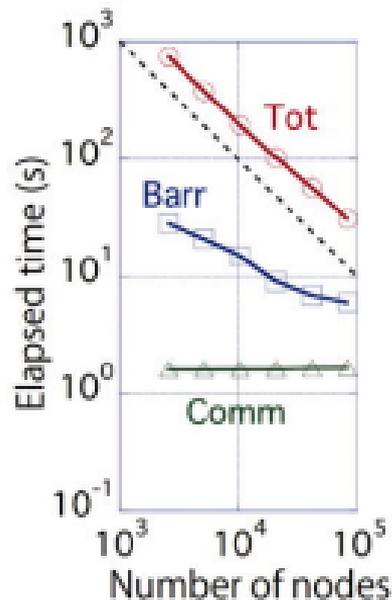


Extremely scalable algorithm for 10^8 -atom quantum material simulation on the full system of the K computer

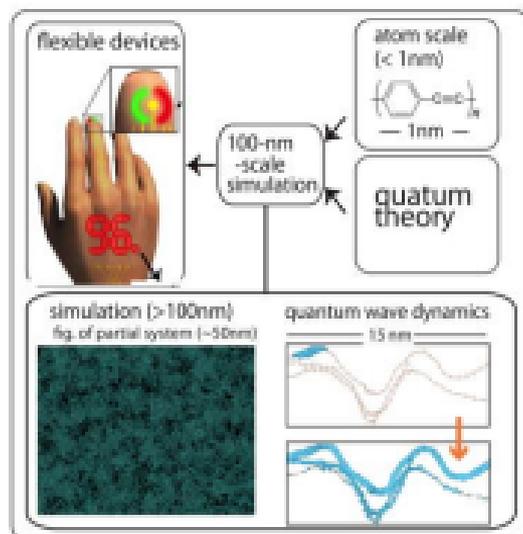
T. Hoshi, H. Imachi (Tottori U),

K. Kumahata, M. Terai, K. Miyamoto, K. Minami and F. Shoji (RIKEN-AICS)

1. Algorithm



2. Application



Acknowledgement :
M. Ishida
(Sumitomo Chemical
Co.)

Application-Algorithm-Architecture co-design

Application : Quantum material simulationn



Algorithm : Numerical linear algebra



Architecture : The K computer



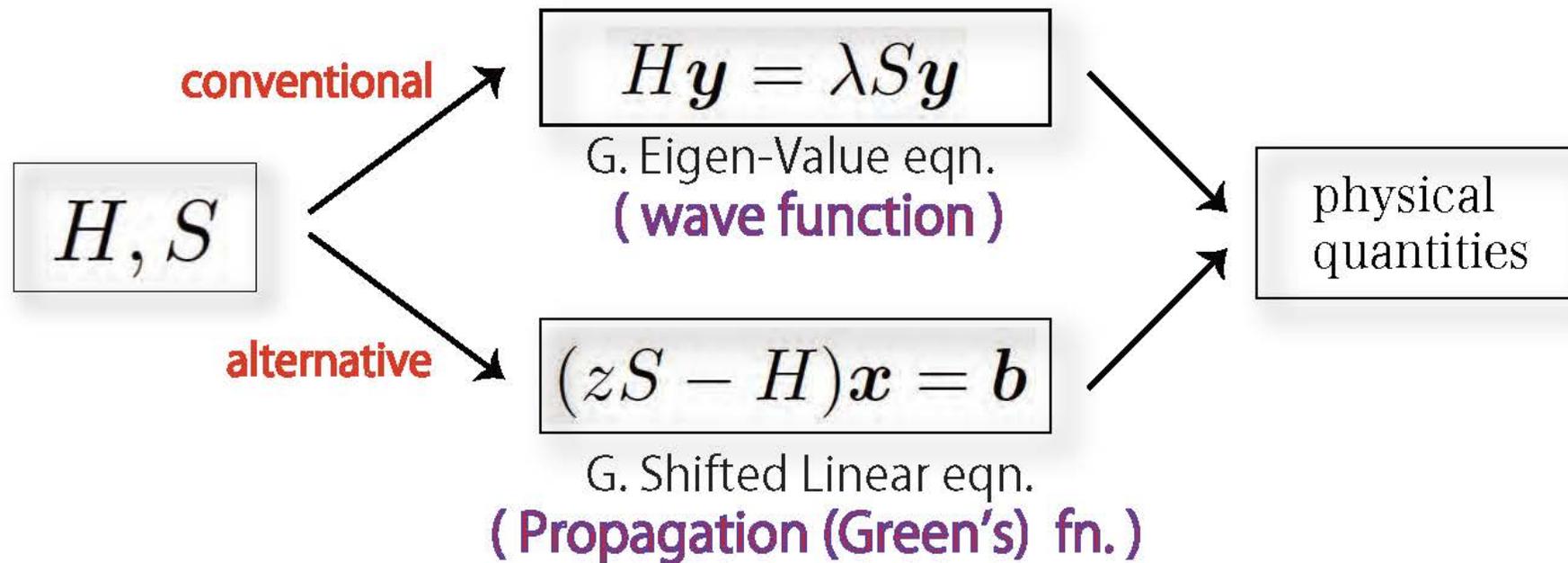
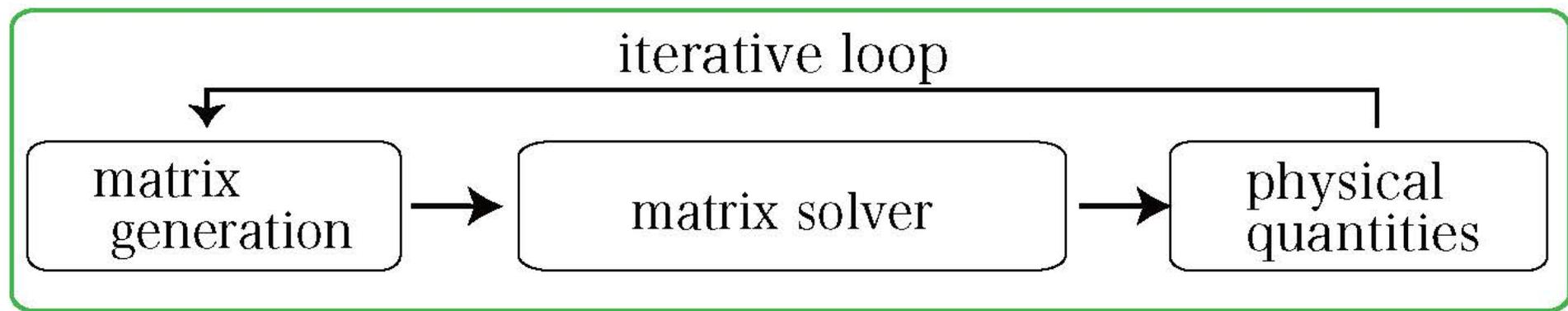
$$Hy = \lambda Sy$$

