Krylov Subspace Methods (KSMs) provide powerful and general-purpose ways to project a given problem into a much smaller one that yields good approximate solutions to the original problem. The variety of applications of this general approach is phenomenal. They range from the well-known uses of KSMs for solving linear systems and eigenvalue problems, to less established ones such as computing approximate spectral densities, solving systems of Ordinary Differential Equations, and dimension reduction in machine learning.

June 4: Tutorials

13-13:30 Registration, coffee and tea

13:30-16:30 Krylov subspace methods

Yousef Saad, University of Minneapolis, MN, USA
This tutorial of two lectures will give an overview of Krylov subspace methods, and discuss the related algorithms, theory, and applications.

13:30-14:45 First lecture

14:45-15:15 Coffee and tea

15:15-16:00 Second lecture

16:00-16:30 Discussions and Q&A

June 5: Colloquium

13-13:30 Registration, coffee and tea

13:30-14:15 Divide and conquer algorithms for large Hermitian eigenvalue problems

Yousef Saad, University of Minnesota, MN, USA

Algorithms based on Divide and conquer paradigms can lead to complex, but efficient and flexible algorithms for solving large Hermitian eigenvalue problems. This talk will discuss how various such strategies can be combined to exploit both ‘spectrum slicing’, i.e., computing slices of the spectrum independently, and domain decomposition. These strategies are independent of each other but both are essential if one has to compute very large parts of the spectrum, as is the case in approaches that deal with excited states in solid state physics. The presentation will begin with an overview of polynomial filtering techniques. This general approach can be quite efficient in the situation where the matrix-vector product operation is inexpensive and when a large number of eigenvalues is sought. We present an algorithm (and package) that combines the Lanczos algorithm with partial reorthogonalization and polynomial filtering. An alternative to polynomial filtering that is generating a growing interest is a class of methods that exploit filtering by rational functions. Good representatives of this general approach are the FEAST eigensolver and the Sakurai-Sugiura algorithm. Here we will argue that the standard way of selecting these rational filters, which is based on using the Cauchy integral, can be substantially improved -- especially when iterative solvers are involved. Finally, the talk will discuss our ongoing work on Domain-Decomposition (DD) type methods that rely on spectral Schur complements combined with Newton's iteration.

14:15-15:00 Unite and Conquer Approach for High Scale Numerical Computation, Application to Krylov Methods
The ability to exploit emerging exascale computational systems will require a careful review and redesign of core numerical algorithms and their implementations to fully exploit multiple levels of concurrency, hierarchical memory structures and heterogeneous processing units available in these computational platforms. In this talk, we highlight the constraints imposed by these architectures allowing the conception of smart co-design algorithms. Following this insight, we present the "unite and conquer" approach to solve linear systems of equations and eigenvalue problems for extreme scale computing. Unite and conquer approach focuses on decreasing the number of restart cycles in restarted numerical methods by coupling either synchronously or asynchronously several restarted methods called co-methods. In the end of a restart cycle, each co-method locally gathers available results of all collaborating co-methods and selects the best one in order to create its restarting information. This can permit the global reduction of the number of cycles to convergence. We discuss the properties of these methods that make them well adapted to large-scale multi-level parallel architectures and highlight the generality of the approach. We present some experiments validating the approach for unite and conquer Krylov methods on several parallel platforms.

15:00-15:30 Coffee and tea

15:30-16:15 Parameter auto-tunings at runtime for Parallel and distributed KSM

Serge Petiton, University of Lille Sciences and Technologies and Maison de la Simulation

The convergence and the efficiencies of parallel and distributed KSM methods, such as GMRES and ERAM, greatly depend on the supercomputers used and on the choice of several parameters, such as the subspace size or the restarting strategies, which are difficult to set efficiently before the computation. Minimizing and avoiding communication strategies may also be developed to minimize several costs. Thus, these methods have a lot of correlated parameters which may be optimized using auto-tuning strategies to accelerate convergence, minimize storage space, data movements, and energy consumption.

In this talk, we will survey some auto-tuning potential strategies for parallel and distributed KSM methods. We'll discuss results obtained on clusters of accelerators concerning auto-tunings of subspace sizes, orthogonalisations and restarting strategies. As a conclusion, we will discuss auto-tuning strategies for KSM on future exascale supercomputers, leading to intelligent KSM methods capable of "smart" decisions during computation.

Contact : julien.derouillat@cea.fr - +33 1 69 08 60 70