FIRST YEAR ANNUAL PERFORMANCE REPORT
DOE Grant DE-FG02-94ER25199
"Linear, Non-Modal Phenomena in Numerical Analysis and Applied Mathematics"

Start date: 2/15/94

Lloyd N. Trefethen
Department of Computer Science
Cornell University
14 November 1994

1. Summary

I have completed the first nine months of research supported by this grant. This report reviews the accomplishments of that period and outlines plans for the future. With this document I request continuation funding for a second year of support, beginning 2/15/95, as envisioned in the original grant.

My research group, supported jointly by this grant and by an NSF grant of roughly the same size, consists of myself, occasional visitors, and currently six PhD students: Toby Driscoll, Jeff Baggett, Kim-chuan Toh, David Bau, Divakar Viswanath, and Jing Huang. Thanks in part to DOE support, this is a lively group with much research activity and a good group spirit.

It seems that our work is achieving considerable visibility. In fluid mechanics, the "non-normal" approach to questions of hydrodynamic stability, which we have advocated together with various others such as Farrell and Henningson [1,4,8], seems in just two years to have moved from being a radical view to being nearly mainstream. Another gratifying sign is that the word "pseudospectra" is beginning to appear in titles of papers by authors unrelated to my group [2,3,6,9,10].

2. Accomplishments during first year

The theme of our research is phenomena related to non-normal matrices and operators. Our main areas of investigation of these phenomena are numerical linear algebra, numerical solution of differential equations, fluid mechanics, and other general and miscellaneous topics. In the grant proposal, I listed 37 possible projects in these areas that we might pursue, emphasizing that I did not expect to make progress on all of them. This list is reproduced on the next page.

During the past nine months, we have made progress on six of these topics, indicated by asterisks in the list.

DISCLAIMER

List of possible research projects from original grant proposal

$*$ = project on which progress has been made; see text

NUMERICAL LINEAR ALGEBRA

* (1) Pseudospectra and Arnoldi/GMRES lemniscates
* (2) Is the GMRES envelope attained? (and related questions from [α])
(3) Ghosts and rounding errors in Lanczos and Arnoldi
(4) Upwind-downwind effects in Gauss-Seidel and SOR
(5) New ideas on nonsymmetric matrix iterations
(6) The Pade-Lanczos connection; expansion of the resolvent at infinity
(7) Polynomial and rational approximation of matrix functions

NUMERICAL DIFFERENTIAL EQUATIONS

(8) More on pseudospectra of spectral methods
(9) Pseudospectra of 1D wave problem with absorbing boundary condition
(10) The accuracy-stability tradeoff ("quantitative CFL")
(11) Convergence of pseudospectra of discretizations
(12) Local Fourier analysis, multigrid, transient effects
(13) Boundary conditions for PDEs (GKS, Beam & Warming,...)
(14) Papkovitch-Fadle operator

FLUID MECHANICS

* (15) Full pseudospectra for pipe Poiseuille flow
(16) Why are streamwise vortices so prevalent in fluid flows?
* (17) Threshold exponent for transition to turbulence
(18) Why secondary instability theory is misleading

GENERAL THEORY

* (19) To what extent do pseudospectra determine behavior?
(20) Nilpotent operators and growth of the resolvent at infinity
(21) Fill the gap in the Kreiss matrix theorem
(22) Non-convex generalization of the numerical range
(23) Density effects; average vs. worst case effects
(24) Geometric questions: what pseudospectra are possible?

