The Top 10 Computational Methods of the 20th Century

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In the January/February 2000 issue of the journal *Computing in Science & Engineering*, a joint publication of the American Institute of Physics and the IEEE Society, the guest editors J. Dongarra and F. Sullivan put together a list they entitled "Top Ten Algorithms of the Century." Their goal was "to assemble the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century." In the May 2000 issue of *SIAM News*, B.A. Cipra briefly described these 10 algorithms. They are: (1) the Monte Carlo method, (2) the Simplex method, (3) Krylov Subspace Iteration method, (4) Householder Matrix Decomposition, (5) the Fortran Compiler, (6) the QR algorithm, (7) the Quicksort algorithm, (8) Fast Fourier Transform (FFT), (9) the Integer Relation Detection algorithm, and (10) the Fast Multipole algorithm.

Researchers and practitioners of *Computational Mechanics* (CM) will surely observe that not all of these algorithms are close to their hearts. On the other hand, undoubtly one can think of algorithms which are extremely important to CM and do not appear in the Dongarra-Sullivan list. Also, the appearance of the Fortran Compiler as an item in the list is puzzling, since as important to scientific computing it may be, Fortran cannot really be regarded as an algorithm. In this light, I thought it would be appropriate to compile a new list, which consists of 20th-century numerical algorithms and methods that have influenced CM the most.

Four of the ten algorithms of the original list are retained in the new list. These greatly influenced CM as well as many other fields of science and engineering. The rest are replaced because their particular impact on CM is felt to be smaller.

Before presenting the new list, four remarks have to be made. First, the items on the list are numerical "methods," not just "algorithms." The difference between the two notions is not clear-cut — both are mathematical procedures to solve a given type of problem by performing a finite number of steps. However, generally the steps of an algorithm are very basic, whereas the steps of a method are more involved; each step of a method may be a known algorithm in itself. Second, we broaden the list even more, such that each item represents a *family* of related methods. The reason is that in most cases it is the combined effect of the whole family that has an impact on CM, not just a single method devised in this family.

Third, the list consists of methods that are believed to have influenced CM greatly; the influence of a method is judged only by how much it is used in current CM work. This influence measure is rather objective, in contrast to the "importance" of a method which is subjective and very hard to judge. Finally, the proposed list is unavoidably biased due

to the author's specific background, knowledge, interpretation and taste. For example, the reader will notice the author's emphasis on techniques that are particularly useful in solid FE analysis...

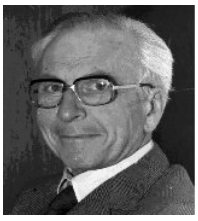
So here is the proposed top-10 list in chronological order.

1. The Finite Element Method (FEM)

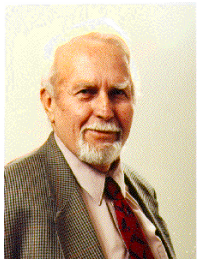
How could FEM be forgotten in the original list? No need to tell the readers of IACM Expressions how central in CM FEM is. It is often claimed that FEM is the single most important invention in computational engineering. FEM can be described as a general method for the approximate solution of partial differential equations based on a variational (or a weak) formulation.

The method was originally devised by the famous applied mathematician R. Courant in 1943 [1], but was totally ignored (mainly because of lack of computers back then) until it was reinvented by engineers in 1956. One of the pioneers was R.W. Clough, who also coined the term 'finite elements' [2]. Other recognized early developers include O.C. Zienkiewicz and J. Argyris. See, e.g., the historical accounts by Oden [3] and Zienkiewicz [4].

R. Courant



J. Argyris



O.C. Zienkiewicz

Closely related to FEM is the *Boundary Element Method (BEM)* which was developed much later, and combined known integral equation techniques and FEM ideas. The first work using BEM in its modern form can be traced back to a seminal paper by T.A. Cruse and F.J. Rizzo in 1968 [5]. See also the historical account by Rizzo [6].

2. Iterative Linear Algebraic Solvers

Almost every single numerical method in CM involves the solution of a linear algebraic system, $\boldsymbol{Ax} = \boldsymbol{b}$. It is well known that direct solution methods like Gaussian Elimination are effective only for small and moderately-large systems, whereas very large systems (say, of dimension larger than 10,000) must be solved iteratively. Since CM very often leads to

very large algebraic systems of equations, iterative linear solvers are extremely important in this domain. Effective iterative schemes exploit the special structure of the matrix $\boldsymbol{A}$, such as symmetry and sparseness.

