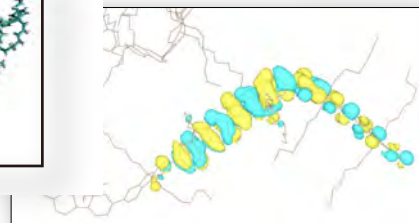
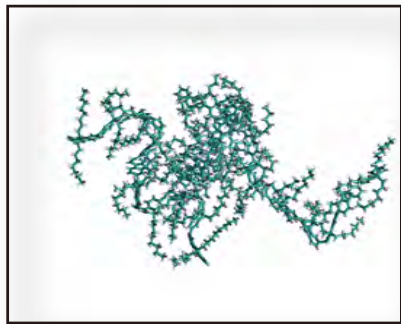


Krylov subspace theories and ultra-large-scale electronic state calculations on the K computer (as an interdisciplenary research between physics and applied mathematics)

T. Hoshi(星健夫)^{1,2}, T. Sogabe(曾我部知広)^{3,2}, T. Miyata(宮田考史)^{4,2}, S.-L. Zhang(張紹良)^{4,2}

1. Tottori University, Japan;
2. Core Research for Evolutional Science and Technology,
Japan Science and Technology Agency (CREST-JST), Japan;
3. Aichi Prefecture University, Japan;
4. Nagoya University, Japan



$$Hy = \lambda Sy$$

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



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4. Performcance issues on the supercomputer

5. For further collaboration

between physics and applied mathematics.

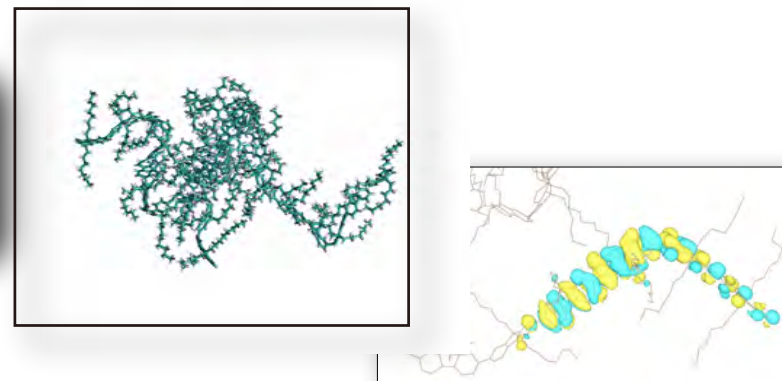
5-a. Interior eigen-pair problem

5-b. 'Open data' for matrix

Overview : Application-Algorithm-Architecture co-design

a common concept in the current computational physics

Application : Materials research
with electronic structure



Algorithm : Numerical linear algebra

$$Hy = \lambda Sy$$

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

Architecture : from top-class supercomputers
to small (personal) computers



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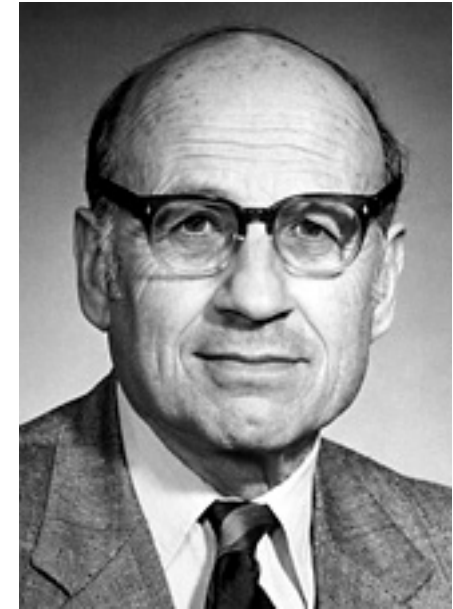
Tutorial : What is electronic structure calculation ?

- (a) quantum-mechanical 'wave' theory for electrons in materials (*)
- (b) basics of many nanomaterial simulations
- effective Schrodinger equation
- generalized Hermitian eigen-value problem (as a typical numerical problem)

$$Hy = \lambda Sy$$

λ : energy for each electron ('eigen energy')
 y : shape of electronic 'wave' ('wavefunction')(**)

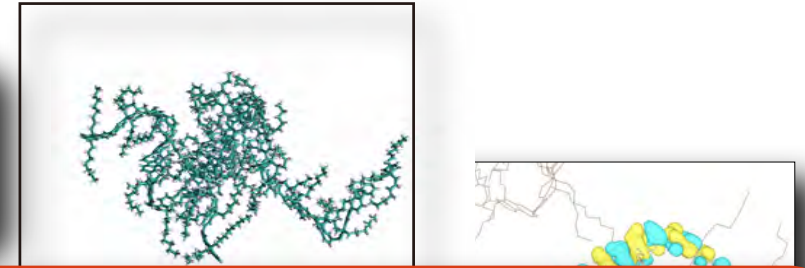
(*)Walter Kohn (1923~)
Nobel Prize in Chemistry 1998



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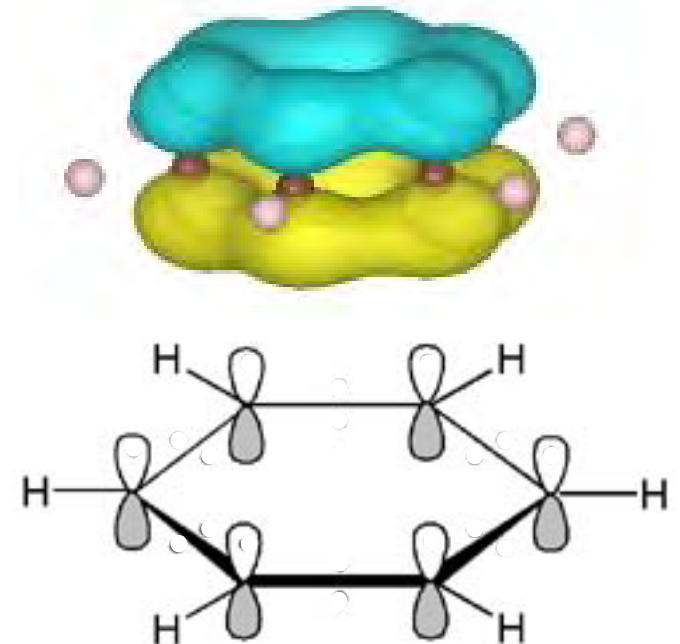
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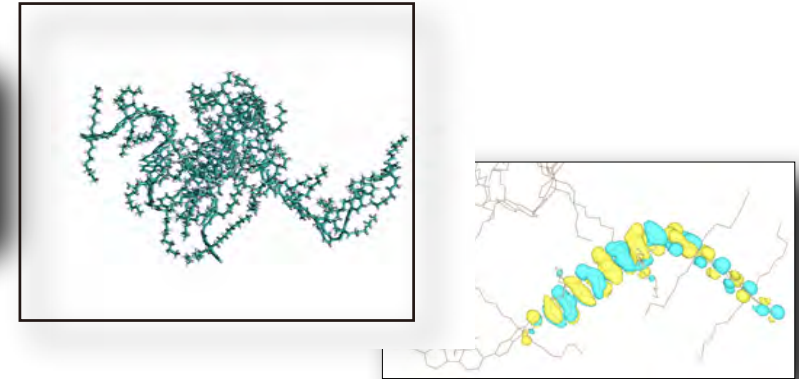
(**) Exmample of electronic 'wave'
(wave function)
→ one of Benzene (C_6H_6)