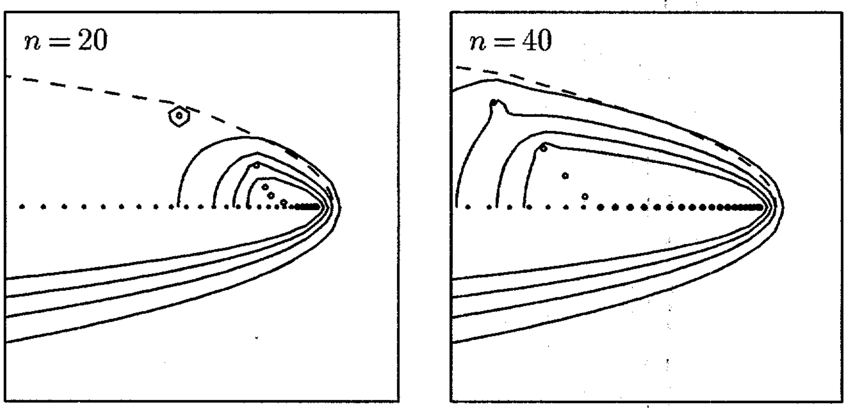
MISCELLANEOUS

* (25) Pseudospectra of random matrices
(26) POD, KLT, SVD, coherent structures, inertial manifolds
(27) History of spectra and physics of pseudospectra
(28) Non-normality and chaos (Lorenz, Henon,...)
(29) The 2x2 nonlinear model of [11] <--> Takens-Bogdanov bifurcation
(30) Connections with scattering theory
(31) Landau damping
(32) Detuning of oscillators and mode localization
(33) Beating, diffusion of a delta pulse, and other normal effects
(34) Complex analysis: pseudo-singularities, extrapolation, crowding
(35) Pseudospectra of interpolation operators
(36) Connections with potential theory, balayage, Stahl, Saff, etc.
(37) Find new physical applications!

(1) Pseudospectra and Arnoldi/GMRES lemniscates

Experiments make it clear that when matrix iterations are applied to certain highly nonnormal matrices, the behavior of the iteration is related in some way to the pseudospectra of the matrix. In [7] we observed that the pseudospectra might be approximated by the lemniscates of the iteration polynomial, and the grant proposal listed this topic for further investigation. During the past year we carried out such an investigation, and found that a perhaps more useful connection is simply between the pseudospectra of A and those of its Hessenberg projections, as computed by an Arnoldi iteration. A similar observation has been considered by Ruhe [10].

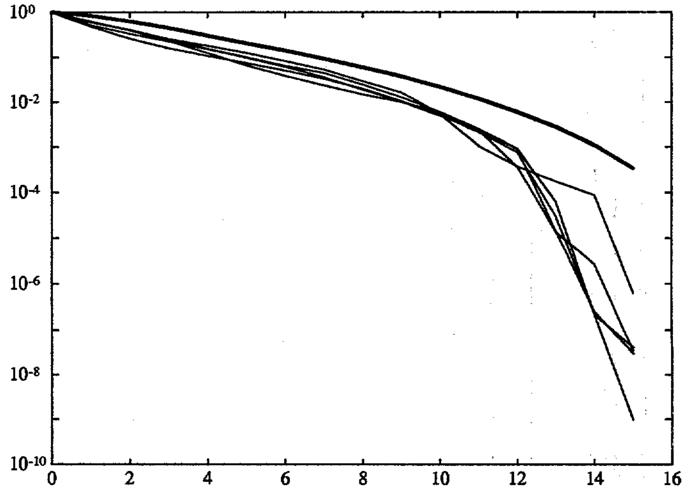
The figure below illustrates the phenomenon in question. The matrix being studied a 100×100 Chebyshev spectral approximation to a univariate convection-diffusion operator with Péclet number 40, as in [β]. In each of the two parts of the figure, the lower half represents the exact ϵ-pseudospectra sought ($\epsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}$) and the upper half represents the same ϵ-pseudospectra of a Hessenberg approximation H_n obtained after n steps of an inverse-Arnoldi iteration (i.e., the Arnoldi iteration applied to A^{-1}).



The approximation of $\Lambda_\epsilon(A)$ by $\Lambda_\epsilon(H_n)$ in figures likes these is impressive. For some practical applications, this phenomenon could speed up calculations enormously when the matrices are large. Kim-chuan Toh and I explored this possibility mainly experimentally, and report our findings in [γ].

(2) Is the GMRES envelope attained?

In [α], Greenbaum and I investigated "ideal Arnoldi" and "ideal GMRES" problems related to minimizing $\|p(A)\|$ over classes of polynomials p. The true Arnoldi or GMRES iterations, by contrast, actually minimize $\|p(A)\,q\|$, where q is an initial vector which we might as well consider to be normalized by $\|q\| = 1$. Thus the ideal iteration provides an upper bound for the true iteration, one which is conceptually simpler since it depends on only a matrix rather than a matrix and a vector. The figure below, from [α], illustrates this relationship for a certain 16×16 example. The upper curve shows the convergence of an ideal GMRES iteration for this matrix, and the lower, lighter curves show convergence of true GMRES iterations for five randomly chosen initial vectors.