$$(zS - H)x = b$$



Ground algorithm design

Workflow of electronic structure calculations



Basic equations

Generalized eigen-value (GEV) equation

$$H\mathbf{y}_k = \varepsilon_k S\mathbf{y}_k$$

H, S : Hermitian, S : positive definite ($S \doteq I$)

wavefunction
formulation

$$G = \sum_k \frac{\mathbf{y}_k \mathbf{y}_k^T}{z - \varepsilon_k}$$

Generalized shifted linear (GSL) equations

$$(zS - H)\mathbf{x} = \mathbf{b} \quad (z : \text{complex energy})$$

non-Hermitian

$$\rightarrow \mathbf{x} = G\mathbf{b}$$

with $G \equiv (zS - H)^{-1}$: the Green's function

the propagation
(Green's) function
formulation

Highly parallelizable mathematical structure

A pioneering work : W. Kohn, Phys. Rev. Lett. (1996) (W. Kohn won the Nobel Prize at 1998.)

Generalized eigen-value problem

$$H\mathbf{y}_k = \lambda_k S\mathbf{y}_k \quad (1)$$

Physical quantity with a given matrix X
(Ex. the case of $X = H$
--> Electronic structure energy)

$$\langle X \rangle \equiv \sum_k f(\lambda_k) \mathbf{y}_k^t X \mathbf{y}_k \quad (2)$$

with a given weight function
(‘Fermi distribution function’)

$$f(\lambda) \equiv \frac{1}{\exp(\beta(\lambda - \mu)) + 1} \quad (3)$$

(β, μ : given parameters)

Physical quantity in trace form

$$\langle X \rangle = \text{Tr}[X\rho] \quad (4)$$

with the density matrix

$$\rho \equiv \sum_k f(\lambda_k) \mathbf{y}_k \mathbf{y}_k^t \quad (5)$$

Decomposition of the trace form

$$\text{Tr}[\rho X] = \sum_j \underbrace{\mathbf{e}_j^t \rho X \mathbf{e}_j}_{\text{‘projected physical quantity’}} \quad (6)$$

**‘projected physical quantity’
calculated in parallelism**

with \mathbf{e}_j (j-th unit vector)

$$\mathbf{e}_j \equiv (0, \dots, 0, 1_j, 0, \dots, 0)^t \quad (7)$$

Highly parallelizable mathematical structure

The trace decomposition

$$\text{Tr}[\rho X] = \sum_j \boxed{e_j^t \rho X e_j} \quad (6)$$

gives the generalized shifted linear (GSL) equations for calculation of projected physical quantities (PPQ).

GSL eqns.

$$(zB - A)\mathbf{x}^{(1)} = \mathbf{e}_1$$

$$(zB - A)\mathbf{x}^{(2)} = \mathbf{e}_2$$

$$(zB - A)\mathbf{x}^{(3)} = \mathbf{e}_3$$

⋮

PPQ

$$\boxed{e_1^T \rho X e_1}$$

$$\boxed{e_2^T \rho X e_2}$$

$$\boxed{e_3^T \rho X e_3}$$

⋮

$$\langle X \rangle = \text{Tr}[\rho X]$$

Highly parallelizable mathematical structure

Simplified explanation

- decomposition of the trace form
- calculation of trace elements as parallel computation

$$\text{Tr}[A] = A_{11} + A_{22} + \dots + A_{MM}$$


The diagram shows a horizontal line with three upward-pointing arrows. The first arrow points to A_{11} , the second to A_{22} , and the third to A_{MM} . A horizontal line connects the bases of these three arrows, with the text "parallel computation" centered below it.

parallel computation

Highly parallelizable mathematical structure

Note on implementation.

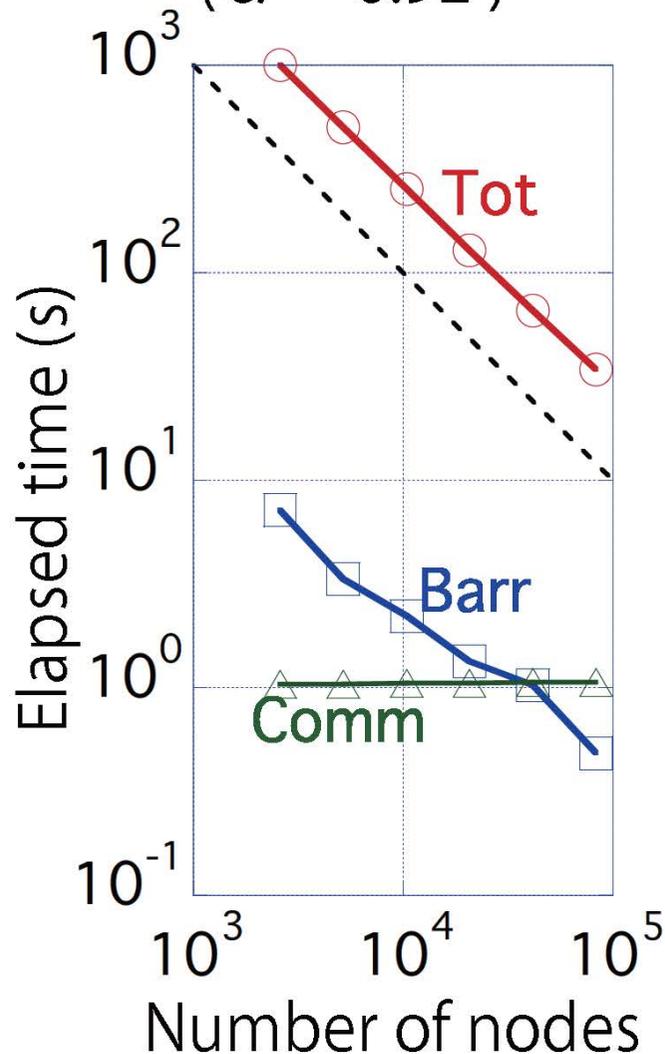
- (a) MPI/OpenMP hybrid parallelism is used and each trace element (A_{jj}) is calculated as single-core (single-thread) computation
- (b) (Max # of parallelism)
 - = (matrix dimension) in principle
 - (# of atoms) in our code
 - ex. 10^8 -atom system → 10^8 -core calculation is possible
- (c) the severest bottleneck of the K computer
 - The limitation of build-in memory size (16 GB / node)
 - ex. 10^8 atom system consumes 9 GB per node
- (d) Flat MPI is also possible in our code
 - but consumes much larger memory

