Current Research Interests

In the last ten years, my research has concentrated on iterative methods for sparse linear systems and eigenvalue problems (primarily, so-called Krylov subspace methods) and on fast direct methods for structured matrices (primarily, Toeplitz and Hankel matrices). These two topics are of high interest in practice. The task of solving huge sparse systems of linear equations comes up in many if not most large-scale problems of scientific computing. In fact, if tasks were judged according to hours spent on them on high-performance computers, the one of solving linear systems might be by far the most important one. And as the problems being solved become larger and larger, iterative methods, in particular those related to conjugate gradients or biconjugate gradients and featuring short recurrences, have a clear competitive advantage.

The two topics of Krylov subspace methods and fast methods for Toeplitz and Hankel matrices may seem unrelated, but, in fact, there is a common theoretical background: the conjugate gradient (CG) and the biconjugate gradient (BiCG) methods (as well as many related ones) have a close connection with orthogonal polynomials, the classical moment problem, Padé approximation, Hankel matrix factorization, and the QD and QR algorithms; likewise, there is an analogue connection between orthogonal polynomials, the trigonometric moment problem, Padé approximation, Toeplitz matrix factorization, and certain less known algorithms of numerical linear algebra. It turned out that these connections, although known for a long time, can still be capitalized upon to make major improvements in the mentioned two topics. The idea of look-ahead steps in Lanczos-type, Levinson-type, and Schur-type methods, necessary to avoid breakdowns and numerical instability in the case of nonsymmetric matrices, originated from making use of these connections. Since 1989 I have been the major promoter of these look-ahead methods and one of the promoters of Lanczos-type product methods, like BiCGStab2, which for non-Hermitian linear systems are the most effective Krylov subspace methods with low memory requirement. The look-ahead Lanczos method, which, as it turned out, I reinvented, has become a crucial part of the QMR method of Freund and Nachtigal. In 1992, I was the first to propose for nonsymmetric Toeplitz matrices stable direct solvers that are under a very weak assumption fast (that is, of cost $\mathcal{O}(N^2)$) or even superfast (that is, of cost $\mathcal{O}(N \log^2 N)$). These Toeplitz solvers have been further discussed and enhanced in a series of papers with Marlis Hochbruck.

Currently, my interests still include Krylov subspace methods and the many interrelations in the circle of areas mentioned above. While I do not expect that we will find a method that converges much faster than the best known ones, there is still a definite need to improve the reliability of these methods, since they are often strongly affected by roundoff errors and since their convergence behavior is not well understood.

In practice, Krylov subspace methods are often applied as inner iterations in the Newton method for large nonlinear systems of equations resulting from the discretization of nonlinear PDEs. A current research project is to further investigate, test, and enhance related nonlinear iterative methods that I have proposed some time ago.

For many particular problems there is also still a strong need to find good preconditioners. By a preconditioner we not only want to reduce the number of iterations of the Krylov subspace method, but we want an overall cost reduction. The best reduction is often attained with preconditioners that are specially adapted to the given problem. Of particular interest are here multiscale methods, where, as in the multigrid example, coarse approximations naturally lead to a preconditioner. Various approaches (classical multigrid, algebraic multigrid, hierarchical bases, wavelets) share this philosophy and have proven to be very effective. However, the application of these approaches to very complex PDEs is often nontrivial and leaves a lot of room for research.

There is, of course, also a need to deal with real-world applications. I am in regular contact with computational scientists from a variety of fields. The area I have been involved with most is that of semiconductor device simulation, where I have profited for many years from collaborations with Prof. W. Fichtner's simulation group. As is well-known, these problems are extremely hard to solve. There is a strong nonlinearity to cope with, and some variables cover an enormous range of scales. Iterative methods are not always so successful, and in fact direct sparse solvers based on the supernode technique are often still competitive. To fit the problem into memory, parallel computing making use of domain decomposition becomes an important issue. So, these are problems that require state-of-the-art numerical methods on all levels. Other applications came up "in-house" in the former Interdisciplinary Project Center for Supercomputing (IPS) and in the former Section for Scientific Projects and Support (SPS) of the Swiss Center for Scientific Computing (CSCS/SCSC): Dr. Philippe de Forcrand, head of the Computational Particle Physics Group, used Krylov subspace methods I proposed in Computational Quantum Chromodynamics (QCD), and PD Dr. Diethelm Würtz, head of the Solid State Physics Group, made use of them in high-temperature superconductivity simulations.