

Numerical linear algebraic problems in large-scale massively parallel electronic state calculations on the K computer

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The present paper presents the numerical linear algebraic problems and their solution algorithms in our large-scale massively parallel electronic state calculations; [1] (i) generalized eigen-value problem ($A\mathbf{y} = \lambda B\mathbf{y}$) for whole [2] and partial [3] eigen pairs, (ii) generalized shifted linear equations ($(zB - A)\mathbf{x} = \mathbf{b}$) [4-6], (iii) Schrödinger-like dynamical equation ($d\mathbf{u}/dt = -iA\mathbf{u}$) or its formal solution ($\mathbf{u}(t + \delta t) := \exp(-i\delta t A)\mathbf{u}(t)$). They appear in structure (molecular dynamics) simulation or quantum transport (hole wave packet dynamics) simulation of nano material applications, such as organic electronic devices. Our simulation code is called 'ELSEs' (=Extra Large-Scale Electronic Structure calculation) [1] and was optimized for the K computer and other massively parallel supercomputers. We prepared a matrix data collection of 'ELSEs Matrix Library', [7] an open database of our real problems for numerical analysis researchers. Several recent papers are listed below and older ones can be found in the papers or the web sites [1].

[1] <http://www.elses.jp/>, <http://www.damp.tottori-u.ac.jp/~hoshi/>

[2] Hiroto Imachi and Takeo Hoshi, Hybrid numerical solvers for massively parallel eigenvalue computation and their benchmark with electronic structure calculations, to appear in IPSJ Trans. ACS 52. Preprint: <http://arxiv.org/abs/1504.06443>; Hiroto Imachi and Takeo Hoshi, Poster in this workshop.

[3] Dongjin Lee, Takafumi Miyata, Tomohiro Sogabe, Takeo Hoshi, Shao-Liang Zhang, An interior eigenvalue problem from electronic structure calculations, Japan J. Indust. Appl. Math. 30, 625 (2013).

[4] Takeo Hoshi, Susumu Yamamoto, Takeo Fujiwara, Tomohiro Sogabe, Shao-Liang Zhang, An order- N electronic structure theory with generalized eigenvalue equations and its application to a ten-million-atom system, J. Phys.: Condens. Matter 24, 165502 (2012); Takeo Hoshi, Keita Yamazaki, Yohei Akiyama, Novel linear algebraic theory and one-hundred-million-atom electronic structure calculation on the K computer, JPS-CP. 1, 016004 (2014).

[5] Tomohiro Sogabe, Takeo Hoshi, Shao-Liang Zhang, Takeo Fujiwara, Solution of generalized shifted linear systems with complex symmetric matrices, J. Comp. Phys. 231, 5669 (2012).

[6] Shigeru Iwase, Takeo Hoshi, Tomoya Ono, Efficient numerical solver for first-principles transport calculation based on real-space finite-difference method, to appear in Phys. Rev. E. Preprint: <http://arxiv.org/abs/1502.00081>.

[7] <http://www.elses.jp/matrix/>