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Parallel Software for Nonlinear Systems of Equations

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Mathematical background for homotopy algorithms.

The nonlinear systems of equations arising in circuit simulation, structural optimization, closed loop optimal control, chemical engineering of distillation systems, combustion chemistry, CAD/CAM modelling, robotics, computer vision, and orbital mechanics have several properties that make them especially amenable to homotopy methods. Even so, the homotopy zero curves are not trivial to track, and sophisticated curve tracking techniques are sometimes required. The size of typical engineering problems also presents some interesting numerical linear algebra challenges, and the supported work has been geared toward developing parallel sparse matrix techniques specifically tailored to the sparsity structures corresponding to the mentioned problem areas, in the context of homotopy algorithms.

The original mathematical model, after some sort of discretization, approximation, or reduction, ultimately leads to a nonlinear system of equations

$$F(x) = 0,$$

where $F : E^n \to E^n$ is assumed to be a C^2 map. Suppose there exists a C^2 map

$$\rho : E^m \times [0,1) \times E^n \to E^n$$

such that

1) the $n \times (m+1+n)$ Jacobian matrix $D\rho(a,\lambda,x)$ has rank n on the set

$$\rho^{-1}(0) = \{(a,\lambda,x) \mid a \in E^m, 0 \le \lambda < 1, x \in E^n, \rho(a,\lambda,x) = 0\},$$

and for any fixed $a \in E^m$, letting $\rho_a(\lambda,x) = \rho(a,\lambda,x)$,

2) $\rho_a(0,x) = 0$ has a unique solution x_0,

3) $\rho_a(1,x) = F(x)$,

4) $\rho_a^{-1}(0)$ is bounded.

Then the supporting theory says that for almost all $a \in E^m$ there exists a zero curve γ of ρ_a, along which the Jacobian matrix $D\rho_a$ has rank n, emanating from $(0,x_0)$ and reaching a zero $\bar{x}$ of F at $\lambda = 1$. γ does not intersect itself and is disjoint from any other zeros of ρ_a. The globally convergent algorithm is to pick $a \in E^m$ (which uniquely determines x_0), and then track the homotopy zero curve γ.

There are many different algorithms for tracking the zero curve γ; the previous proposal discussed three such algorithms: ordinary differential equation based, normal flow, and augmented Jacobian matrix. The descriptions of these algorithms are now in the literature for the software package HOMPACK, so will not be repeated here. The development of sparse homotopy algorithms within HOMPACK specifically tailored for various parallel machines (e.g., distributed memory, shared memory, and vector) and problem areas (e.g., circuit simulation, structural optimization, optimal control, and combustion chemistry) was the central theme of this research.

Accomplishments under DOE Grant DE-FG05-88ER25068.

The most recent annual report, DOE/ER/25068-4, for this project summarized the accomplishments through February, 1995, and provided a historical perspective on progress on the various project tasks. At that point in time, DOE support had contributed to over 60 theses, refereed conference papers, and refereed journal papers. Rather than recapitulate that annual report, this section will simply list publications since the beginning of the current funding period, March 1, 1995. These are:

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Conversion of HOMPACK to FORTRAN 90.

The entire HOMPACK package has been redone in FORTRAN 90, taking full advantage of high level array operations, automatic arrays, pointers, and dynamic memory allocation. Along with this conversion, various improvements to the HOMPACK algorithms were incorporated. For example, a new end game (see the ACM TOMS paper by Sosonkina cited above) has been added, and new, more general, data structures and preconditioners are being employed in the sparse codes. This conversion to FORTRAN 90 was a major undertaking, requiring several years, but the improvement in readability, portability, and ease of use was spectacular.

Some users of HOMPACK have suggested that HOMPACK be redone using the reverse call protocol. Many users of mathematical software are unfamiliar with reverse call, nor is it the consensus preference of computer scientists. Therefore, the FORTRAN 90 version of HOMPACK still uses forward calling (FORTRAN 90 modules obviate most of the advantages of reverse calling, anyway), but several "expert" routines using reverse call were added. STEPNX is a reverse call stepping subroutine, designed to be used in lieu of any of the six stepping routines STEPDF, STEPNF, STEPQF, STEPDS, STEPNS, or STEPQS. STEPNX returns to the caller for all linear algebra, all function and derivative values, and can deal gracefully with situations such as the function being undefined at the requested steplength.

