jh130011-NA07

星健夫 (鳥取大学, JST-CREST(Post Peta))

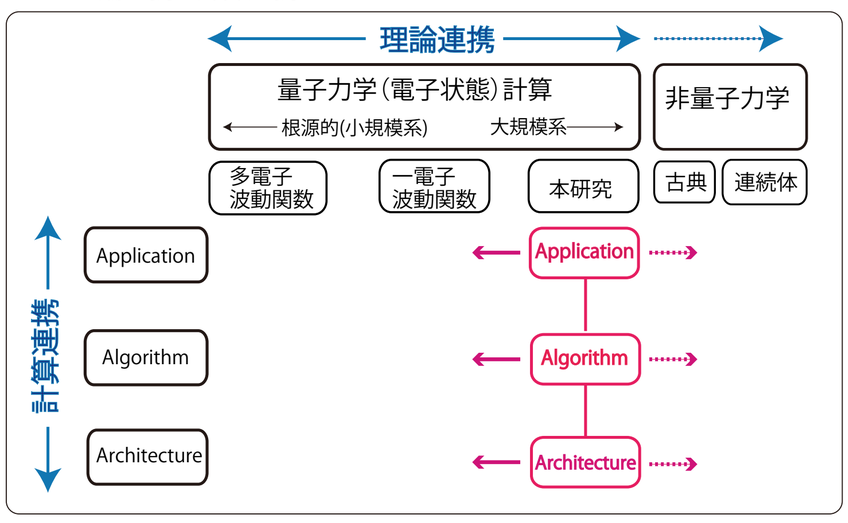
超大規模超並列電子状態計算を中核とした物理・数理・HPCの融合研究

参加者：曽我部知広[1,2](副代表), 張 紹良[3,2], 宮田考史[3,2], 山元進[4], 西野信也[5], 井町宏人[5], 川居佳史[6], 秋山洋平[6], 山﨑渓太[6]
[1]愛知県立大, [2]JST-CREST(Post Peta), [3]名古屋大, [4]東京工科大, [5]東大, [6]鳥取大,

