

## 「京」での100ナノ電子状態計算にみる、数理と物質科学の融合

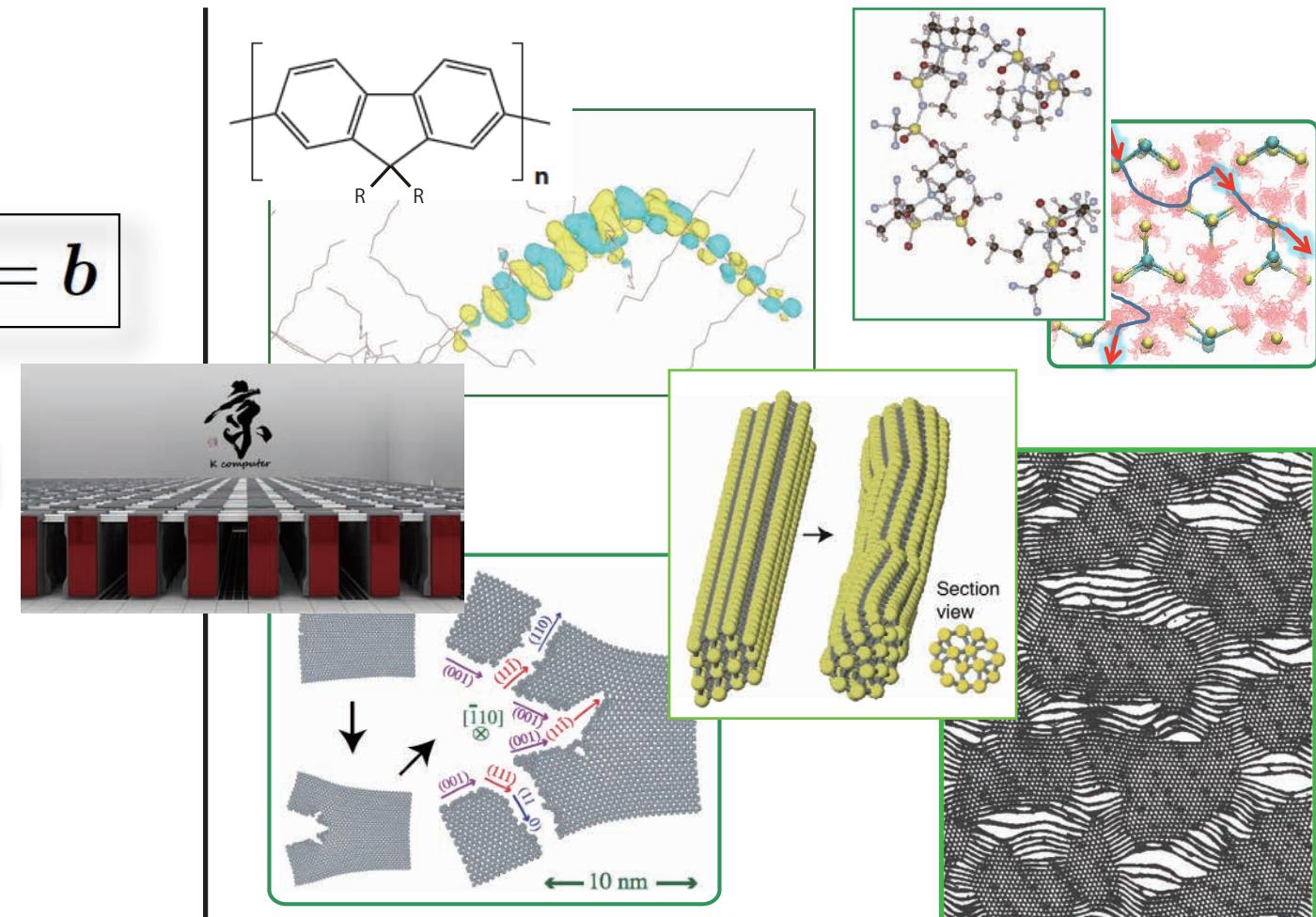
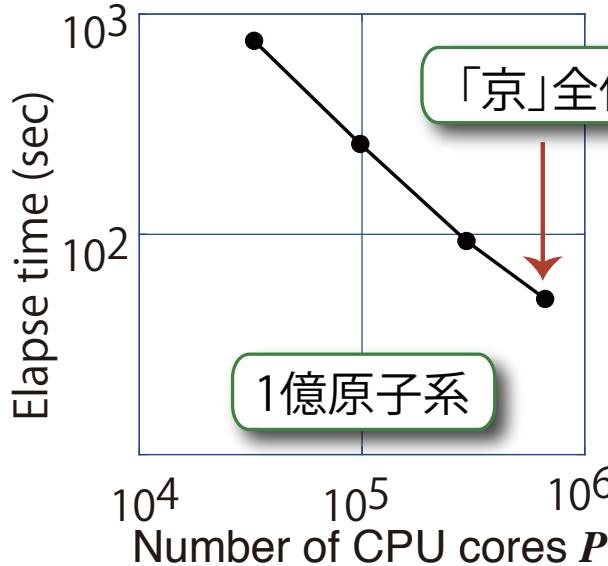
星健夫 (鳥取大学工学研究科応用数理工学講座)

出身: 東京大学工学部物理工学科

主な所属学会: 物理学会、応用数理学会、応用物理学会

$$H\mathbf{y} = \lambda S\mathbf{y}$$

$$(zS - H)\mathbf{x} = \mathbf{b}$$



# 内容など

1. 全体の概要
2. 計算:並列計算への入門
3. 応用:ヘリカル金ナノワイヤ
4. 応用:シリコン脆性  
-----(以上が前回)-----
5. 数理: (a)大行列数理への入門  
          (b) シフト型クリロフ部分空間理論  
          (新しい超並列型アルゴリズム)
6. 応用:ナノ複合カーボン
7. 応用:有機デバイス系への展望

5/13

10:45-12:15

13:30-15:00

レポート課題:

締切:5月末日。

提出先:星にPDF(3MB以内)をメールで送付。氏名と学生番号を明記すること。

星のアドレス:hoshi@damp.tottori-u.ac.jp

内容:問題(1)自身の研究内容の概略(1ページ以内)