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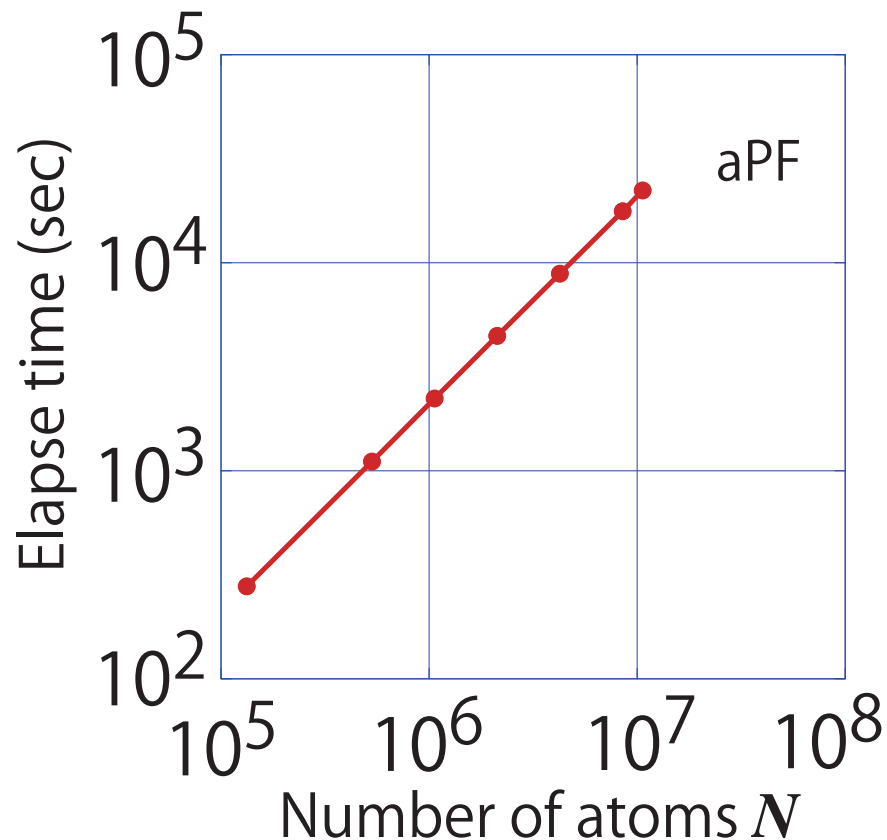
'ELSES' : Our code for 'order- N ' electronic state calculations

Hoshi et al., JPCM24, 165502 (2012); JPSJ 82, 023710 (2013).

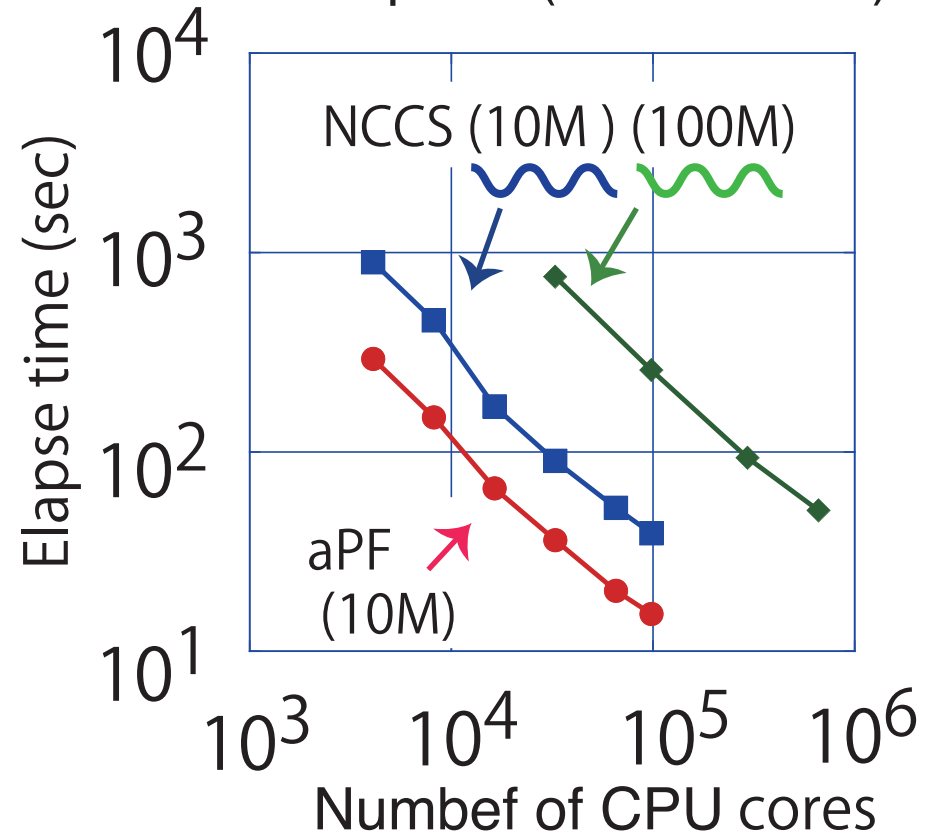
Benchmark with nanomaterials ($\sim 100\text{M}$ atoms \rightleftharpoons Si : $(120\text{nm})^3$ region)

aPF : amorphous-like conjugated polymer, poly-(9,9 dioctyl-fluorene),
NCCS: sp²-sp³ nano composite carbon solid

(a) Order- N scaling



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

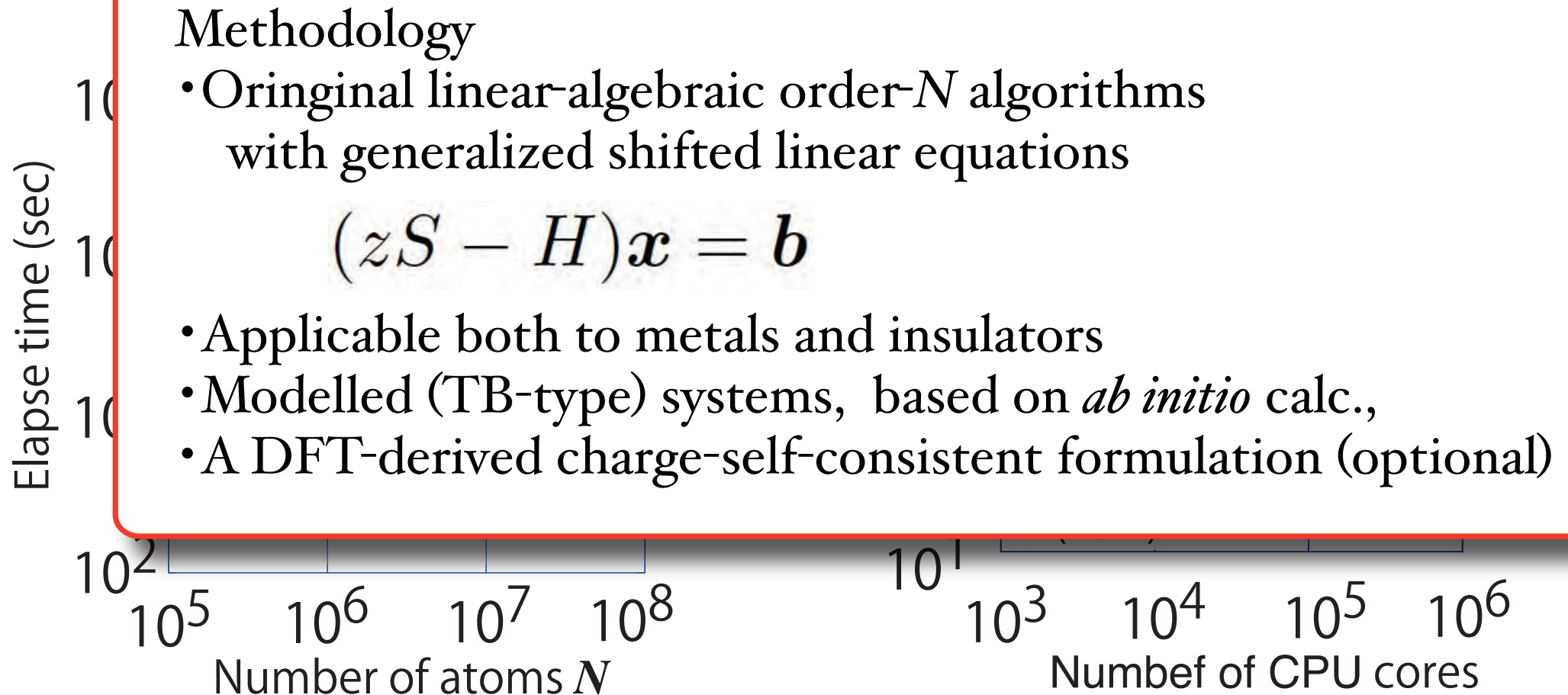


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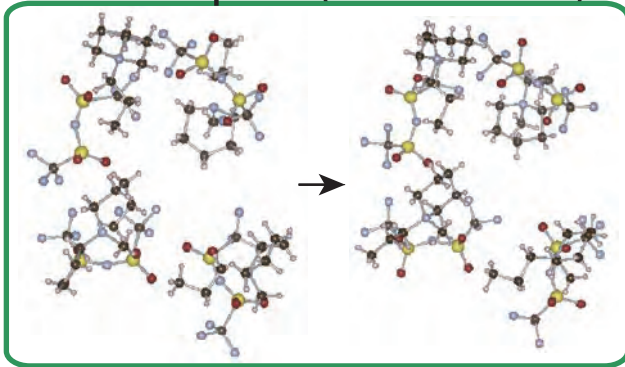


