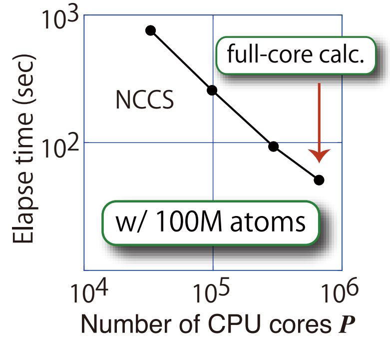
「京」での1億原子電子状態計算 ～物質科学と数理科学の接点として～

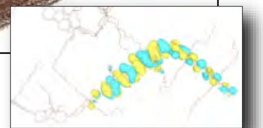
星健夫、井町宏人(鳥取大, CREST)

1. Overview: Application-Algorithm-Architecture co-design
2. 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. 「京」での1億原子(100ナノスケール)電子状態計算
4. 数理ソルバー：クリロフ部分空間法
5. 複合数理原理ソルバーと「ミドルウェア」開発
6. まとめ



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

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



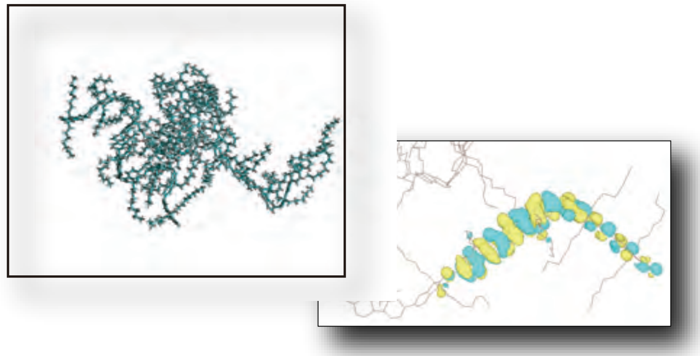
謝辞(予算)
JST-CREST(PostPeta領域),
科研費新学術領域(コンピューティクス)
JST-ASTEP, 構造材料元素戦略、科研費(一般)、など

Overview

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



↕

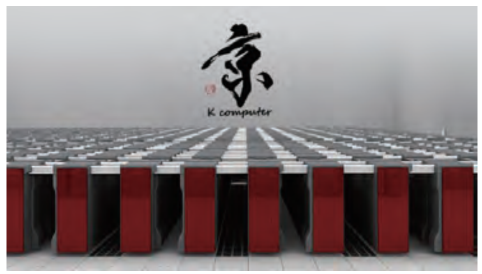
Algorithm : numerical linear algebra

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

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

↕

Architecture : (post-)petascale supercomputers



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Application : qu r

Algorithm : nu

Architecture : (

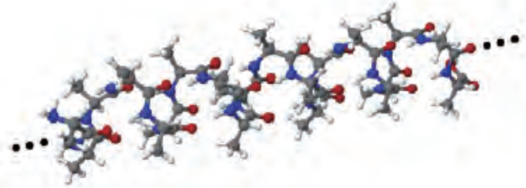
電子状態計算ソサエティとの強い連携によって、
新しい数理(固有値問題)ソルバーが生まれた例

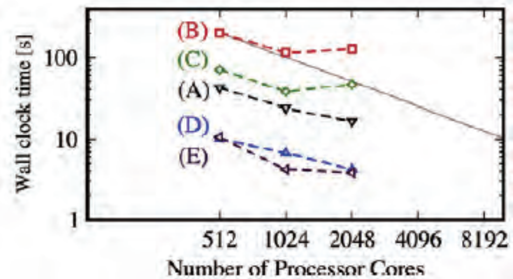
- 国内→今日の話
- 海外

(1) ELPA (http://elpa.rzg.mpg.de/)

T. Auckenthaler, Parallel Comput. 37, 783 (2011)

A. Marek, J. Phys.: Condens. Matter 26, 213201 (2014)





(2) FEAST (http://www.ecs.umass.edu/~polizzi/feast/)

E. Polizzi, Phys. Rev. B79, 115112 (2009)

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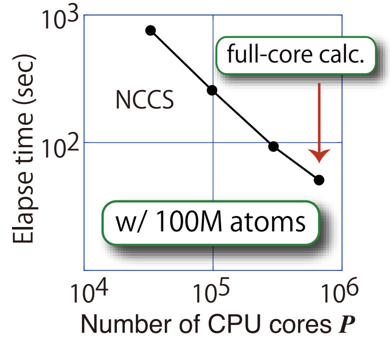

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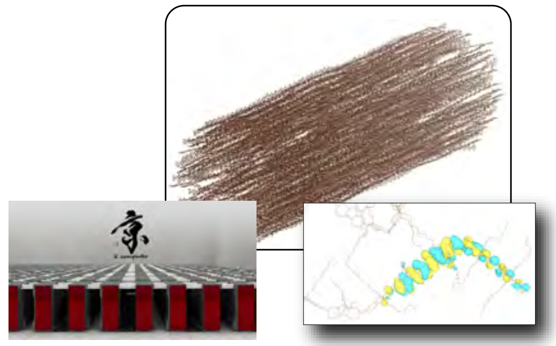

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チュートリアル：物理からみた大行列数理ソルバー(の入り口)

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

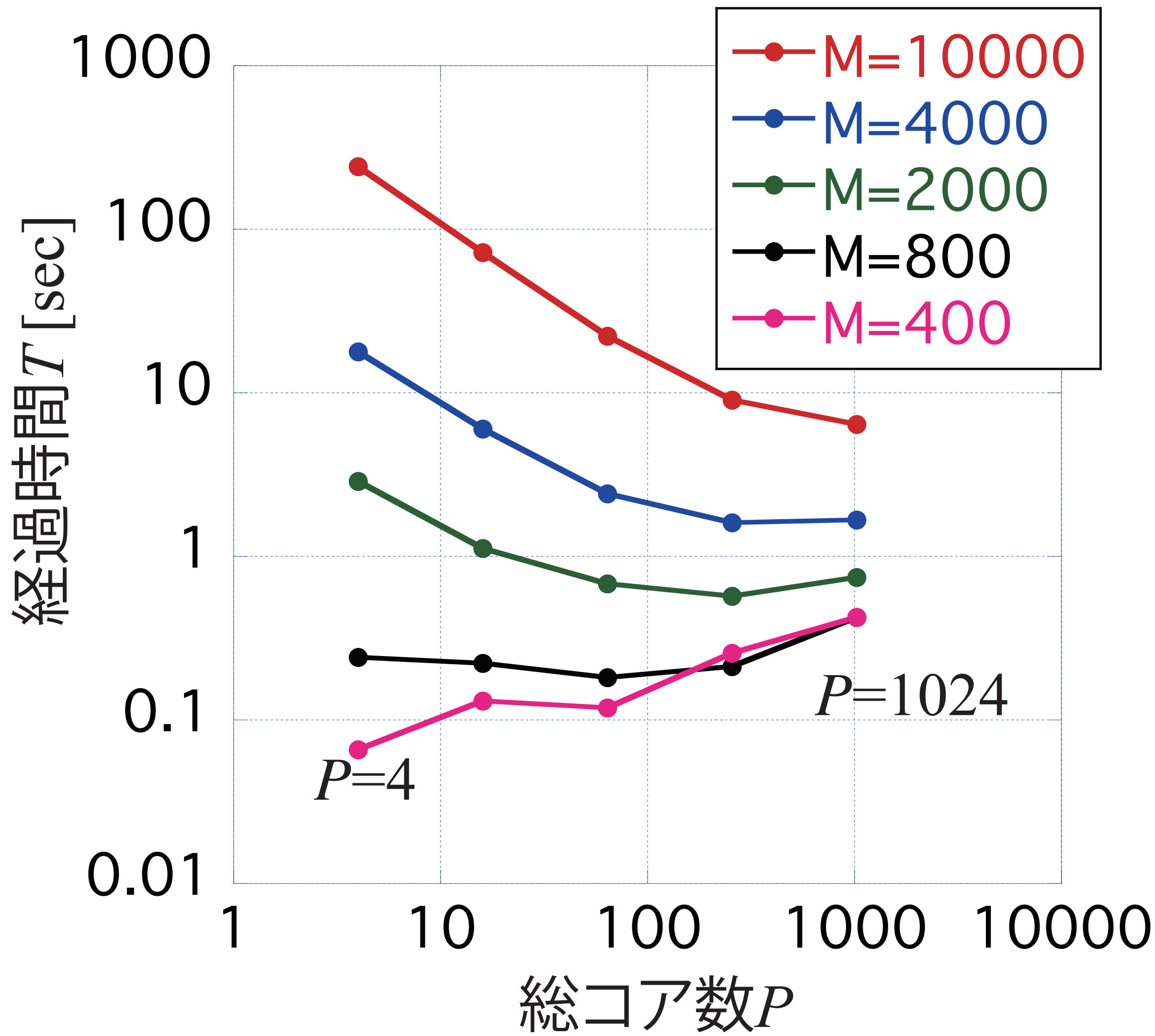
(iii) 行列の種類

「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 x 1K x 1K = 8 MB
(b) M=1万だと
8B x 10K x 10K = 0.8GB (約1GB)
(c) M=10万だと
8B x 100K x 100K = 80 GB

例：中小規模行列の全固有対計算(*)



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

Strategies of matrix solvers

Krylov (iterative) solvers
- ‘projection’ strategy
- (mainly) sparce matrices
- basics of O(N) calculation

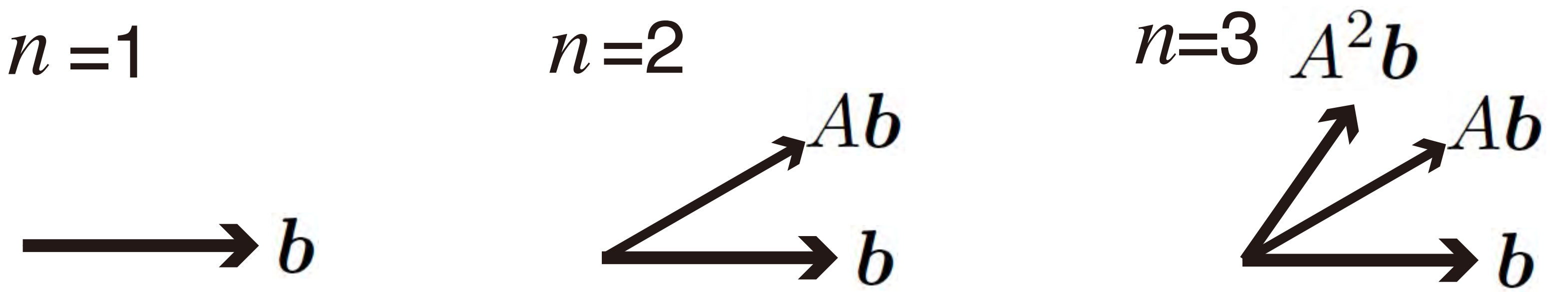
ex. CG algorithm

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

‘projection’ on the Krylov subspace of

$$K_n(A;\boldsymbol{b}) \equiv \mathrm{span}\left\{\boldsymbol{b}, A\boldsymbol{b}, A^2\boldsymbol{b}, \ldots, A^{n-1}\boldsymbol{b}\right\}$$

n : subspace dimension (iteration number)