Iterative methods for the solution of $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ started to appear in 1950, with the invention of the method of *Krylov spaces* and the method of *Conjugate Gradients* by Hestenes and Stiefel [7] for symmetric matrices. Since then these methods have been improved significantly, and many new iterative methods have been invented, such as *GMRES* by Saad and Shultz (1986) [8] for non-symmetric matrices, which is widely used today in CM applications.

3. Algebraic Eigenvalue Solvers

Both the standard eigenvalue problem $\boldsymbol{K}\boldsymbol{d} = \lambda\boldsymbol{d}$ and the generalized eigenvalue problem $\boldsymbol{K}\boldsymbol{d} = \lambda\boldsymbol{M}\boldsymbol{d}$ occur often in CM, e.g., in free vibration or buckling analyses. Often the matrices $\boldsymbol{K}$ and $\boldsymbol{M}$ are large and sparse.

A powerful method that solves both types of problems has been devised in 1950 by *Lanczos* [9]. About ten years later, J.G.F. Francis has developed the now well-known *QR algorithm* for computing eigenvalues [10]. During the 60's and 70's the QR method has dominated the field, because in contrast to the Lanczos method which was invented to compute a few extreme eigenpairs, the QR method finds all the eigenvalues of a reasonably small matrix almost as fast as a few. However, in the 80's, when large eigenvalue problems started to attract attention in CM, the Lanczos algorithm has had a glorious "come-back" because it is particularly appropriate for such problems, and enables the efficient computation of a small portion of the eigenmodes.

C. Lanczos

4. Matrix Decomposition Methods

Many algebraic solution techniques (for both linear-system solvers and linear-eigenvalue solvers) in use today are heavily based on matrix decomposition (or factorization), namely on the ability to express a matrix as a product of simpler matrices. The simpler matrices may be diagonal, triangular, symmetric, skew-symmetric, orthogonal, etc. In the context

of CM, the decomposition often has a physical meaning as well. Examples include spectral decomposition and polar decomposition.

The pioneer in this area is *Householder* that has shown, in a sequence of papers starting in 1951, why matrix decomposition is very useful and has developed factorization algorithms. The most accessible reference on this work is Householder's book from 1964 [11].

A. Householder

5. Finite Difference Methods for Wave Problems

In the early days of CM, systems of ordinary differential equations emanating from (hyperbolic) wave problems were solved by the classical Euler time-integration techniques. However, in the late 50's the CM community realized that special methods developed directly for wave problems were in need.

Two early time-integration methods that are still commonly used today are the family of schemes developed by *Newmark* in 1959 [12] for structural dynamics, and the *Lax-Wendroff* scheme devised in 1960 [13] for the solution of 1st-order hyperbolic systems. Later many other schemes were proposed, with some improved properties. We mention for example the *Hilber-Hughes-Taylor* scheme from 1978 with improved numerical dissipation.

One important issue that arises in the computational solution of hyperbolic and parabolic-hyperbolic problems is that of discontinuity capturing, and especially capturing of shock waves. The classical finite difference methods could not resolve discontinuities properly. S.K. Godunov was the first to recognize the difficulty and in 1959 proposed, for problems in fluid dynamics, the now well-known *Godunov* scheme [14]. This opened the way to various *upwinding* and *flux-splitting* schemes proposed by van Leer (1974, 1982), Steger and Warming (1979), Roe (1980) and others, which can be found today in many of the modern production codes. Related methods have been developed in the context of the Finite Volume Method and FEM as well.

6. Nonlinear Algebraic Solvers

Most problems in CM are nonlinear. Discretization in space and time leads to a nonlinear system of algebraic equations. When large-scale problems have started to be considered it

was realized that classical nonlinear solvers, like Bisection, Secant or even Newton are either not powerful enough or are inefficient.

One important family of improved solvers is that of *Quasi Newton (QN)* schemes. The first QN method was suggested by Davidon in 1959 [15], and was later publicized and improved by Fletcher and Powell. A QN method which became famous is the *BFGS* scheme which was developed in 1970 independently by each of Broyden, Fletcher, Goldfarb and Shanno. A totally different approach to nonlinear problems with nonlinearity of a non-monotone nature is represented by *Arclength* methods (called 'continuation methods' by mathematicians). The first Arclength methods in the context of CM were proposed by G.A. Wempner (1971) [16] and E. Riks (1972) [17].