Examples of nano-material studies with 'ELSES'

Motivations

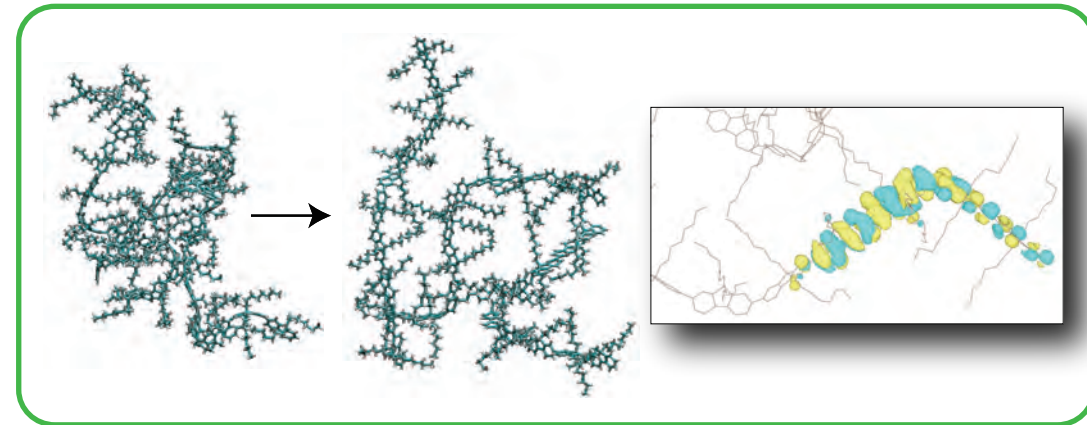
- (i) industrial application
- (ii) new material (from Japan)
- (iii) standard material

Ionic liquid (PP13-TFSI)

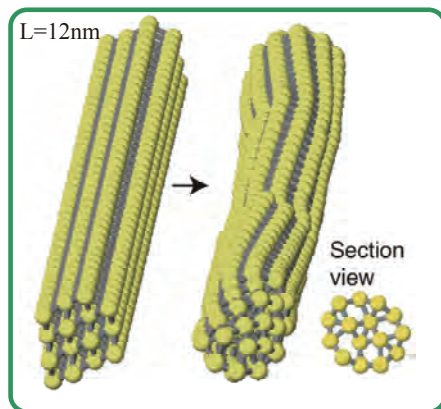


Li^+ diffusion
in solids
(Nishino et al.)

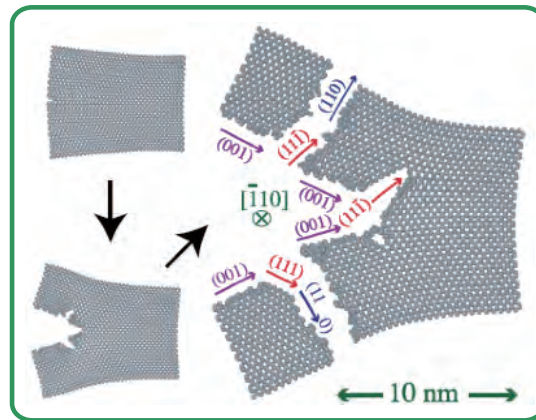
Amorphous-like conjugated polymer (poly-(9,9 dioctyl fluorene))



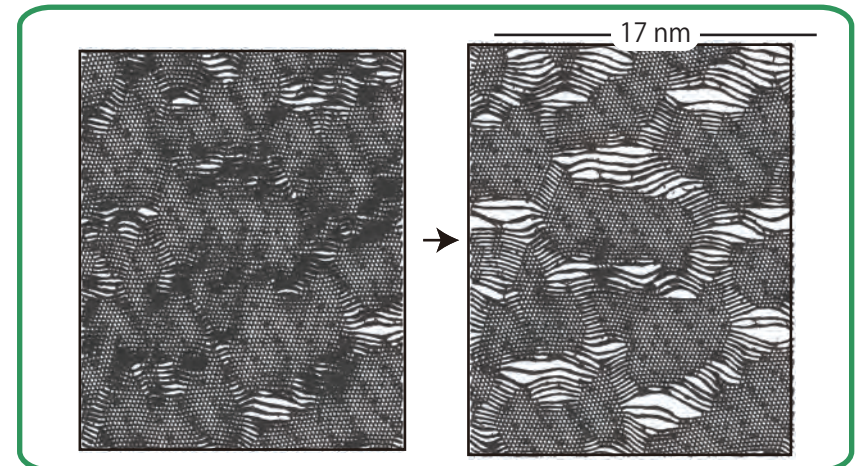
helical gold nanowire



silicon brittle fracture



sp²-sp³ nano-composite carbon solid (for nano-polycrystalline diamond)

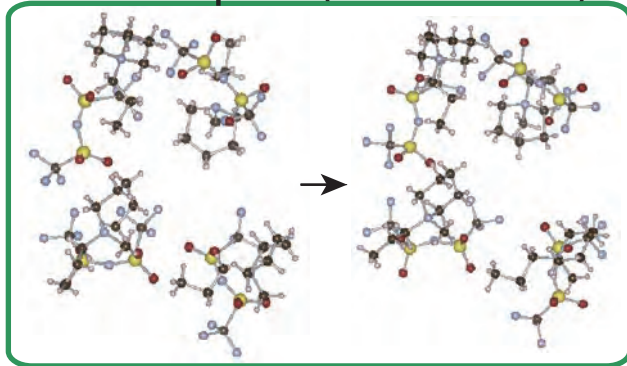


Examples of nano-material studies with 'ELSES'

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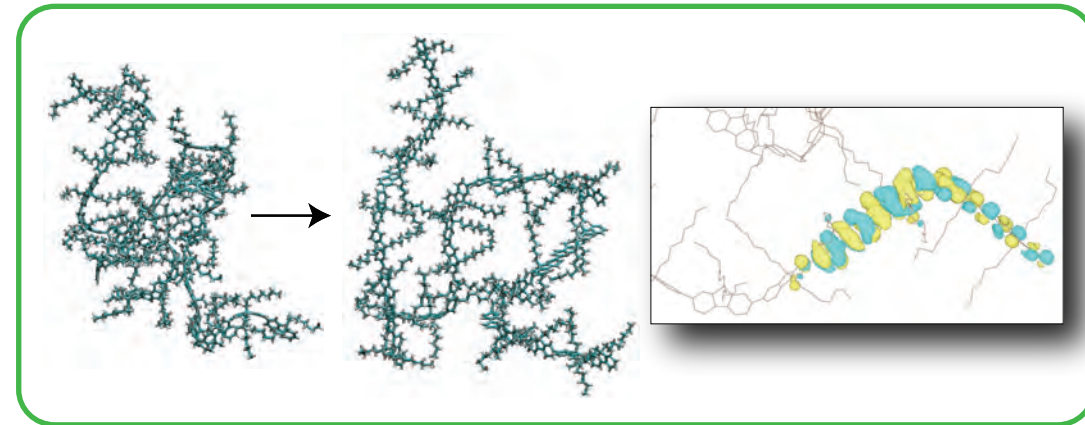
Ionic liquid (PP13-TFSI)



Li⁺ diffusion
in solids

Recent paper :
S. Nishino (U Tokyo)
T. Fujiwara (U Tokyo),
H. Yamasaki (Toyota),
S. Yamamoto (Tokyo U. Tech.),
T. Hoshi (Tottori U),
Solid State Ionics 225,
22–25 (2012).