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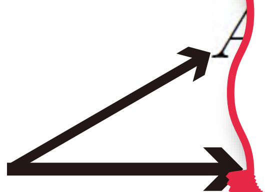
'projection' on the Krylov subsp

$$K_n(A;\boldsymbol{b}) \equiv \mathrm{span}\{\boldsymbol{b}, A\boldsymbol{b},$$

n : subspace dim

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:

注:第1版(1973)には、
クリロフ部分空間法の章なし。

Strategies of matrix solvers

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ex. CG algorithm

Direct solvers

ex. CG algorithm for $A\boldsymbol{x} = \boldsymbol{b}$

→ the n-th step solution $\boldsymbol{x}_n$ is given by

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

‘projection’ on the Krylov subspace of

$$K_n(A;\boldsymbol{b}) \equiv \mathrm{span}\left\{\boldsymbol{b}, A\boldsymbol{b}, A^2\boldsymbol{b}, \ldots, A^{n-1}\boldsymbol{b}\right\}$$

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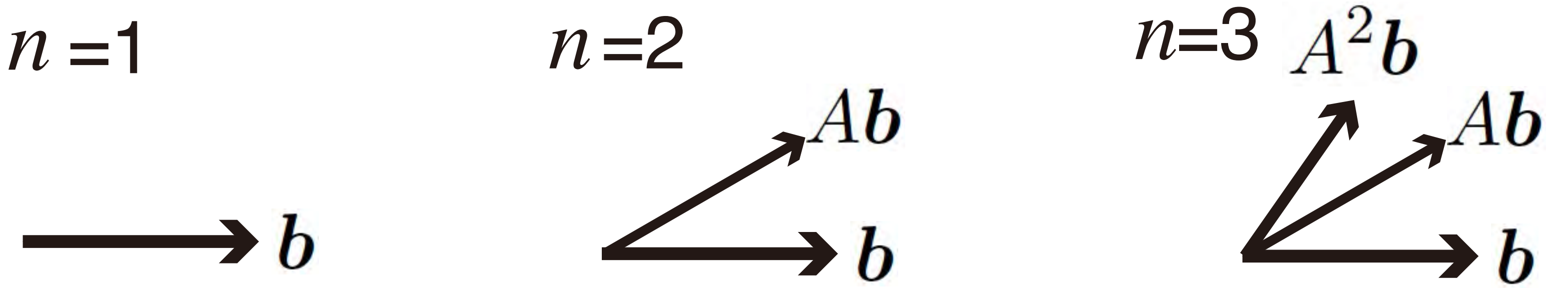

Strategies of matrix solvers

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Direct solvers

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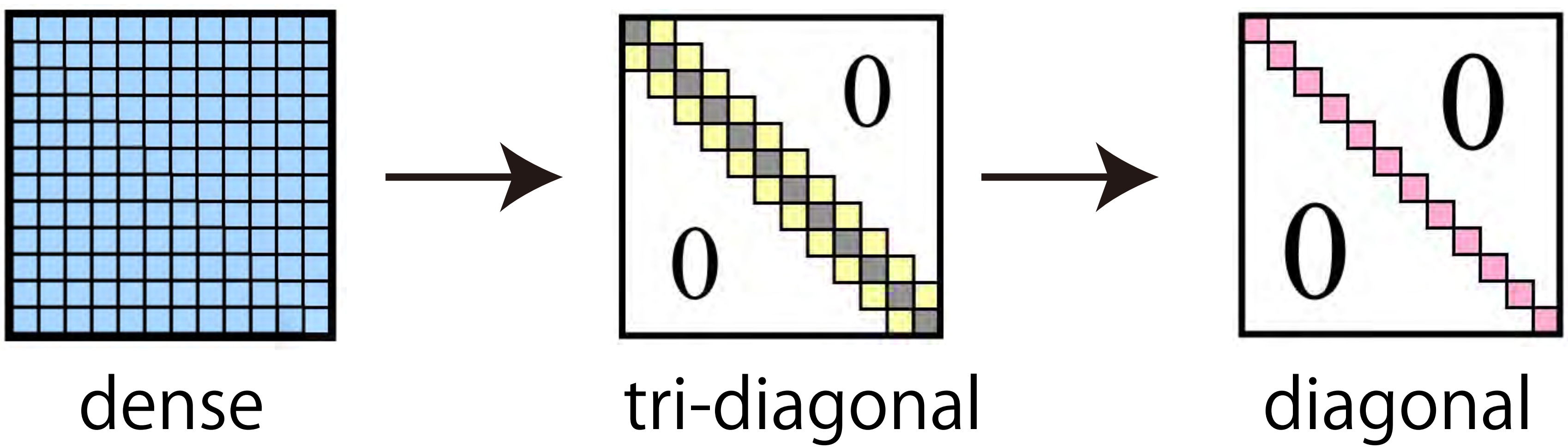
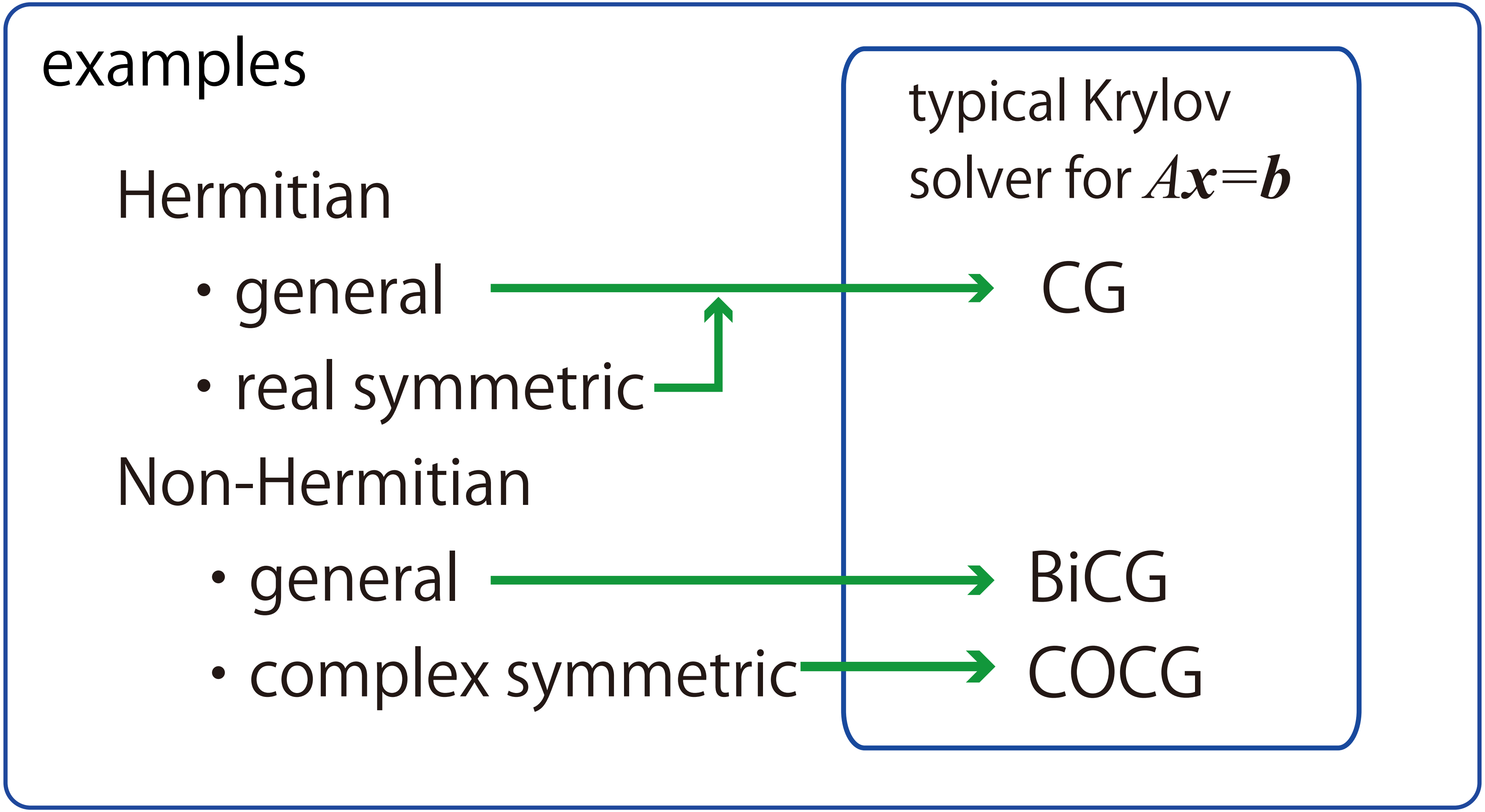
- (mainly) dense matrices
- O(N^3) calculation

‘transformation’ of the whole space

Example



行列の種類による分類


examples
Hermitian
・general
・real symmetric
Non-Hermitian
・general
・complex symmetric
typical Krylov
solver for $\boldsymbol{Ax}=\boldsymbol{b}$
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)

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(ii) 解法の基盤的戦略

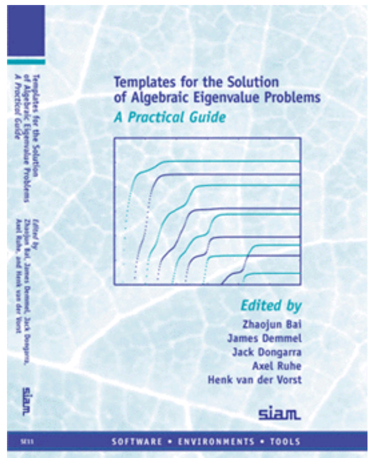
→「射影」と「変換」

(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)

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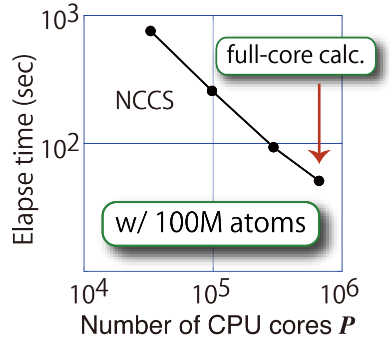

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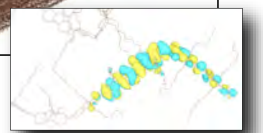

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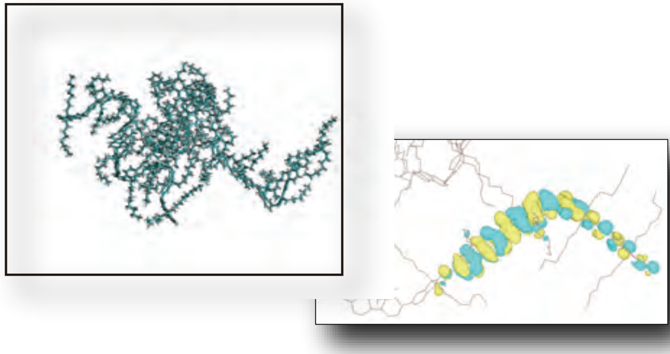

