日本応用数理学会(2013年9月)「ペタスケール環境における固有値解法」セッション

京コンピュータにおける超大規模量子物質シミュレーション

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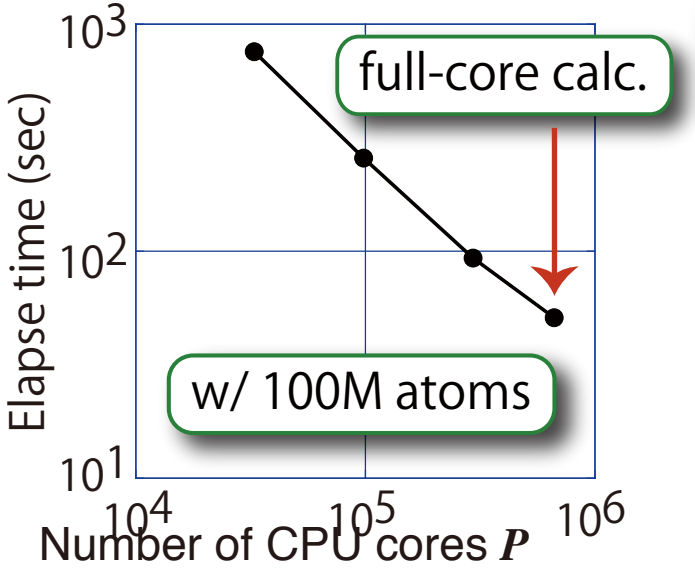
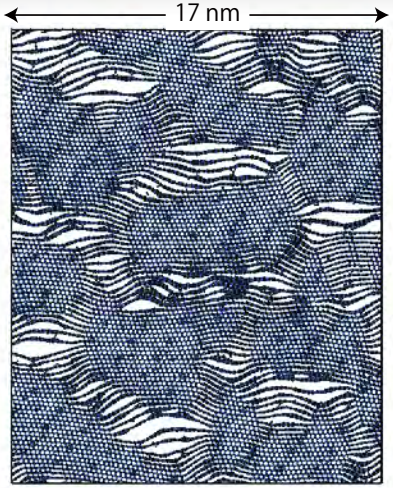
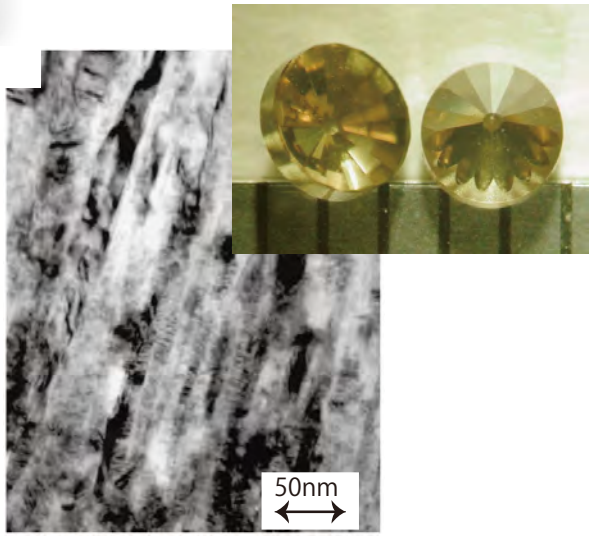
1. 概要:Application-Argorithm-Architecture co-design
2. 理論(クリロフ部分空間など)
3. 「京」での1億原子（100nmスケール)系計算
4. 展望:Petaからpost-petaへ
5. まとめ