1

Overview : 計算物質科学における2種類の連携軸

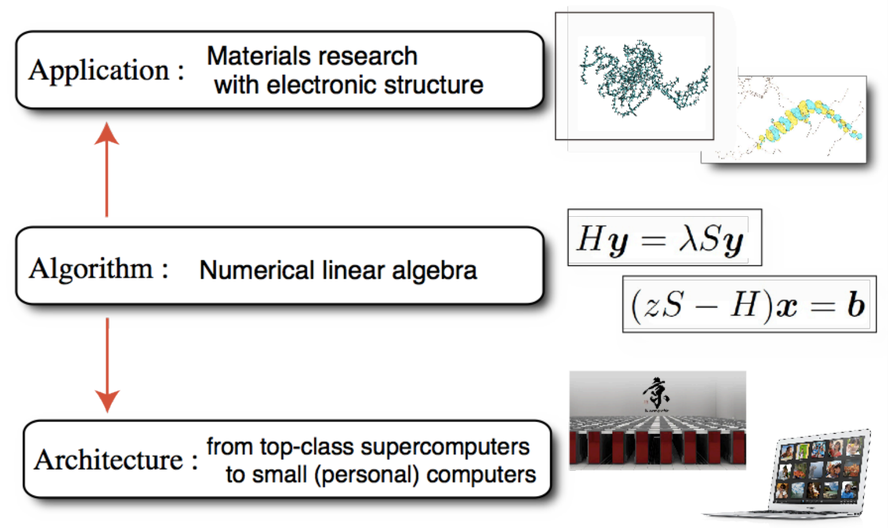
→理論連携と計算連携



2

Overview : Application-Algorithm-Architecture co-design

a common concept in the current computational physics



3

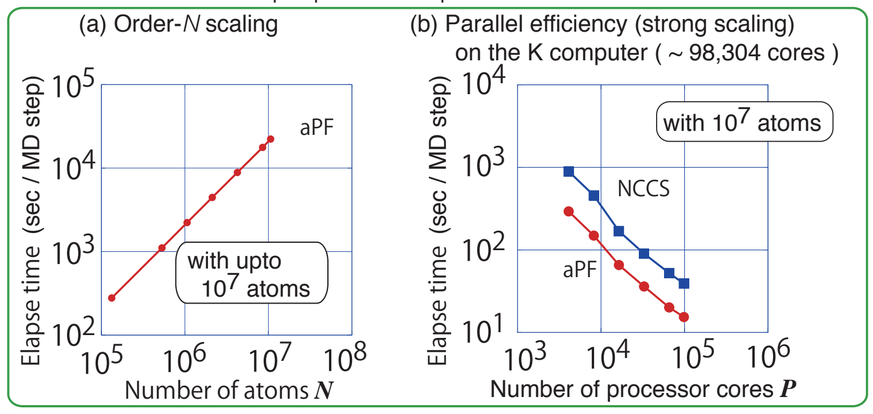
http://www.elses.jp

'ELSES' : Our code for 'order-*N*' electronic structure calculations

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

Benchmark with nanomaterials (~10^7 atoms ⇄ Si : $(70\text{nm})^3$region)

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

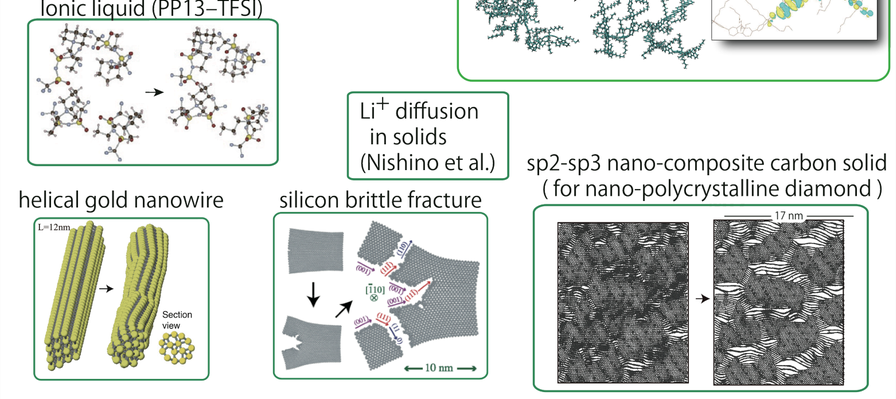


4

http://www.elses.jp

Examples of nano-material studies with 'ELSES'

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



5

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

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

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

6

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

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

non-hermitian

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

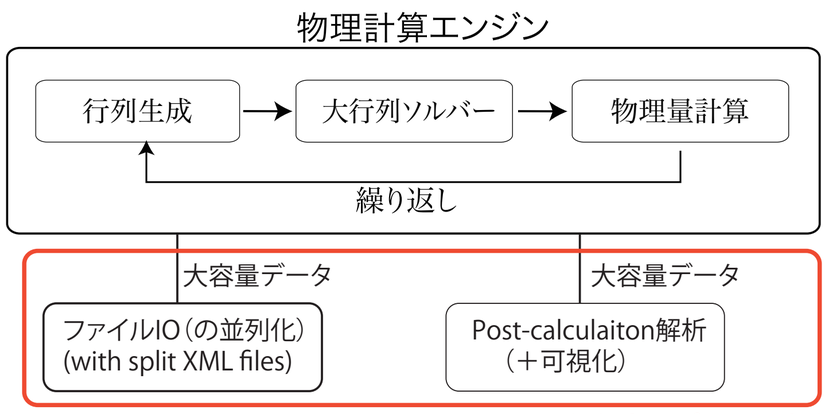
*Takayama *et al*., JPSJ73, 1519 (2004); Takayama et al. PRB 73, 165108(2006); Sogabe et al. ETNA31, 126 (2008)

7

(物理学を抜いた説明)

「物理計算エンジン」(というコンセプト)

→「行列生成+数値計算＋物理量計算」(の繰り返し)を一体として、アルゴリズム構築。



8

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

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