Research Activities in Computing Science at Umeå University with focus on Scientific and Parallel Computing

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Abstract

In this presentation, we give an overview of research activities at the Department of Computing Science, Umeå University with focus on Scientific, Parallel and High-Performance Computing. The first part of the talk will give a brief general overview. The second part will illustrate some of the current research directions of my students, myself and colleagues. I plan to review some recent results in the following areas.

- Recursive Blocked Algorithms and Hybrid Data Structures for Dense Matrix Library Software (with Erik Elmroth, Fred Gustavson, and Isak Jonsson, see *SIAM Review*, Vol. 46, No. 1, 2004, pp. 3-45.)
- Matrix Equations (with Robert Granat and Isak Jonsson)
  - RECSY - A high performance library for Sylvester-type matrix equations
  - ScaLAPACK-style algorithms and software for Sylvester-type matrix equations
- Parallel, Blocked and Multishift Variants of the QZ Algorithm for Regular Matrix Pairs (with Björn Adlerborn and Daniel Kressner, TU-Berlin)
- Robust Computation of Canonical Structure Information of Matrices and Matrix Pencils - from Staircase Algorithms to Orbit and Bundle Stratifications (with Erik Elmroth, Pedher Johansson, Stefan Johansson, and earlier Jim Demmel and Alan Edelman)
- Periodic Systems - Matrix Equations, Perturbation Theory and Applications (with Robert Granat, Isak Jonsson, Daniel Kressner, Jiguang Sun, and Andras Varga, DLR, Germany)
  - Reordering of eigenvalues in the periodic Schur form (PSF) of a product of matrices
  - Computation of subspaces and condition estimation

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Some additional background

Research in Computing Science is conducted in a broad range of fields and is based on fundamental, interdisciplinary and applied scientific issues. Several ongoing research projects are interdisciplinary and involve university departments from different faculties and international collaboration. Examples of such areas include image processing, bioinformatics, medical informatics, computer communications, real-time physics simulations, scientific visualization, and virtual reality (VR) environments.

Our research in scientific computing and parallel computing is well established internationally and focuses on theory, model, method, and software development(s). Scientific computing is advancing rapidly, and its focus often shifts as the technical development of computers continues. Faster computers allow the study of new complex problems and new computer architectures with complex memory hierarchies require new algorithms, tools and techniques to achieve maximum effectiveness. At the same time, the development of models and methods goes hand in hand with a deepened mathematical understanding. Important examples are ill-posed problems and inverse problems for which different types of regularization are necessary.

In addition to intradisciplinary investigations of problems such as numerical linear algebra, differential equations, and optimization, research is also focused on applications in engineering and science. Examples include chemical equilibrium processes, kinetic analysis, and radio stereometry (RSA).

Research groups participate in international projects and EU-funded efforts including NICONET, a thematic network for numeric analysis in automatic control engineering with industrial applications. In collaboration with High Performance Computing Center North (HPC2N), we also make important contributions to international software libraries for high-performance and parallel computer systems (LAPACK, ScaLAPACK, SLICOT, ESSL etc.) and for generic Web and Grid computing environments and portals.

In collaboration with VRlab/HPC2N, we are conducting research in real-time physics simulations (Kenneth Holmlund, Claude Lacoursièré, and Krister Wiklund). Ongoing projects include Visual Interactive Simulation—Tools and Applications (VISTA, EU Structural Funds) and Interactive Simulation of Complex Materials. In VISTA, we study high performance and robust numerical methods for dry frictional contact problems in multibody systems, leading to the solution of so called mixed linear complementary problems (MLCP). The latter project is focusing on the simulation of granular material and interaction between rigid bodies and such material using particle methods (e.g., the smoothed particle hydrodynamics (SPH) method).

Our research in Bioinformatics (FL Jeanette Tångrot, graduate student, in collaboration with Uwe Sauer at the Umeå Center for Molecular Pathogenesis (UCMP)) is focused on the use of structural information to improve biological sequence similarity searches using so called structure-anchored Hidden Markov Models (saHMMs).