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



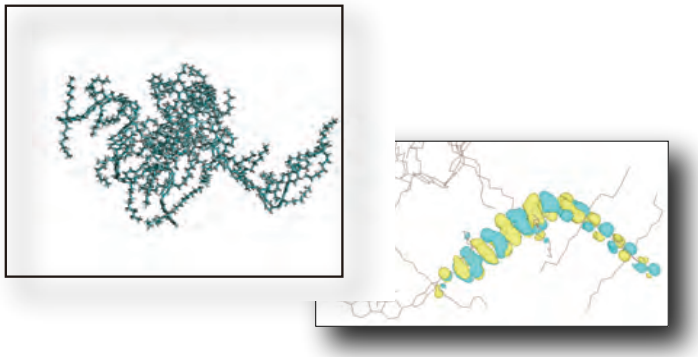


Overview

Application-Algotirhm-Architecture co-design

→新しいアイディアとその組み合わせでブレークスルーを

Application : electronic state calculation

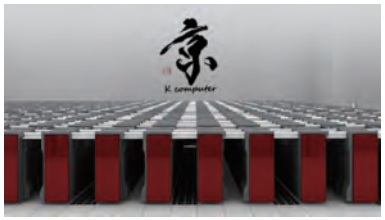


Algorithm : numerical linear algebra

$$Hy = \lambda Sy$$

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

Architecture : from supercomputers to personal computers



Overview

Application-Algotirhm-Architecture co-design

→新しいアイディアとその組み合わせでブレークスルーを

Tutorial : What is electronic state calculation ?

→ (a) quantum-mechanical 'wave' theory
for electrons in materials

(b) basics of quantum material simulations

→ effective Schrödinger equation

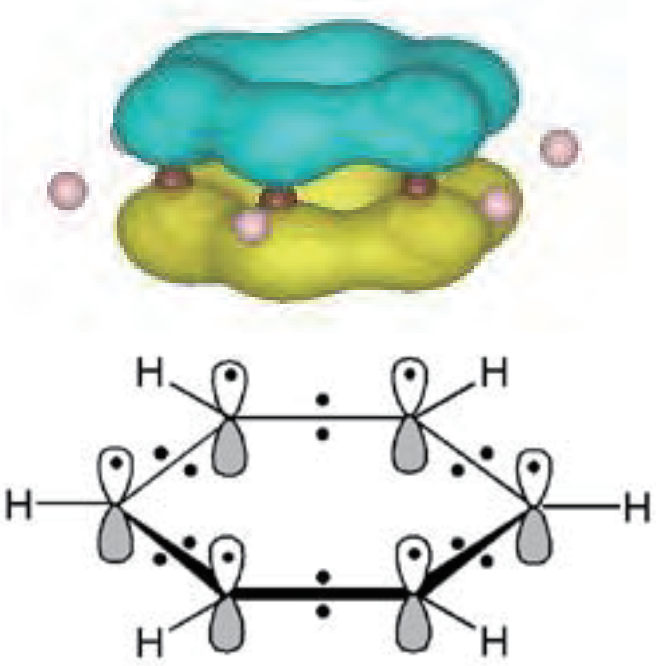
→ generalized Hermitian eigen-value problem
(as a typical numerical problem)

$$H\boldsymbol{y} = \lambda S\boldsymbol{y} \quad (\ S \approx I\ )$$

λ : energy for each electron ('eigen energy')

$\boldsymbol{y}$: shape of electrnic 'wave' ('wavefunction')(*)

