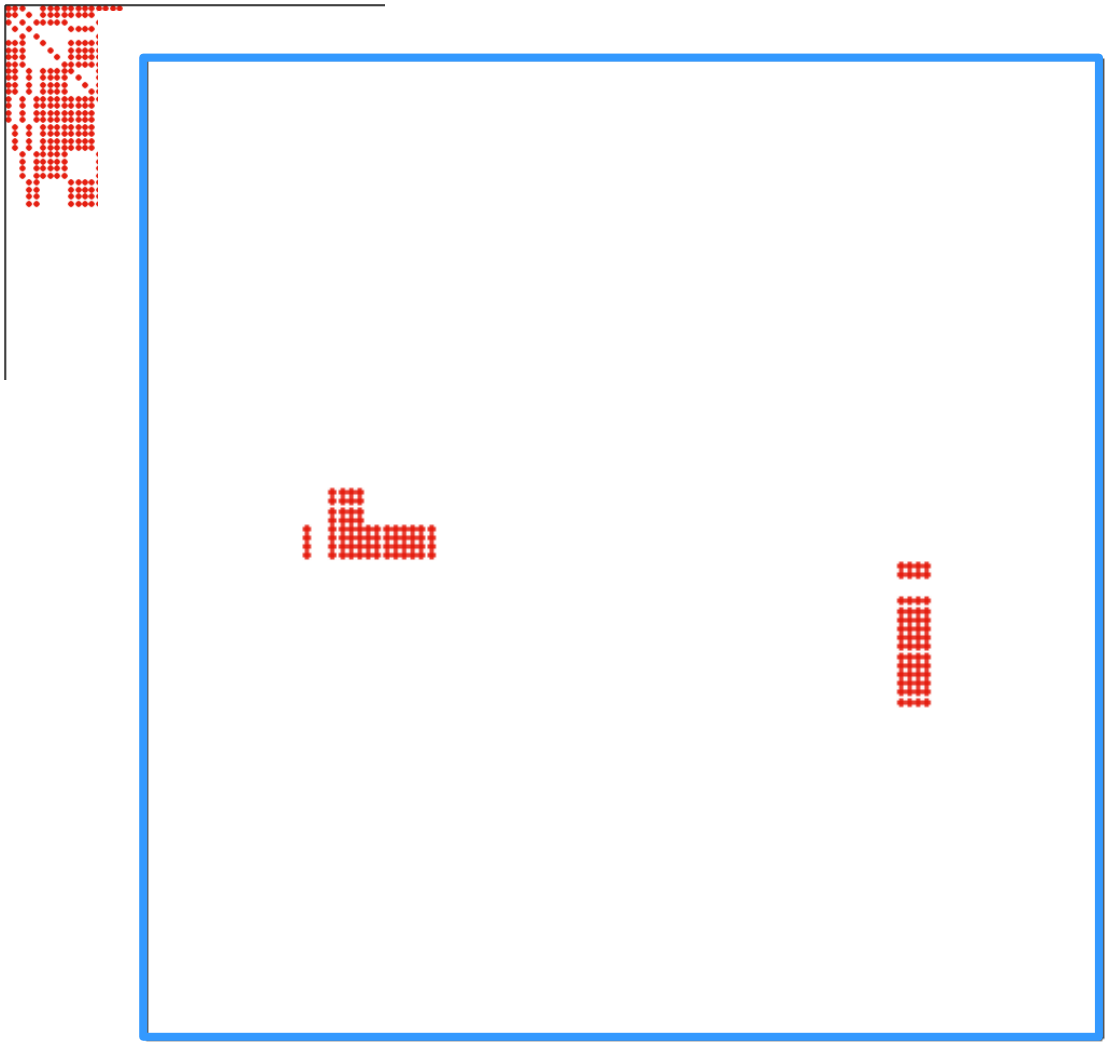
Summary

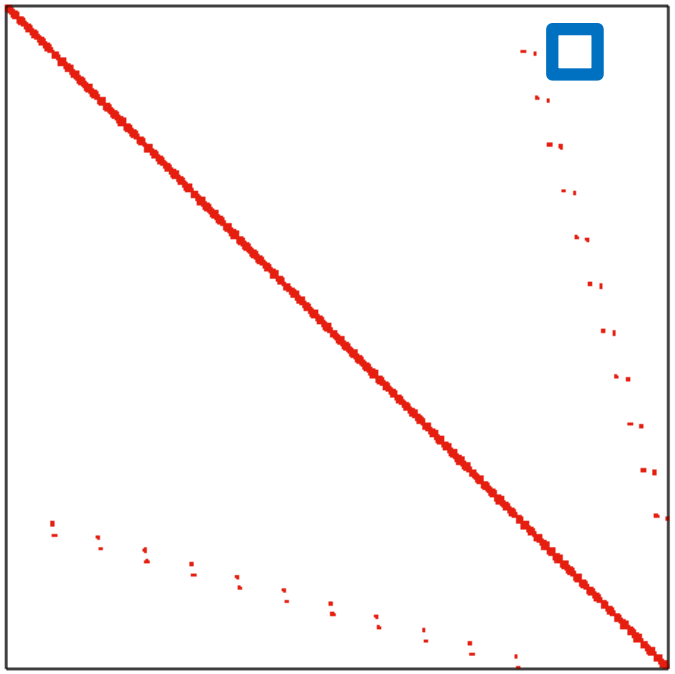
- One-way dissection ordering was applied to parallelize LU decomposition for a linear system with sparse symmetric matrix.
  - Thread parallelization had good scalability, in case that an appropriate division of computational region was taken.
  - Implementation with CCS representation is quite good for the solution of the Poisson equation.

Further studies

- Hybrid parallelization should be implemented and evaluated.
- Electronic structure calculation of organic polymer materials will be carried out. Comparison with iterative solvers should be considered.

Application of one-way dissection ordering to the matrix *H*





# of sub-regions	11
# of elements in sub-regions	252
# of elements in boundaries	72x10

Thank you for your attention!