問題(2)本講義の感想(半ページ以上上限はなし。図表を付しても可)。

注:講義時間内に問題が追加される可能性もある。

# 大行列数理への入門

# チュートリアル: 物理からみた大行列数理ソルバー(の入り口)

3つの視点から分類

- (i) 行列サイズ: 大行列とはどの程度の大きさか?
- (ii) 解法の基盤的戦略
- (iii) 行列の種類

# 「大規模行列」とは、どの程度のサイズか？

→M=1万次元くらいが  
「中規模行列」

実行列のデータ容量

(a) M=1000だと

$$8B \times 1K \times 1K = 8 \text{ MB}$$

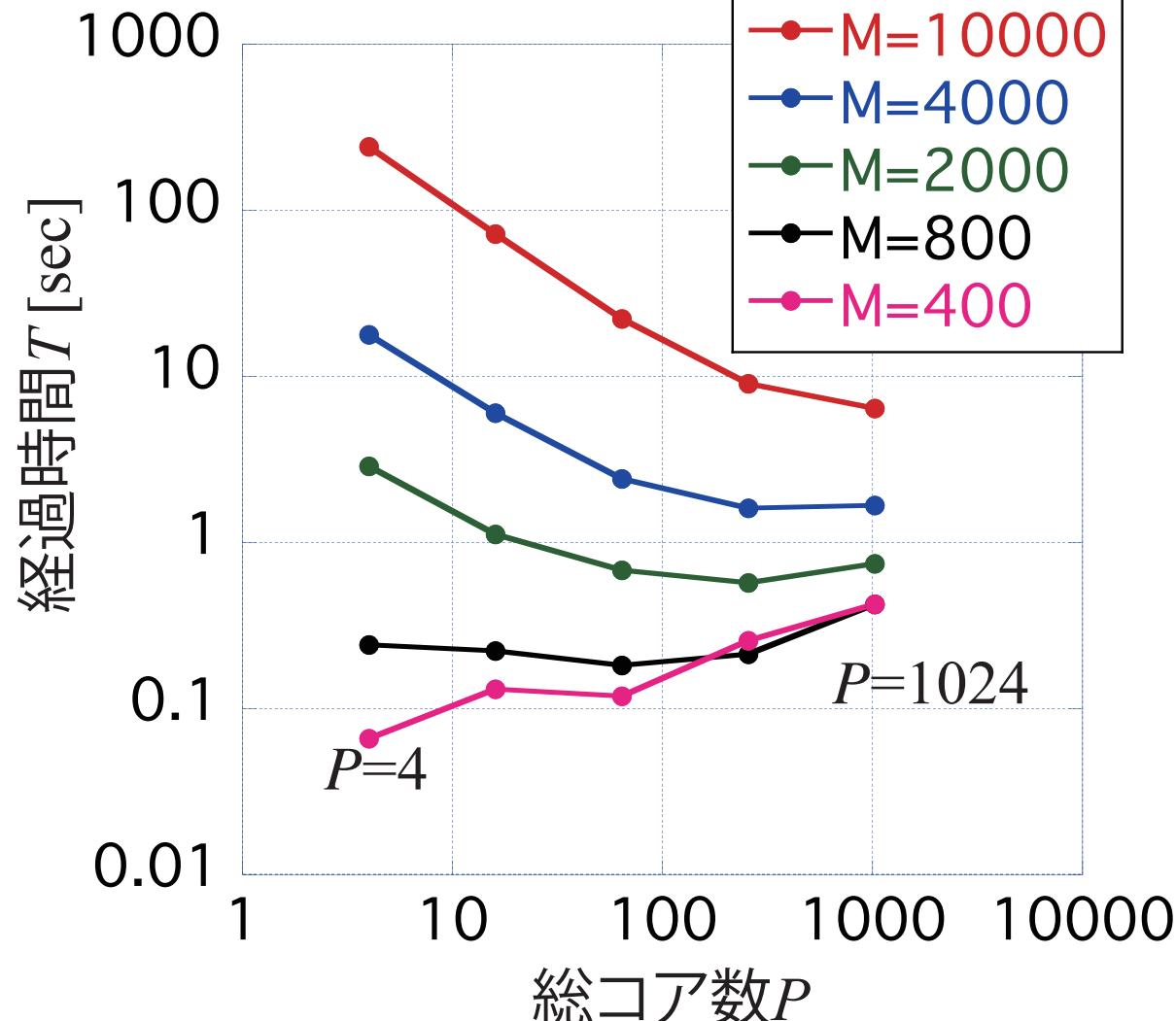
(b) M=1万だと

$$8B \times 10K \times 10K = 0.8\text{GB} \text{ (約1GB)}$$

(c) M=10万だと

$$8B \times 100K \times 100K = 80 \text{ GB}$$

例：中小規模行列の全固有対計算(\*)



(\*) Intel Xeon (SGI Altix @ISSP), 實対称, ScaLAPACK

# Strategies of matrix solvers

## Krylov (iterative) solvers

- ‘projection’ strategy
- (mainly) sparse matrices
- basics of  $O(N)$  calculation

ex. CG algorithm

## Direct solvers

- ‘transformation’ strategy
- (mainly) dense matrices
- $O(N^3)$  calculation

‘projection’ on the Krylov subspace of

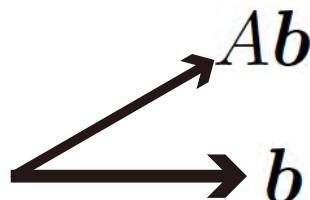
$$K_n(A; \mathbf{b}) \equiv \text{span} \{ \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^{n-1}\mathbf{b} \}$$

$n$  : subspace dimension (iteration number)

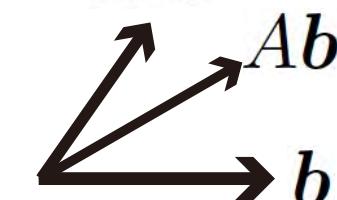
$$n=1$$



$$n=2$$



$$n=3$$



# Strategies of matrix solvers

## Krylov (iterative) solvers

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- (mainly) sparse matrices
- basics of  $O(N)$  calculation

ex. CG algorithm

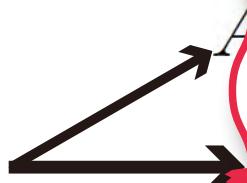
‘projection’ on the Krylov subspace

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

$n$  : subspace dimension

$n=1$

$n=2$



クリロフ部分空間  
→数値解析の基礎

森正武「数値解析」共立出版,  
第2版 (2002). 目次:

第1章 連立1次方程式

1.15 共役勾配法

1.16 クリロフ部分空間法

1.17 前処理付き共役勾配法

第2章 非線形方程式

第3章 行列の固有値問題

第4章 関数近似

第5章 数値積分

第6章 常微分方程式

注: 第1版(1973)には、  
クリロフ部分空間法の章なし。

# Strategies of matrix solvers

## Krylov (iterative) solvers

- ‘projection’ strategy
- (mainly) sparse matrices
- basics of  $O(N)$  calculation

ex. CG algorithm

## Direct solvers

ex. CG algorithm for  $A\mathbf{x} = \mathbf{b}$   
→ the  $n$ -th step solution  $\mathbf{x}_n$  is given by

$$\mathbf{x}_n \in K_n(A; \mathbf{b})$$

‘projection’ on the Krylov subspace of

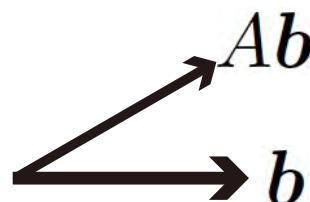
$$K_n(A; \mathbf{b}) \equiv \text{span} \{ \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^{n-1}\mathbf{b} \}$$

