Optimized PC-Linux Configurations for Theoretical Calculation
(*Lecture in Technical Workshop on Computational Chemistry*)

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In the lecture, the performance of programs in computational chemistry compiled by various configurations of compilers and numerical libraries on PC-Linux platforms are demonstrated. These results are additionally correlated with SPEC CPU2000 floating-point benchmark. According to the evaluation the most optimized configurations for computational chemistry in PC-Linux systems are concluded. The topics of free discussion include, but are not limited to the experiences in Linux for scientific computing, setup and management of clusters, performance tuning, and problems in theoretical calculations.

計算化學的軟體在 PC-Linux 的環境下使用不同的程式編譯器與數值函式庫會對浮點效能產生可觀的影響。經由系統化的評估程序，可以找出最佳運算效能的執行環境；同時與工業標準的 benchmark 軟體(SPEC CPU2000) 浮點測試結果作比較，可以得到完全的相關性。交流討論的主題包括但不限於 Linux 平台上的效能最佳化與計算經驗分享、叢集工作站系統的架設與管理、以及計算化學相關的各種問題等。

Related Publications

[1] J.-S. K. Yu, J.-K. Hwang, C. Y. Tang and C.-H. Yu, J. Chem. Inf. Comput. Sci. 44, 635 (2004).
[2] J.-S. K. Yu and C.-h. Yu, J. Chem. Inf. Comput. Sci. 42, 673 (2002).
[3] J.-S. K. Yu and C.-h. Yu, J. Chem. Inf. Comput. Sci. 37, 1111 (1997).