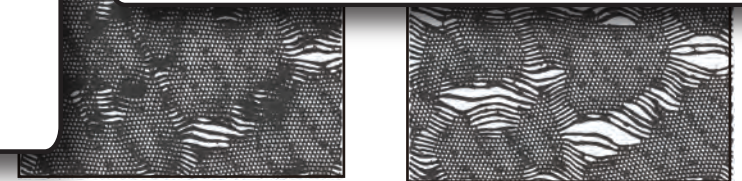
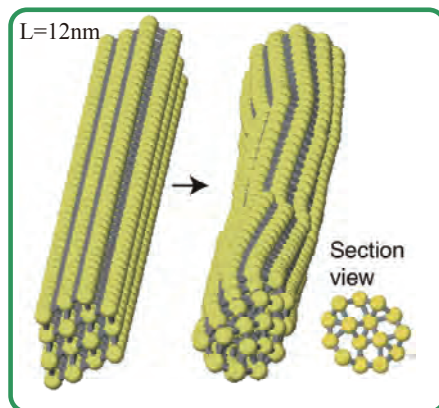
Amourphous-like conjugated polymer (poly-(9,9 dioctyl fluorene))



Recent paper :

T. Hoshi, S. Yamamoto,
T. Fujiwara, T. Sogabe,
S-L Zhang, J. Phys.: CM 24,
165502 (2012) ;
(Acknowl. : M. Ishida
(Sumitomo Chemical Co.))

helical gold nanowire



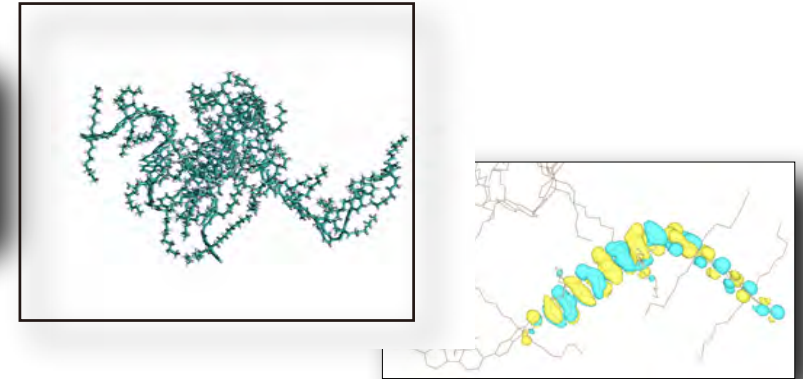
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a common concept in the current computational physics

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Algorithm : Numerical linear algebra

$$Hy = \lambda Sy$$

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

Architecture : from top-class supercomputers
to small (personal) computers



Application-Algorithm-Architecture co-design

→ algorithm design for the entire calculation procedure;
as the iterative loop of
(matrix generation) + (matrix solver) + (calculation of physical quantities)

matrix
generation



matrix solver



calculation of
physical quantities

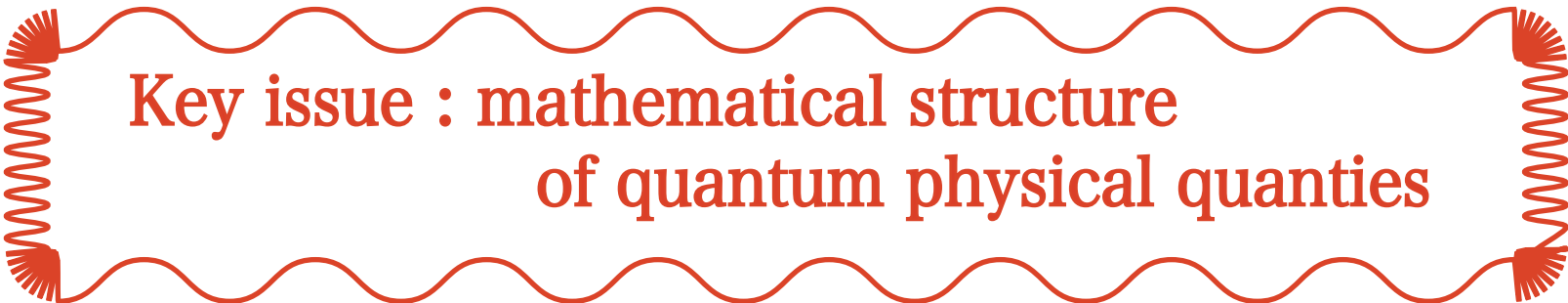
(G. Eigen-Value eqn. or
G. Shifted Linear eqn.)



iterative loop



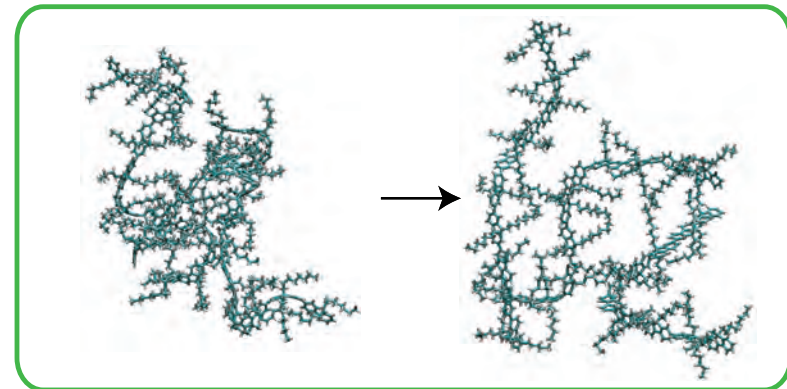
**Key issue : mathematical structure
of quantum physical quantities**



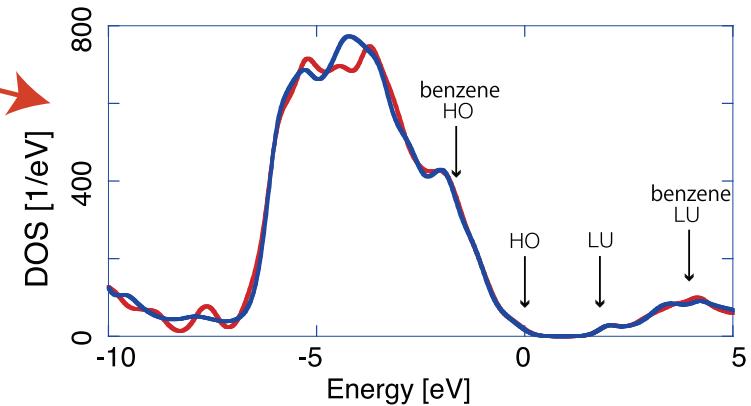
Typical types of quantum physical quantities

- (1) Energy and force
(for structure-dynamics simulation)
→ physical quantity in trace form

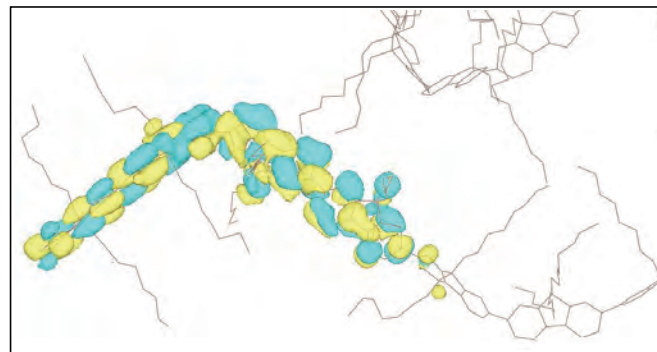
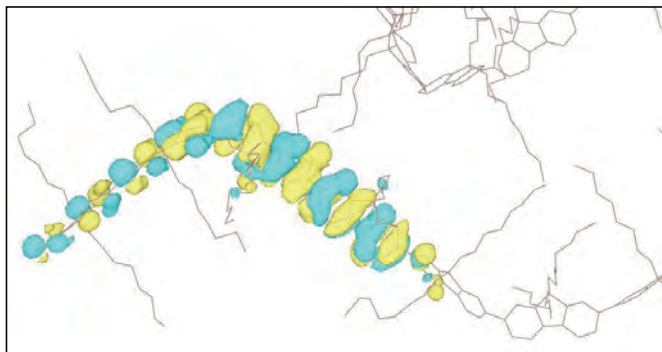
focused here