$n$  : subspace dimension (iteration number)

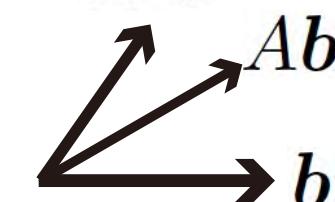
$$n=1$$



$$n=2$$



$$n=3$$



# Strategies of matrix solvers

## Krylov (iterative) solvers

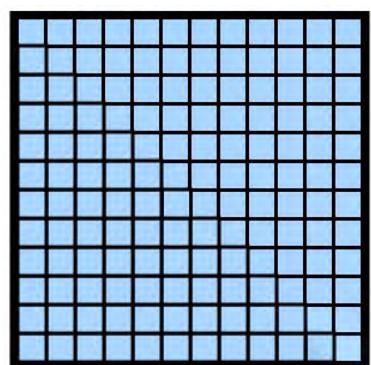
- ‘projection’ strategy
- (mainly) sparse matrices
- basics of  $O(N)$  calculation

## Direct solvers

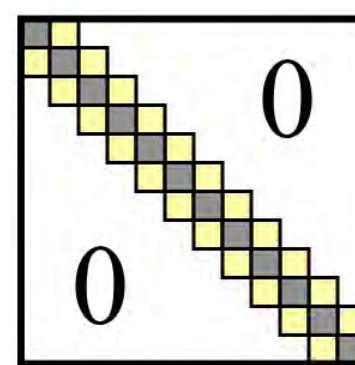
- ‘transformation’ strategy
- (mainly) dense matrices
- $O(N^3)$  calculation

‘transformation’ of the whole space

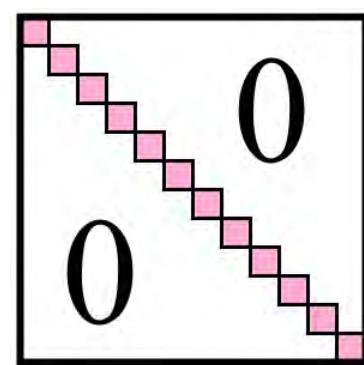
Example



dense



tri-diagonal



diagonal

# 行列の種類による分類

## examples

Hermitian

- general
- real symmetric

Non-Hermitian

- general
- complex symmetric

typical Krylov  
solver for  $Ax=b$

CG

BiCG

COCG

# まとめ: 物理からみた大行列数理ソルバー(の入り口)

→3つの視点から分類

(i) 行列サイズ: 大行列とはどの程度の大きさか?

→ $M=1$ 万次元が「中規模」行列

(ii) 解法の基盤的戦略

→「射影」と「変換」

(iii) 行列の種類

→エルミート・(特殊な)非エルミート、

疎行列・帯行列・ブロック行列、などなど

## 有用な教科書

[1] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe and H. van der Vorst, ed.

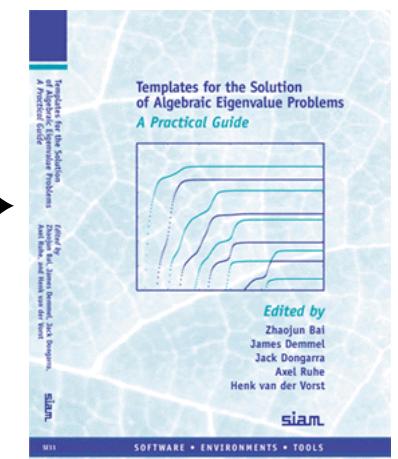
“Templates for the solution of Algebraic Eigenvalue Problems:

A Practical Guide” . SIAM, Philadelphia (2000) →

( available online: <http://web.cs.ucdavis.edu/~bai/ET/contents.html> )

[2] G. H. Golub, C. F. Van Loan,

"Matrix Computations", Johns Hopkins Univ.; 4.ed. (2012)

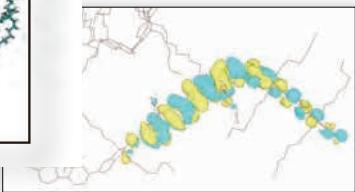
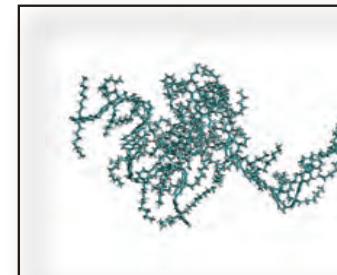


# シフト型クリロフ部分空間理論

# Application-Algotirhm-Architecture co-design

→ 応用(計算物質科学)分野・数理分野・高速計算技術(HPC)分野の連携研究

Application : quantum  
material simulationn



Algorithm : numerical linear algebra

$$H\mathbf{y} = \lambda S\mathbf{y}$$

$$(zS - H)\mathbf{x} = \mathbf{b}$$



Architecture : (post-)petascale  
supercomputers



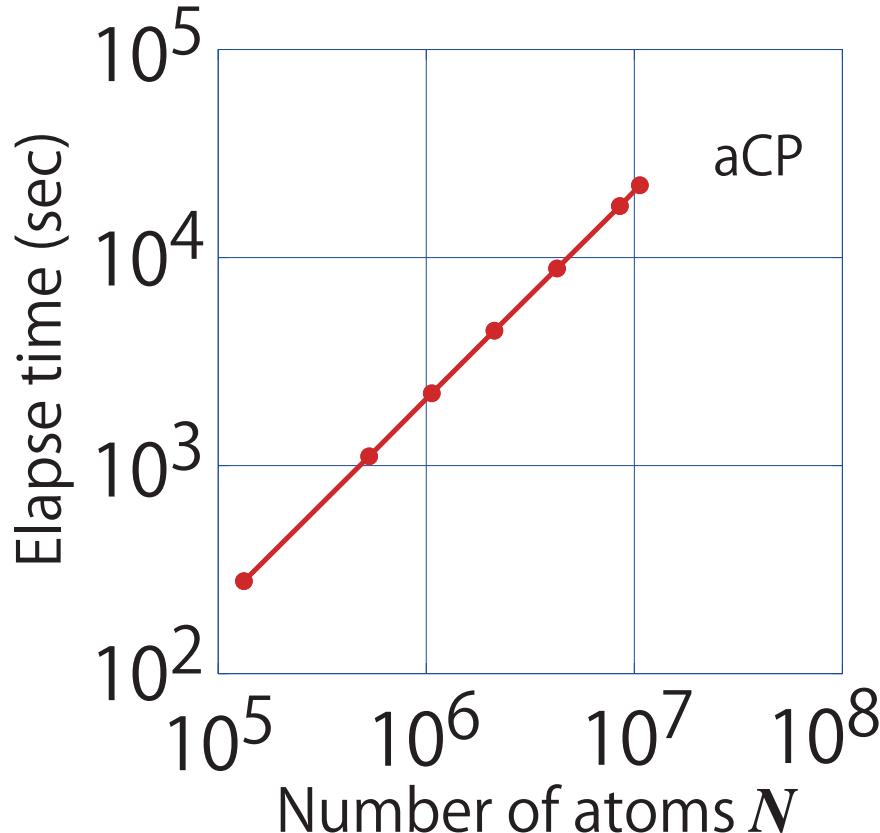
## ELSES, our electronic-structure calculation code