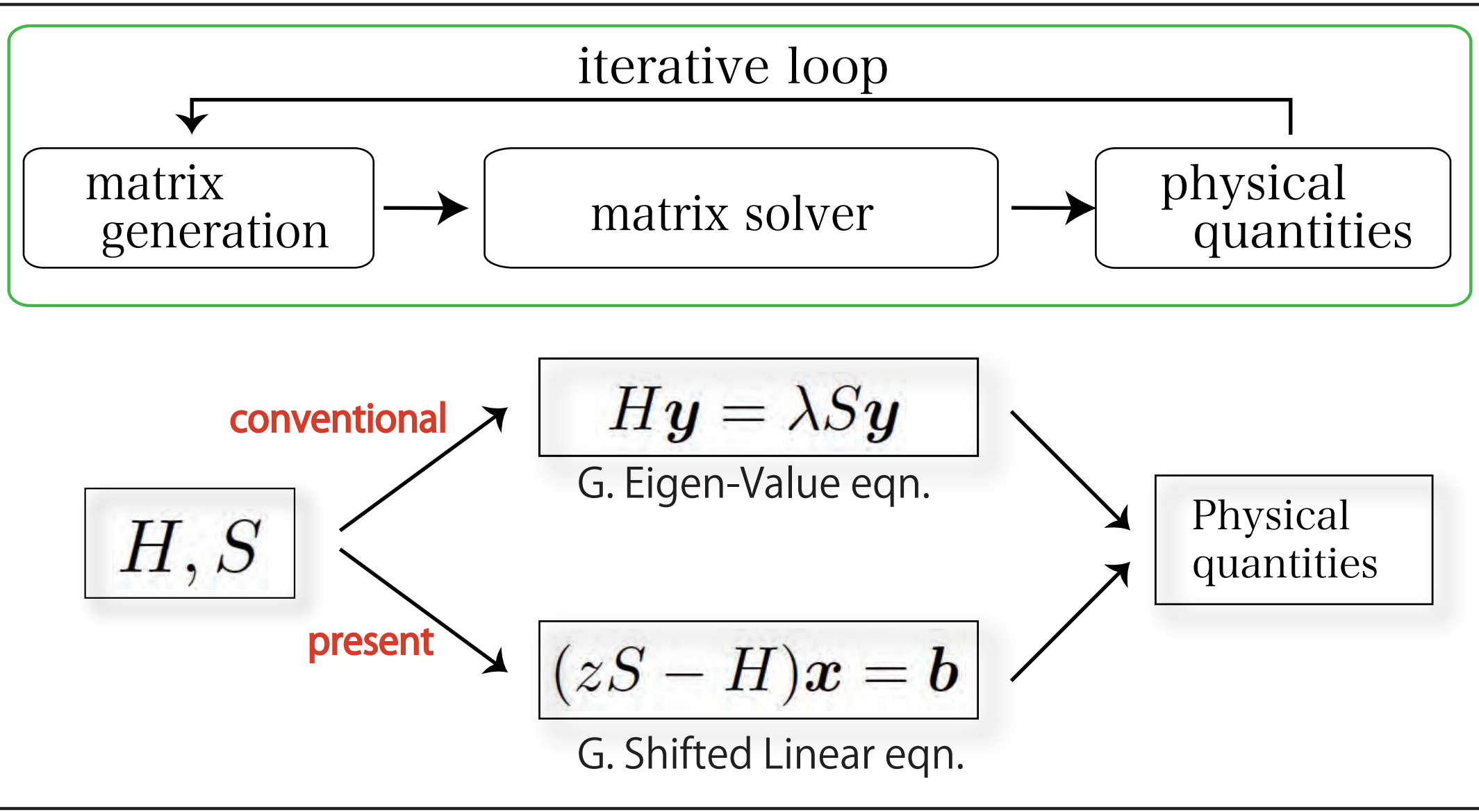
(*) An electronic 'wave'
(wave function)
of Benzene (C_6H_6)



Overview

Application-Algotirhm-Architecture co-design

→ 目的物理量ごとに、最適な計算手順(workflow)を構築



Theory and methodology

(1) One of our novel linear-algebraic solvers

→ multiple Arnoldi algorithm(*) for generalized shifted linear eq.

$$(H - zS)\boldsymbol{x} = \boldsymbol{b} \quad (\ S \approx I\ )$$

→ the use of multiple Krylov subspaces of

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

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

(*)T. Hoshi, S. Yamamoto, T. Fujiwara, T. Sogabe, S.-L. Zhang, J. Phys.: Condens. Matter 24, 165502 (2012)

(2) HPC issues on the K computer

→ Balance operation, communication and memory costs

(3) Other details

- Applicable both to metals and insulators
- Modelled (TB-type) systems, based on ab initio calculation
- A DFT-derived charge-self-consistent formulation (optional)