- (2) Electronic spectrum
(density of states, and so on)
→ weighted eigen-value histogram



- (3) Specific eigen states
(Fig. HOMO and LUMO)
→ interior eigen-pair problem



ex. π conjugated polymer:
poly-(9,9 dioctil fluorene)
Ref. Hoshi, et al. JPCM 24,
165502 (2012)

Mathematical structure of quantum physical quantities

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)

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

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

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

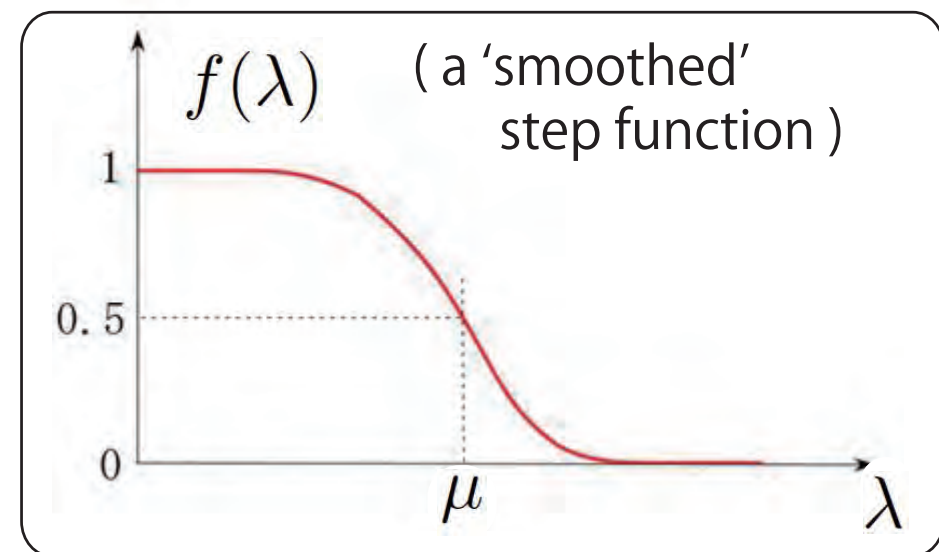
(β, μ : given parameters)

Physical quantity in trace form

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

with the density matrix

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



Quantum physical quantities in trace form

Sparse property of physical quantity

When we calculate a physical quantity

$$\text{Tr}[X\rho] = \sum_{i,j} X_{ij} \rho_{ji}$$

(X : a sparse matrix)

We need the selected elements of $\{\rho_{ji}\}$ only among the (i, j) pairs with $X_{ij} \neq 0$, even if ρ is a dense matrix.

→ “Quantum locality”

or “Nearsightedness principle”

W. Kohn, Phys. Rev. Lett, 76, 3168 (1996)

Simplest example

$$X = \begin{pmatrix} 0 & X_{12} & 0 \\ X_{21} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



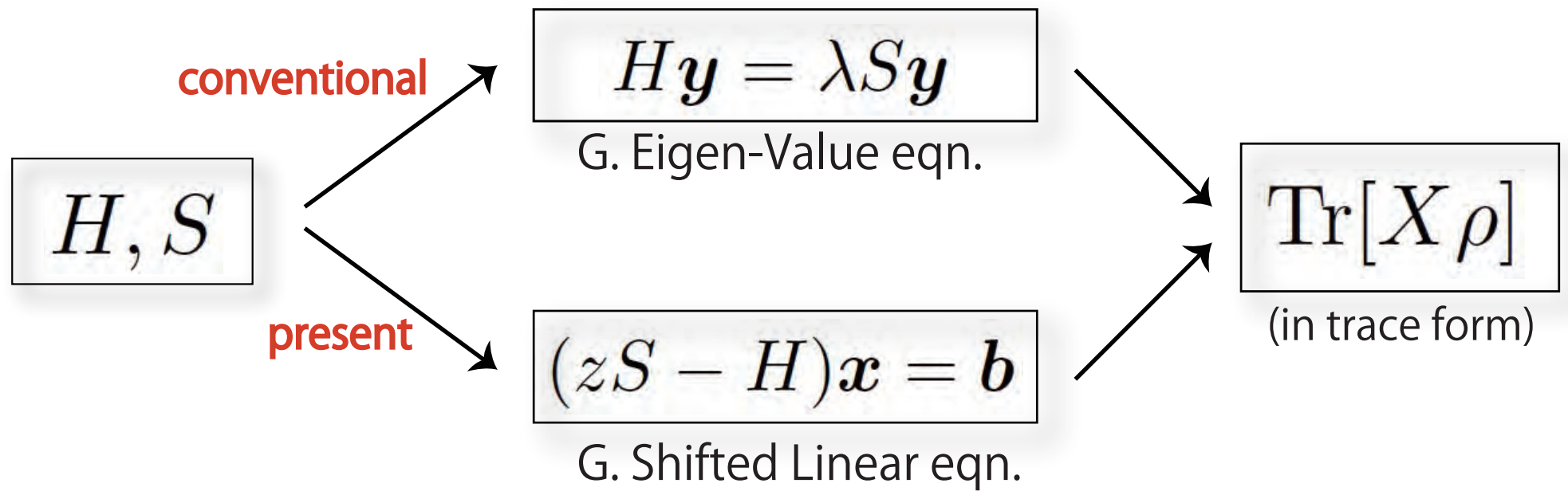
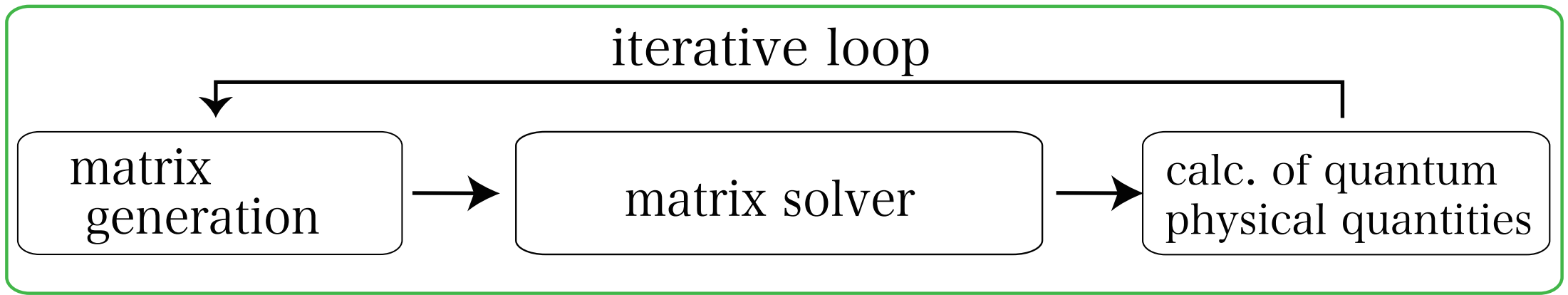
$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{pmatrix}$$

We need only
these elements !!

Conclusion of 'Application-Algorithm-Architecture co-design'

Algorithm design for the entire calculation process

→ We are focusing on the calculation of 'physical quantities in trace form'



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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

Novel linear algebraic algorithms

- [1] Teng et al., PRB 83, 165103 (2011); [2] Hoshi et al, JPCM 24, 165502 (2012).
[3] Sogabe JCP 231, 5669 (2012); [4] Yamashita et al., Trans. JSIAM 21, 241 (2011).