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

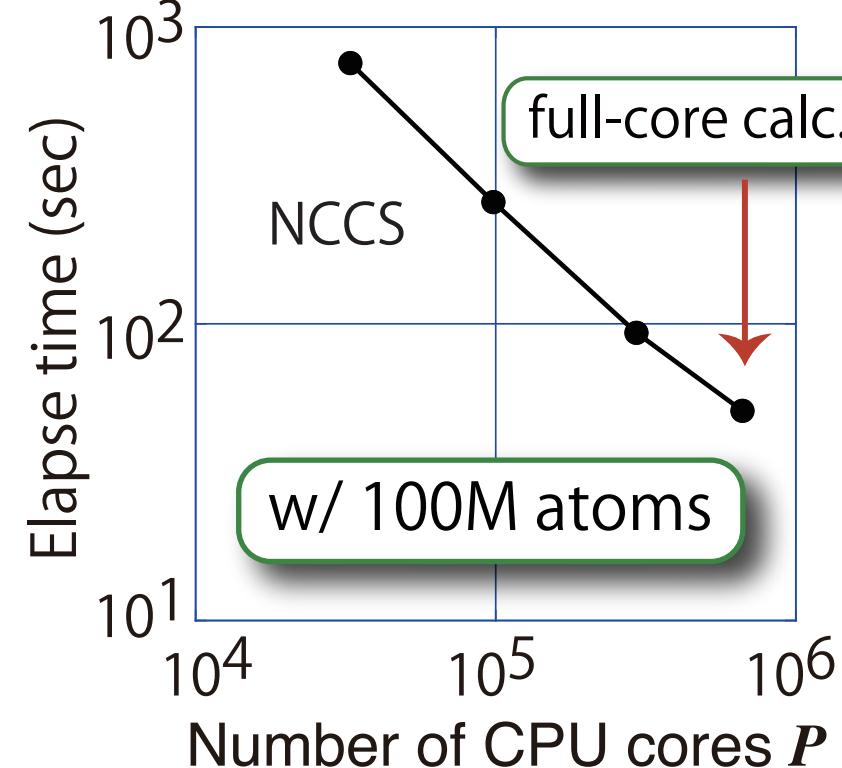
( Hoshi et al., JPCM24, 165502(2012) JPSJ 82, 023710 (2013); JPSCP. 1, 016004 (2014) )

aCP :amourphous-like conjugated polymer, poly-(9,9 dioctil-fluorene),  
NCCS: sp<sub>2</sub>-sp<sub>3</sub> nano composite carbon solid

(a) Order- $N$  scaling



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



## ELSES, our electronic-structure calculation code

Benchmark with upto 100M atoms(  $\rightleftharpoons$  Si : (126nm)<sup>3</sup>region)

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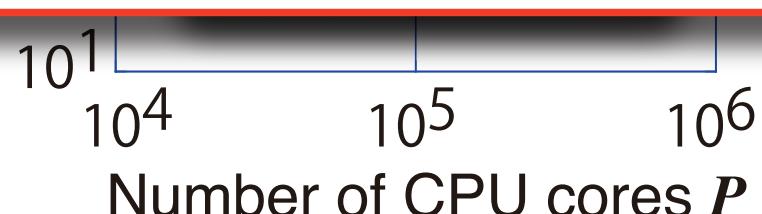
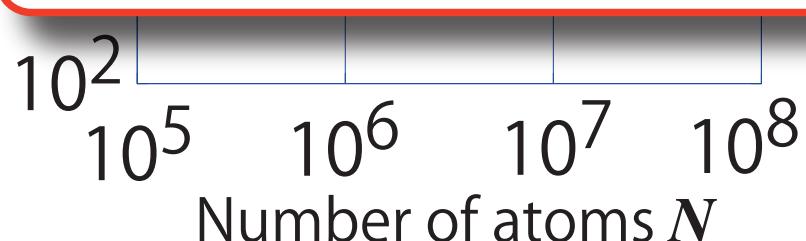
### Methodology

- Original linear-algebraic order- $N$  algorithms with generalized shifted linear equations

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

- Applicable both to metals and insulators
- Modelled (TB-type real-space) systems based on *ab initio* calc.,
- Options:
  - DFT-derived charge-self-consistent formulation
  - van-der-Waals correction

Elapsed time (sec)



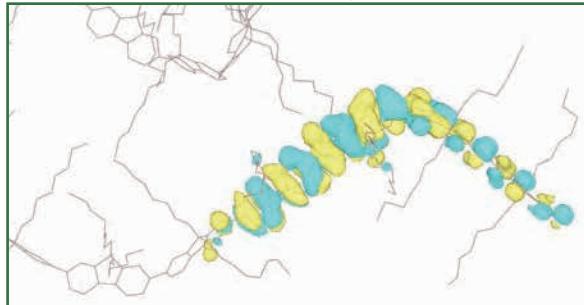
# Application studies with ELSES

<http://www.elses.jp/>

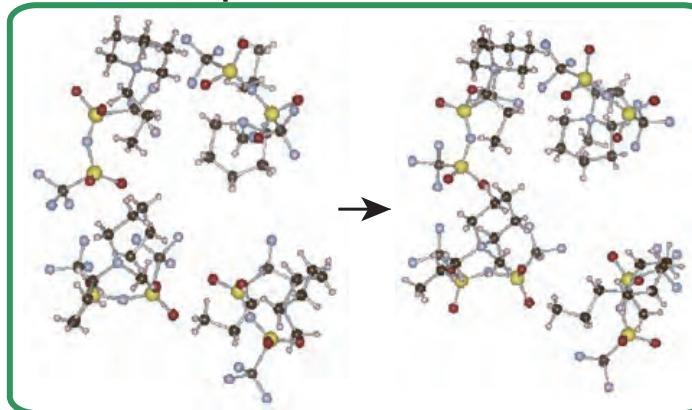
Acknowledgement (coworkers, data provision) :

S. Nishino (U Tokyo, Hulinks Inc.), T. Fujiwara (U Tokyo), S. Yamamoto(TEU),  
H. Yamasaki(Toyota) , Y. Zempo(Hosei U), M. Ishida(Sumitomo Chem. Co.)

