

slide for ICIAM2015 (PP-A01-6)

# Novel Krylov-subspace Solver of Generalized Shifted Linear Equations for Massively Parallel Quantum Material Simulations

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Note: The present slide appears as

[http://www.damp.tottori-u.ac.jp/~hoshi/info/slide\\_hoshi\\_201508\\_ICIAM\\_lt.pdf](http://www.damp.tottori-u.ac.jp/~hoshi/info/slide_hoshi_201508_ICIAM_lt.pdf)

## abstract

Novel Krylov-subspace algorithms were developed for massively parallel quantum material simulations or electronic structure calculations. The method solves the generalized shifted linear equations  $((zS-H) x = b)$ , instead of conventional generalized eigen-value equation. The paper presents the algorithms and the results of 100-nm-scale or one-hundred-million-atom materials on the K supercomputer with a high parallel efficiency.

The paper also presents recent linear-algebraic algorithms based on time-dependent Schrodinger-type equations and its application to organic electronics materials

Note: a recent review: T. Hoshi, et al., PoS 020, 65 (2014)

[http://pos.sissa.it/archive/conferences/202/065/IWCSE2013\\_065.pdf](http://pos.sissa.it/archive/conferences/202/065/IWCSE2013_065.pdf)

# 1. ELSES, our quantum material simulation code

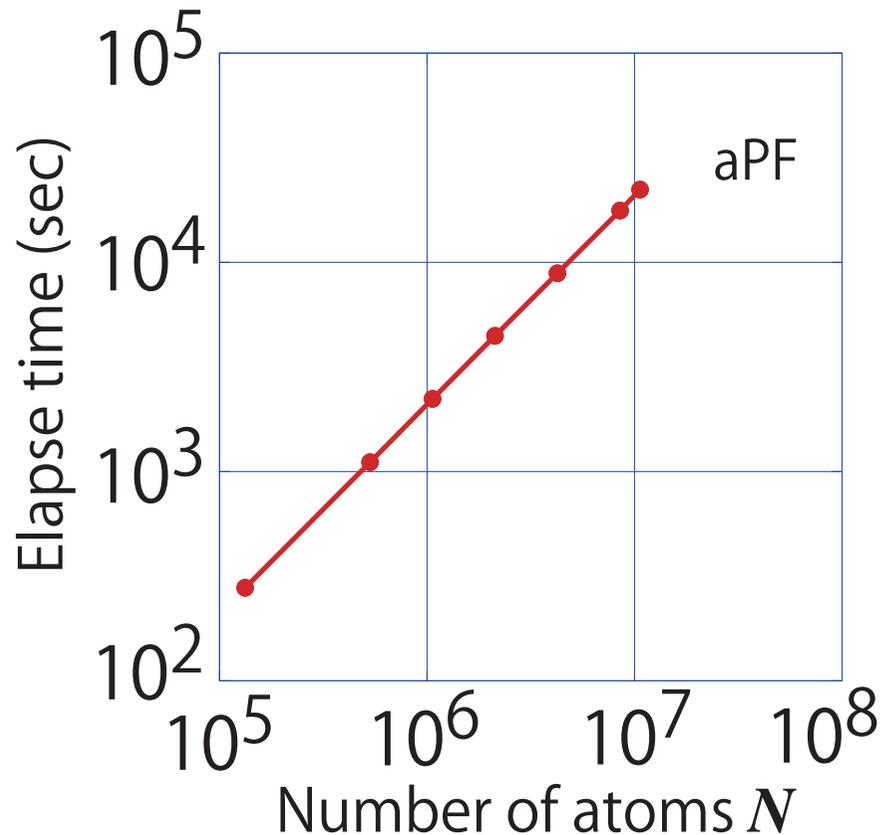
(ELSES = Extra-Large-Scale Electronic Structure calculation code)

Benchmark with upto 100M atoms(  $\rightleftharpoons$  Si :  $(126\text{nm})^3$  region)