→ Iterative (Krylov subspace) solvers for generalized shifted linear equation

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

Mathematical principles	$S \neq I$	$S = I^*$
Gerlerkin Principle	gLanczos, gArnoldi, mArnodi, Arnoldi (M;W;G)	subs. diag.
Collinear Residual	gsCOCG, gsQMR	sCOCG, sQMR

*Takayama *et al.*, JPSJ73, 1519 (2004); Takayama et al. PRB 73, 165108(2006); Sogabe et al. ETNA31, 126 (2008)

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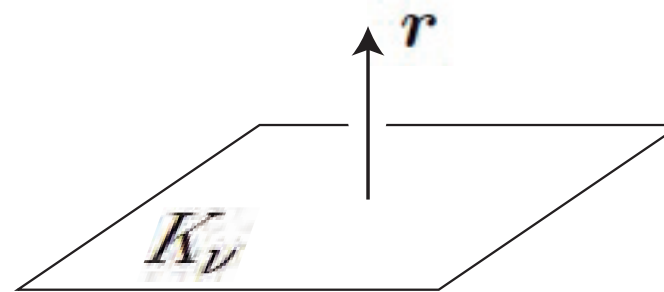
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(2-a) Gerlerkin Principle

→ "Orthogonality" principle on the residual vector

$$r \perp K_\nu = \text{span}\{u_1, u_2, \dots, u_\nu\}$$

$$u_i^t S u_j = \delta_{i,j}$$



Mathematical principles		
Gerlerkin Principle		
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Mathematical principles		<p>(2-b) Collinear Residual Theorem*</p> <p>from the shift invariance of Krylov subspace</p> $K_\nu(A + \sigma I; b) = K_\nu(A; b)$ <p>→ drastic reduction of mat-vec multiplications</p> <p>*Frommer, Computing 70, 87 (2003)</p>	
Gerlerkin Principle	g		
Collinear Residual	m		
		gsQMR	sQMR

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Overview of multiple Arnoldi method (1/2)

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

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

Def.: multiple Krylov subspace

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

Def.: subspace eigen pair : $(\varepsilon_\alpha, \mathbf{v}_\alpha)$ (3)

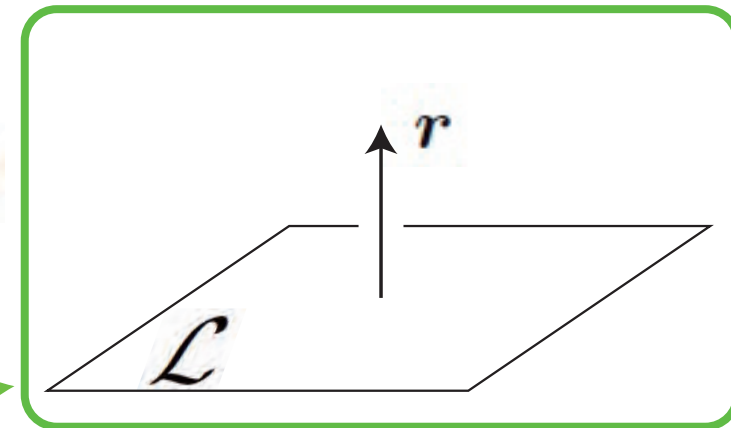
$$(\mathbf{v}_\alpha \in \mathcal{L}, \alpha := 1, 2, \dots, p + q)$$

Def.: residual vector: $\mathbf{r}_\alpha \equiv (H - \varepsilon_\alpha S)\mathbf{v}_\alpha$ (4)

Galerkin principle : $\mathbf{r} \perp \mathcal{L}$ (5)

so as to determine the subspace eigen pair of $(\varepsilon_\alpha, \mathbf{v}_\alpha)$

→ standard eigen-value equation within the subspace



Overview of multiple Arnoldi method (detailed formulation)

Original problem

$$H\mathbf{y} = \lambda S\mathbf{y} \quad (\text{a})$$

Subspace

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

with 'S'-orthogonal bases: $\{\mathbf{u}_m\}$

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

(generated by
the Gram-Schmidt procedure)

Subspace eigen pair : $(\varepsilon_\alpha, \mathbf{v}_\alpha)$ ($\mathbf{v}_\alpha \in \mathcal{L}$)

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

The Galerkin principle ($\varepsilon_\alpha, \{C_{n\alpha}\}_n$)
determines as

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

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

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

The subspace Green function

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

Overview of multiple Arnoldi method (2/2)

Why multiple subspace? $\mathcal{L} \equiv K_p(H; \mathbf{b}) \oplus K_q(H; S^{-1}\mathbf{b})$ ($\nu \equiv p + q$)

→ Exact reproduction of some physical properties within the subspace

Def.: density matrix

in the fully-filled limit (FFL):

$$\Omega \equiv \sum_{\alpha}^{\nu} \mathbf{u}_{\alpha} \mathbf{u}_{\alpha}^{\text{T}} \quad (6)$$

(\mathbf{u}_{α} : subspace eigen vectors)

Def.: Projected physical quantity

in the FFL: $\mathbf{b}^{\text{T}} \Omega X \mathbf{b}$ (7)

X : arbitrary real-symmetric matrix

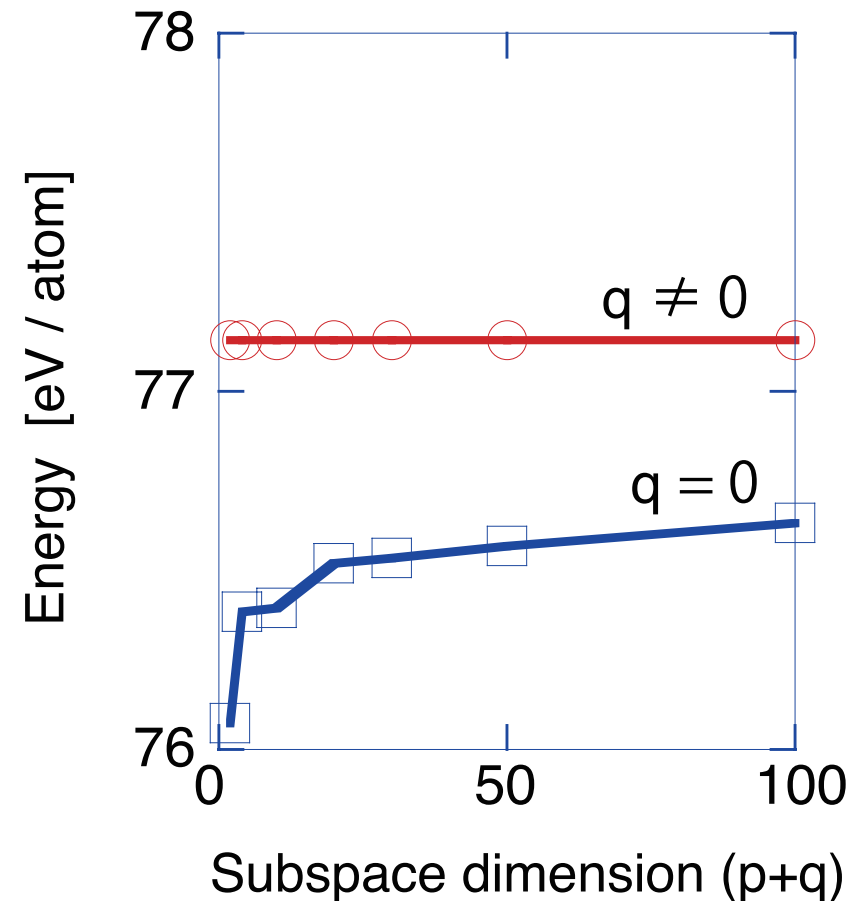
(ex. $X = H$: the case of energy)

Theorem:

If $q \neq 0$, then $\mathbf{b}^{\text{T}} \Omega X \mathbf{b} = (\text{exact})$ (8)

Note: $\Omega \neq (\text{exact})$ (9)

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



Summary of novel Krylov subspace methods

Six solvers for generalized shifted linear equation

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

→ See the reference list in the abstract for details

Summary of multiple Arnoldi method

- The original matrix equation

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

is reduced into a smaller matrix equation within the multiple Krylov subspace of

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

- The multiple Krylov subspace of (2) is used, because of the exact conservation law of fully-filled-limit (FFL) projected physical quantities

$$\mathbf{b}^T \Omega X \mathbf{b} = (\text{exact}) \quad (3)$$

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Post-calculation analysis method

.....is crucial, so as to obtain physical conclusions from huge electronic-structure data

Large-scale calculation
by massively-parallel computers



Huge electronic structure data
(as the Green's function)