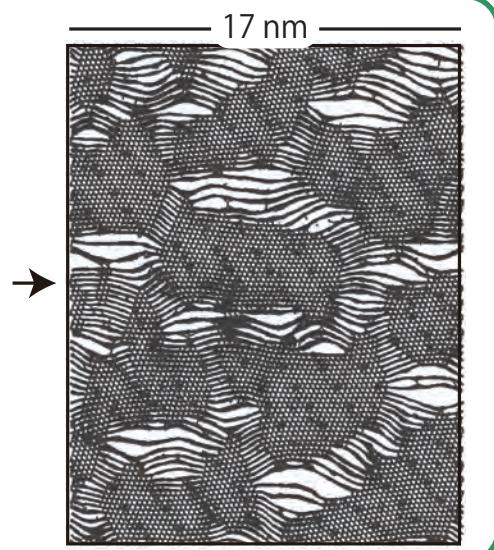
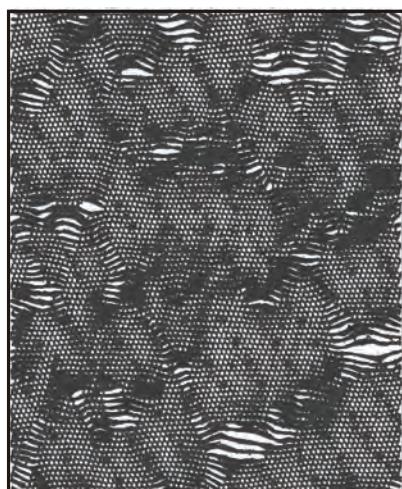
Organic materials  
(amorphous-like  
conjugated polymer)



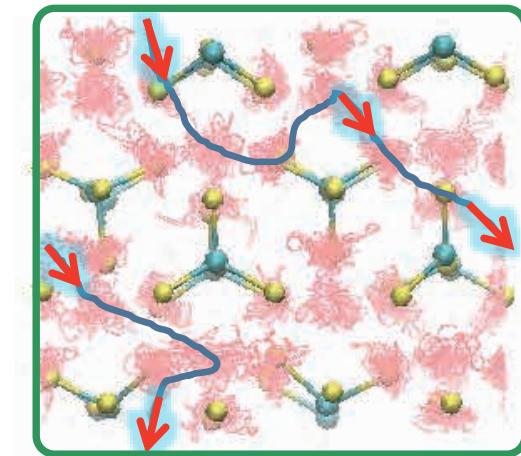
Ionic liquid



sp<sub>2</sub>-sp<sub>3</sub> nano-composite carbon solid

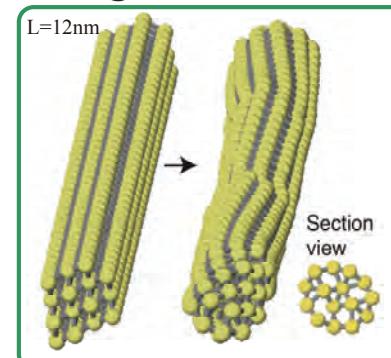


Li ion diffusion

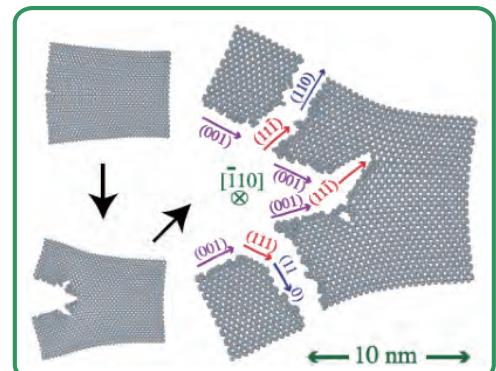


Nishino et al. PRB90,  
024303, (2014)

helical gold nanowire

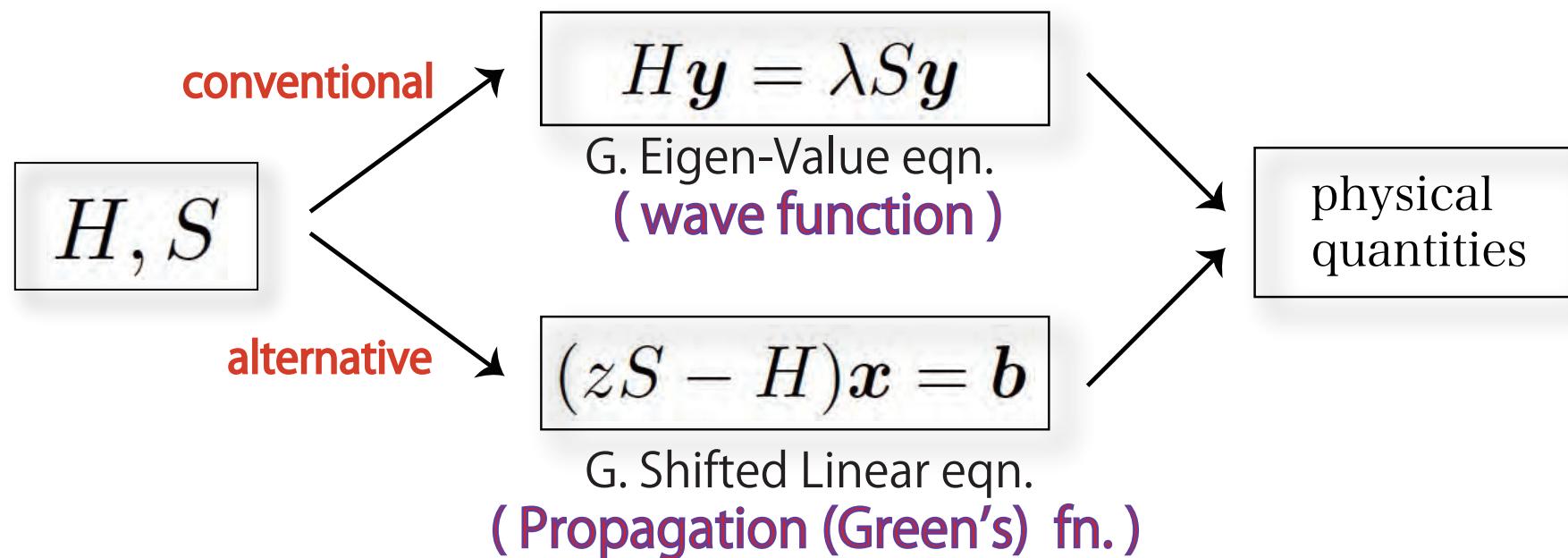
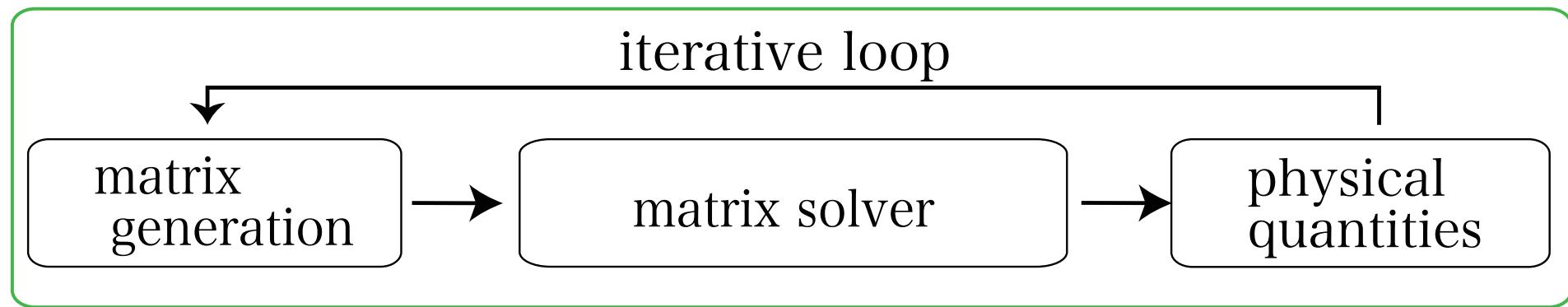