↕

Algorithm : numerical linear algebra

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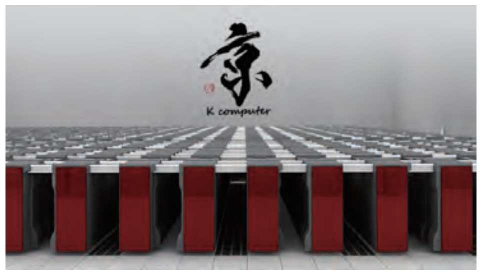
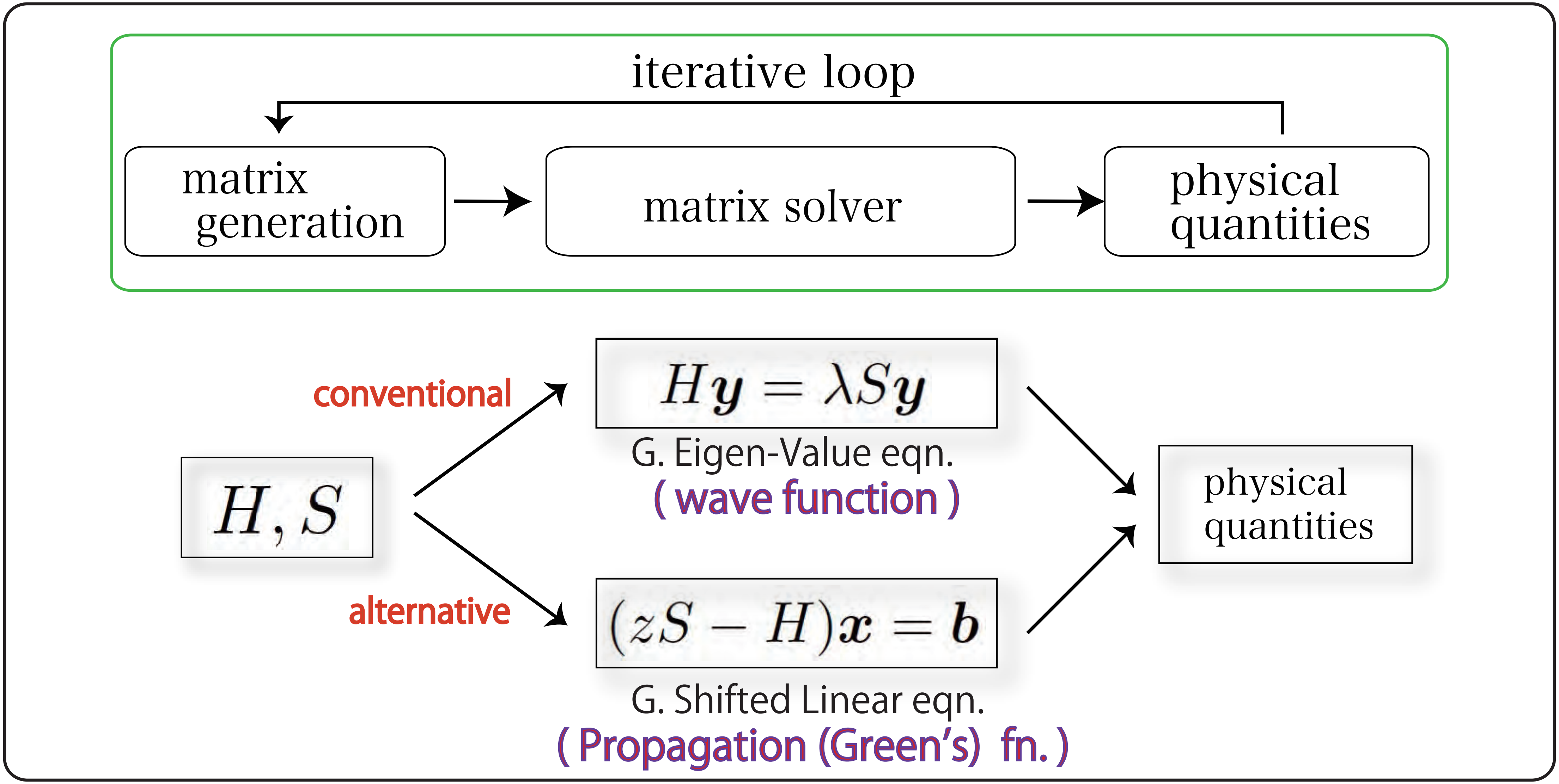
Architecture : (post-)petascale supercomputers



Overview

Application-Algotirhm-Architecture co-design

Workflow



Basic equations

Generalized eigen-value (GEV) equation

wavefunction formulation

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

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

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

Generalized shifted linear (GSL) equations

the propagation (Green's) function formulation

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

non-Hermitian

→ $$\boldsymbol{x} = G\boldsymbol{b}$$

with $G \equiv (zS - H)^{-1}$: the Green's function http://www.elses.jp

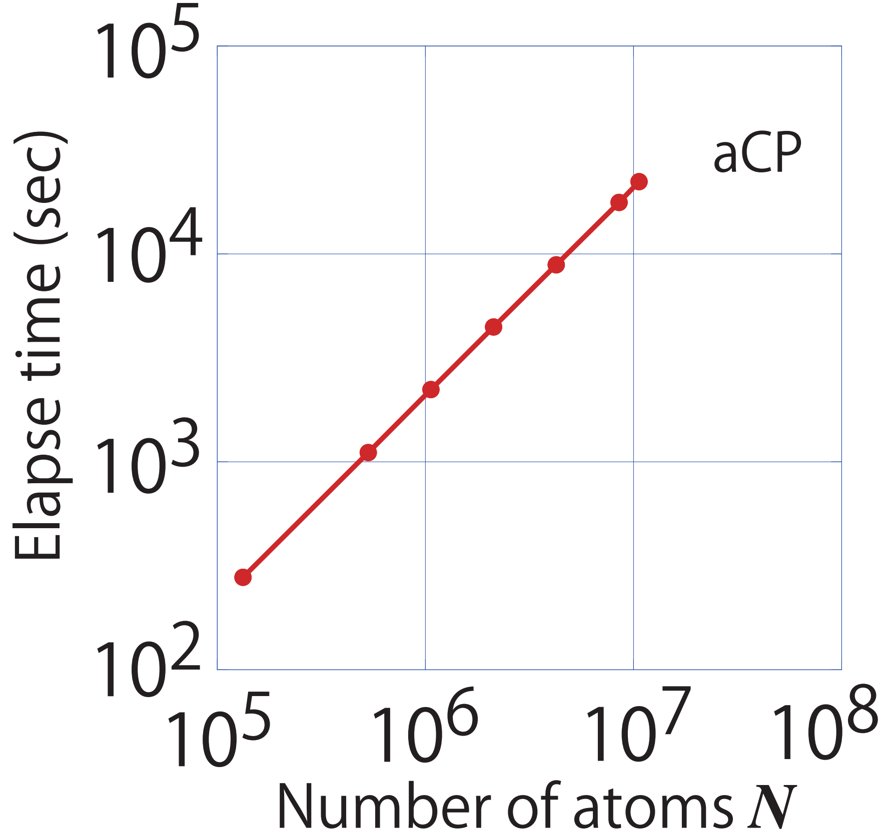
ELSES, our electronic-structure calculation code

Benchmark with upto 100M atoms(⇄ Si : (126nm)^{3}region)

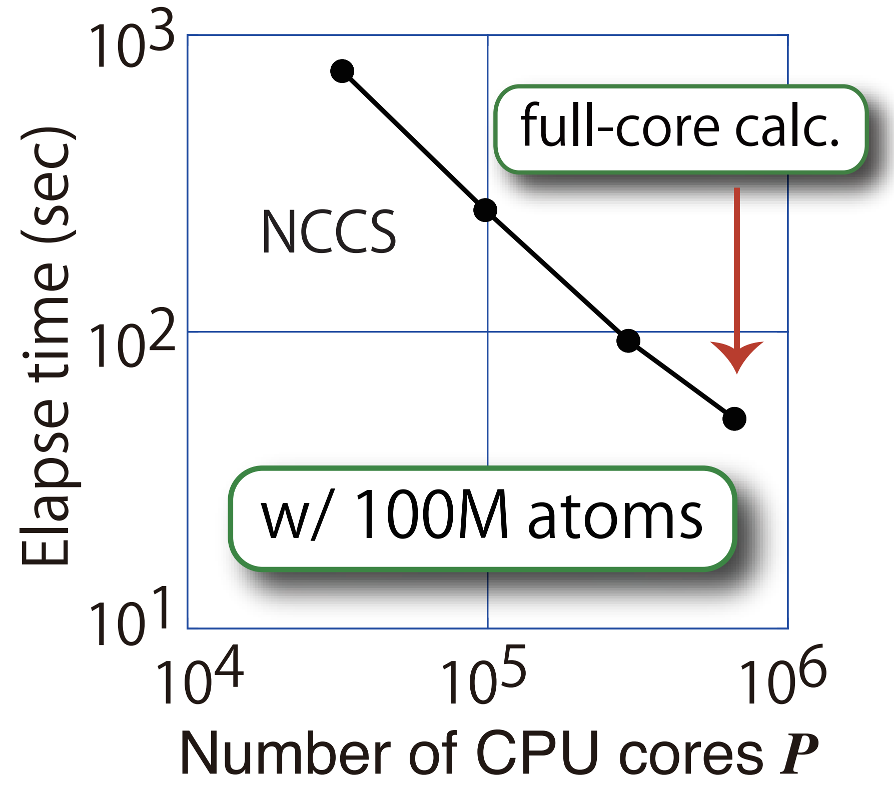
(Hoshi et al.,JPCM24, 165502(2012) JPSJ 82, 023710 (2013); JPSCP. 1, 016004 (2014))

aCP :amourphous-like conjugated polymer, poly-(9,9 dioctil-fluorene),
NCCS: sp2-sp3 nano composite carbon solid

(a) Order-*N* scaling



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



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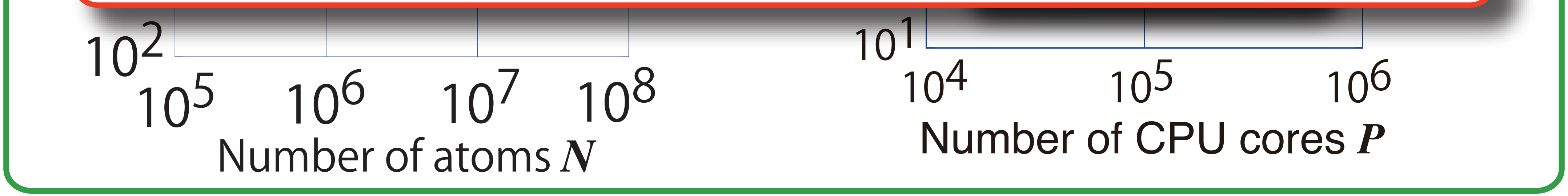
aPF :amourphous-like conjugated polymer, poly-(9,9 dioctil-fluorene),

Methodology

- Oringinal linear-algebraic order-N algorithms with generalized shifted linear equations

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

- 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

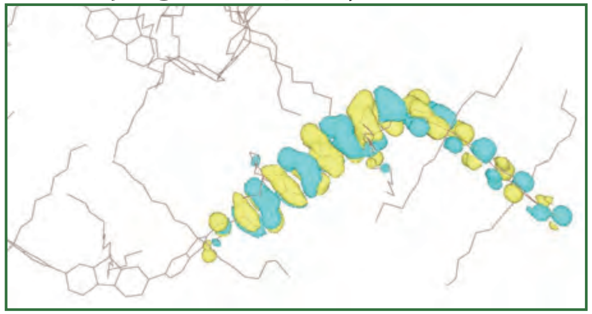


Application studies with ELSES

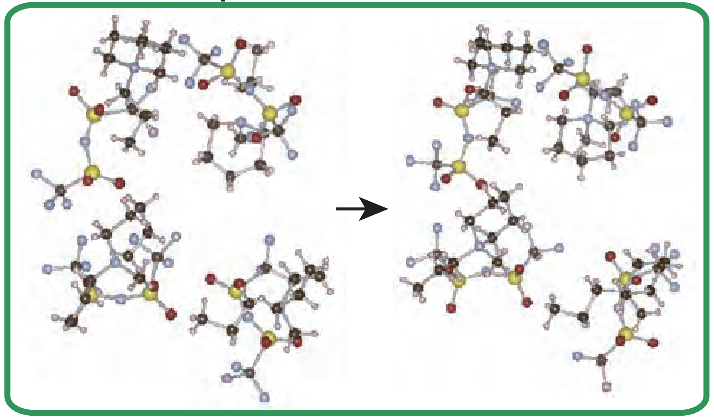
http://www.elses.jp/

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.)

