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## The Hong Kong University of Science and Technology

#### **Department of Mathematics**

# **Seminar on Applied Mathematics**

### A Parallelizable Algorithm for Orthogonally Constrained Optimization Problems

by

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#### <u>Abstract</u>

To construct a parallel approach for solving orthogonally constrained optimization problems is usually regarded as an extremely difficult mission, due to the low scalability of orthogonalization procedure. In this talk, we propose an infeasible algorithm for solving optimization problems with orthogonality constraints, in which orthogonalization is no longer needed at each iteration, and hence the algorithm can be parallelized. We also establish a global subsequence convergence and a worst-case complexity for our proposed algorithm. Numerical experiments illustrate that the new algorithm attains a good performance and a high scalability in solving discretized Kohn-Sham total energy minimization problems.

Date: Wednesday, 4 October 2017 Time: 4:00p.m. – 5:00p.m. Venue: Room 4472, Academic Building (near Lifts 25 & 26), HKUST All are welcome!