Result : strong scaling upto the full system of the K computer

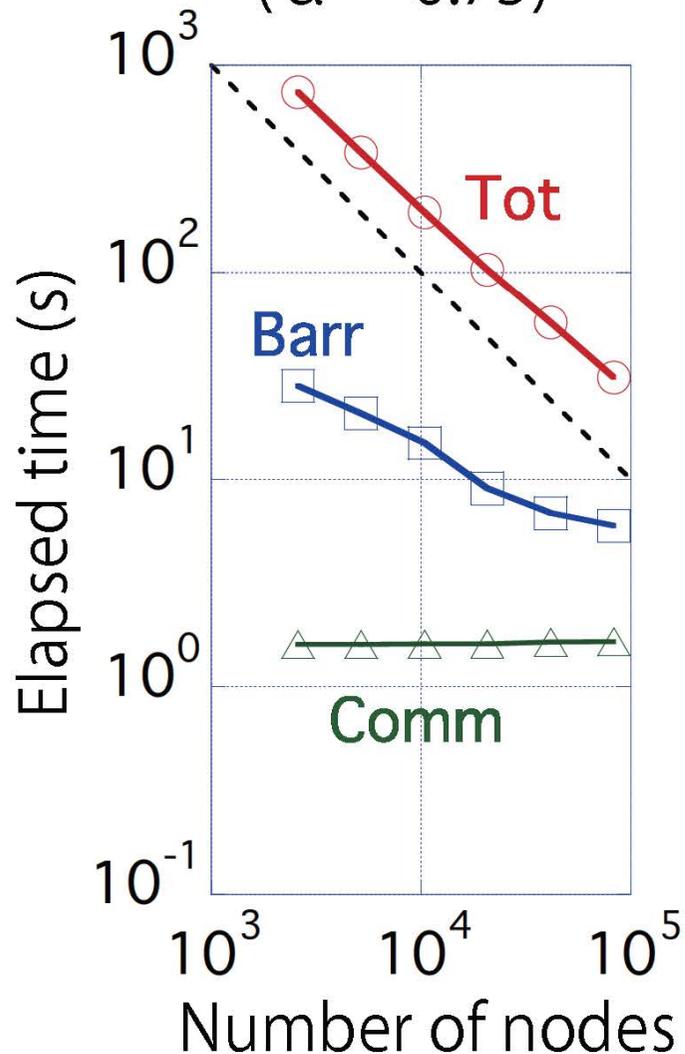
100-nm-scale or 10^8 atoms calculations

parallel efficiency ratio α is determined with the reference data with 2,592 nodes.

(a) ideal diamond crystal
($\alpha = 0.92$)



(b) condensed polymer
($\alpha = 0.75$)



Tot : total elapsed time
Barr: barrier time
Comm: MPI communication time

Result : strong scaling upto the full system of the K computer

100-nm-scale or 10^8 atoms calculations

parallel efficiency ratio α is determined with the reference data with 2,592 nodes.

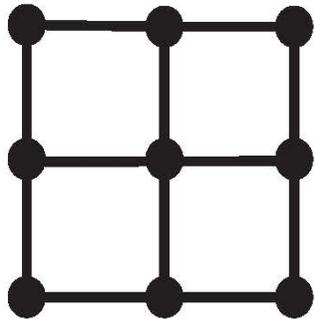
(a) ideal diamond crystal
($\alpha = 0.92$)

(b) condensed polymer
($\alpha = 0.75$)

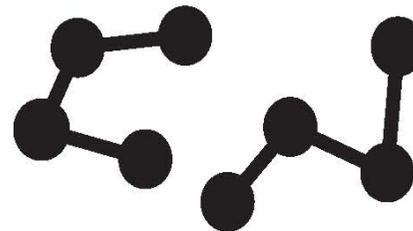
Note

A higher parallel efficiency ($\alpha = 0.92$) appears in (a) the ideal diamond case, because the atomic structure is ideal or exactly periodic and the tasks are equivalent among nodes.

(a) ideal crystal (schematic)



(b) condensed polymer (schematic)