The ODE-based (D), normal flow (N), and quasi-Newton augmented Jacobian matrix (Q) routines provide complete algorithmic "coverage," but the D and Q routines are rarely used in practice, because the N routines are usually (but not always!) more efficient. Whether the Jacobian matrix is sparse or dense is the expert user's problem—hence only one expert reverse call routine, STEPNX, is needed.

ROOTNX provides an expert reverse call end game routine. ROOTNX has the same protocol as STEPNX, and generalizes the ROOT* routines by finding a point on the zero curve where $g(\lambda, x) = 0$, as opposed to just the point where $\lambda = 1$. Thus ROOTNX can find turning points, bifurcation points, and other "special" points along the zero curve. The combination of STEPNX and ROOTNX will provide considerable flexibility for an expert user.

Nonlinear systems with large, sparse Jacobian matrices.

Among all the Krylov subspace methods for solving a linear system $Ax = b$ with a nonsymmetric invertible coefficient matrix A, the generalized minimal residual algorithm (GMRES) and the quasi-minimal residual algorithm (QMR) are considered the most robust. Similar to the classical conjugate gradient method, GMRES produces approximate solutions x_k which are characterized by a minimization property over the Krylov subspaces span$\{r_0, Ar_0, A^2r_0, \ldots, A^{(k-1)}r_0\}$, where $r_0 = ||b - Ax_0||$ and k is the iteration number. However, unlike the conjugate gradient algorithm, the work and memory required by GMRES grow proportionately to the iteration number. In practice, the restarted version GMRES(k) is used, where the algorithm is restarted every k iterations until the residual norm is small enough. The restarted version may stagnate and never reach the solution.

QMR reduces the computational effort by employing a short-term recursion for building the Lanczos basis. An implementation of QMR based on the look-ahead Lanczos process avoids breakdowns associated with Lanczos-type algorithms. However, a QMR iterate is a relaxed version of a minimal residual iterate, which results in more iterations than GMRES(k) (that may or may not take more time than GMRES(k)). The QMR algorithm may also behave erratically.

The essence of the adaptive GMRES strategy in HOMPACK90 is to adapt the parameter k to the problem, similar in spirit to how a variable order ODE algorithm tunes the order k.

With FORTRAN 90, which provides pointers and dynamic memory management, dealing with the variable storage requirements implied by varying k is not too difficult. k can be both increased and decreased—an increase-only strategy is described below.

Though GMRES(k) cannot break down, it can stagnate. A test of stagnation developed by H. Walker detects an insufficient residual norm reduction in the restart number (k) of steps. Precisely, GMRES(k) is declared to have stagnated and the iteration is aborted if at the rate of progress over the last restart cycle of steps, the residual norm tolerance cannot be met in some large multiple (*bgv*) of the remaining number of steps allowed (*itmax* is a bound on the number of steps permitted). Slow progress of GMRES(k), which indicates an increase in the restart value k is needed, may be detected with a similar test. The near-stagnation test uses a different, smaller multiple (*smv*) of the remaining allowed number of steps. If near-stagnation occurs, the restart value k is incremented by some value m and the *same* restart cycle continues. Restarting would mean repeating the nonproductive iterations that previously resulted in stagnation, at least in the case of complete stagnation (no residual reduction at all). Such incrementing is used whenever needed if the restart value k is less than some maximum value *kmax*. When the maximum value for k is reached, adaptive GMRES(k) proceeds as GMRES(*kmax*).

Pseudo code for an adaptive GMRES(k) is:

choose $x, tol, itmax, kmax, m$;

$r := b - Ax$; $\quad itno := 0$;

while $\|r\| > tol$ **do**

begin

$r^{old} := r$; $\quad v_1 := r/\|r\|$; $\quad j := 0$;

A: $\quad j := j + 1$;

$itno := itno + 1$;

for $i = 1$ **step** 1 **until** j **do** $h_{i,j} := (Av_j, v_i)$;

$$\tilde{v}_{j+1} := Av_j - \sum_{i=1}^{j} h_{i,j} v_i;$$

$h_{j+1,j} := \|\tilde{v}_{j+1}\|$;

$v_{j+1} := \tilde{v}_{j+1} \;/\; h_{j+1,j}$;