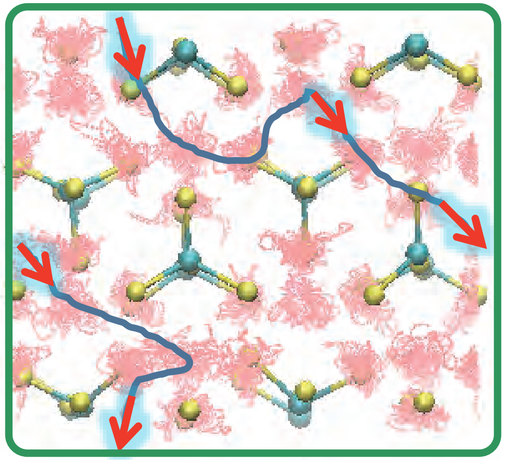
Organic materials
(amourphous-like
conjugated polymer)



Ionic liquid

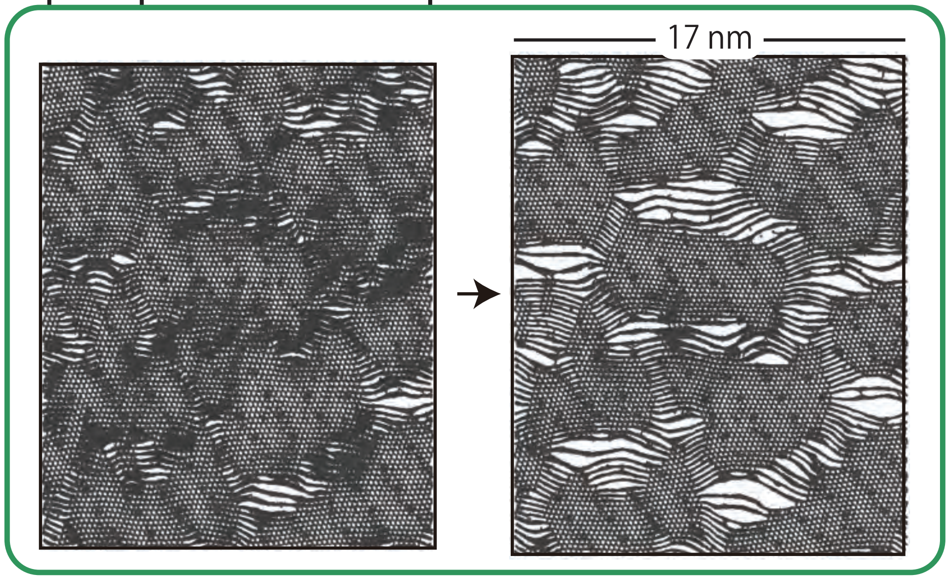


Li ion diffusion

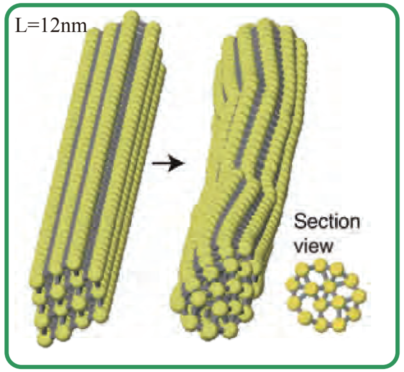


Nishino et al. PRB90, 024303, (2014)

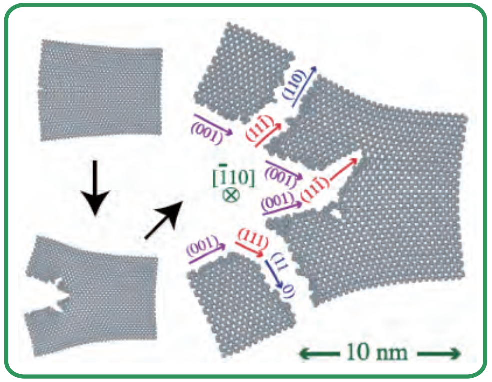
sp2-sp3 nano-composite carbon solid



helical gold nanowire



Si brittle fracture



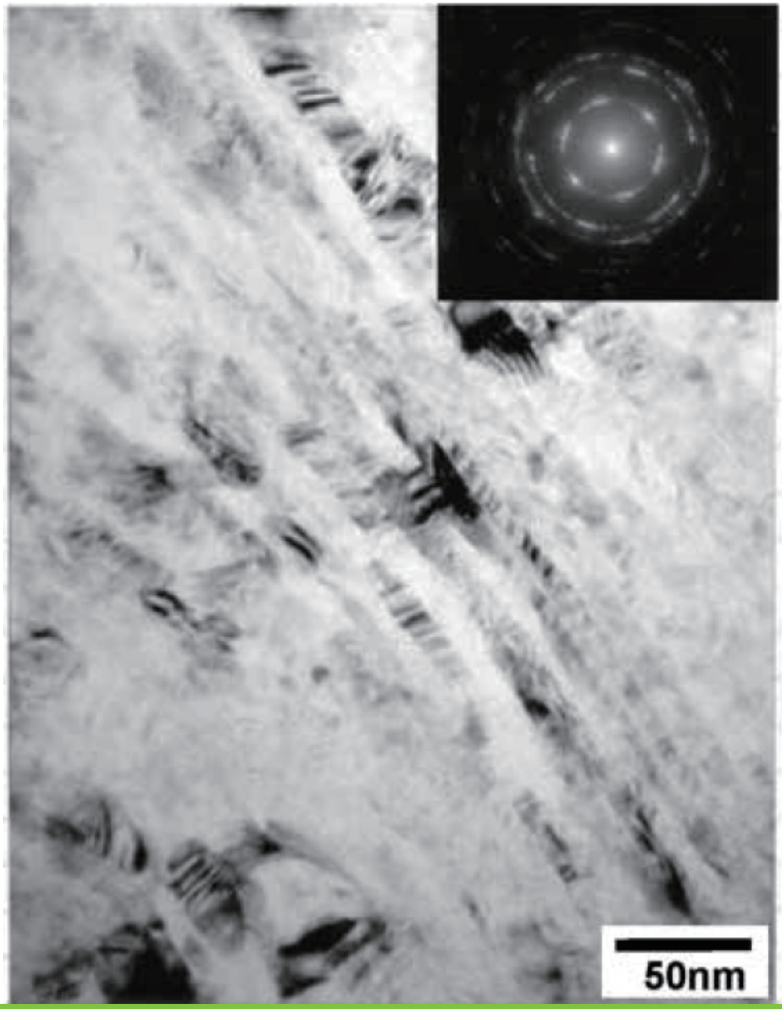
Nano-polycrystalline diamond (NPD)

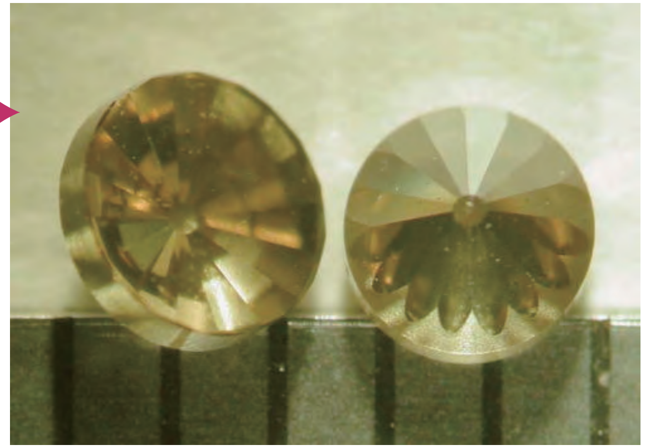
→ novel ultra-hard material

T. Irifune, et al. , Nature 421, 599（2003）(@ Ehime Univ.)

→ harder than conventional diamond crystals

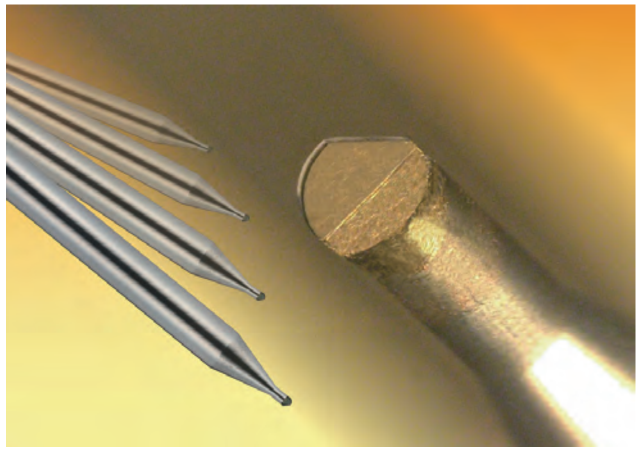
100-nm-scale structure





macroscale sample

1 mm



industrial product (2012)
(Sumitomo Electric Industries)

Hoshi et al, JPSJ 82, 023710 (2013).