Tot : tot elapsed

er time

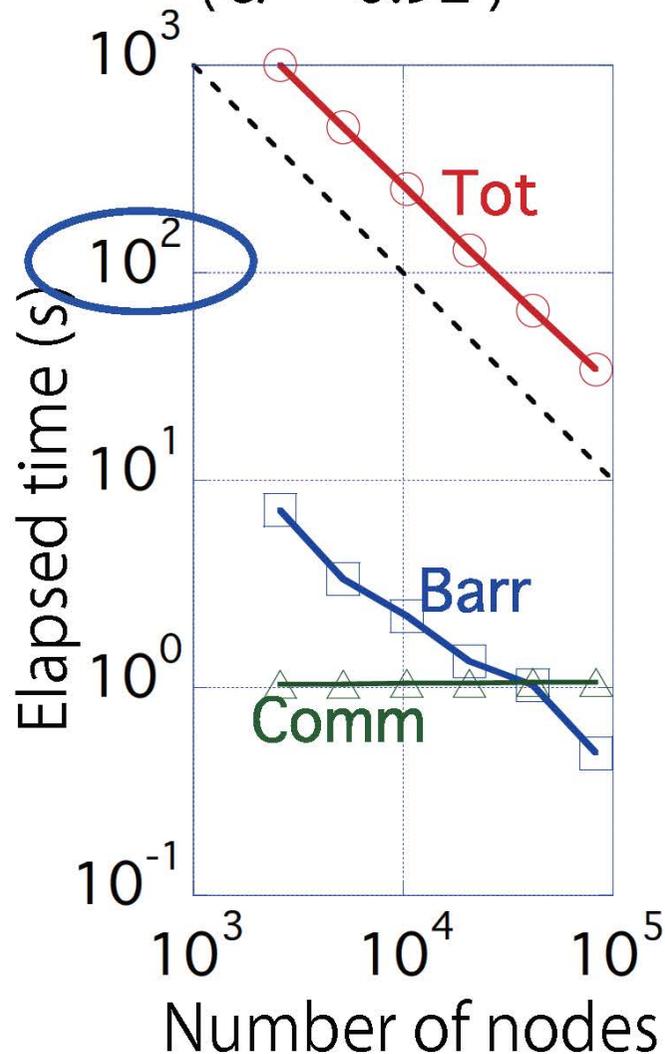
ation time

Result : strong scaling upto the full system of the K computer

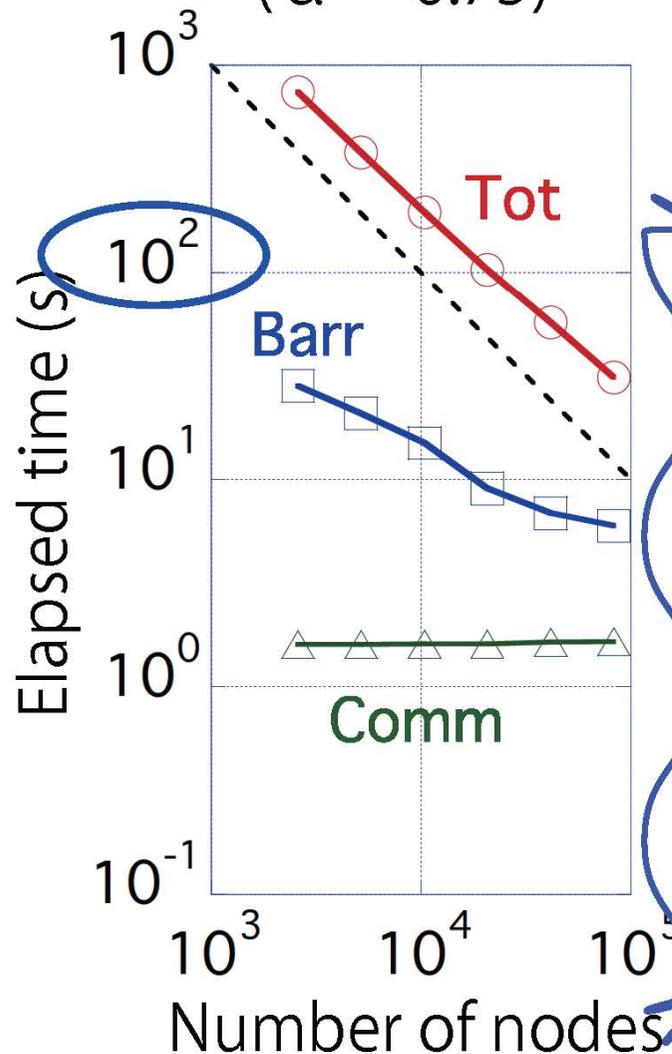
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Note:

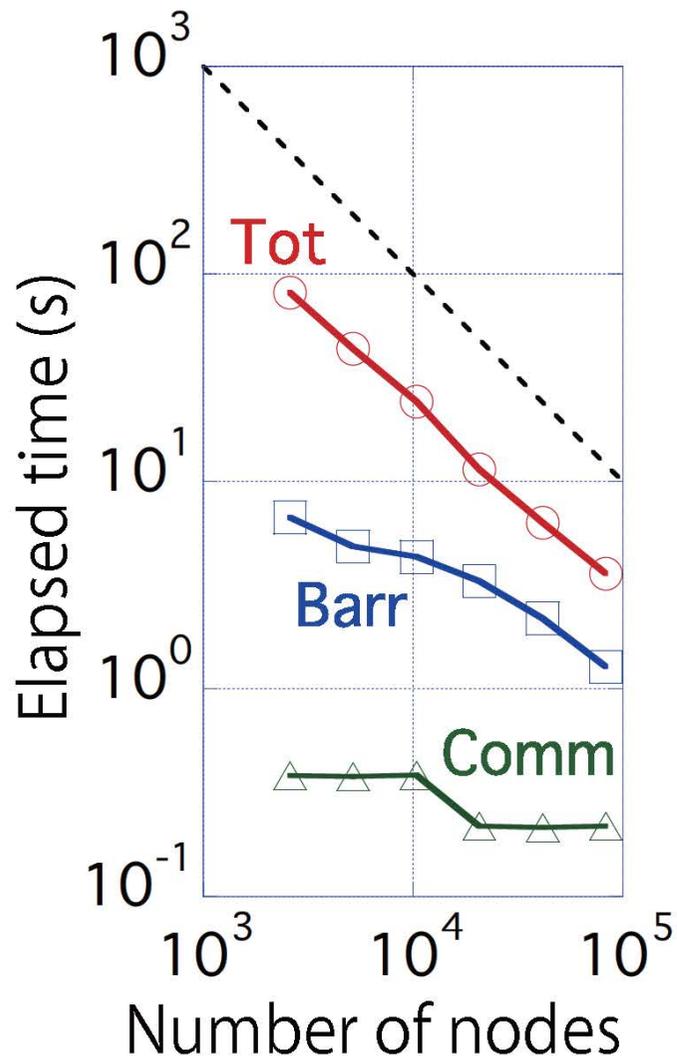
Elapsed time of 10^2 sec is a qualified time-to-solution in real research.

Ex. quantum mechanical MD with 10^3 time steps
→ Total simulation time is $10^2 \times 10^3 = 10^5$ sec
≐ 1day

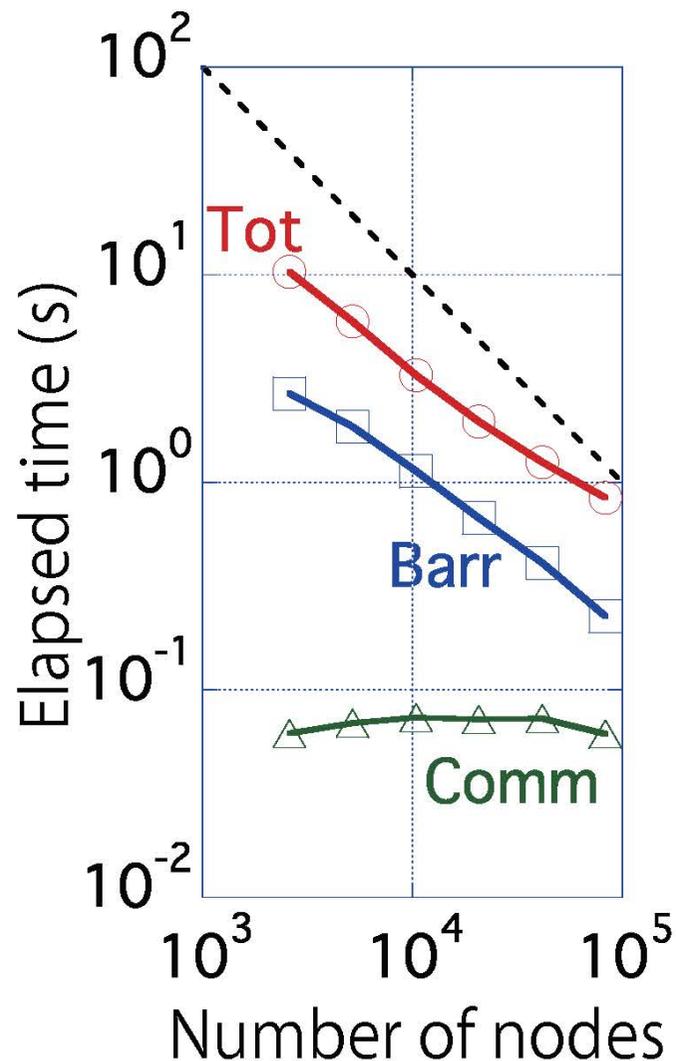
Result : strong scaling upto the full system of the K computer

Smaller samples of condensed polymers

(c) 10^7 -atom system
($\alpha = 0.71$)