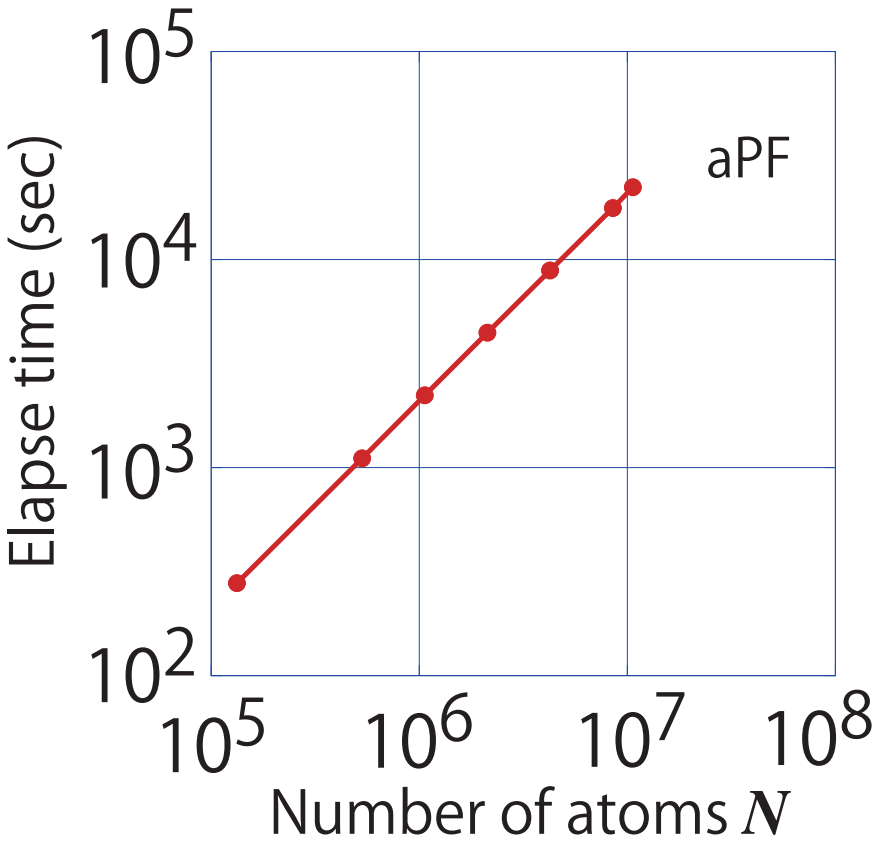
ELSES, our electronic-structure calculation code

Hoshi et al.,JPSJ 82, 023710 (2013); Hoshi et al., Preprint (http://arxiv.org/abs/1307.3218)

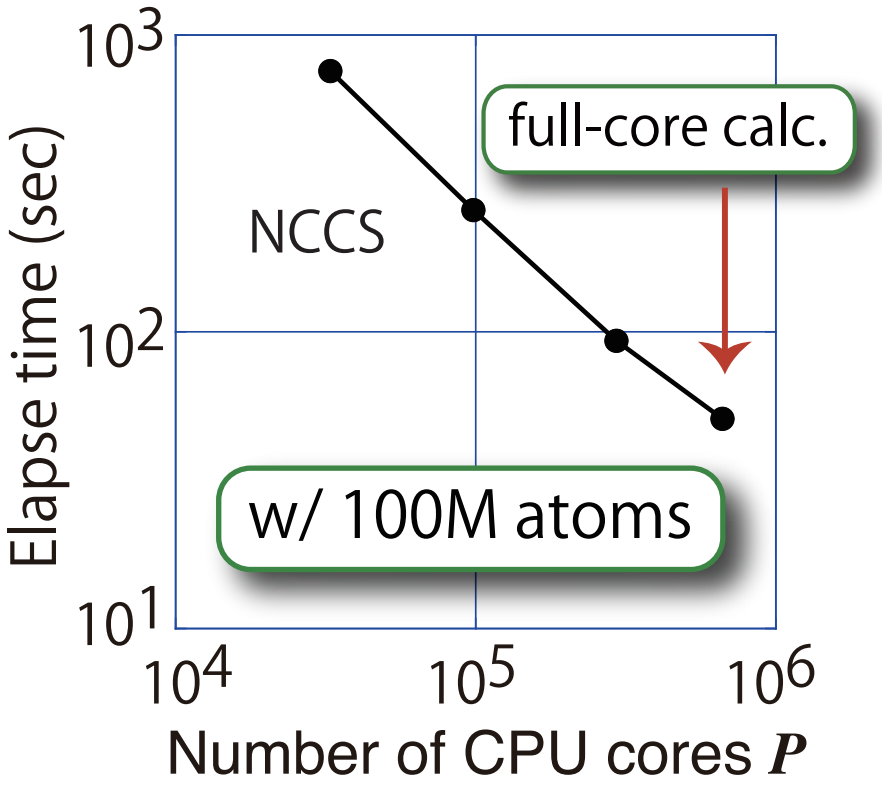
Benchmark with upto 100M atoms(⇄ Si : $(126\text{nm})^3$region)

aPF :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)