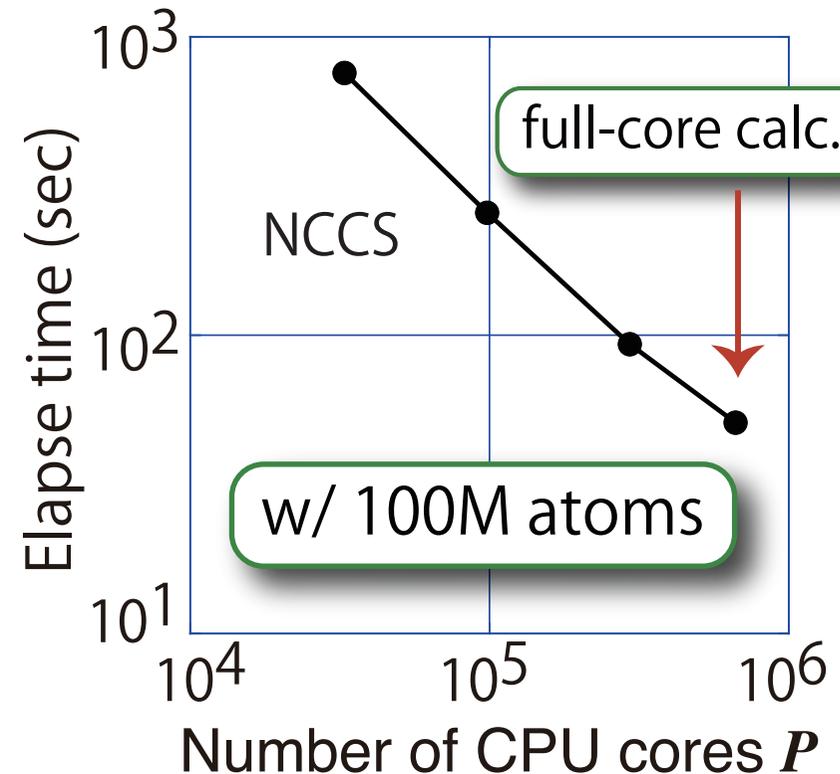
aPF : amorphous-like conjugated polymer, poly-(9,9 dioctyl-fluorene),

NCCS: sp<sup>2</sup>-sp<sup>3</sup> nano composite carbon solid

(a) Order- $N$  scaling



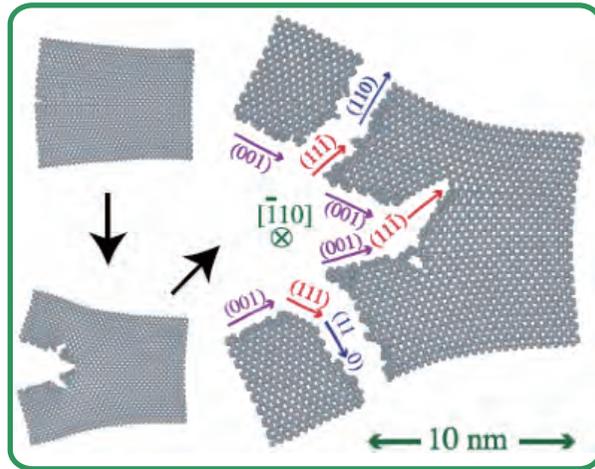
(b) Parallel efficiency (strong scaling) on the K computer (  $\sim$  all nodes )



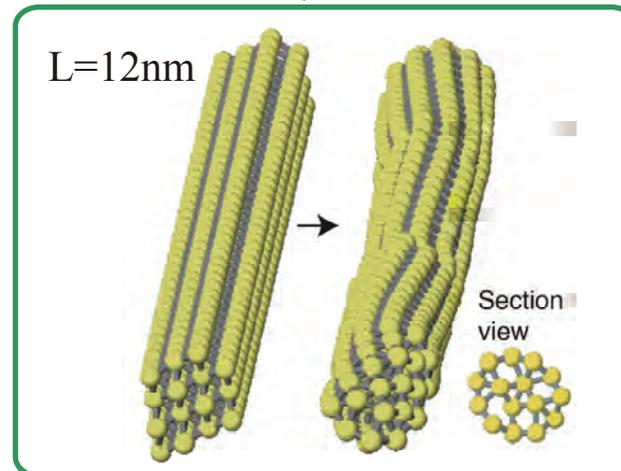
## 2. Nano-material studies with ELSEES ( <http://www.elses.jp/> )

Acknowledge (co-worker, data supply) : S. Nishino, T. Fujiwara (U. Tokyo), S. Yamamoto (Tokyo Eng U)  
H. Yamasaki (Toyota), Y. Zempo (Hosei U), M. Ishida (Sumitomo Chem.)