Si brittle fracture



# Application-Algotirhm-Architecture co-design

## Workflow



# Basic equations

Generalized eigen-value (GEV) equation

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

wavefunction formulation

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

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

Generalized shifted linear (GSL) equations

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

**non-Hermitian**

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

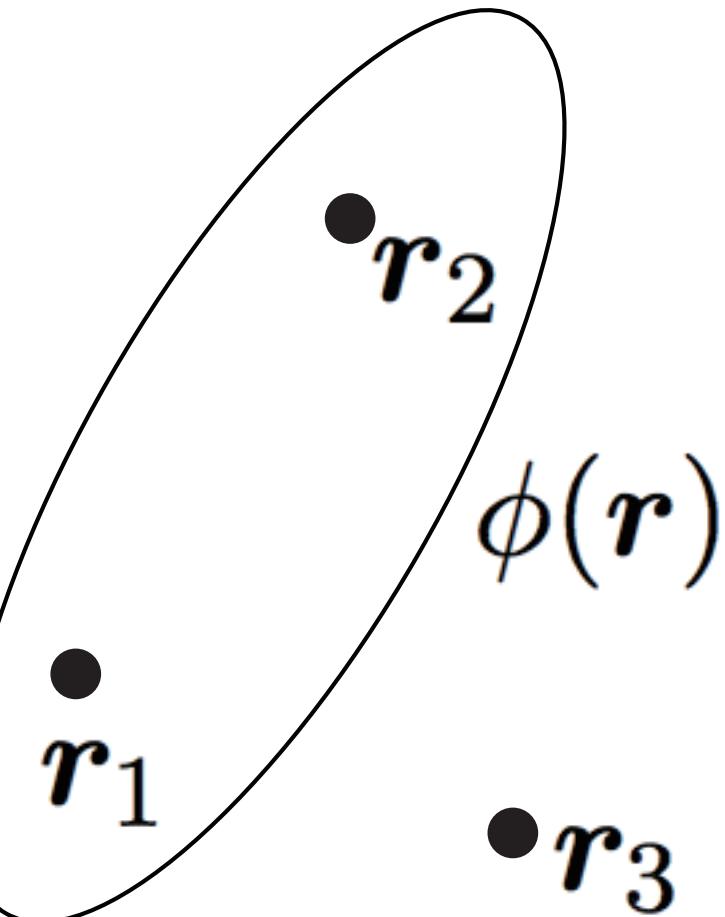
the propagation (Green's) function formulation

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

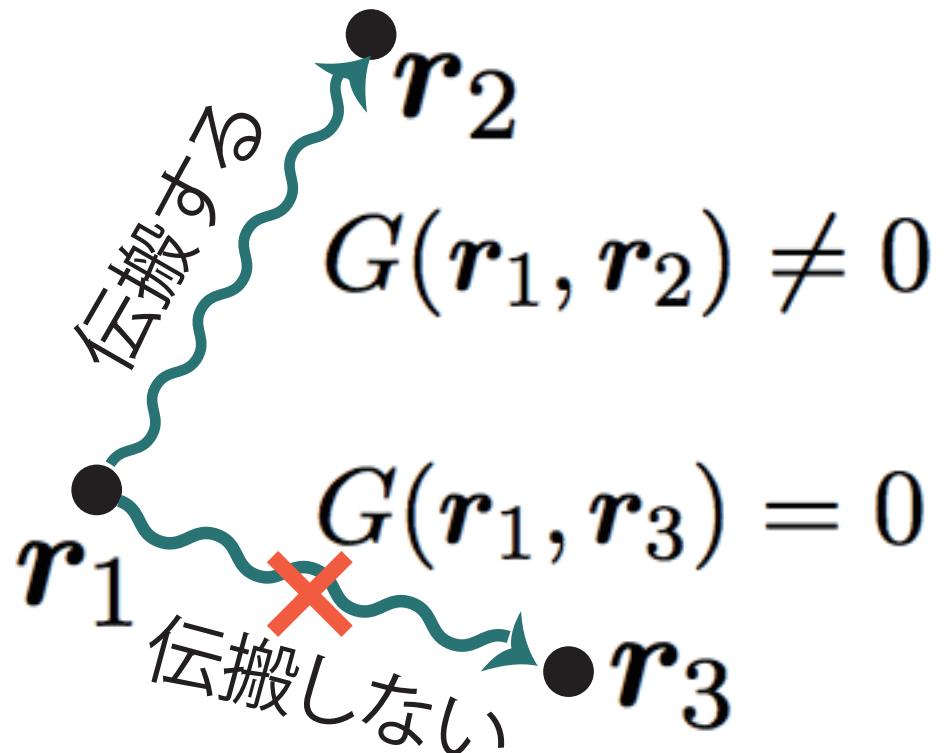
# チュートリアル: 波動関数と伝搬(グリーン)関数

波動関数描像  $\longleftrightarrow$  伝搬関数描像

空間的広がり



伝搬の可否



# 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)

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

with a given weight function  
('Fermi distribution function')