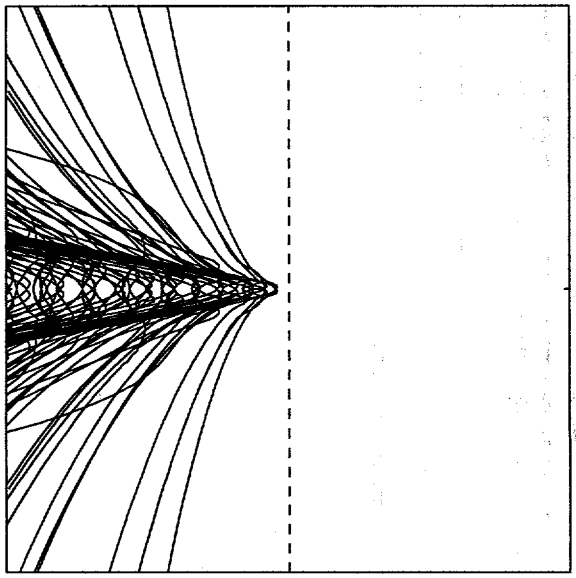


We conjectured in [α] that for any GMRES iteration, "the envelope is attained" in the sense that for every iteration number n, there is an initial vector q whose corresponding step-n GMRES residual norm $\|p(A)q\|$ matches the matrix norm $\|p(A)\|$ for the ideal GMRES polynomial. Last year, in work not yet published, Faber and Joubert and Knill and Manteuffel constructed an example that showed that our conjecture was false. In their example, the ratio of the two critical quantities is greater than 0.9999! That made for a puzzling situation indeed, suggesting almost that their example might be an artifact of rounding errors (though it wasn't).

Recently, Kim-chuan Toh and I have found a much simpler counterexample than that of Faber, et al., which leads to a much more convincing ratio of less than 0.95. This new example is so simple that we hope we can build upon it in later work and thereby obtain improved insight into the general problem of convergence of nonsymmetric matrix iterations. We have not yet written up this work for publication.

(15) Full pseudospectra for pipe Poiseuille flow

In the proposal, I proposed to carry out large-scale computations to determine spectra and pseudospectra for the problem of stability of pipe Poiseuille flow (flow in a pipe), to carry forward to the pipe problem the kind of computations we reported for flows in channels in [11]. About half of this work has now been done. Using IBM and Intel parallel machines, my wife Anne Trefethen and I have now determined spectra and pseudospectra for this problem at several Reynolds numbers. These are large computations, and a typical result looks like this:



This figure represents the spectrum of the linearized pipe Poiseuille flow operator at Reynolds number $R = 3000$—a collection of curves in the left half of the complex plane.

Besides their visual appeal, these results have immediate implications for stability of these flows and transition to turbulence. Since the spectrum is in the left half-plane, the flow is technically stable. However, the pseudospectra of the same operator (not shown) extend substantially into the right half-plane, implying that initial perturbations may be greatly amplified by a linar mechanism. This is just what we expected to find, and provides further evidence of the non-modal nature of transition to turbulence under real laboratory conditions.

A preliminary report on this work has been prepared [G], but we need to do much more before submitting it for publication.

(17) Threshold exponent for transition to turbulence

Among the most exciting developments of this year has been continued work by Jeff Baggett, Toby Driscoll, and myself and the problem of transition to turbulence of canonical shear flows such as flow in a pipe. In [11], we suggested a simple 2×2 matrix model of the transition process, making the claim that although of course it did not match the Navier-Stokes equations in any detail, it nontheless retained some important features of subcritical transition. In particular, we made two conjectures: that the amplitude of perturbations required to trigger transition decreases faster than inverse linearly with the Reynolds number R, a phenomenon we called "bootstrapping"; and that the transition process could be understood qualitatively by viewing the nonlinear terms in the

Navier-Stokes equations as arbitrary, even random, rather than analyzing them in detail.

The first of these conjectures, regarding threshold exponents, seems to have been borne out by computational work of Reddy, Henningson and others. This is ongoing work, however, and nobody yet has a good idea of what the exponent is, aside from the fact that it seems to be less than -1, as we conjectured.

Our new development is on the second matter, the study of nonlinear terms as "random" energy mixers. This past summer, Baggett, Driscoll and I took this idea a step further, moving to a 3×3 model and investigating truly random nonlinear perturbations. We found that in our model, close to 100% of all randomly chosen nonlinear mixing terms led to a dynamical process analogous to transition to turbulence. Moreover, bootstrapping occurred in all of these cases, and the early stages of the "transition" process were largely independent of whether the ultimate "turbulent" state was a finite fixed point, a fixed point at infinity, a limit cycle, or chaos. Related observations have been made simultaneously and independently by Gebhard and Grossmann [5]. Our own work has been written up as [B] and already accepted for publication.

(19) To what extent do pseudospectra determine behavior?

This is a large topic, where I have many more unanswered questions than firm answers. However, one nice development occurred this year in collaboration with my student Jeff Baggett. He investigated the question of when the spectrum of a Hilbert space operator A does, or does not, determine the asymptotic behavior of $\|\exp(tA)\|$ as $t\to\infty$. There is a theorem by Prüss that answers this question, which we realized can be viewed as a condition on pseudospectra: the asymptotic growth or decay rate of $\|\exp(tA)\|$ is equal not to the spectral abscissa of A, but to the limit as $\epsilon\to 0$ of the ϵ-pseudospectral abscissas.