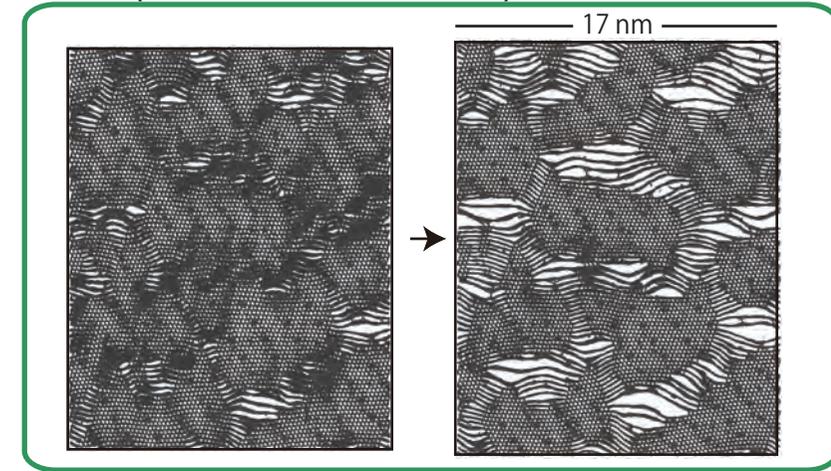
(a) silicon fracture  
(material strength)



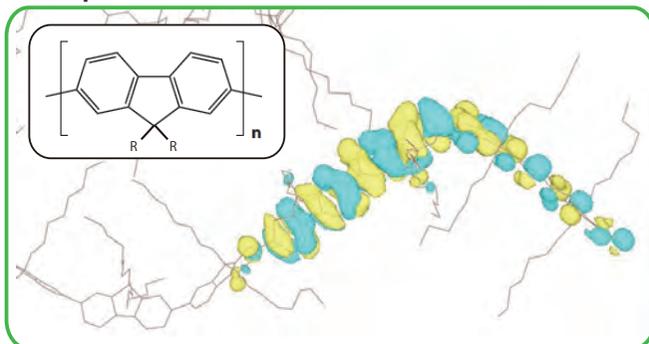
(b) helical multishell gold nanowire (nano electronics)



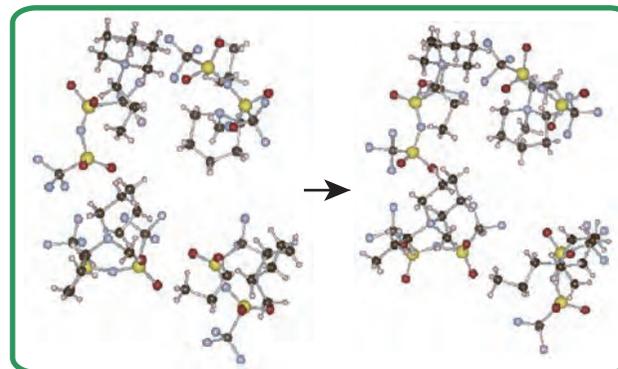
(c) sp<sup>2</sup>-sp<sup>3</sup> nano-composite carbon (Ultra-hard material)



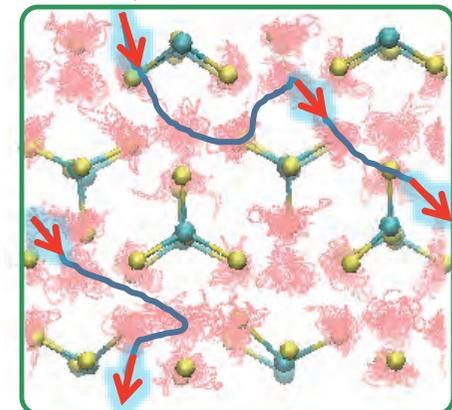
(d) Amorphous-like conjugated polymer:  
poly (9,9) dioctyl-fluorene  
(opto-electronics material)



(e) Ionic liquid : PP13-TFSI  
(battery problem)



(f) Li<sup>+</sup>-ion diffusion in solid  
(battery problem)