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

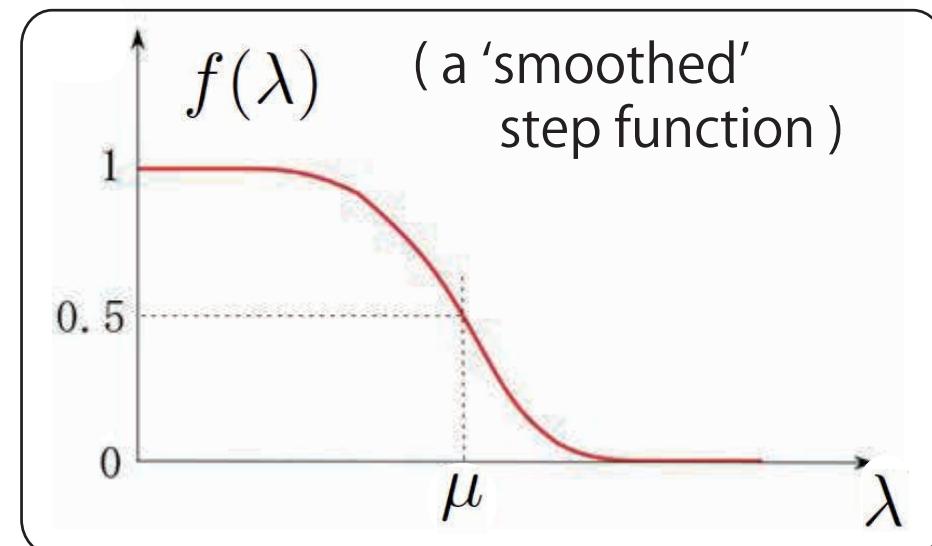
(  $\beta, \mu$  : given parameters )

Physical quantity in trace form

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

with the density matrix

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



# The work flow

$$(H, S) \rightarrow G \rightarrow \mu \rightarrow \rho$$

$\mu$  :chemical potential  
(determined by the bisection method)  
 $\rho$  :density matrix (calculated from  $G$  &  $\mu$ )

$$\rho_{ij} = \frac{-1}{\pi} \int f(\varepsilon) G_{ij}(\varepsilon + i0) d\varepsilon$$

# Studies on novel linear algebraic algorithms

Collaboration with applied mathematics researchers:

T. Sogabe (Aichi Pref. U), S.-L. Zhang, T. Miyata (Nagoya U)

Studies for (generalized) shifted linear equations:  $(zS - H)\mathbf{x} = \mathbf{b}$

[1] Use of the collinear residual theorem;

R. Takayama, et al., Phys. Rev. B 73, 165108 (2006)

→ Theoretical extensions:

T. Sogabe, et al, ETNA 31, 126 (2008)

H. Teng, et al, Phys. Rev. B 83, 165103 (2011)

T. Sogabe, et al, J. Comp. Phys. 231, 5669 (2012) ]

**non-Hermitian  
(complex symmetric)**

[2] Krylov subspace theory with exact physical conservation law;

T. Hoshi, et al, J. Phys.: Condens. Matter 24, 165502 (2012)

Studies for generalized eigen-value problem:  $H\mathbf{y} = \lambda S\mathbf{y}$

[3] Use of Sylvester's theorem of inertia;

D. Lee, et al, Japan J. Indust. Appl. Math. 30, 625 (2013)

# Shift invariance of Krylov subspace

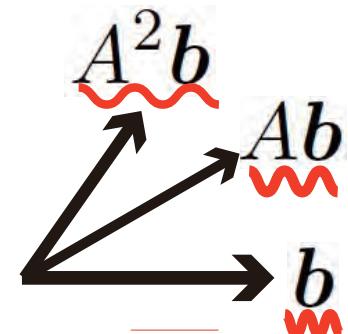
$$K_n(A + \sigma I; \mathbf{b}) = K_n(A; \mathbf{b})$$

ex.  $n = 3$

$$(A + \sigma I)^0 \mathbf{b} = \mathbf{b}$$

$$(A + \sigma I)^1 \mathbf{b} = \sigma \mathbf{b} + A \mathbf{b}$$

$$(A + \sigma I)^2 \mathbf{b} = \sigma^2 \mathbf{b} + 2\sigma A \mathbf{b} + A^2 \mathbf{b}$$



# Shifted conjugate-orthogonal conjugate gradient (sCOCG) method

Shifted linear equations:  $(A + \sigma I) \mathbf{x}^{(\sigma)} = \mathbf{b}$  ( $\sigma := 0, \sigma_1, \sigma_2, \dots$ )

## Collinear residual theorem

→ One can construct the Krylov subspace method with the following property

$\mathbf{x}_n^{(\sigma)}$  : solution vector at the n-th iterate

Residual vector at the '**seed**' eq. ( $\sigma = 0$ )

$$\mathbf{r}_n^{(0)} \equiv A\mathbf{x}_n^{(0)} - \mathbf{b} (\rightarrow \mathbf{0}) \quad (1)$$

Residual vector at the '**shifted**' eq. ( $\sigma \neq 0$ )

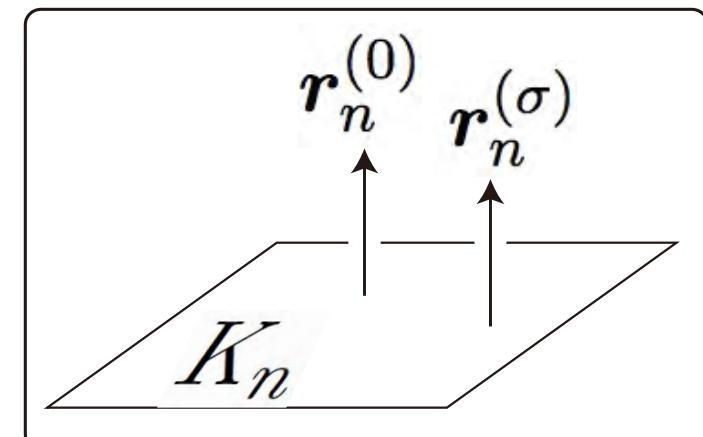
$$\mathbf{r}_n^{(\sigma)} \equiv (A + \sigma I)\mathbf{x}_n^{(\sigma)} - \mathbf{b} (\rightarrow \mathbf{0}) \quad (2)$$

A. Frommer, Computing 70, 87 (2003)

Collinear residual theorem  
(between origina and shifted eqns.)