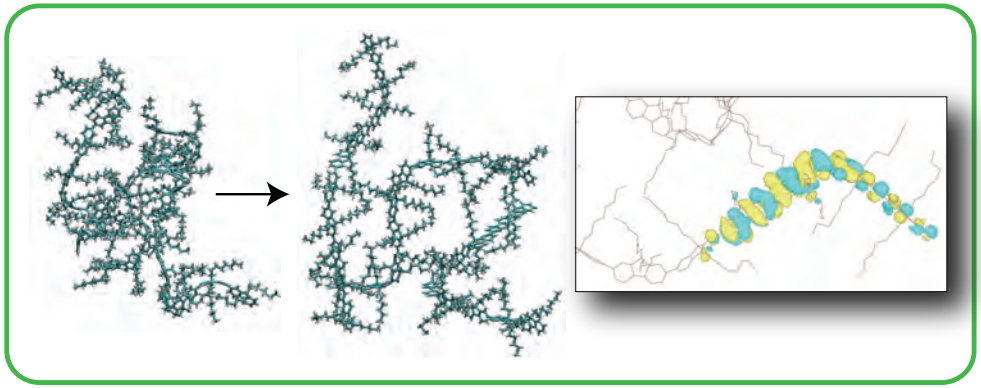


結果

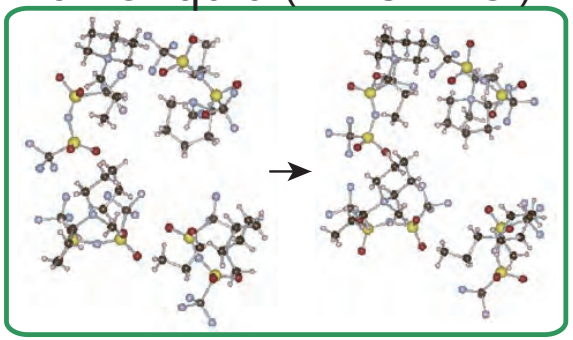
ELSES:物質研究の例(「京」利用の前)

方針 (i) 産業利用
(ii) 新物質(日本発)
(iii) 基準物質

Amourphous-like conjugated polymer
(poly-(9,9 dioctyl fluorene) [有機EL]

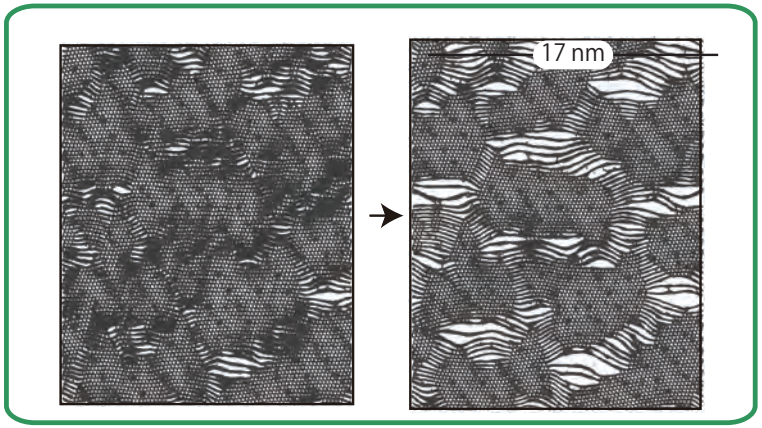


Ionic liquid (PP13–TFSI)

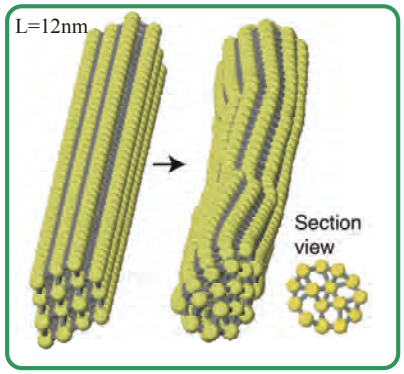


Li^+ diffusion
in solids
(Nishino et al.)