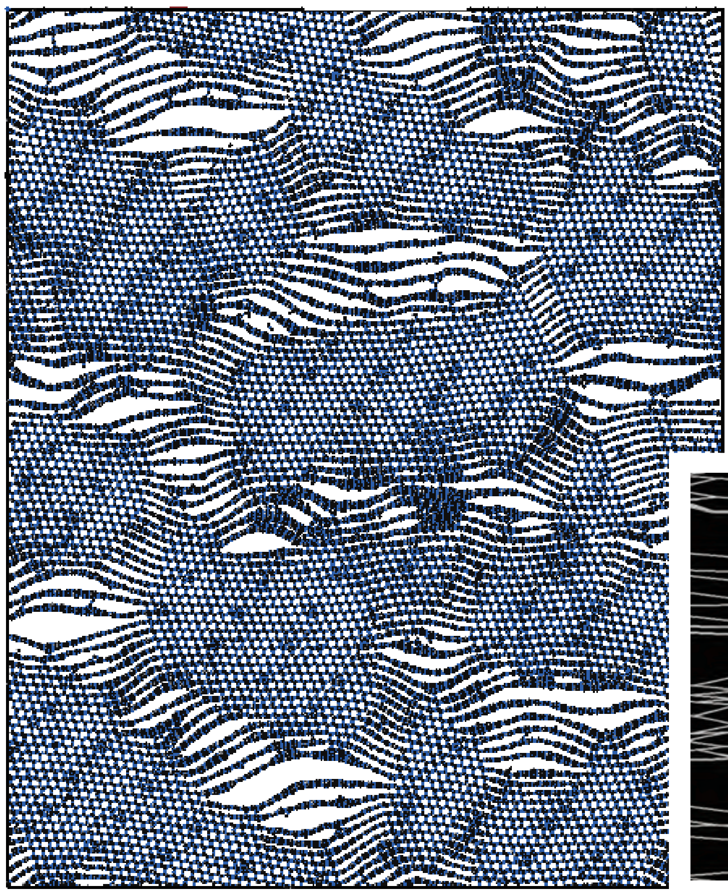
Visualization analysis in sp2-sp3 nano-composite carbon solids

Research on nano-polycrystalline diamond
→ nano-composite carbon with local Green's function analysis (πCOHP) theory
→ distinction between sp2 and sp3 domains
with characteristic domain shape and domain boundaries

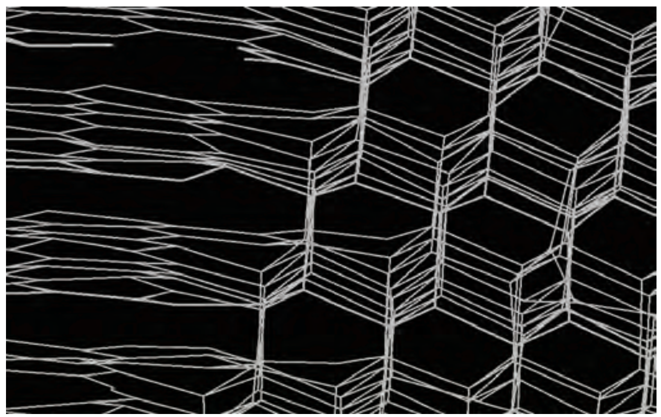
(a) Visualization
for sp2 and sp3 domains

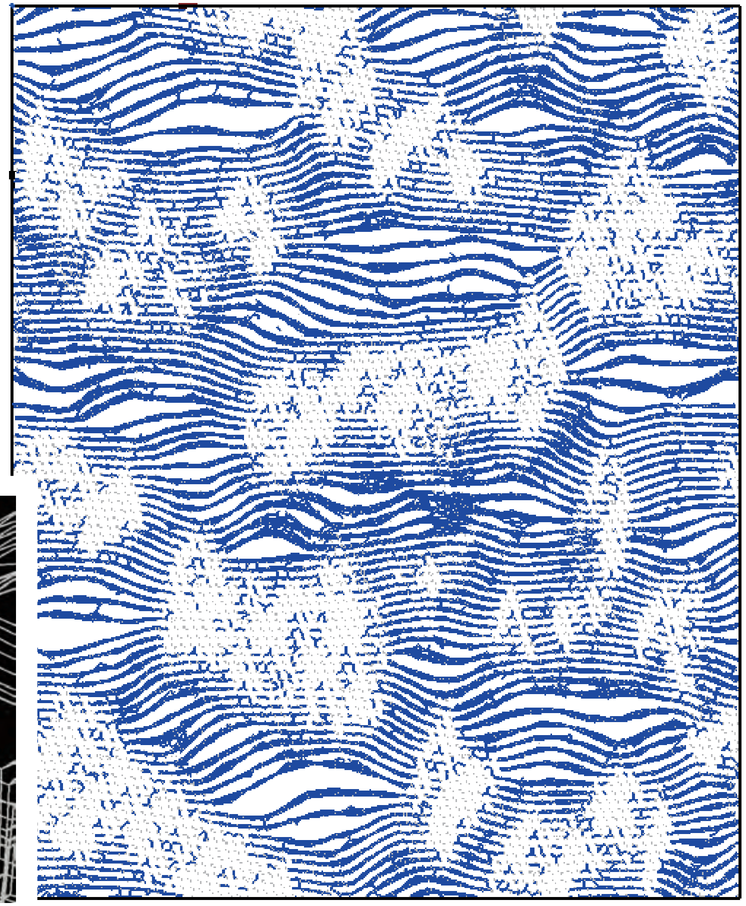
(b) Visualization
only for sp2 domains

17 nm



sp2-sp3 domain
boundary ↓



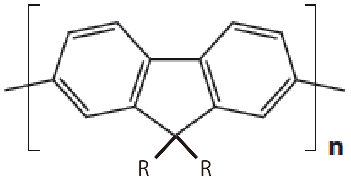


Recent results on organic materials

T. Hoshi, et al., J. Phys.: CM 24, 165502 (2012); JPS-CP. 1, 016004, (2014); unpublished

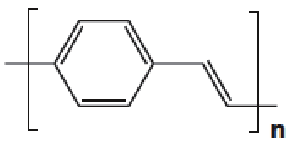
[Acknowledgement : M. Ishida (Sumitomo Chemical Co.)]

conjugated polymer (CP)



PFO

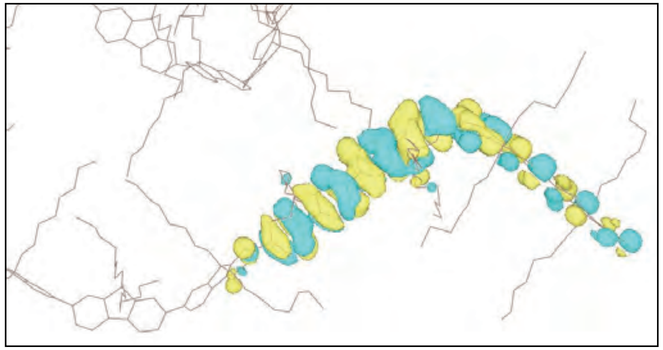
(R = C_8H_{17})

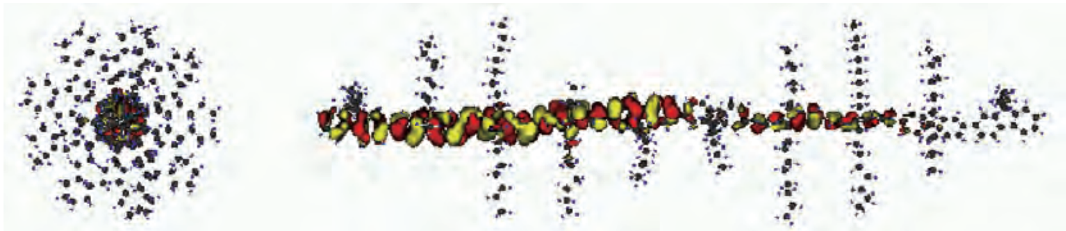


PPV

finite temperature calculation
→ non-ideal structure with localized π states
(cf. J. Terao, Nature Comm, 4., 1691 (2013))

amourphous-like PFO
with thermal motion

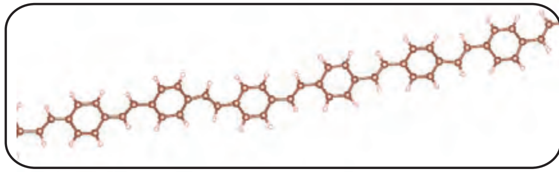




HOMO wfn of the PFO single chain (n=10)
with thermal motion

(preliminary) PPV bundle
(L≒ 40 nm)
for π-stacking domains

close-up



今後の展望:
有機エレクトロニクス系
(電気伝導計算)

「京」での1億原子電子状態計算 〜物質科学と数理科学の接点として〜

星健夫、井町宏人(鳥取大, CREST)

1. Overview: Application-Algorithm-Architecture co-design
2. 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. 「京」での1億原子(100ナノスケール)電子状態計算
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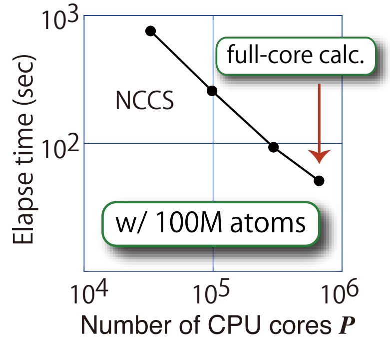
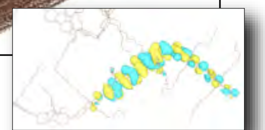
5. 複合数理原理ソルバーと「ミドルウェア」開発
6. まとめ



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

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

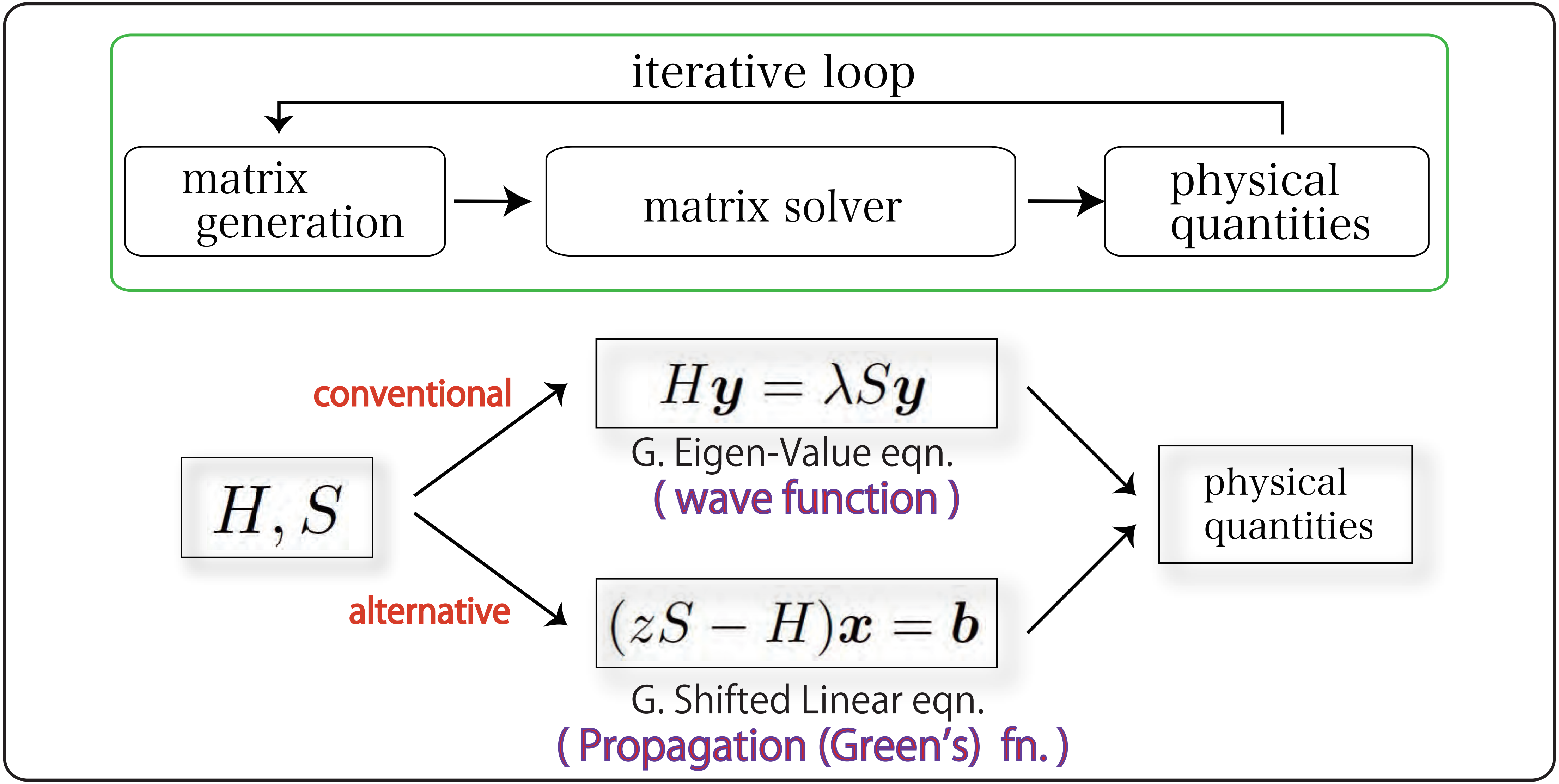


謝辞(予算)
JST-CREST(PostPeta領域),
科研費新学術領域(コンピューティクス)
JST-ASTEP, 構造材料元素戦略、科研費(一般)、など

Overview

Application-Algotirhm-Architecture co-design

Workflow



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

non-Hermitian
(complex symmetric)