(d) 10^6 -atom system
($\alpha = 0.38$)

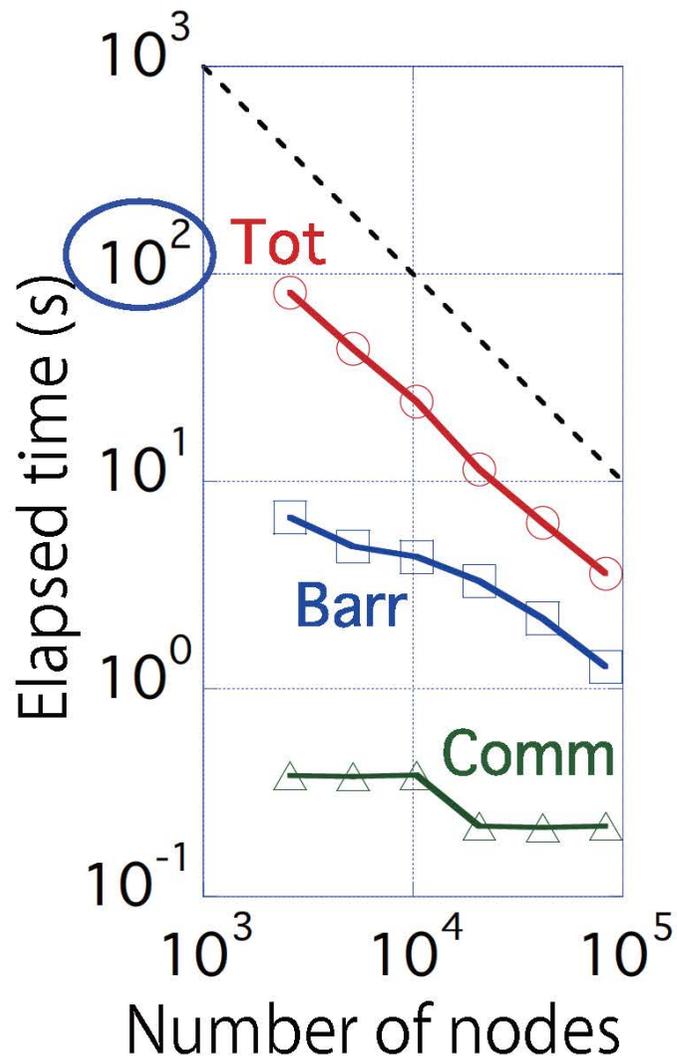


Tot : total elapsed time
Barr: barrier time
Comm: MPI communication time

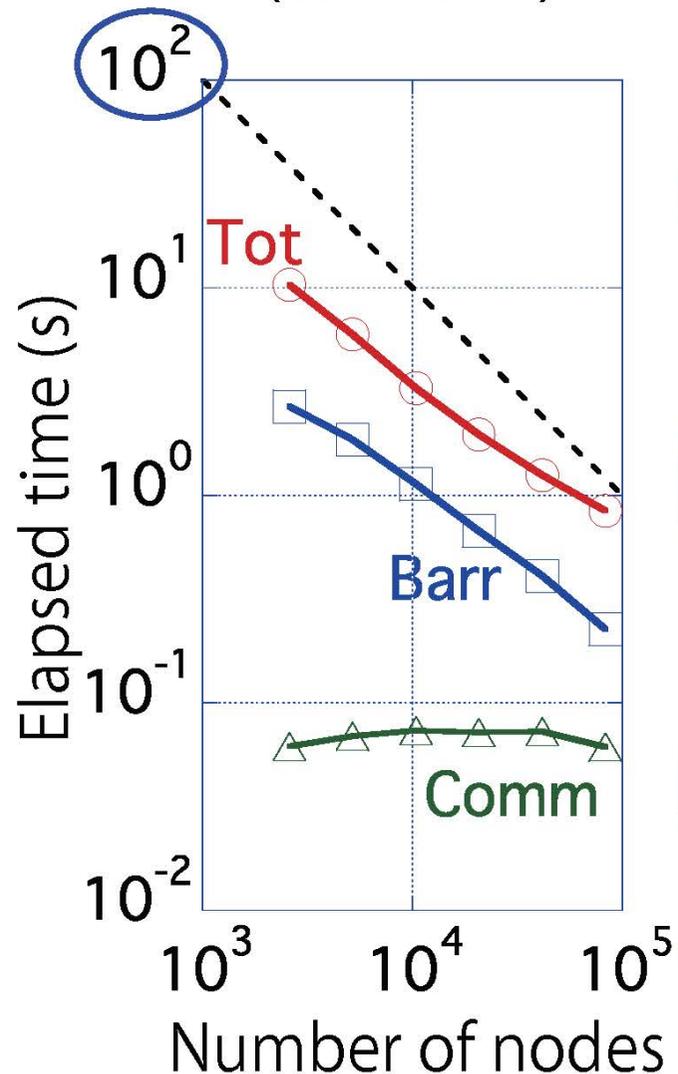
Result : strong scaling upto the full system of the K computer

Smaller samples of condensed polymers

(c) 10^7 -atom system
($\alpha = 0.71$)



(d) 10^6 -atom system
($\alpha = 0.38$)



Tot: total elapsed

Note:

The parallel efficiency ratio α is smaller than 10^8 -atom system, but the result shows the qualified time-to-solution ($< 10^2$ sec).