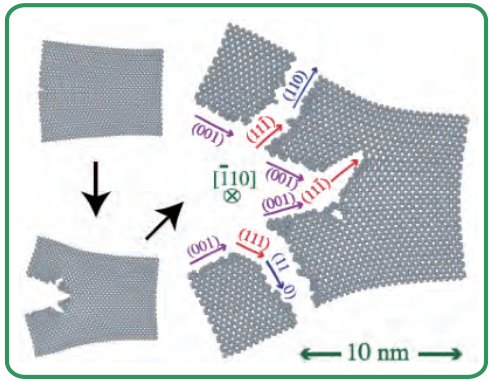
sp2-sp3 nano-composite carbon solid
(for nano-polycrystalline diamond)



helical gold nanowire



silicon brittle fracture



謝辞(共同研究・データ提供) 西野信也・藤原毅夫(東大), 山元進(東京工科大),
山崎久嗣(トヨタ自動車), 善甫康成(法政大), 石田雅也(住友化学)

展望

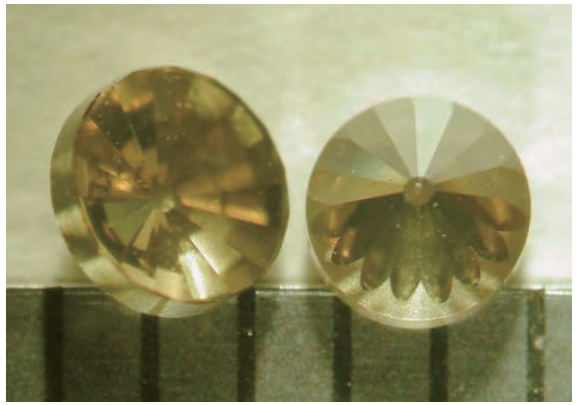
PetaからPost-petaへ：100nmスケール(1億原子以上)計算へのニーズ

→複合的ナノ物質（ナノドメイン・ドメイン境界の複合）→従来物質にない機能

例：ナノ多結晶ダイヤモンド・・・日本発の革新的超強度物質*

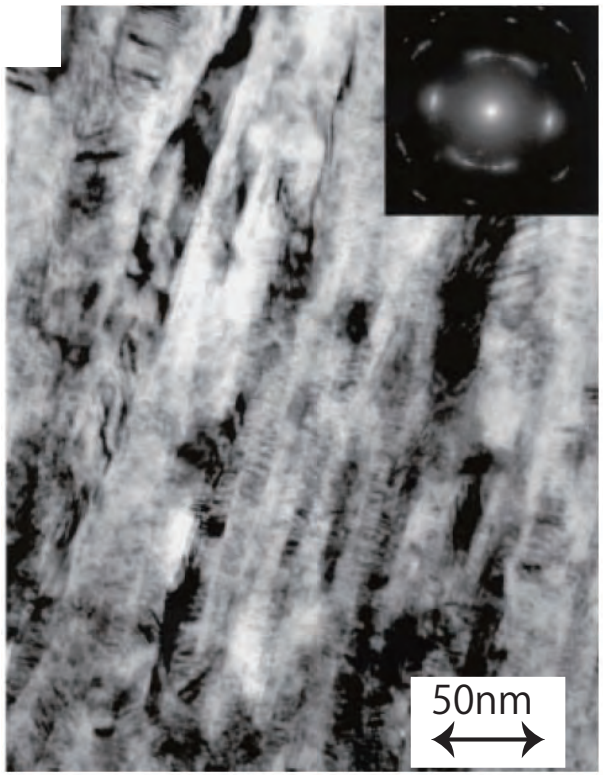
(*)Irifune et al., Nature 421, 599（2003); (**) Hoshi et al.,JPSJ 82, 023710 (2013)