[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)]

[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: $H\boldsymbol{y} = \lambda S\boldsymbol{y}$

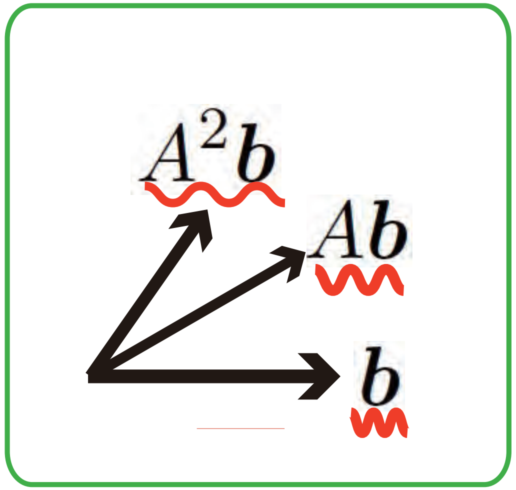
[3] Use of Sylvester's theorem of inertia;
D. Lee, et al, Japan J. Indust. Appl. Math. 30, 625 (2013)

Shift invariance of Krylov subspace

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

ex. $n = 3$

$$(A+\sigma I)^0\boldsymbol{b} = \boldsymbol{b}$$
$$(A+\sigma I)^1\boldsymbol{b} = \sigma\boldsymbol{b} + A\boldsymbol{b}$$
$$(A+\sigma I)^2\boldsymbol{b} = \sigma^2\boldsymbol{b} + 2\sigma A\boldsymbol{b} + A^2\boldsymbol{b}$$



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

Shifted conjugate-orthogonal conjugate gradient (sCOCG) method

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

Collinear residual theorem

A. Frommer, Computing 70, 87 (2003)

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

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

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

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

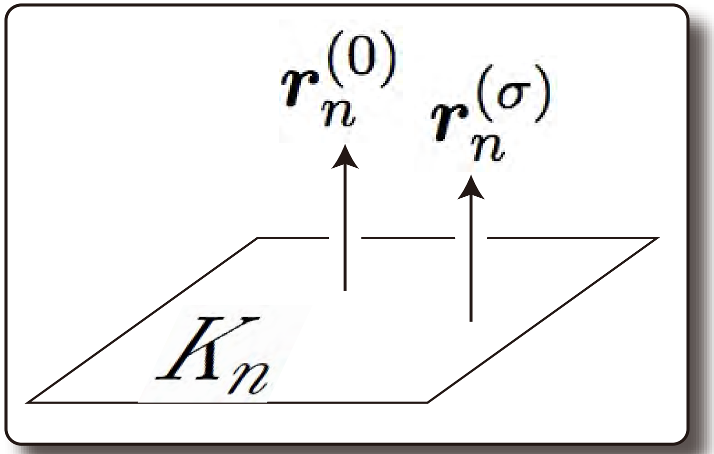
Residual vector at the **'shifted'** eq. $(\sigma \neq 0)$

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

Collinear residual theorem
（between origina and shifted eqns.）

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

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



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Collinear residual theorem
(between origina and shifted eqns.)

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

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

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

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

Shifted COCG method

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

$$\boldsymbol{x}_0 = \boldsymbol{x}_0^\sigma = \boldsymbol{p}_{-1} = \boldsymbol{p}_{-1}^\sigma = 0,$$
$$\pi_0 = \pi_{-1}^\sigma = 1, \boldsymbol{r}_0 = \boldsymbol{b},$$
$$\beta_{-1} = 0, \alpha_{-1} = 1$$

do $n = 0, 1, \cdots$

$$\boldsymbol{p}_n = \boldsymbol{r}_n + \beta_{n-1}\boldsymbol{p}_{n-1} \quad (1)$$
$$\alpha_n = \frac{\boldsymbol{r}_n^{\mathrm{T}}\boldsymbol{r}_n}{\boldsymbol{p}_n^{\mathrm{T}} A \boldsymbol{p}_n} \quad (2)$$
$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \alpha_n \boldsymbol{p}_n \quad (3)$$
$$\boldsymbol{r}_{n+1} = \boldsymbol{r}_n - \alpha_n A \boldsymbol{p}_n \quad (4)$$
$$\beta_n = \frac{\boldsymbol{r}_{n+1}^{\mathrm{T}}\boldsymbol{r}_{n+1}}{\boldsymbol{r}_n^{\mathrm{T}}\boldsymbol{r}_n} \quad (5)$$

enddo

Collinear residual theorem

$$\boldsymbol{r}_n \equiv A\boldsymbol{x}_n - \boldsymbol{b} \to \boldsymbol{0} \quad \text{(a)}$$
$$\boldsymbol{r}_n^{(\sigma)} \equiv (A + \sigma I)\boldsymbol{x}_n^{(\sigma)} - \boldsymbol{b}$$
$$= \frac{1}{\pi_n^{(\sigma)}}\boldsymbol{r} \quad \to \boldsymbol{0} \quad \text{(b)}$$

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

$$\pi_{n+1}^\sigma = (1 + \alpha_n \sigma)\pi_n^\sigma + \frac{\alpha_n \beta_{n-1}}{\alpha_{n-1}}(\pi_n^\sigma - \pi_{n-1}^\sigma) \quad (6)$$
$$\beta_{n-1}^\sigma = \left(\frac{\pi_{n-1}^\sigma}{\pi_n^\sigma}\right)^2 \beta_{n-1} \quad (7)$$
$$\alpha_n^\sigma = \frac{\pi_n^\sigma}{\pi_{n+1}^\sigma}\alpha_n \quad (8)$$
$$\boldsymbol{p}_n^\sigma = \frac{1}{\pi_n^\sigma}\boldsymbol{r}_n + \beta_{n-1}^\sigma \boldsymbol{p}_{n-1}^\sigma \quad (9)$$
$$\boldsymbol{x}_{n+1}^\sigma = \boldsymbol{x}_n^\sigma + \alpha_n^\sigma \boldsymbol{p}_n^\sigma \quad (10)$$

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

Shifted COCG method

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

$$\boldsymbol{x}_0 = \boldsymbol{x}_0^\sigma = \boldsymbol{p}_{-1} = \boldsymbol{p}_{-1}^\sigma = 0,$$
$$\pi_0 = \pi_{-1}^\sigma = 1, \boldsymbol{r}_0 = \boldsymbol{b},$$
$$\beta_{-1} = 0, \alpha_{-1} = 1$$

do $n = 0, 1, \cdots$

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

Collinear residual theorem

$$\boldsymbol{r}_n \equiv A\boldsymbol{x}_n - \boldsymbol{b} \to \boldsymbol{0} \quad \text{(a)}$$
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$$\boldsymbol{p}_n^\sigma = \frac{1}{\pi_n^\sigma}\boldsymbol{r}_n + \beta_{n-1}^\sigma\boldsymbol{p}_{n-1}^\sigma \quad (9)$$
$$\boldsymbol{x}_{n+1}^\sigma = \boldsymbol{x}_n^\sigma + \alpha_n^\sigma\boldsymbol{p}_n^\sigma \quad (10)$$

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

[1] A. Frommer, Computing 70, 87 (2003) (原論文) → QCD

[2] R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. Fujiwara, Phys. Rev. B 73, 165108 (2006). →大規模電子状態計算(本研究)

[3] S. Yamamoto, T. Fujiwara, and Y. Hatsugai, Phys. Rev. B 76, 165114 (2007); S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang and T. Fujiwara, J. Phys. Soc. Jpn., 77,114713 (2008).

→ 多体問題 [full-CI型計算, 多軌道拡張ハバードモデル, $La_{3/2}Sr_{1/2}NiO_4$]

→ Lanczos (基底状態) + シフト型クリロフ (excitation spectrum)

[4] 実空間グリッド型第一原理量子電気伝導計算(RSPACE)

小野倫也(筑波大)・岩瀬滋(阪大)との共同研究(論文準備中)

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

→ Shell model 計算

[6] Y. Futamura, H. Tadano and T. Sakurai, JSIAM Letters 2, 127 (2010).

→ 実空間グリッド型第一原理計算(RSDFT)

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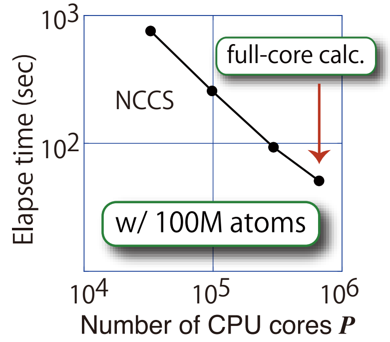

$$Hy = \lambda S y$$

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JST-ASTEP, 構造材料元素戦略、科研費(一般)、など

Strategies of matrix solvers

Krylov (iterative) solvers

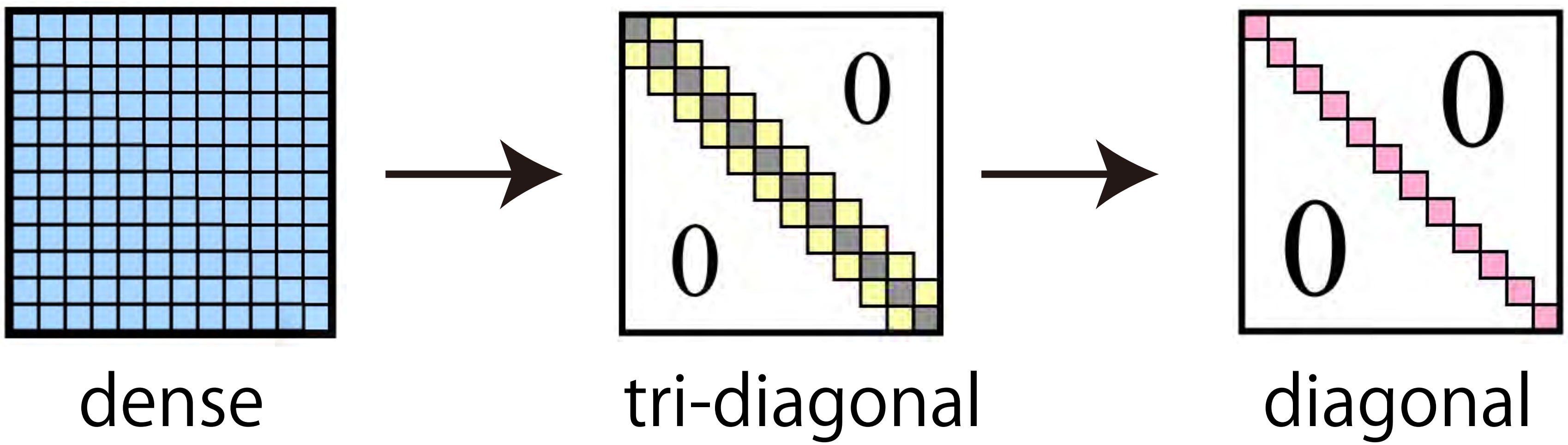
- ‘projection’ strategy
- (mainly) sparce matrices
- basics of O(N) calculation