→ satisfactory to real research

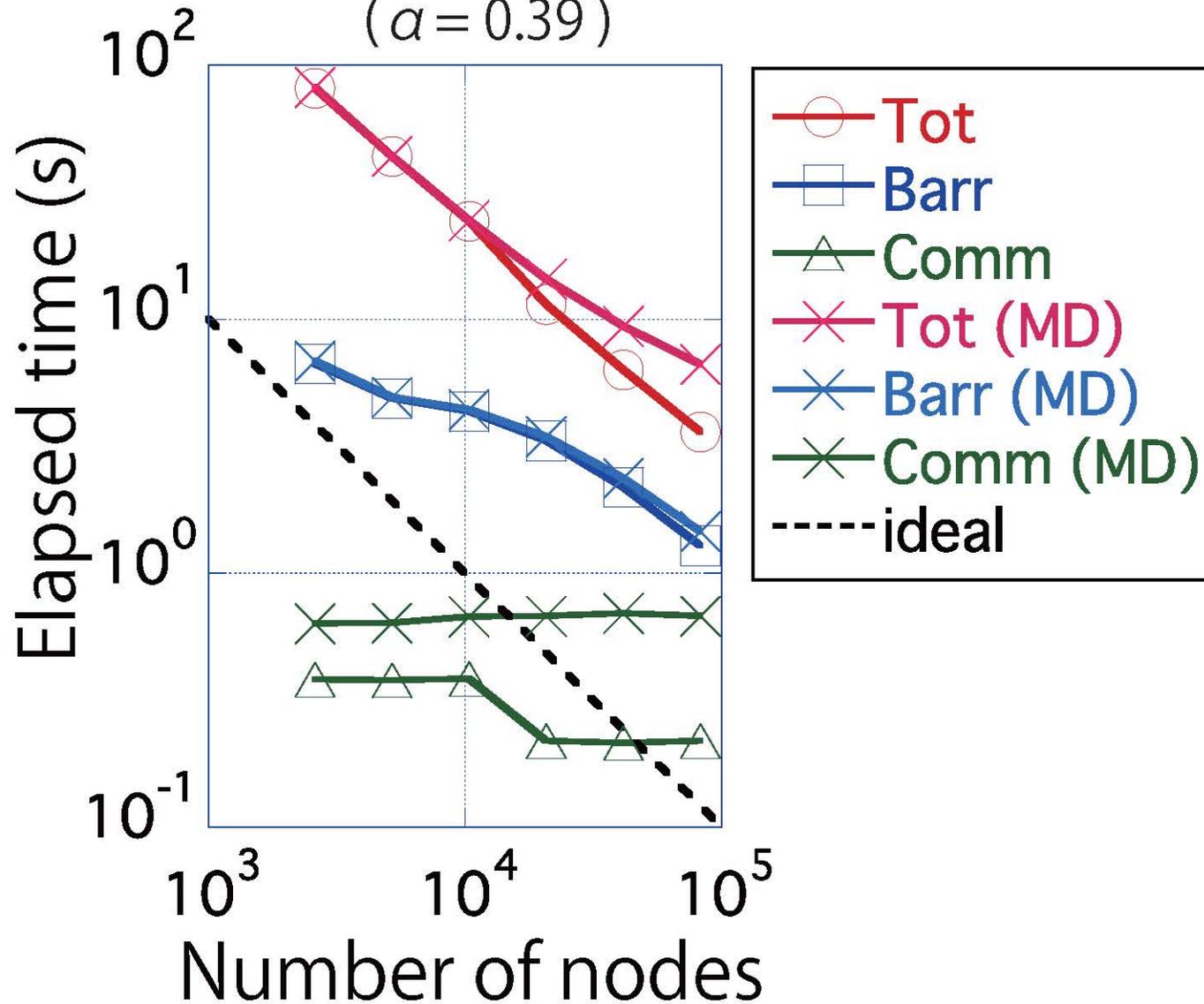
Result : strong scaling upto the full system of the K computer

Bench mark with quantum mechanical MD simulation

→ additional time and memory costs for calculation of force and velocity

Condensed polymer with 10^7 atoms

($\alpha = 0.39$)



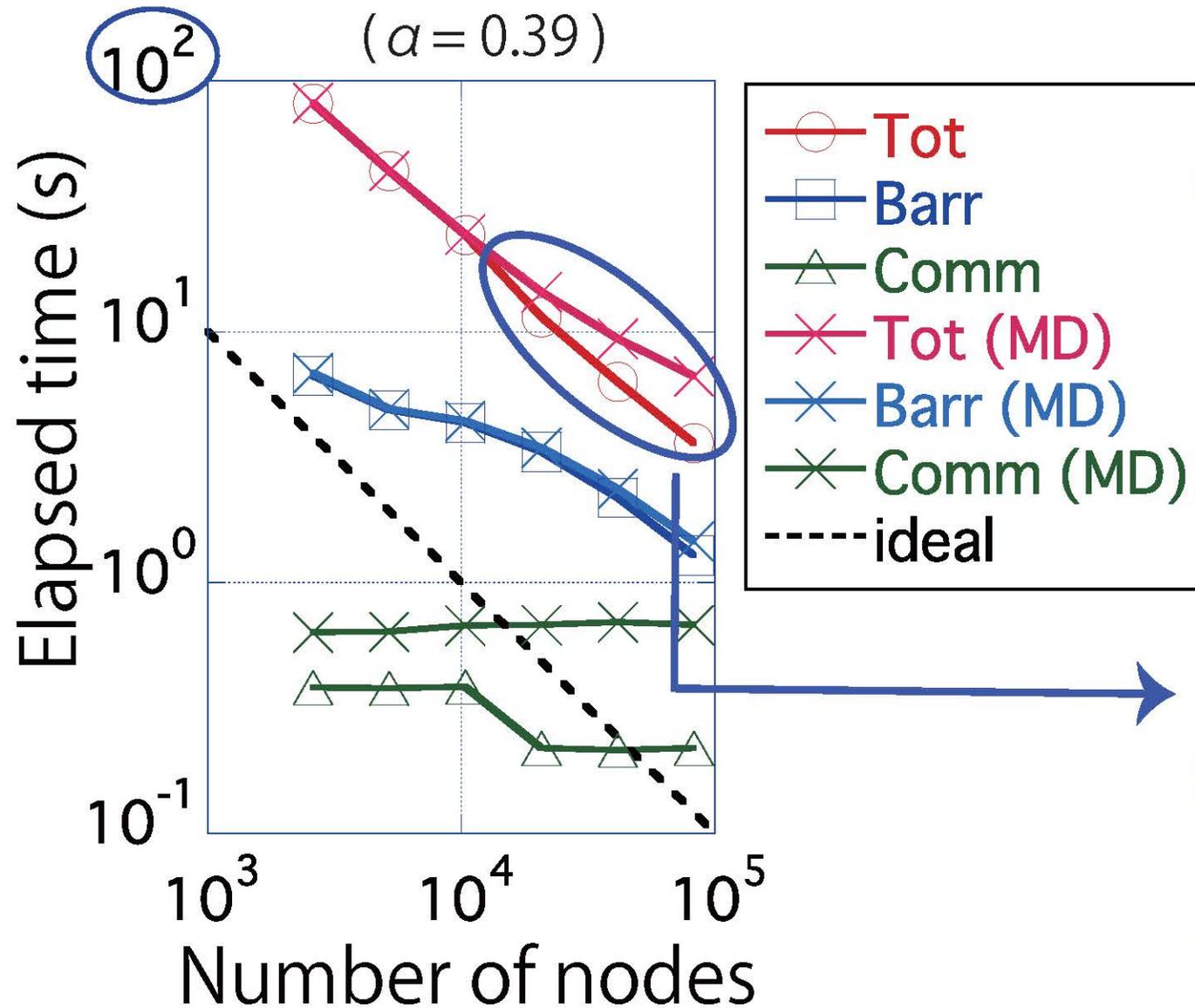
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Bench mark with quantum mechanical MD simulation

→ additional time and memory costs for calculation of force and velocity

Condensed polymer with 10^7 atoms

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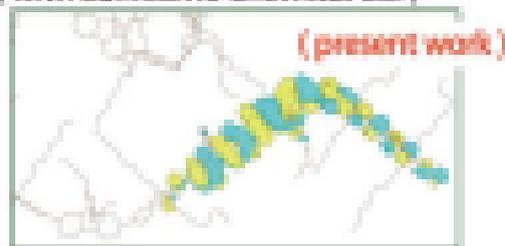
Note:

The additional time cost is not negligible, when ($\#$ node) $> 2 \times 10^4$.