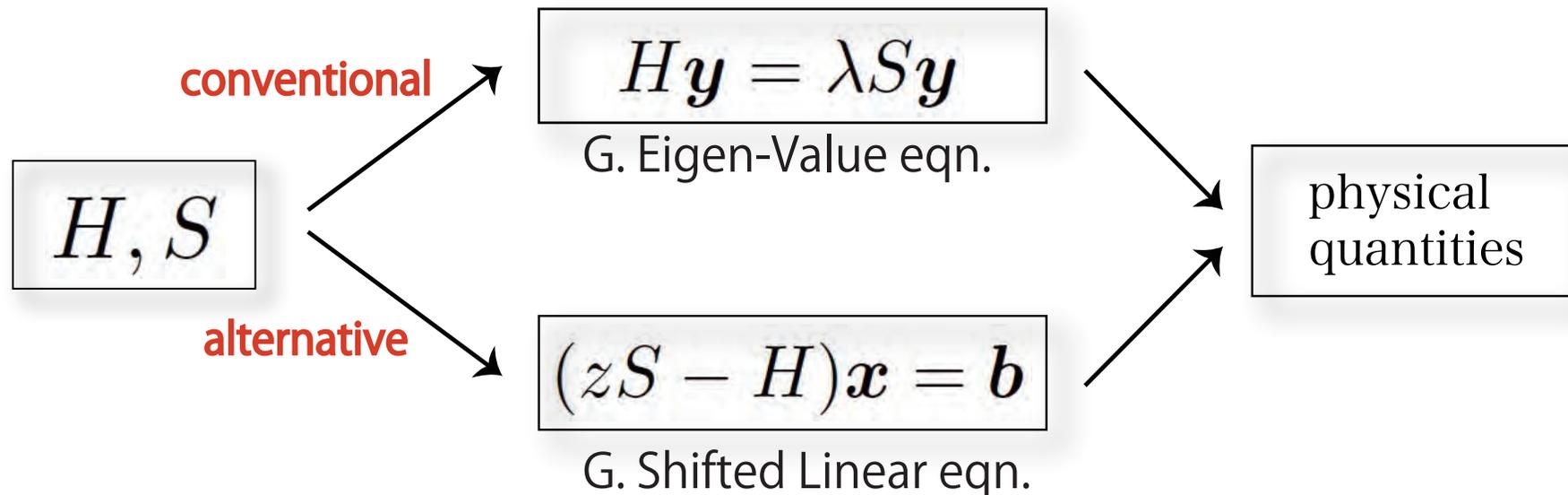
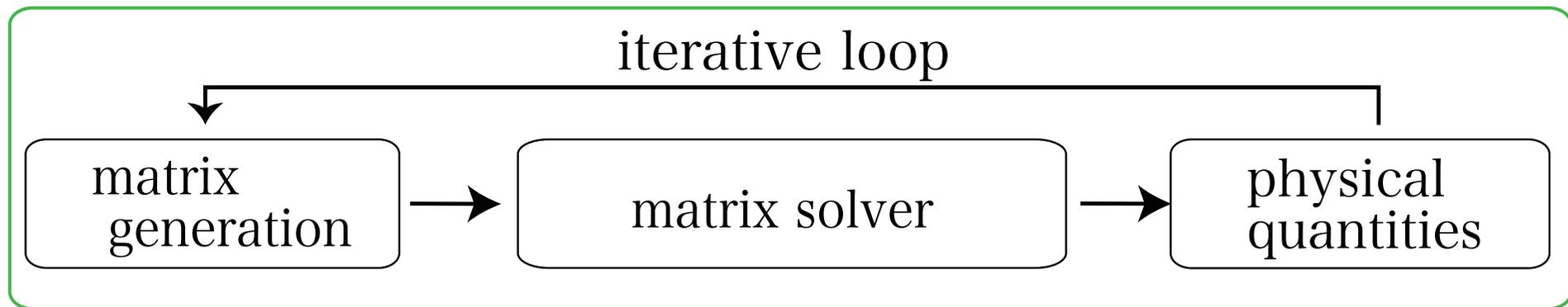


Note: calculations with modelled (TB-type) quantum theories based on ab initio calculation

