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超大規模超並列電子状態計算を中心とした物理・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

example

Application

Algorithm

Architecture

soft/middle/hardware software

middle-ware solver hardware

co-design

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.

iterative loop

matrix generation → matrix solver → physical quantities

$H\mathbf{y} = \lambda S\mathbf{y}$ G. Eigen-Value eqn. (wavefunction)

H, S conventional

$(zS - H)\mathbf{x} = b$ alternative G. Shifted Linear eqns. (Green's function)

physical quantities

3 ELSES, our quantum material simulation code
(ELSES = Extra-Large-Scale Electronic Structure calculation code)
Benchmark with upto 100M atoms(\approx Si; (126nm) 3 region)
(Ref. Hoshi, et al., JPS-CP 1, 016004 (2014), <http://www.elses.jp/>)

(a) Order- N scaling

Elapsed time (sec) vs Number of atoms N

(b) Parallel efficiency (strong scaling) on the K computer (~ full-core calc.)

Elapsed time (sec) vs Number of CPU cores P

aPF : amorphous-like conjugated polymer, poly-(9,9 diocetyl-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

$(H - zS)\mathbf{x} = b$ non-hamiltonian	Solvers with Galerkin Principle	Solvers with Collinear Residual Theorem
g Lanczos, g Arnoldi, m Arnoldi(M,W,G)	gs COCG, gs QMR	

Note: The case of $\square =$, 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 latest preprint: <http://arxiv.org/abs/1402.7285>

(a) silicon brittle fracture (MEMS) (b) helical multishell gold nanowire (electronics) (c) sp2-sp3 nano-pomposite carbon (for industrial ultra-hard material)

(d) Amorphous-like conjugated polymer: poly(9,9 diocetyl-fluorene) (opto-electronics material) (e) Ionic liquid : PP13-TFSI (battery problem)

(f) Quantum transport of d-band metal nanowire (electronics)

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

Application

Quantum material simulation

Algorithm (Numerical linear algebra)

Hybrid solver

Architecture (various)

Top-class SC Middle-class SC WS/PC

Iterative (Krylov) Direct

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

7 A recent result: domain-boundary wavefunction 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.

17 nm

Close up of sp2-sp3 domain boundary

Composite of graphite-like and diamond-like domains in a study of Nano-Poly-crystalline Diamond [1][2], an ultra hard material (for novel industrial product [3]) [1] T. Iritani, et al., Nature, 421, 599 (2003) (@ Ehime U)

[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

PFO ($n=10$) at finite temperature

HOMO

2nd HOMO

3rd HOMO

bundle-like PPV $L \approx 40$ nm ($n=50$)

拡大図

Elapsed time (sec) vs Number of CPU cores

Benchmark on FX10: bundle-like PPV with 120K atoms