(a) マクロスケール

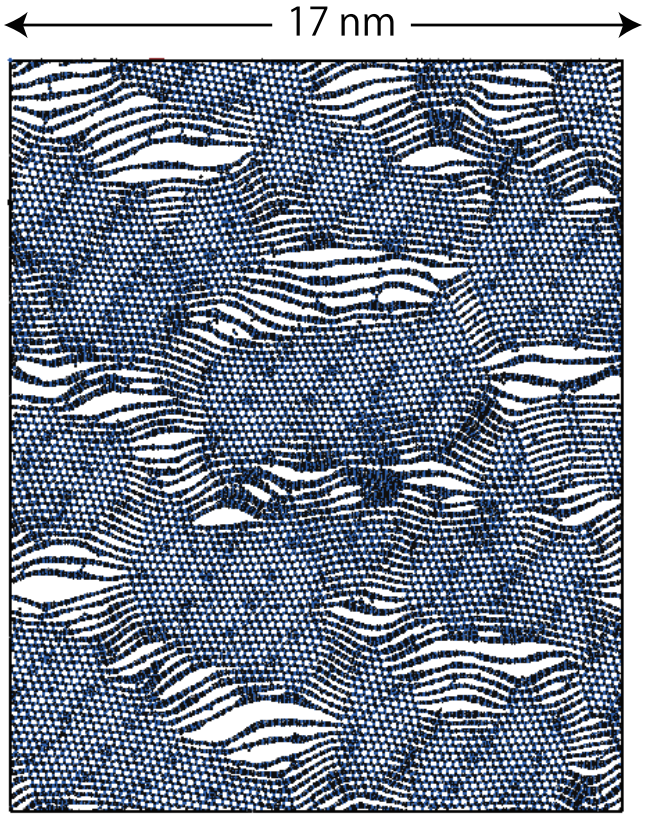


→2012年
住友電工が製品利用

(b) 実験(100nmスケール)*



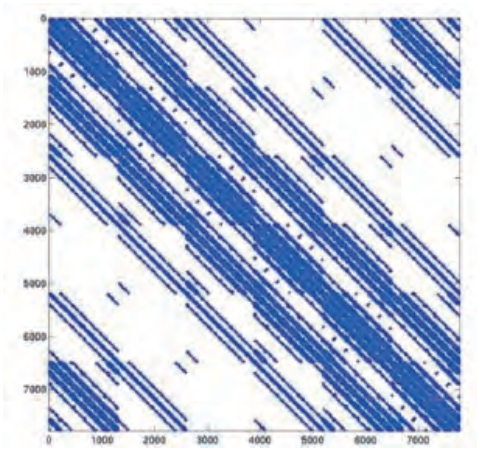
(c) 従来計算**：10万原子系

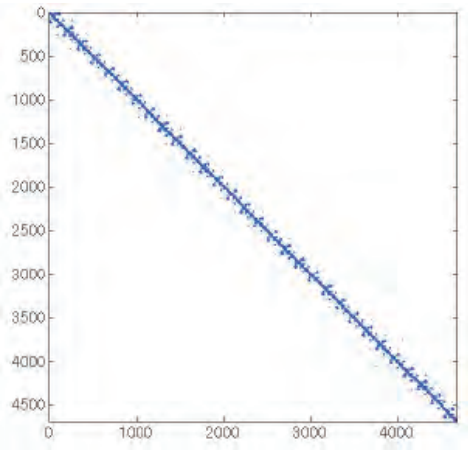


展望

物質科学と応用数学のさらなる連携研究のために

・データ共有
→実問題の大規模疎行列データを
　ライブラリ化して公開(~100万次元)
　: ELSES matrix library :
　　http://www.elses.jp/matrix/





・コード共有
→行列ソルバーの擬似(ミニ)アプリ
　: Eigen Test (α状態) : http://www.damp.tottori-u.ac.jp/~hoshi/eigen_test/

・研究：複合数理原理によるソルバー(hybrid solver)*
→(密行列ソルバー的アイディア)+(疎行列ソルバー的アイディア)

*例：内部固有値問題; D. Lee, T. Miyata, T. Sogabe, T. Hoshi, S.-L. Zhang, EASIAM, 2013; to appear in Japan J. Indust. Appl. Math.