### 3. Application-Algorithm-Architecture co-design

Large-scale quantum material simulation (electronic structure calculation)

→ Construct an optimal workflow for each target physical quantity



## 4. 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

the propagation  
(Green's) function  
formulation

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

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

## 5. Novel linear algebraic algorithms

→ Krylov subspace solvers for generalized shifted linear equation

$$\underbrace{(H - zS)}_{\text{non-hermitian}} x = b$$

Solvers with Galerkin Principle	Solvers with Collinear Residual Theorem(*)
gLanczos, gArnoldi, mArnodi, Arnoldi(M,W,G)	gsCOCG, gsQMR

(\*) A. Frommer,  
Computing 70, 87 (2003)

Our recent papers

- [1] H. Teng, et al., Phys. Rev. B 83, 165103 (2011).
- [2] T. Hoshi, et al, J. Phys. Cond. Matt. 24, 165502 (2012).
- [3] T. Sogabe, et al., J. Comp. Phys. 231, 5669 (2012).
- [4] S. Iwase et al., Phys. Rev. E 91, 063305 (2015).

The other papers can be found in our webpage:

<http://www.damp.tottori-u.ac.jp/~hoshi/>

## 6. Example : multiple Arnoldi (mArnoldi) method

Original problem :  $H\mathbf{y} = \lambda S\mathbf{y}$  (generalized eigen-value equation) (1)

$H, S$  : real-symmetric,  $S$  : positive definite

Use of 'multiple Krylov subspaces', for obtaining the approximate eigen vectors,

$$\mathcal{L} \equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b}) \quad (2)$$

$$= \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_\nu\} \quad (\mathbf{u}_i^T S \mathbf{u}_j = \delta_{i,j}) \quad (\nu \equiv p + q)$$

Tutorial: Krylov subspace

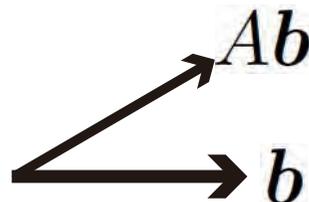
$$K_n(A; \mathbf{b}) \equiv \text{span}\{\mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^{n-1}\mathbf{b}\}$$

$n$  : subspace dimension (iteration number)

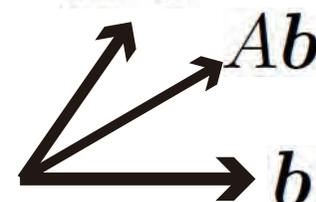
$n=1$



$n=2$



$n=3$



## Details of the multiple Arnoldi method (1)

Original problem :  $H\mathbf{y} = \lambda S\mathbf{y}$  (1)

Def: Subspace

$$\begin{aligned} \mathcal{L} &\equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b}) \\ &= \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_\nu\} \quad (2) \\ &\quad (\nu \equiv p + q) \end{aligned}$$

with the 'S'-orthogonality of  $\{\mathbf{u}_m\}$

$$\mathbf{u}_i^T S \mathbf{u}_j = \delta_{i,j} \quad (3)$$

Def: Subspace (approximate)

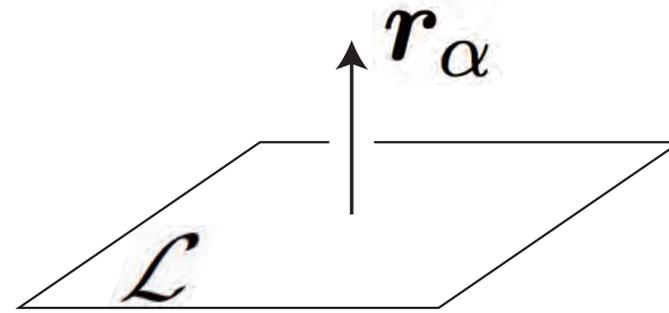
eigen pairs of  $(\varepsilon_\alpha, \mathbf{v}_\alpha)$  ( $\mathbf{v}_\alpha \in \mathcal{L}$ )

$$\mathbf{v}_\alpha = \sum_n^{\nu} C_{n\alpha} \mathbf{u}_n \quad (4)$$

Def: The residual vector

$$\mathbf{r}_\alpha \equiv (H - \varepsilon_\alpha S) \mathbf{v}_\alpha \quad (5)$$