7. Fast Fourier Transform (FFT)

Spectral methods in CM often rely on the discrete Fourier transform. The most important step in this context is the calculation of the first N Fourier coefficients of a function when its values at N points are given. A straight forward calculation of the Fourier coefficients requires $O(N^2)$ floating-point operations. The FFT is an algorithm for doing this calculation with only $O(N \log N)$ operations.

The FFT method was invented in 1965 [18] by J.W. Cooley from IBM and J.W. Tukey from Princeton University and AT&T Bell Labs. The method had an immediate enormous impact on signal processing, but its contribution to CM and other branches of computational science is very important as well.

J. Tukey

8. Nonlinear Programming

The Simplex method appearing in the Dongarra-Sullivan list is a very well-known algorithm, invented by G. Dantzig, for linear programming, namely for optimization problems with linear objective function and linear inequality constraints. However, most optimization problems encountered in CM are associated with *nonlinear* objective functionals. On the discrete level, the simplest problems of this type are *Quadratic Programming (QP)* problems, with quadratic objective function and linear constraints. Such problems arise in various fields

of CM, including elastic contact and plasticity. This class of problems is very important also because the solution of more complicated problems can be approached by considering a sequence of QP problems.

Early work on Nonlinear Programming is due to Goldfarb (1969) [19], Murtagh and Sargent (1969) [20], McCormick (1970), Fletcher (1971) and Murray (1971). Methods for large scale optimization (variations of which are used today in some optimization packages) are due to Griffith and Stewart (1961) and Murtagh and Saunders (1978).

9. Soft Computing Methods

Traditionally, CM has been based on 'rigorous' classical mathematical procedures that draw on PDE theory, theoretical mechanics, numerical analysis, functional analysis, etc. However, since the early 80's new families of computational methods, which are sometimes collectively termed "soft computing" methods, have been applied. These types of schemes are based on a heuristic approach rather than on rigorous mathematics and draw on concepts of Artificial Intelligence (AI). Despite the fact that these methods were initially received with suspicion, they have turned out in many cases to be surprisingly powerful, and their use in various areas of CM keeps increasing. The three main techniques that had an important impact on CM are *Neural Networks*, *Genetic Algorithms* and *Fuzzy Logic*. All three types of methods can be thought of as general optimization techniques, but they are based on totally different methodologies.

Traces of soft computing ideas can be found already in the 40's. Pioneers include McCulloch and Pitts in Neural Networks, Holland in Genetic Algorithms and Zadeh in Fuzzy Logic — although some claim that Fuzzy Logic was invented by Buddha! In the 60's and 70's the area was advanced by computer scientists, but only since the early 80's application of soft computing methods in CM have started to appear. See, e.g., the books [21, 22] and the review paper [23].

Buddha

10. Multiscale Methods

Many problems in CM involve more than one length scale. Moreover, in some cases the different length scales interact with each other in a complicated way. This may occur in two levels: the physical level, where the phenomenon under consideration involves both a micro scale and a macro scale (two examples are aeroacoustics and fracture mechanics), and the numerical level, where poor resolution in one scale causes the deterioration of accuracy in another scale. Methods that address these issues are collectively called Multiscale Methods.

One famous multiscale technique is the *Multigrid* method which can be thought of as an iterative linear algebraic solver requiring only $O(N)$ operations. The chief inventor is A. Brandt, in 1977 [24]. Another approach is that of *Wavelets*, which, like simple sines and cosines, constitute building blocks of general functions, but are local and have special translation and dilation properties which allow them to resolve different scales. Wavelets have origins already in 1909 (in the thesis of A. Haar) but were formulated in the way familiar today in 1985 and later, by each of S. Mallat [25], Y. Meyer and I. Daubechies.

Research in Multiscale Methods is still very dynamic. To end with a futuristic note, let us mention, in the context of FEM, the very recent Variational Multiscale method proposed by T.J.R. Hughes [26], the Partition of Unity Method of J.M. Melenk and I. Babuška [27], and the Hierarchical Modeling approach of J.T. Oden's group [28]. All these methods are very promising but are still evolving and only time will tell what impression they will leave on CM.

T.J.R. Hughes

I. Babuška

J.T. Oden

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