Update $\|r\|$;

if $\|r\| \leqq tol$ **then goto** B

if $j < k$ **then goto** A

$test := k \times \log[tol/\|r\|] \;/\; \log\left[\|r\|/((1.0+\epsilon)\|r^{old}\|)\right]$;

if $k \leqq kmax - m$ **and** $test \geqq smv \times (itmax - itno)$ **then**

begin

$k := k + m$;

goto A

end

elseif $k \geqq kmax$ **and** $test \geqq bgv \times (itmax - itno)$ **then**

Abort

end if

B: $e_1 := (1, 0, \ldots, 0)^T$;

Solve $\min_y \left\| \|r\|e_1 - \bar{H}_j y \right\|$ for y_j;

$V_j := [v_1, \ldots, v_j]$; $\quad x := x + V_j y_j$; $\quad r := b - Ax$

end

In practice, the modified Gram-Schmidt process is used for the construction of an orthogonal basis of the Krylov subspace. Some numerical experience has been obtained on sequences of linear systems arising from the application of homotopy algorithms to circuit design and simulation problems. The sparse matrices involved in circuit problems are nonsymmetric, indefinite, and unstructured. Following the conclusions of the PIs' earlier work, ILU(0) (right) preconditioning is used, the initial vector x is zero, and $itmax = 5n$.

For five circuit problems from McQuain, Melville, Ribbens, and Watson (cited above), the table shows the minimum, maximum, and average number of iterations along the homotopy zero curve, and the CPU time in seconds for the algorithms. The notation for the algorithms is: AGILU—adaptive GMRES(k) preconditioned with ILU(0) (for AGILU the table also shows the largest k reached); GILU—GMRES(k) preconditioned with ILU(0); FGILU—flexible GMRES(k), each iteration of which is preconditioned with one restart cycle of GMRES(k)/ILU(0); QMR—three-term recursion QMR. An asterisk indicates failure to converge.

Problem		rli13b, $n = 31$	ups01a, $n = 59$	bgatt, $n = 125$	is7a, $n = 468$	is7b, $n = 1854$
AGILU	min	1	6	32	178	1178
$m = 2$	max	72	130	245	1004	5656
	avg	14.58	35.56	104.14	355	3643
	time	0.23	0.22	0.66	3.14	161.61
	max k	6	6	9	15	48
AGILU	min	1	6	32	178	704
$m = 4$	max	50	55	124	1004	3383
	avg	11.75	20.48	82.00	355	2497.80
	time	0.19	0.14	0.53	3.17	111.73
	max k	6	6	9	15	48
AGILU	min	1	6	32	178	558
$m = 6$	max	50	55	120	1004	4344
	avg	10.6	17.76	74.50	355	2732.20
	time	0.17	0.12	0.48	3.13	124.05
	max k	6	6	11	15	50
GILU	min	*	*	*	178	*
	max	*	*	*	1004	*
	avg	*	*	*	355	*
	time	*	*	*	3.15	*
FGILU	min	*	*	35	86	66
	max	*	*	124	205	126
	avg	*	*	85.29	113.40	95.6
	time	*	*	1.95	3.60	209.38
QMR	min	1	8	24	70	*
	max	12	15	27	91	*
	avg	7.08	10.48	25.14	76.20	*
	time	1.21	0.84	2.12	7.76	*

The values of k (2, 2, 5, 15, 20, respectively) for the problems are chosen to compare AGILU with GILU when: (1) GMRES(k) does not exhibit near stagnation behavior (is7a); (2) near stagnation is detected for *some* matrices (rli13b, ups01a, bgatt); (3) near stagnation causes an increase in k for *all* the matrices (is7b). In the first case, AGILU and GILU perform the same. In the second case, GILU stagnates on the matrices where AGILU increases the restart value and then converges. No final solution is reached by GILU in the third case.

The optimal choice of increment values is an open question. The table shows that even a small increment in the restart value may lead to the convergence. However, if an increment is too small, an increase occurs more than once, the cost of which is, often, one extra restart cycle executed. If m is too large, for large problems (is7b), the cost of the last few added iterations becomes significant and may degrade the performance.

It is clear from the data presented that AGILU outperforms both FGILU and QMR. Contributors to the poor performance of the QMR algorithm are a significant overhead, and two matrix-vector products per iteration as opposed to one in AGILU. The failure of the QMR algorithm on problem is7b is due to the sensitivity of the QMR algorithm to starting points; for some starting vectors, QMR converges. Whenever FGILU converges, it requires more work per iteration than AGILU, since a new GMRES(k)/ILU(0) preconditioner is computed in each iteration of GMRES(k). Other variations of FGILU also appear very expensive in the context of homotopy algorithms.