Direct solvers

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

‘transformation’ of the whole space

Example



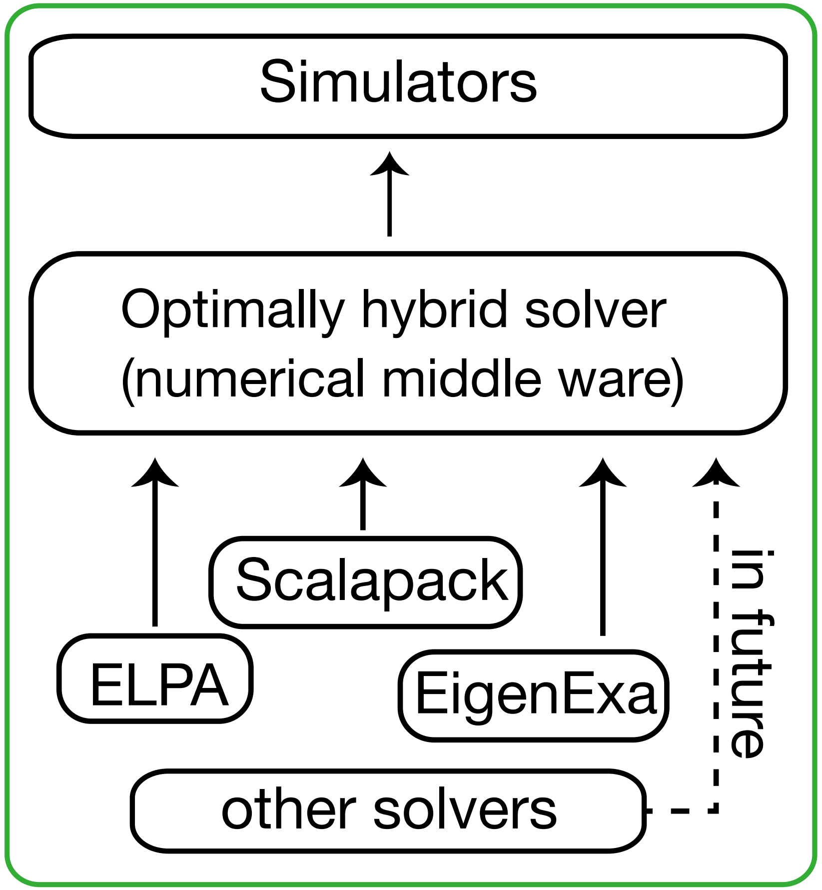
Optimally hybrid solver, as a 'numerical middle ware'

Ex. Direct solver for generalized eigen-value problem
(The midlleware code will appear online) (H. Imachi, T. Hoshi, in prep.)

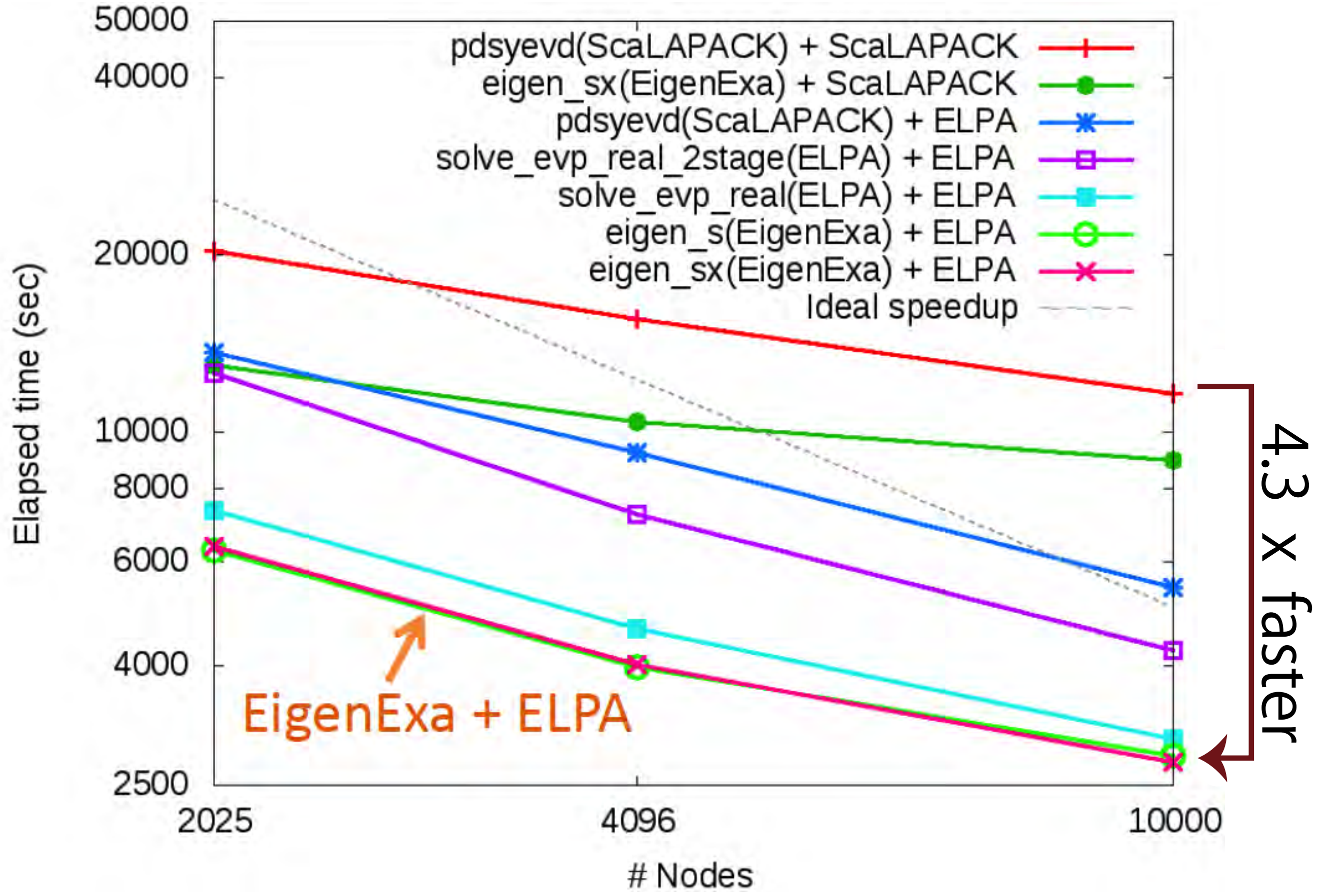
→ Hybrid among three direct solver libraries with (1) ScaLAPACK, (2) ELPA, and (3) EigenExa (RIKEN-AICS, Imamura)http://www.aics.riken.jp/labs/lpnctrt/

[Acknowledgement: T. Imamura and T. Fukaya (RIKEN-AICS)]

Concept

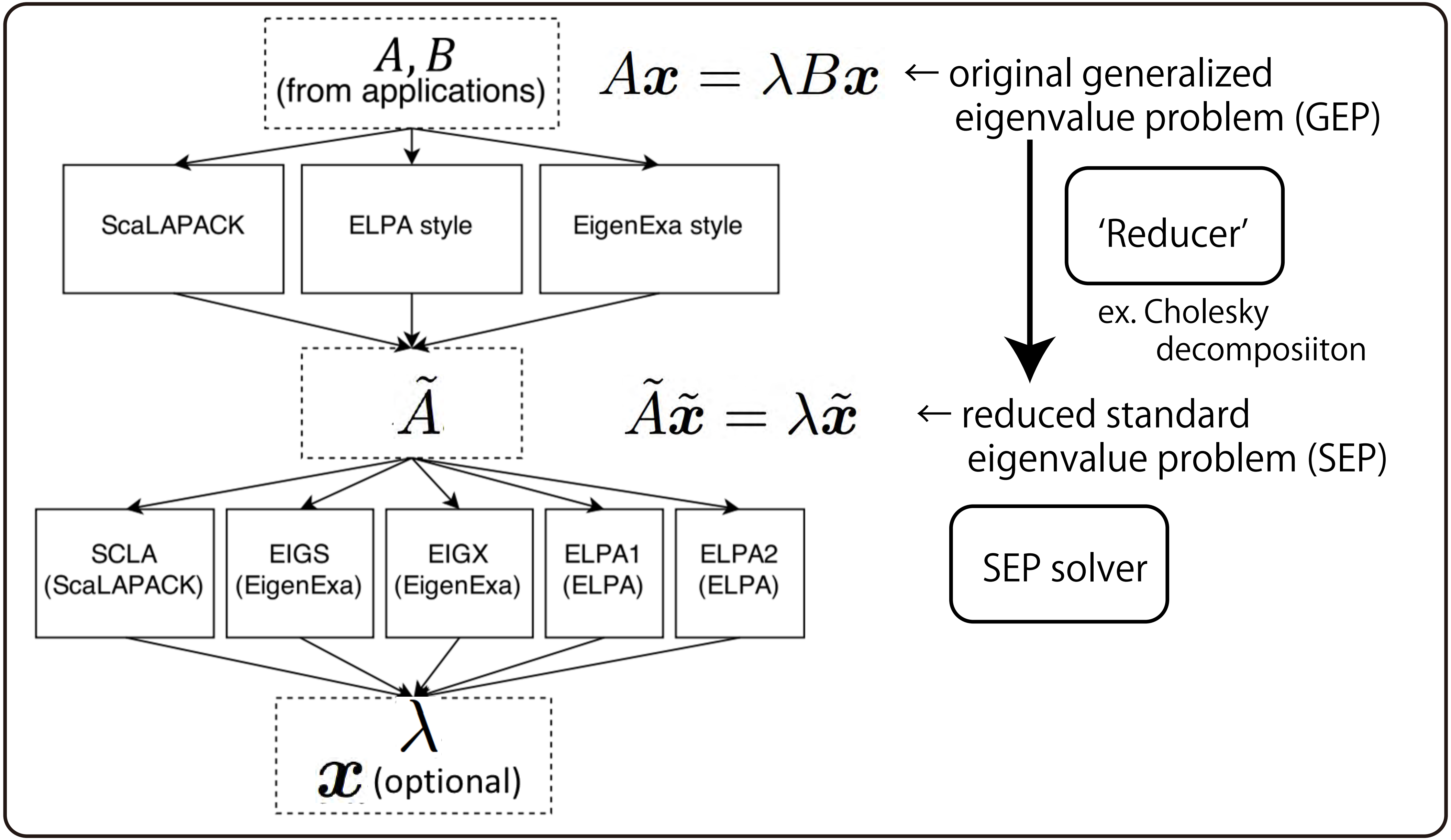


Strong scaling (on K) with *M*= 430,000 by upto 10^4 nodes



Optimally hybrid solver, as a 'numerical middle ware'