まとめ

1. Overview: Application-Algorithm-Architecture co-design
   → 新しいアイディアとその組み合わせでブレークスルーを
   → 目的物理量ごとに最適な計算手順(workflow)を構築
2. 新しいクリロフ部分空間アルゴリズム
   → 一般化シフト型線形方程式

$$(H - zS)\boldsymbol{x} = \boldsymbol{b} \quad (\ S \approx I\ )$$

3. 「京」フルノードでの超並列計算
   → 1 億原子(100nmスケール) 系
4. 展望
   (a) PetaからPost-petaへの物質科学的展望
   （ナノドメインの複合した物質→物質設計）
   (b) 物質科学と応用数学のさらなる協調研究へ
   (行列データ集、擬似アプリ、複合数理原理)

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

Overview of multiple Arnoldi method (2/2)

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

→ Exact reproduction of physical conservation laws within the subspace

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

$$\Omega \equiv \sum_{\alpha}^{\nu} \boldsymbol{u}_\alpha \boldsymbol{u}_\alpha^{\mathrm{T}} \qquad (6)$$

($\boldsymbol{v}_\alpha$: subspace eigen vectors)

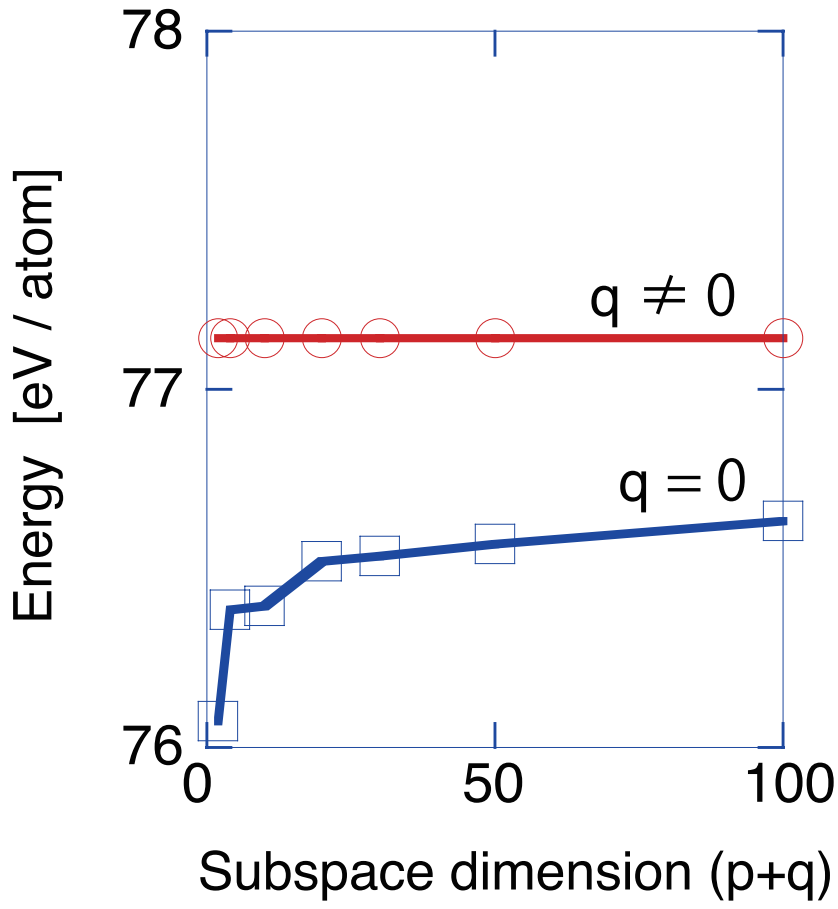
Def.: Projected physical quantity
in the FFL : $\boldsymbol{b}^{\mathrm{T}}\Omega X \boldsymbol{b}$ (7)

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

Theorem:
If $q \neq 0$, then $\boldsymbol{b}^{\mathrm{T}}\Omega X \boldsymbol{b} = (\mathrm{exact})$ (8)

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

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



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

$$\rightarrow \quad \boldsymbol{x} = G\boldsymbol{b}$$

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