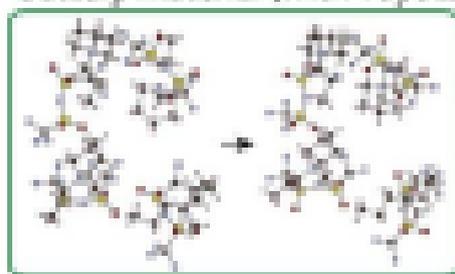
We have not yet well investigated in this point. We can say, however, the elapsed time shows the qualified time-to-solution ($< 10^2$ sec)

Applications with ELSEES (<http://www.elses.jp>), our software

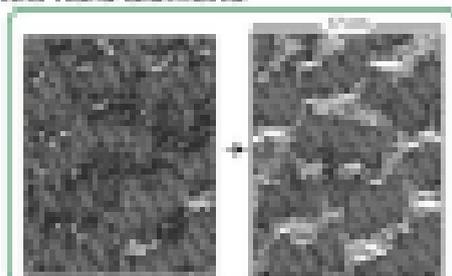
Organic device materials
(with Sumitomo Chemical Co.)



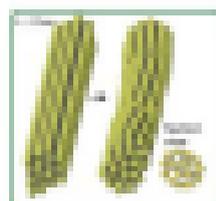
Battery material (with Toyota)



Ultra-hard diamond



helical metal
nanowire



silicon fracture



Detailed method:

Modelled (transferable tight-binding) theory based on first-principles calculations

The algorithmic strategy of the use of the (generalized) shifted linear eqns, instead of eigen-value equations, is general and was applied to many scientific areas with large computation. Here is the examples of the papers

[1] (**QCD**) A. Frommer, Computing 70, 87 (2003)

[2] (**large scale electronic structure calc.**)

R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. Fujiwara, PRB 73, 165108 (2006)

[3] (**many-body wavefunction theory**)

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang and T. Fujiwara,

J. Phys. Soc. Jpn., 77,114713 (2008).

→ Software 'K ω ' : <https://github.com/issp-center-dev/Komega>, (v.0.1 Oct. (2016))

[4] (**ab initio transport calculation**)

S. Iwase, T. Hoshi, T. Ono, Phys. Rev. E 91, 06330 (2015).

[5] (**GW calculation**)

F. Giustino, M. L. Cohen, S. G. Louie, Phys. Rev. B. 81, 115105 (2010)

[6] (**nuclear physics**)

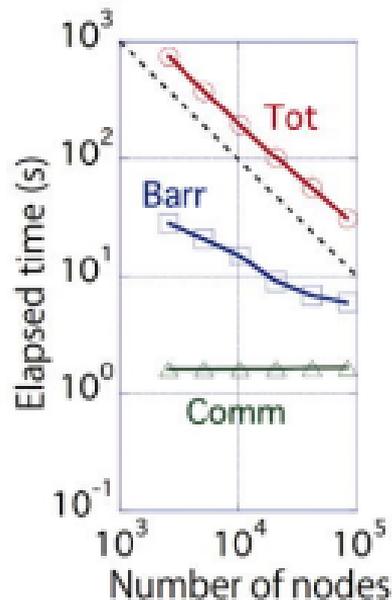
T. Mizusaki, K Kaneko, M. Honma, T. Sakurai, Phys. Rev.C 82, 024310 (2010)

Extremely scalable algorithm for 10^8 -atom quantum material simulation on the full system of the K computer

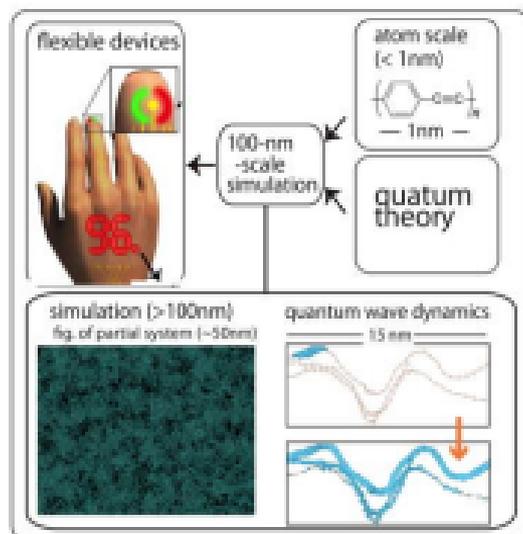
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1. Algorithm



2. Application

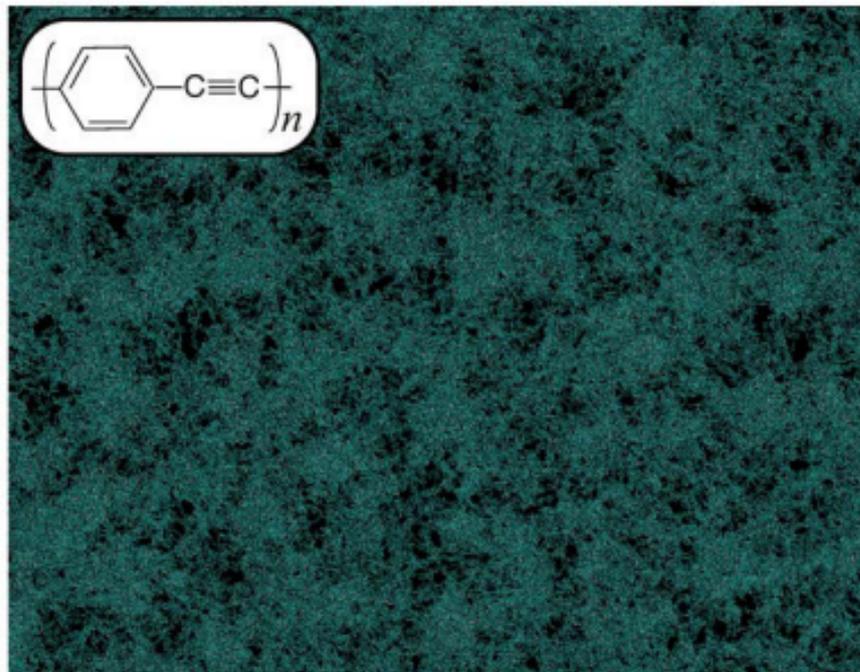


Acknowledgement :
M. Ishida
(Sumitomo Chemical
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100-million-atom caulation of condensed organic polymers