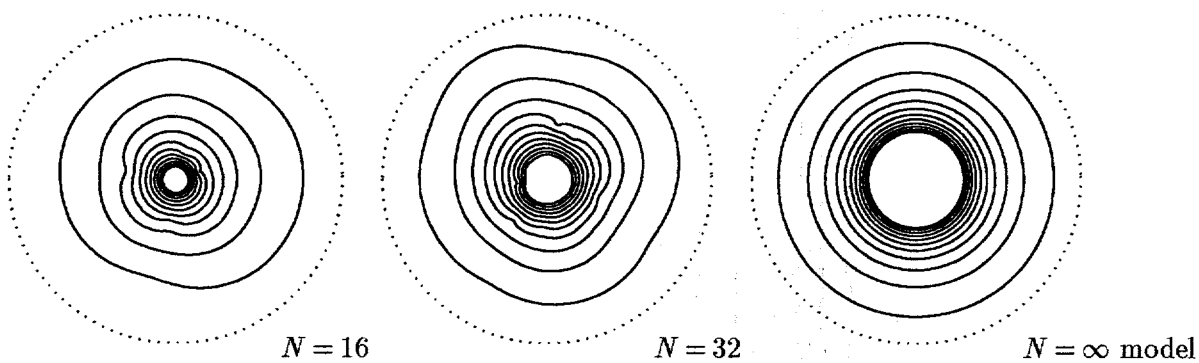
This much is known mathematics, though not as well known as it should be. What is new is that Baggett was able, through large-scale calculations, to compute the numbers to visualize this result in the case of the original example of such phenomena introduced by Hille and Phillips in the 1950s. He also treated a more elementary subsequent example due to Zabczyk. The result is a beautiful paper [A] which I hope will convey eloquently that geometric intuition can be applied to resolve what look like deeps mathematical problem. Potential applications are by no means just in pure mathematics; the distinction between the spectral abscissa and the "growth abscissa" arises in convection-diffusion processes, in hydrodynamic stability problems, and possibly in dynamos such as those that create the magnetic fields of the stars and planets.

(25) Pseudospectra of random matrices

This is a favorite, admittedly not very applied topic of mine on which, unexpectedly, I made some progress during the past year. A central question is, why do random triangular matrices have such huge inverses? Since the eigenvalues are not small, this is a matter of non-normality, and easily demonstrated by experiments. Recently, I realized that this problem can be analyzed by means of random recurrence relations. This leads to a back-of-the-envelope estimate for the norm of the resolvent of a strictly lower-triangular matrix L with random elements from the complex normal distribution of standard deviation $N^{-1/2}$:

$$\|(zI-L)^{-1}\| \approx |z|^{-2}e^{|z|^{-2}/2}.$$

The plots below compare this model to the pseudospectra of randomly selected matrices of dimensions 16 and 32. (In each plot we have $\epsilon = 10^{-2}, 10^{-3}, \ldots, 10^{-12}$, and the dotted curve is the circle about the origin of radius 1/2.) The agreement is good enough that it seems quite possible that the formula above is valid in the limit $N \to \infty$. So far, I have not worked out all the details or written a paper on this subject.



(–) Schwarz-Christoffel conformal mapping.

Finally, I mention a topic unrelated to non-normality and not included in the grant proposal, on which we have made exciting progress. In the 1980s, I produced a Fortran package SCPACK for computing Schwarz-Christoffel conformal maps of polygons. In the past year, my student Toby Driscoll put a large amount of time into writing a similar package for Matlab, which is a better environment for such calculations because it combines high-quality numerics with built-in graphics. Driscoll produced a "Schwarz-Christoffel Toolbox" that goes far beyond what I achieved in Fortran. It has many features not included in SCPACK, both interactive and mathematical, illustrating nicely how far programming environments have advanced in the last decade. Driscoll's work is described in [D] and [E], and the software is available electronically (`driscoll@cam.cornell.edu`). Judging by my own experience with SCPACK, this is a product that will find many users in the upcoming years.

3. Plans for second year

I will not give details about plans for the second year, as they have not changed significantly since the proposal was written. Ongoing work related to fluid mechanics is certainly a high priority, as well as work related to nonsymmetric matrix iterations. Our team is moving along at a good clip these days, and I anticipate an exciting year ahead.