$$\mathbf{r}_n^{(\sigma)} = \frac{1}{\pi_n^{(\sigma)}} \mathbf{r}_n^{(0)} \quad (3)$$

$\pi_n^{(\sigma)}$  : scalar



# Shifted conjugate-orthogonal conjugate gradient (sCOCG) method

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A. Frommer, Computing 70, 87 (2003)

Collinear residual theorem  
( between origina and shifted eqns. )

$$\mathbf{r}_n^{(\sigma)} = \frac{1}{\pi_n^{(\sigma)}} \mathbf{r}_n^{(0)} \quad (3)$$

$\pi_n^{(\sigma)}$  : scalar

Eq.(2) is replaced by Eq.(3)  
→ The matrix-vector multiplication is replaced  
by the scalar-vector multiplication  
→ Drastic reduction of operation cost

# Shifted COCG method

'seed' eq. :  $A \mathbf{x} = \mathbf{b}$

$$\mathbf{x}_0 = \mathbf{x}_0^\sigma = \mathbf{p}_{-1} = \mathbf{p}_{-1}^\sigma = 0,$$

$$\pi_0 = \pi_{-1}^\sigma = 1, \mathbf{r}_0 = \mathbf{b},$$

$$\beta_{-1} = 0, \alpha_{-1} = 1$$

do  $n = 0, 1, \dots$

$$\mathbf{p}_n = \mathbf{r}_n + \beta_{n-1} \mathbf{p}_{n-1} \quad (1)$$

$$\alpha_n = \frac{\mathbf{r}_n^T \mathbf{r}_n}{\mathbf{p}_n^T A \mathbf{p}_n} \quad (2)$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \alpha_n \mathbf{p}_n \quad (3)$$



$$\mathbf{r}_{n+1} = \mathbf{r}_n - \alpha_n A \mathbf{p}_n \quad (4)$$

$$\beta_n = \frac{\mathbf{r}_{n+1}^T \mathbf{r}_{n+1}}{\mathbf{r}_n^T \mathbf{r}_n} \quad (5)$$

enddo

## Collinear residual theorem

$$\mathbf{r}_n \equiv A \mathbf{x}_n - \mathbf{b} \rightarrow \mathbf{0} \quad (a)$$

$$\begin{aligned} \mathbf{r}_n^{(\sigma)} &\equiv (A + \sigma I) \mathbf{x}_n^{(\sigma)} - \mathbf{b} \\ &= \frac{1}{\pi_n^{(\sigma)}} \mathbf{r} \rightarrow \mathbf{0} \end{aligned} \quad (b)$$

'shifted' eq. :  $(A + \sigma I) \mathbf{x}^{(\sigma)} = \mathbf{b}$

$$\pi_{n+1}^\sigma = (1 + \alpha_n \sigma) \pi_n^\sigma + \frac{\alpha_n \beta_{n-1}}{\alpha_{n-1}} (\pi_n^\sigma - \pi_{n-1}^\sigma) \quad (6)$$

$$\beta_{n-1}^\sigma = \left( \frac{\pi_{n-1}^\sigma}{\pi_n^\sigma} \right)^2 \beta_{n-1} \quad (7)$$

$$\alpha_n^\sigma = \frac{\pi_n^\sigma}{\pi_{n+1}^\sigma} \alpha_n \quad (8)$$

$$\mathbf{p}_n^\sigma = \frac{1}{\pi_n^\sigma} \mathbf{r}_n + \beta_{n-1}^\sigma \mathbf{p}_{n-1}^\sigma \quad (9)$$

$$\mathbf{x}_{n+1}^\sigma = \mathbf{x}_n^\sigma + \alpha_n^\sigma \mathbf{p}_n^\sigma \quad (10)$$

# Shifted COCG method

'seed' eq. :  $A \mathbf{x} = \mathbf{b}$

$$\mathbf{x}_0 = \mathbf{x}_0^\sigma = \mathbf{p}_{-1} = \mathbf{p}_{-1}^\sigma = 0,$$

$$\pi_0 = \pi_{-1}^\sigma = 1, \mathbf{r}_0 = \mathbf{b},$$

$$\beta_{-1} = 0, \alpha_{-1} = 1$$

do  $n = 0, 1, \dots$

$$\mathbf{p}_n = \mathbf{r}_n + \beta_{n-1} \mathbf{p}_{n-1} \quad (1)$$

$$\alpha_n = \frac{\mathbf{r}_n^T \mathbf{r}_n}{\mathbf{p}_n^T A \mathbf{p}_n} \quad (2)$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \alpha_n \mathbf{p}_n \quad (3)$$



$$\mathbf{r}_{n+1} = \mathbf{r}_n - \alpha_n A \mathbf{p}_n \quad (4)$$

$$\beta_n = \frac{\mathbf{r}_{n+1}^T \mathbf{r}_{n+1}}{\mathbf{r}_n^T \mathbf{r}_n} \quad (5)$$

enddo

## Collinear residual theorem

$$\mathbf{r}_n \equiv A \mathbf{x}_n - \mathbf{b} \rightarrow \mathbf{0} \quad (a)$$

$$\begin{aligned} \mathbf{r}_n^{(\sigma)} &\equiv (A + \sigma I) \mathbf{x}_n^{(\sigma)} - \mathbf{b} \\ &= \frac{1}{\pi_n^{(\sigma)}} \mathbf{r} \rightarrow \mathbf{0} \end{aligned} \quad (b)$$

'shifted' eq. :  $(A + \sigma I) \mathbf{x}^{(\sigma)} = \mathbf{b}$

$$\pi_{n+1}^\sigma = (1 + \alpha_n \sigma) \pi_n^\sigma + \frac{\alpha_n \beta_{n-1}}{\alpha_{n-1}} (\pi_n^\sigma - \pi_{n-1}^\sigma) \quad (6)$$

$$\beta_{n-1}^\sigma = \left( \frac{\pi_{n-1}^\sigma}{\pi_n^\sigma} \right)^2 \beta_{n-1} \quad (7)$$

$$\alpha_n^\sigma = \frac{\pi_n^\sigma}{\pi_{n+1}^\sigma} \alpha_n \quad (8)$$

$$\mathbf{p}_n^\sigma = \frac{1}{\pi_n^\sigma} \mathbf{r}_n + \beta_{n-1}^\sigma \mathbf{p}_{n-1}^\sigma \quad (9)$$

$$\mathbf{x}_{n+1}^\sigma = \mathbf{x}_n^\sigma + \alpha_n^\sigma \mathbf{p}_n^\sigma \quad (10)$$

# 共線残差定理を用いたシフト型クリロフ部分空間理論の物理への応用例

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