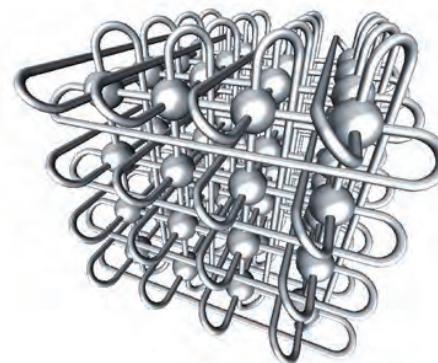


Post-calculation analysis



Physical conclusions

distributed among nodes



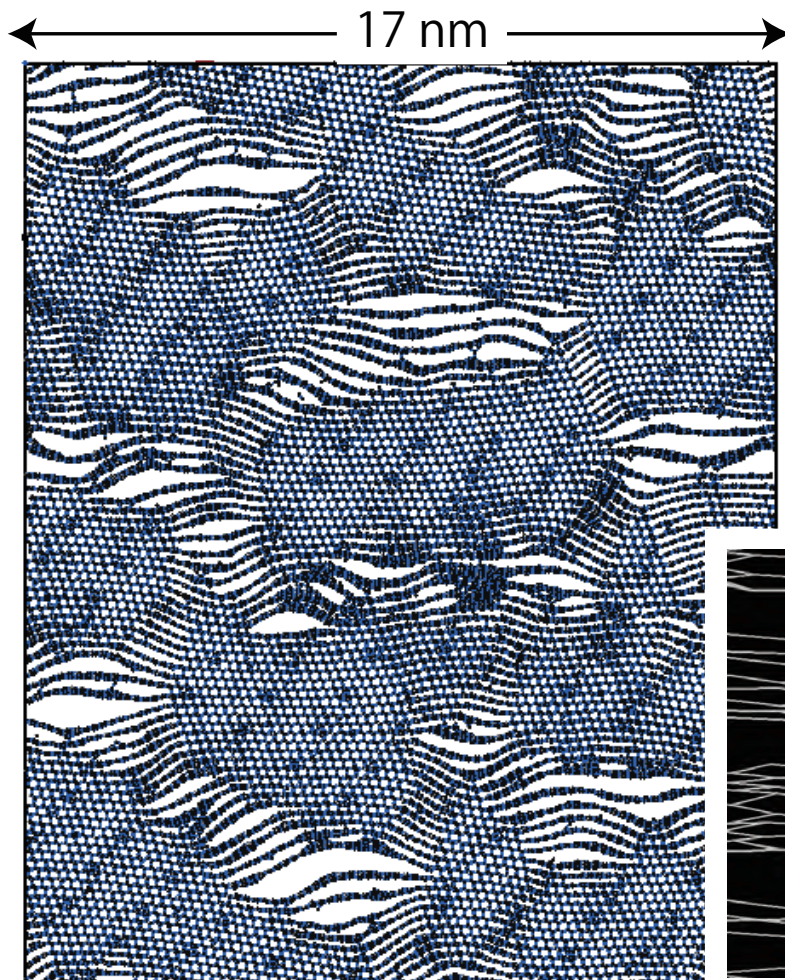
ex. (π)COHP analysis
→next page

Visualization with massively parallel data analysis
based on the Green-function theory (π -COHP*)

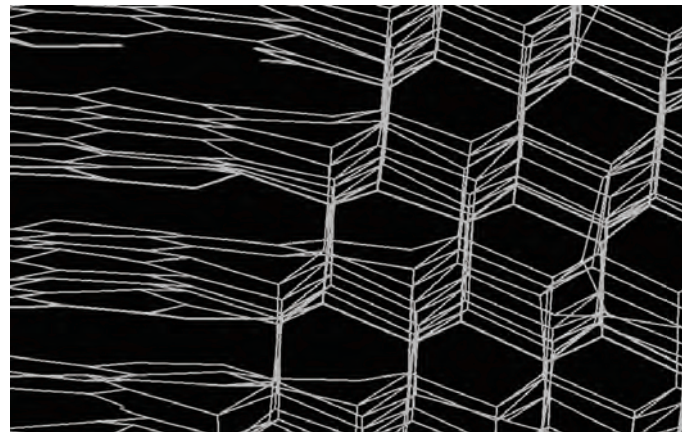
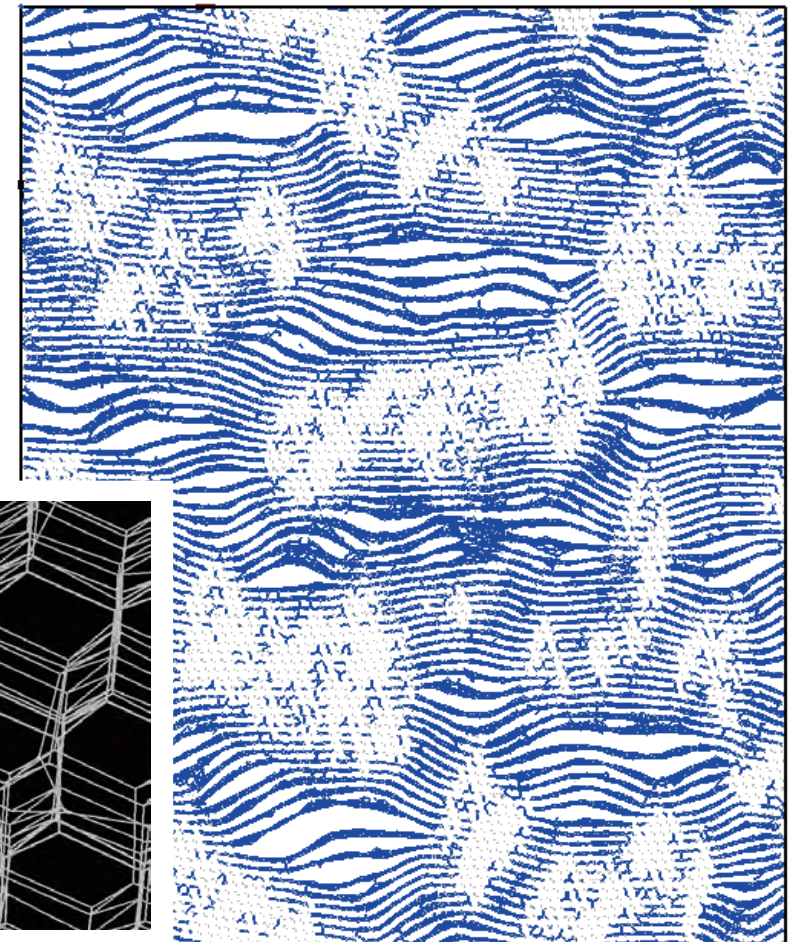
Ex. sp² and sp³ nano composite carbon solid with 100K atoms
→ the distinction of sp² and sp³-domains

(A) Visualize sp² and sp³ domains

(B) Visualize only sp² domains



sp²-sp³
domain
boundary



Krylov subspace theories and ultra-large-scale electronic state calculations on the K computer (as an interdisciplenary reseach between physics and applied mathematics)

1. Overview : Application-Algorithm-Architecture co-design
 - 1-a. Overview from physics
 - 1-b. ELSEES : our code
 - 1-c. Overview from mathematics
2. Krylov-subspace theories
for generalized shifted linear equation
3. 'Big data' (post-simulation) analysis.
4. Perforcance issues on the supercomputer
5. For further collaboration
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 - 5-a. Interior eigen-pair problem
 - 5-b. 'Open data' for matrix

Architecture-related issues

→ Better performance on the supercomputers, such as the K computer

1. Optimal balance between

operation cost, communication cost and memory cost.