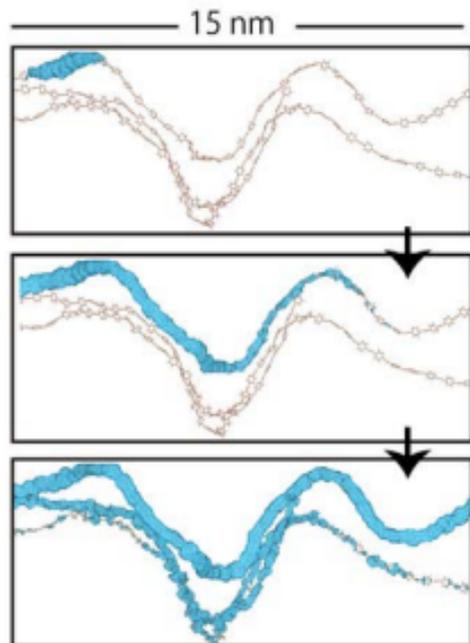
Investigation on wave propagation mechanism (for device property)

- (a) material: poly-(phenylene-ethynylene) (PPE)
(size \approx 200nm, $P=100,000$ polymers)
Figure of a partial reton (~ 50 nm)



- (b) Quantum dynamics

Fig: Charge dynamics with 1 ps



100-million-atom caulation of condensed organic polymers

Investigation on wave propagation mechanism (for device property)

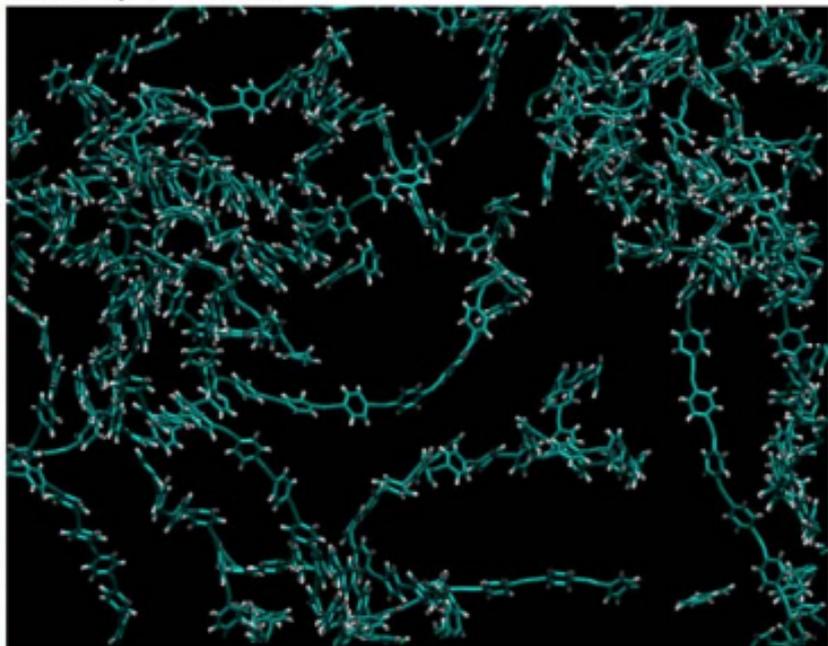
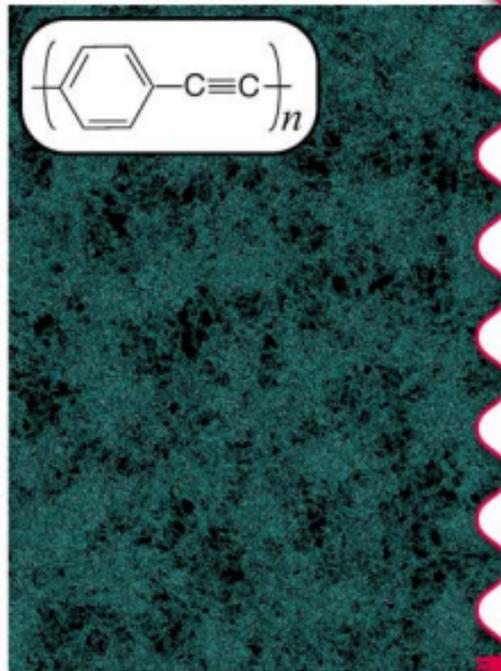
(a) material: poly-(phenylene-ethynylene) (PPE)

(size \approx 200nm, P=100,000 polymers)

Figure of a partial reton (~ close-up (~10nm)

(b) Quantum dynamics

Fig. Charge dynamics with 1 ps



100-million-atom caulation of condensed organic polymers

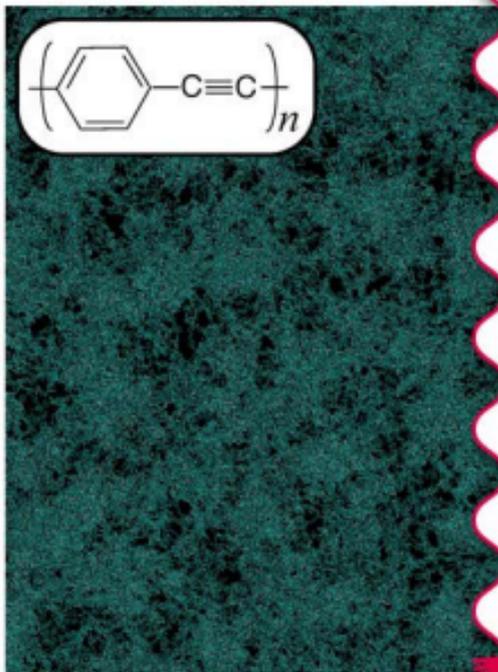
Investigation on wave propagation mechanism (for device property)

(a) material: poly-(phenylene-ethynylene) (PPE)
(size \approx 200nm, P=100,000 polymers)

(b) Quantum dynamics

Fig. Charge dynamics with 1 ps

Figure of a partial reton (~



Quantum mechanical analysis

- (1) calculation of the propagation function
- (2) construct a coarse-grained system
→ network between polymer
(Matrix size) = (# polymers) = 10^5
- (3) eigen-value analysis for propagation
pathbetween polymers
- (4) quantum dynamics
(wave propagation simulation)
for confirmation
of the propagation mechanism

Conclusion

- A novel linear algebraic algorithm realizes 10^8 atom or 100-nm-scale quantum material simulations with an extreme scalability and a qualified time-to-solution on the full system of the K computer
- The highly parallelizable mathematical structure comes from the quantum mechanics not in wavefunction formula but in propagation function formula.
- The idea is general and is applicable to many materials and now we focus on the flexible (organic polymer) device materials for next generation Internet-of-Things (IoT) products, such as display, sensor and battery.

Acknowledgement : M. Ishida (Sumitomo Chemical Co.)
for the collaboration work with organic polymer devices