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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

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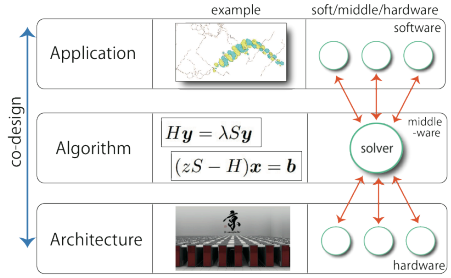
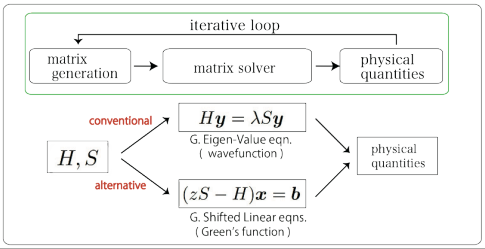
1 Application-Algotirhm-Architecture co-design

→ Concept : Integrating new ideas for breakthrough
→ Code : Sharing mathematical solvers as middlewares



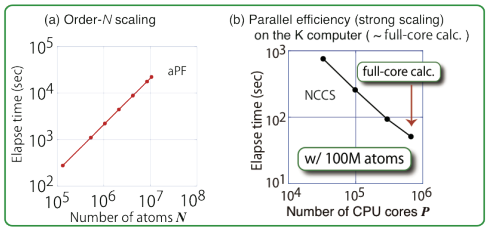
2 Application-Algotirhm-Architecture co-design

Large-scale quantum material simulation (electronic structure calculation)
→ Construct an optimal workflow for each target physical quantity with generalized eigen-value eqn. or generalized shifted linear eqns.



3 ELSES, our quantum material simulation code

(ELSES = Extra-Large-Scale Electronic Structure calculation code)
Benchmark with upto 100M atoms(⇄ Si : (126nm)^{3}region)
(Ref. Hoshi, et al., JPS-CP 1, 016004 (2014), http://www.elses.jp/)



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

4 Our novel linear algebraic solver 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 equations

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

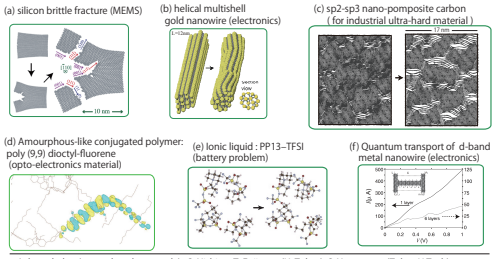
Solvers with Galerkin Principle	Solvers with Collinear Residual Theorem
gLanczos, gArnoldi, mArnodi, Arnoldi(M,W,G)	gsCOCG, gsQMR

Note: The case of $S=I$, the theories are reduced to the previous ones; Takayama et al., JPSJ73, 1519 (2004);PRB73, 165108(2006); Sogabe et al. ETNA31, 126 (2008)

Other (not mathematical) details
- Applicable both to metals and insulators
- Modelled (tight-binding-form) systems, based on *ab initio* calculation
- A *ab initio*-derived charge-self-consistent formulation, van der Walls interaction (optional)

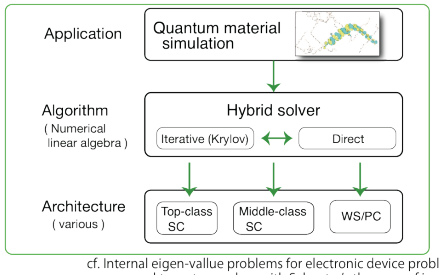
5 Nano-material studies with ELSES

References are listed in out latest preprint: http://arxiv.org/abs/1402.7285



Acknowledge (co-worker, data supply) : S. Nishino, T. Fujiwara (U. Tokyo), S. Yamamoto (Tokyo U Tech)
H. Yamasaki (Toyota), Y. Zempo (Hosei U), M. Ishida (Sumitomo Chem.) and (fomer) students

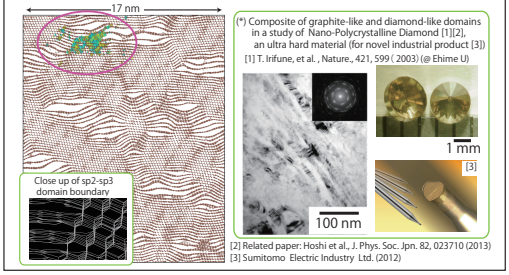
6 (This year~) Hybrid solver for various physical quantities



cf. Internal eigen-vallue problems for electronic device problem
→ novel two-stage solver with Sylvester's theorem of inertia;
D. Lee, et al. JJIAM 30, 625 (2013)

7 A recent result; domain-boundary wavefuntion in sp2-sp3 nano-composite carbon solid

→ 'EigenExa', a novel direct eigen-value solver, was used (Imamura @ AICS)
The matrix size is M = 430,080. The FX10 was used.



[2] Related paper: Hoshi et al., J. Phys. Soc. Jpn. 82, 023710 (2013)
[3] Sumitomo Electric Industry Ltd. (2012)

8 Preliminary results : organic electronics materials

10-nm- and 100-nm-scale non-ideal systems
→ huge π -electron network