Workflow of hybrid solver (H. Imachi and T. Hoshi, in prep.)
= standard eigenvalue problem (SEP) solver + 'Reducer'



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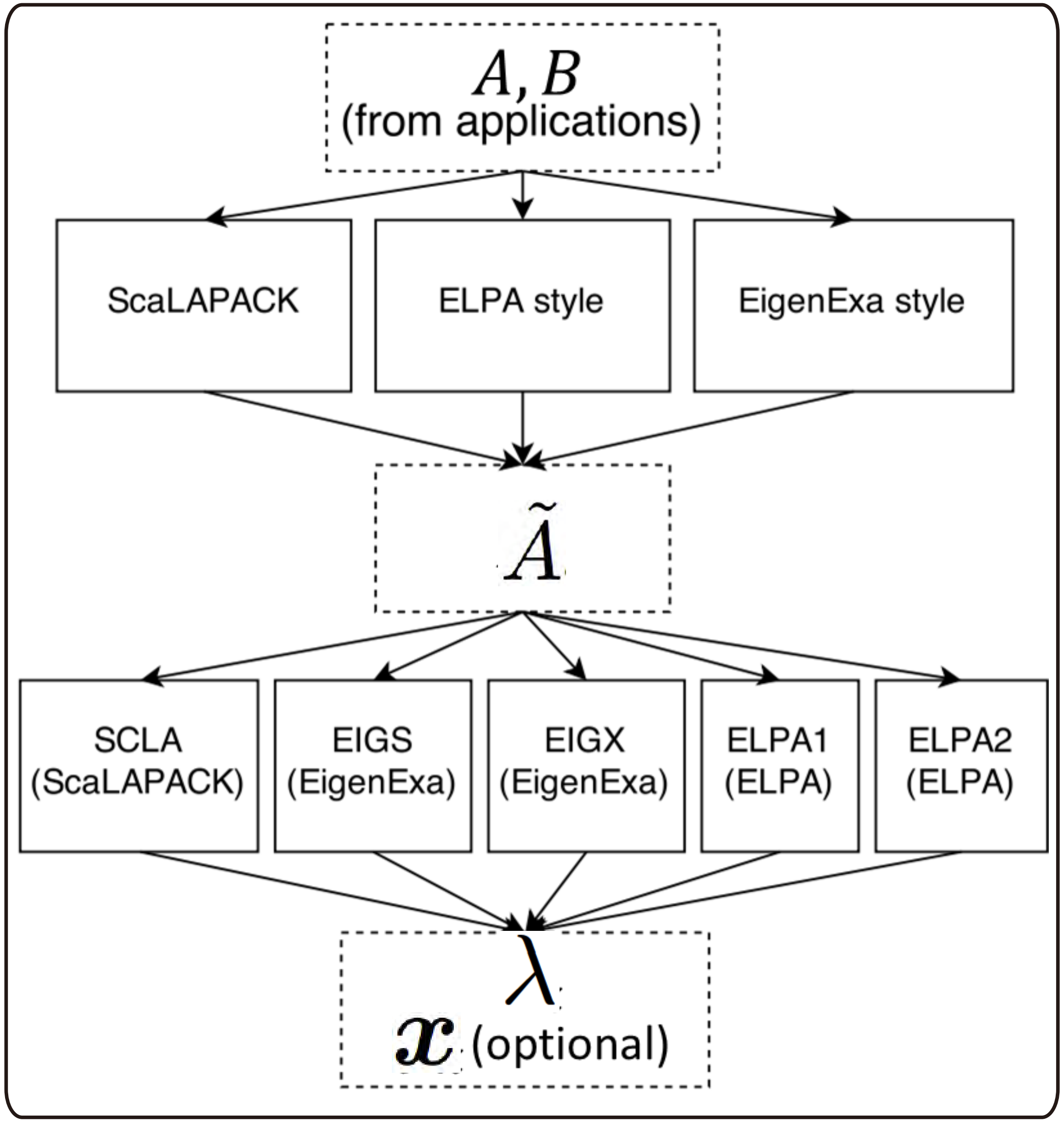

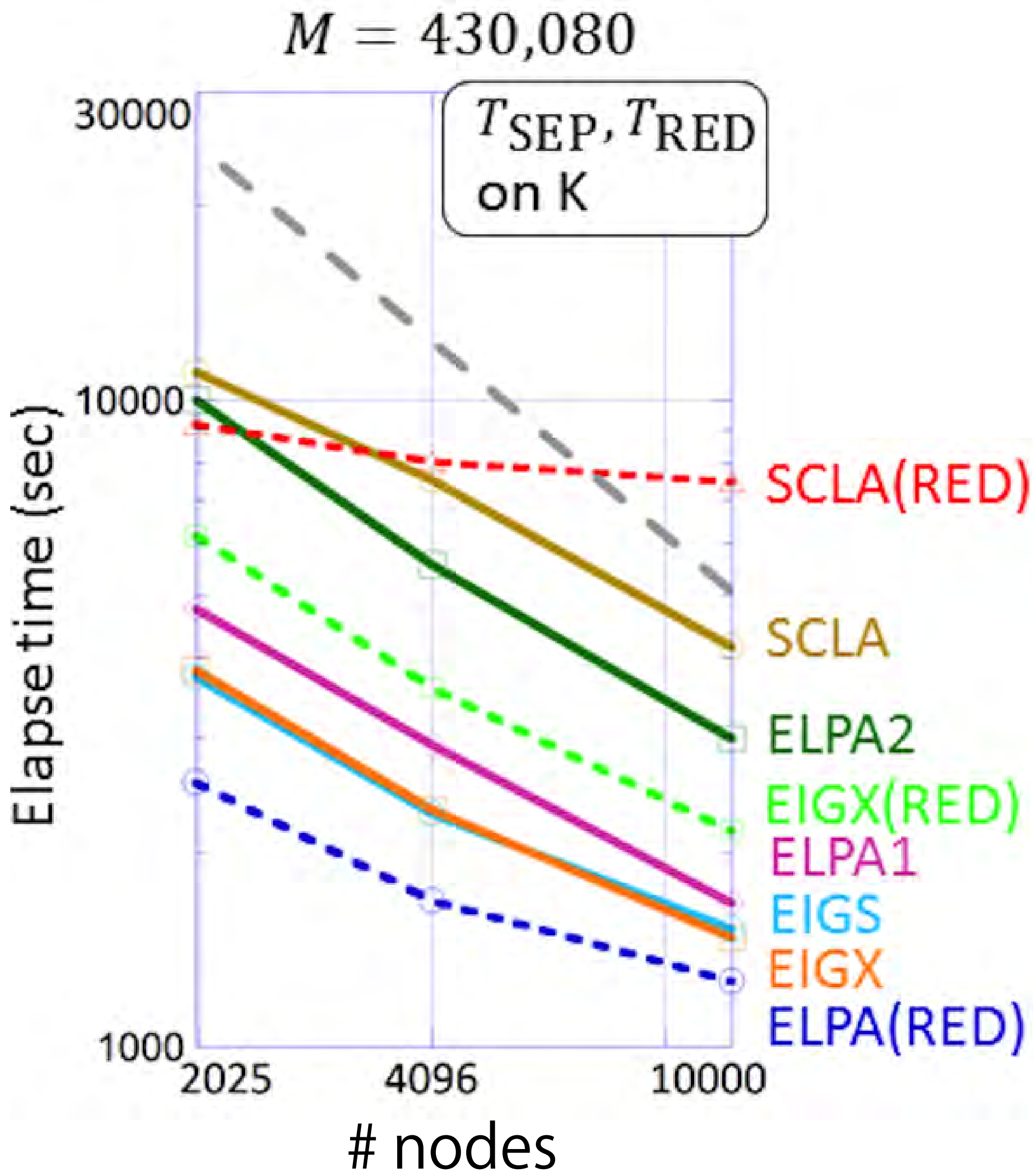

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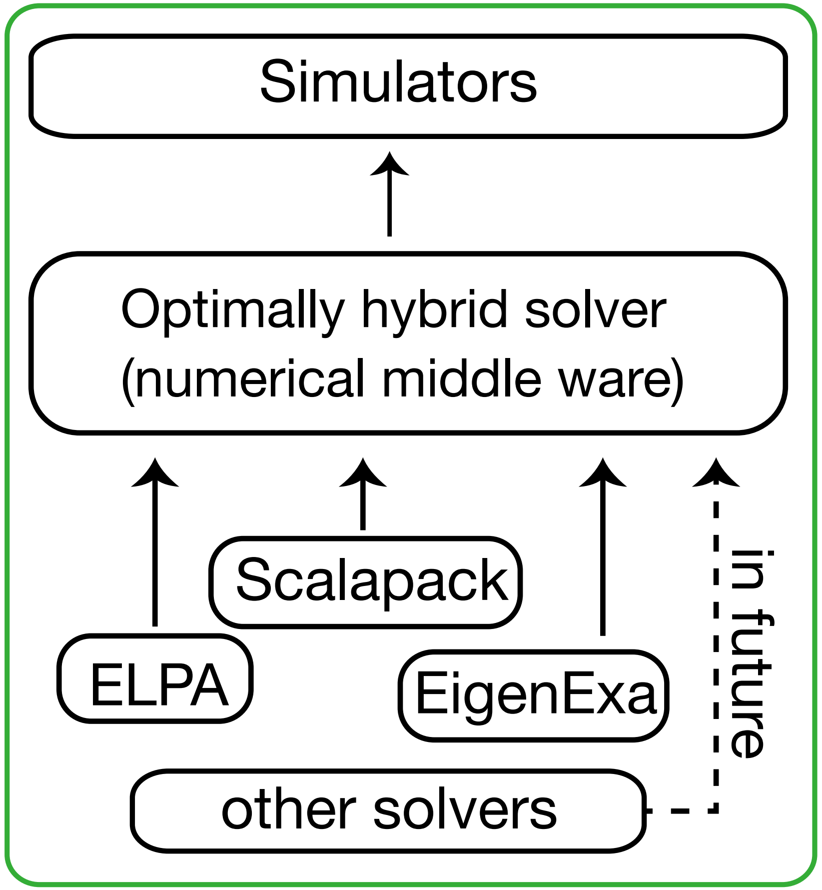

複合数理原理ソルバー(ミドルウェア)の展開
→さらに広範囲の複合化
→候補
- シフト型クリロフ(今日の話)
- ブロックヤコビ法(山本有作(電通大))
(Talk at ISC-QSD2014, Tokyo. Dec. 2014)
iterative local 'transformation' strategy
scalable at M=10^4 with 10^4 nodes

まとめ

1. Overview: Application-Algorithm-Architecture co-design
2. 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つの視点で分類
   →サイズ、解法戦略(「射影」・「変換」)、行列の種類
3. 「京」での1億原子(100ナノスケール)電子状態計算
   →「京」全ノードまでの強スケーリング性
   →展望：有機エレクトロニクス系（電気伝導計算）
4. 数理ソルバー：クリロフ部分空間法
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   →さまざまな分野での応用
5. 複合数理原理ソルバーと「ミドルウェア」開発
   →展望：Postpeta時代むけて、共有化
   (注：未達成な要素：性能予測、自動チューニング)