→ ex. memory-saving workflow

2. Parallel file IO

hardware : built-in parallel file IO function on the K computer

software : use of split XML files

Memory-saving workflow

.... reduces the memory size drastically;
ex. 28GB→1.6GB (with 100 K atom)

The data array for the Green's function, the biggest one,
is not stored in the memory but recalculated

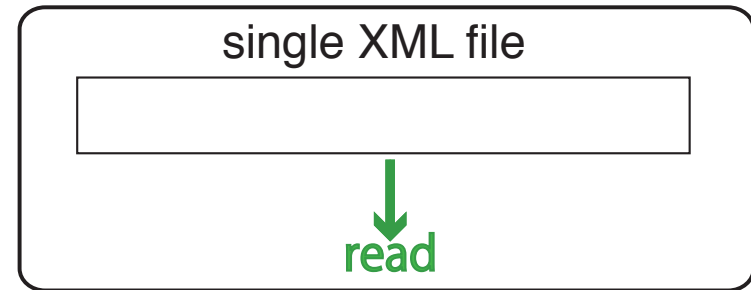
$$(H, S) \Rightarrow G \Rightarrow \mu \Rightarrow (\text{recalc. of } G) \Rightarrow \rho$$

Parallel file IO with split XML file

ex. Accerlation in the initial procedure with 10M atoms

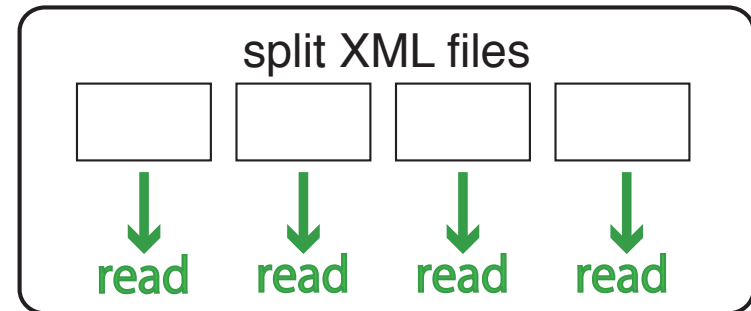
(a) with non-parallel file reading

→ $T = 1426.6$ sec



(b) with parallel file reading

→ $T = 69.6$ sec



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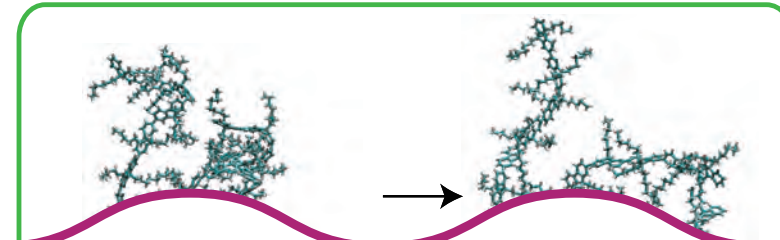
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Typical types of quantum physical quantities

(1) Energy and force
(for structure-dynamics simulation)
→ physical quantity in trace form

(2) Electronic spectrum
(density of states, and so on)
→ weighted eigen-value histogram

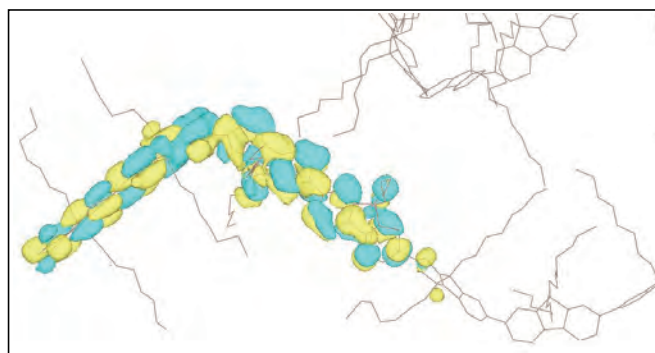
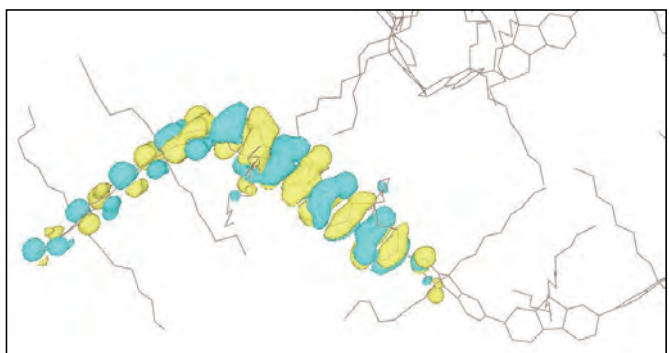
(3) Specific eigen states
(Fig. HOMO and LUMO)
→ interior eigen-pair problem



Problem :
the calculation of the k -th eigen pair
for a given value of k

For specific electrons
responsible for material properties in
electronics and optics

cf. D. Lee et al., 19. on this conference



ex. π conjugated polymer:
poly-(9,9 dioctil fluorene)
Ref. Hoshi, et al. JPCM 24,
165502 (2012)

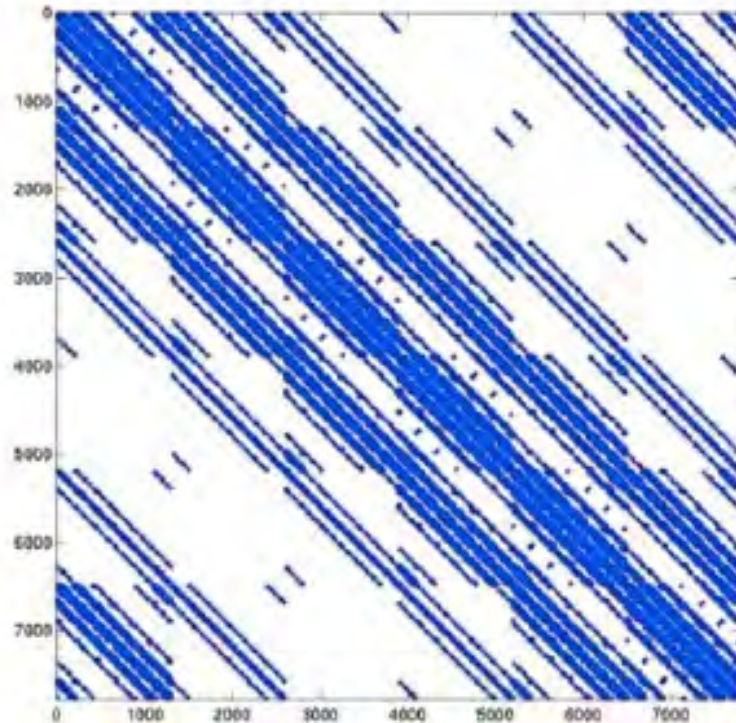
'Open Data' : ELSES matrix library

→Matrix data in our real problem with the matrix size of $M = 10^2 \sim 10^6$

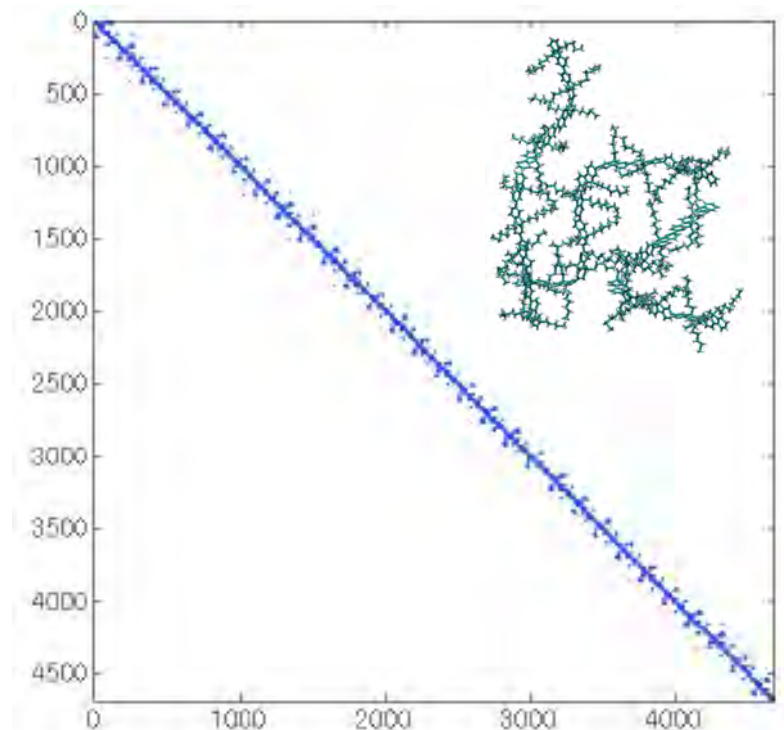
→For further collaboration between physics and applied mathematics

Note : Matrix property is significantly different among materials.

(a) Solid gold



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



Summary

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