The Galerkin principle ( $\mathbf{r}_\alpha \perp \mathcal{L}$ )



determines the subspace eigen pairs by the standard eigen-value problem of

$$\sum_n^{\nu} \mathcal{H}_{mn} C_{n\alpha} = \varepsilon_\alpha C_{m\alpha} \quad (6)$$

with the 'reduced' ( $\nu \times \nu$ ) matrix

$$\mathcal{H}_{mn} \equiv \mathbf{u}_n^T H \mathbf{u}_m \quad (7)$$

The subspace Green function is given by

$$G^{(b)} \equiv \sum_\alpha^{\nu} \frac{\mathbf{v}_\alpha \mathbf{v}_\alpha^T}{z - \varepsilon_\alpha} \quad (8)$$

## Details of the multiple Arnoldi method (2)

Why multiple subspace?  $\mathcal{L} \equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b}) \quad (\nu \equiv p + q)$   
 $= \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_\nu\} \quad (\mathbf{u}_i^T S \mathbf{u}_j = \delta_{i,j})$

→ Exact reproduction of physical conservation laws within the subspace

Def.: fully-filled limit density matrix (FFL-DM)

$$\Omega \equiv \sum_{\alpha}^{\nu} \mathbf{u}_{\alpha} \mathbf{u}_{\alpha}^T \quad (9)$$

Def.: Projected physical quantity in the FFL:  $\mathbf{b}^T \Omega X \mathbf{b} \quad (10)$

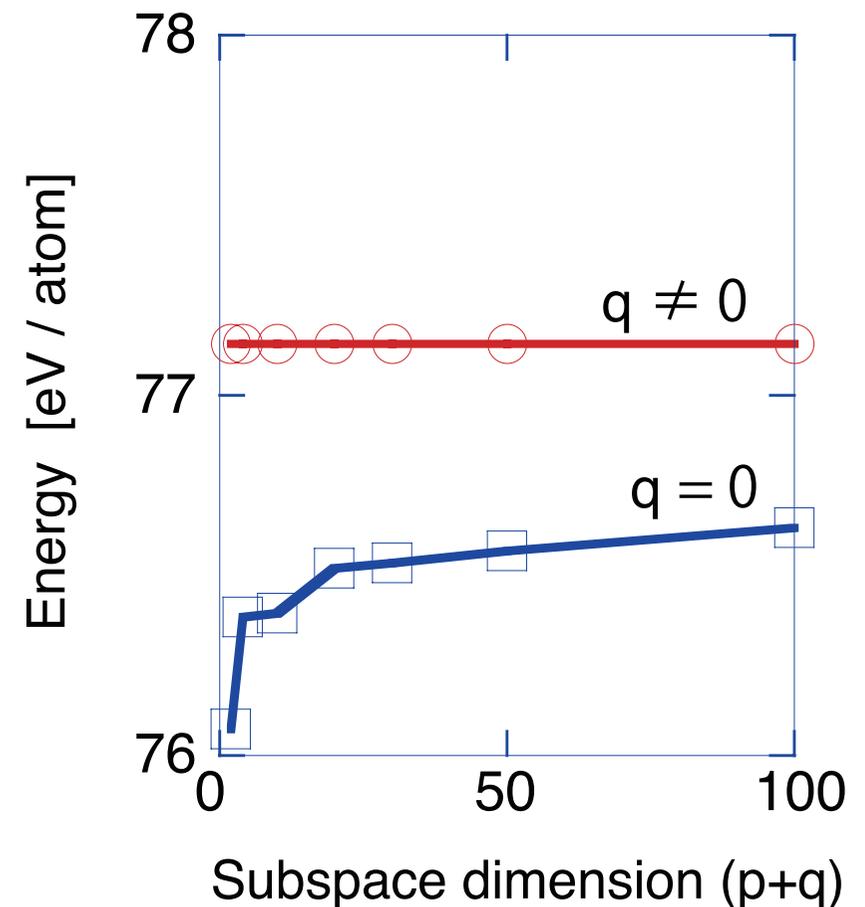
$X$ : arbitrary real-symmetric matrix  
(ex.  $X = H$ : the case of energy)

Theorem:

If  $q \neq 0$ , then  $\mathbf{b}^T \Omega X \mathbf{b} = (\text{exact}) \quad (11)$

Note:  $\Omega \neq (\text{exact}) \quad (12)$

Ex.  $\mathbf{b}^T \Omega X \mathbf{b}$  with  $X = H$



## Details of the multiple Arnoldi method (3) : Proof of 'projection theorem'

Def. : subspace

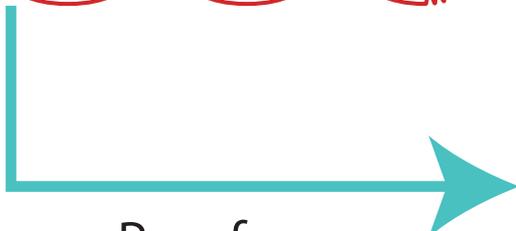
$$\begin{aligned}\mathcal{L} &\equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b}) \\ &= \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_\nu\} \\ &\quad (\mathbf{u}_i^T S \mathbf{u}_j = \delta_{i,j})\end{aligned}$$

Def. : Density matrix in the FFL

$$\Omega \equiv \sum_{\alpha}^{\nu} \mathbf{u}_{\alpha} \mathbf{u}_{\alpha}^T$$

Theorem for physical quantity:

If  $q \neq 0$ , the  $\mathbf{b}^T \Omega X \mathbf{b} = (\text{exact})$

Proof 

'projection theorem' :

$$\Omega S \gamma = \gamma \quad (\text{a})$$

for any vector in the subspace

$$(\gamma \in \mathcal{L})$$

Note:  $\Omega = S^{-1}$  (b)

in the exact solution.

If  $q \neq 0$ , then  $S^{-1}\mathbf{b} \in \mathcal{L}$

and the 'projection' theorem of (a) gives

$$\Omega S(S^{-1}\mathbf{b}) = (S^{-1}\mathbf{b}) \quad (\text{c})$$

$$\text{or} \quad \Omega \mathbf{b} = S^{-1}\mathbf{b} \quad (\text{d})$$

Therefore

$$\mathbf{b}^T \Omega X \mathbf{b} = \mathbf{b}^T S^{-1} X \mathbf{b} \quad (\text{exact}) \quad (\text{e})$$

## 7. Another problem : Recent study for organic electronics device

(a) Original PDE: quantum 'wave' dynamics with a Schrödinger-type equation

$$\partial_t u = -iHu \quad (1)$$

(b) Discretization with given functions  $\{f_i(\mathbf{r})\}$  ( localized near atoms )

$$u(\mathbf{r}, t) \Rightarrow \mathbf{u}(t) \equiv (u_1, u_2, \dots, u_N)^T \quad (2)$$

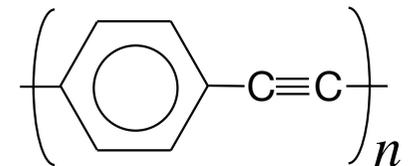
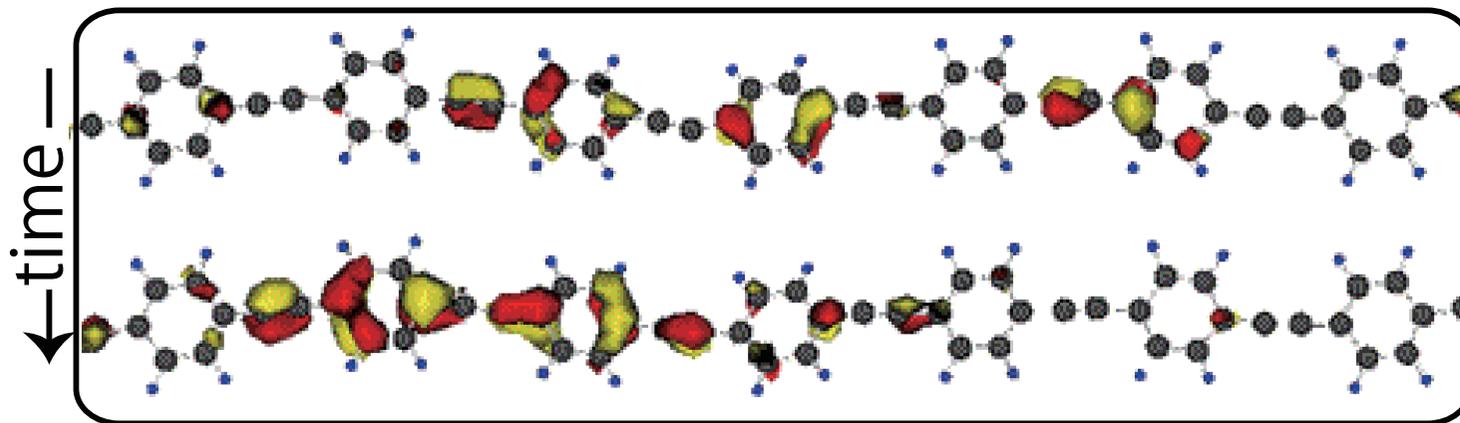
→ its formal solution ( → linear algebraic problems )