4. Papers written in 1994

[A] Jeffrey S. Baggett, *Pseudospectra of an operator of Hille and Phillips,* IPS Rep. 94-15, Interdisciplinary Project Center for Supercomputing, Swiss Federal Inst. of Tech., Zurich, July, 1994, and SIAM J. Math. Anal., submitted.

[B] Jeffrey S. Baggett, Tobin A. Driscoll, and Lloyd N. Trefethen, *A mostly linear model of transition to turbulence,* IPS Rep. 94-17, Interdisciplinary Project Center for Supercomputing, Swiss Federal Inst. of Tech., Zurich, August, 1994, and and Phys. Fluids A, to appear.

[C] David Bau, *Faster SVD for matrices with small m/n,* TR 94-1414, Dept. of Comp. Sci., Cornell U., March, 1994, and SIAM J. Sci. Comp., submitted.

[D] Tobin A. Driscoll, *Schwarz-Christoffel Toolbox User's Guide,* TR 94-1422, Dept. of Comp. Sci., Cornell U., May, 1994.

[E] Tobin A. Driscoll, *A MATLAB toolbox for Schwarz-Christoffel mapping,* IPS Rep. 94-14, Interdisciplinary Project Center for Supercomputing, Swiss Federal Inst. of Tech., Zurich, July, 1994, and and ACM Trans. Math. Software, submitted.

[F] Kim-chuan Toh and Lloyd N. Trefethen, Calculation of pseudospectra by the Arnoldi iteration, Rep. CTC94TR179, Advanced Computing Res. Inst., Cornell U., May, 1994 and SIAM J. Sci. Comp., submitted.

[G] Anne E. Trefethen, Lloyd N. Trefethen, and Peter J. Schmid, *Spectra and pseudospectra for pipe Poiseuille flow,* IPS Rep. 94-16, Interdisciplinary Project Center for Supercomputing, Swiss Federal Inst. of Tech., Zurich, August, 1994.

5. Papers that appeared in 1994

[α] Anne Greenbaum and Lloyd N. Trefethen, *GMRES/CR and Arnoldi/Lanczos as matrix approximation problems,* SIAM J. Sci. Comput. 15 (1994), 359–368.

[β] Satish C. Reddy and Lloyd N. Trefethen, *Pseudospectra of the convection-diffusion operator,* SIAM J. Appl. Math., to appear in Dec. 1994.

[γ] Kim-chuan Toh and Lloyd N. Trefethen, *Pseudozeros of polynomials and pseudospectra of companion matrices,* Numerische Math. 68 (1994), 403–425.

[δ] Elias Wegert and Lloyd N. Trefethen, *From the Buffon needle problem to the Kreiss Matrix theorem,* Amer. Math. Monthly 101 (1994), 132–139.

6. Other references

[1] L. Boberg and U. Brosa, *Onset of turbulence in a pipe,* Zeit. Naturforschung 43a (1988), 697–726.

[2] D. Borba, et al., *The pseudospectrum of the resistive magnetohydrodynamics operator: resolving the resistive Alfvén paradox,* Phys. Plasmas 1 (1994), 3151–3160.

[3] Albrecht Böttcher, *Pseudospectra and singular values of large convolution operators,* J. Int. Eqs. Applics., to appear.

[4] Kathryn M. Butler and Brian F. Farrell, *Three-dimensional optimal perturbations in viscous shear flow,* Phys. Fluids A 4 (1992), 1637–1650.

[5] Thomas Gebhardt and Siegfried Grossmann, *Chaos transition despite linear stability,* Phys. Rev. D, to appear.

[6] S. H. Lui, Computation of pseudospectra by continuation, draft report, Dept. of Math., U. Science and Tech., Hong Kong, 1994.

[7] Noël M. Nachtigal, Lothar Reichel, and Lloyd N. Trefethen, *A hybrid GMRES algorithm for nonsymmetric linear systems,* SIAM J. Matrix Anal. Applics. 13 (1992), 796–825.

[8] Satish C. Reddy and Dan S. Henningson, *Energy growth in viscous channel flows,* J. Fluid Mech. 252 (1993), 209–238.

[9] Kurt S. Riedel, *Generalized epsilon-pseudospectra,* SIAM J. Numer. Anal. 31 (1994), 1219–1225.

[10] Axel Ruhe, *Showing the resolvent norms (pseudospectra) of large matrix pencils using the Rational Krylov algorithm,* talk delivered at Householder Symposium on Linear Algebra, Lake Arrowhead, California, July, 1993.

[11] Lloyd N. Trefethen, Anne E. Trefethen, Satish C. Reddy, and Tobin A. Driscoll, *Hydrodynamic stability without eigenvalues,* Science 261 (1993), 578–584.

preprints removed. ds