
High performance numerical linear algebra: trends and new challenges

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Résumé

The emergence of applications to exploit the enormous data sets that are now becoming available, brings new, interesting, and often challenging, linear algebra problems. In fact, one can say that data mining and machine learning are now beginning to shape a "new chapter" in numerical methods, replacing Computational Fluid Dynamics and Partial Differential Equations as the main source of 'model' linear algebra problems. The talk will start with a survey of the classical high-performance problems and the related state of the art algorithms to solve them. We will cover sparsity, standard Krylov methods, preconditioners, and eigenvalue problems. The second part of the talk will essentially discuss the new 'numerical linear algebra', bringing data related applications to the fore. We will cover key concepts and discuss dimension reduction methods which play a major role. These concepts will be illustrated with a few applications, such as information retrieval, face recognition and matrix completion for recommender systems. The presentation will end with an important emerging application in 'materials informatics'. The synergy between high-performance computing, efficient electronic structure algorithms, and data mining, may potentially lead to major discoveries in materials. We will report on our preliminary experiments in 'materials informatics', a methodology that blends data mining and materials science.

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