$$\mathbf{u}(t + \delta t) := e^{-i\delta t H} \mathbf{u}(t) \quad (3)$$

$$u(\mathbf{r}, t) \equiv \sum_i u_i f_i(\mathbf{r}) \quad (4)$$

→ A preliminary result on a polymer

Fig(below) : The real part is drawn by the two isosurfaces (  $\text{Re}[u(\mathbf{r}, t)] = \pm C$  )



poly-  
(phenylene-ethynylene)(\*)

(\*) Experiment and theory : J. Terao, et al., Nature Comm. 4, 1691 (2013)

## Appendix: 'ELSES matrix library' ( <http://www.elses.jp/matrix/> )

A sparse matrix collection arising in our real problems

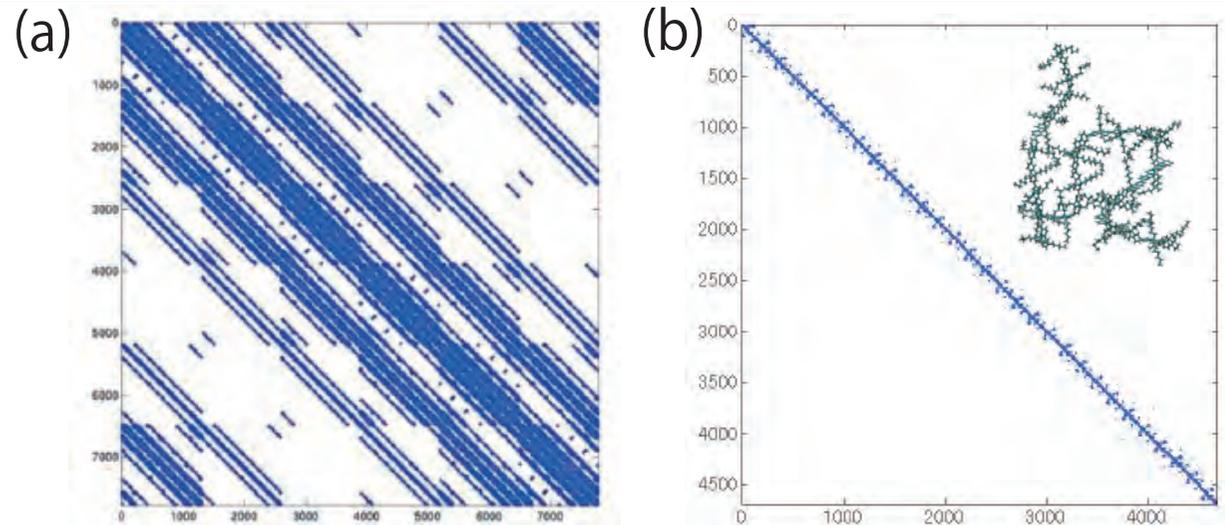
⇒ Prepared for future numerical analysis researches

⇒ The matrix sizes :  $M = 10^2 \sim 10^6$  / The data format: the Matrix Market format

### Examples

(a) Solid gold (within a super cell)

(b) amorphous-like  
conjugated polymer  
poly-((9,9) dioctyl-fluorene)



Notice: a related talk in this conference

CP-Th-D-14-5:

'Parallel generalized eigenvalue computation with hybrid solvers  
and their benchmark on supercomputers'

H. Imachi and T. Hoshi (Tottori U)