

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心とした物理・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, 山崎渓太⁶
¹愛知県立大, ²JST-CREST(Post Peta), ³名古屋大, ⁴東京工科大, ⁵東大, ⁶鳥取大,

<p>1 Overview : 計算物質科学における2種類の連携軸</p> <p>→理論連携と計算連携</p>	<p>2 Overview : Application-Algorithm-Architecture co-design a common concept in the current computational physics</p> <p>Application : Materials research with electronic structure</p> <p>Algorithm : Numerical linear algebra</p> <p>Architecture : from top-class supercomputers to small (personal) computers</p>									
<p>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 (~10⁷ atoms \supseteq Si : (70nm)³region) aPF : amorphous-like conjugated polymer, poly-(9,9 diethyl fluorene), NCCS: sp₂-sp₃ nano composite carbon solid</p> <p>(a) Order-N scaling (b) Parallel efficiency (strong scaling) on the K computer (~ 98,304 cores) with upto 10⁷ atoms</p>	<p>4 http://www.elses.jp Examples of nano-material studies with 'ELSES'</p> <p>Motivations (i) industrial application (ii) new material (from Japan) (iii) standard material</p> <p>Amorphous-like conjugated polymer (poly-(9,9 diethyl fluorene)) </p> <p>Ionic liquid (PP13-TFSI) </p> <p>Li⁺ diffusion in solids (Nishino et al.) </p> <p>helical gold nanowire </p> <p>silicon brittle fracture </p> <p>sp₂-sp₃ nano-composite carbon solid (for nano-polycrystalline diamond) </p>									
<p>5 Basic equations</p> <p>Generalized eigen-value (GEV) equation $H\mathbf{y}_k = \varepsilon_k S\mathbf{y}_k$ H, S: Hermitian, S: positive definite ($S \doteq I$)</p> <p>wavefunction formulation</p> <p>$G = \sum_k \frac{\mathbf{y}_k \mathbf{y}_k^T}{z - \varepsilon_k}$</p> <p>Generalized shifted linear (GSL) equations $(zS - H)\mathbf{x} = \mathbf{b}$ (z: complex energy)</p> <p>non-Hermitian</p> <p>$\rightarrow \mathbf{x} = G\mathbf{b}$ with $G \equiv (zS - H)^{-1}$: the Green's function</p>	<p>6 Novel linear algebraic algorithms</p> <p>[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).</p> <p>→ Iterative (Krylov subspace) solvers for generalized shifted linear equation</p> <p>$(H - zS)\mathbf{x} = \mathbf{b}$ non-hermitian</p> <table border="1"> <thead> <tr> <th>Mathematical principles</th> <th>$S \neq I$</th> <th>$S = I^*$</th> </tr> </thead> <tbody> <tr> <td>Gerlerkin Principle</td> <td>g Lanczos, g Arnoldi, m Arnoldi (M;W;G)</td> <td>subs. diag.</td> </tr> <tr> <td>Collinear Residual</td> <td>gs COCG, gs QMR</td> <td>s COCG, s QMR</td> </tr> </tbody> </table> <p>*Takayama et al., JPSJ 73, 1519 (2004); Takayama et al. PRB 73, 165108(2006); Sogabe et al. ETNA 31, 126 (2008)</p>	Mathematical principles	$S \neq I$	$S = I^*$	Gerlerkin Principle	g Lanczos, g Arnoldi, m Arnoldi (M;W;G)	subs. diag.	Collinear Residual	gs COCG, gs QMR	s COCG, s QMR
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<p>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)</p> <p>→「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。</p> <p>物理計算エンジン</p> <p>行列生成 → 大行列ソルバー → 物理量計算</p> <p>繰り返し</p> <p>大容量データ 大容量データ</p> <p>ファイルIO (の並列化) (with split XML files)</p> <p>Post-calculaiton解析 (+可視化)</p> <p>これらも実アプリには必須</p>	<p>8 *Hoshi, et al., JPSJ 82, 023710 (2013)</p> <p>Visualization with massively parallel data analysis based on the Green-function theory (π-COHP*)</p> <p>Ex. sp₂ and sp₃ nano composite carbon solid with 100K atoms → the distinction of sp₂ and sp₃-domains</p> <p>(A) Visualize sp₂ and sp₃ domains </p> <p>(B) Visualize only sp₂ domains </p> <p>sp₂-sp₃ domain boundary</p>									