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New Parallel Divide-and-Conquer Algorithm for Computing Full Spectrum of Polyacetylene YIHUA BAI, Indiana State University, BOB WARD, University of Tennessee at Knoxville, GUOPING ZHANG, Indiana State University

— The Su-Schrieffer-Heeger (SSH) model is a simple tight-binding model that includes nearest neighbors and is frequently used to study the fundamental properties of trans-polyacetylene (trans-PA), as well as many other materials. In these studies, the essential and most time consuming step is the computation of the eigen-decomposition of the Hamiltonian matrix. In this poster, we present a new scalable parallel algorithm that efficiently computes the full spectrum of Hamiltonian matrices to a prescribed accuracy. Given an accuracy tolerance τ and Hamiltonian matrix A, which is a real symmetric dense matrix, our parallel algorithm fully exploits the structure of the Hamiltonian matrix and computes eigen-solutions in two steps: (a) Construct a block-tridiagonal matrix that approximates the original dense matrix; (b) Use the highly efficient block-tridiagonal divide-and- conquer algorithm to compute approximate eigen-solutions. The computed approximate eigen-solutions satisfy the following conditions: 1) $||A - V\Lambda V^T|| \leq O(\tau||A||)$; and 2) $||(VV^T - I)|| \leq O(n\epsilon_{mach})$, where ϵ_{mach} is the machine precision. Performance tests show that this algorithm is extremely efficient for the computation of electronic spectrum of trans-PA compared to traditional dense eigensolvers. In many tests, the savings is several orders of magnitude!

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