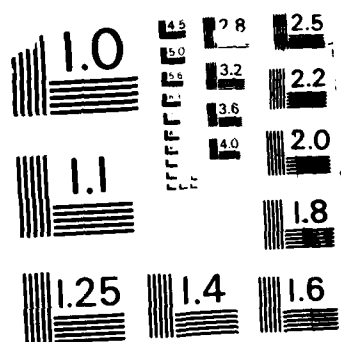AD-A177 171   COMPUTATIONAL FLUID DYNAMICS(U) PITTSBURGH UNIV PA INST   1/1
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Interim Technical Report

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Period: 1 June 1984 through 31 May 1986

Title: Computational Fluid Dynamics

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A. ACCOMPLISHMENTS TO DATE

The following is a brief summary of accomplishments to date under Grant AFOSR-84-0131.

1. The Reduced Basis Method for Algebraic Systems

1.1 Subspace-Projector Pairings. Implementation of the reduced basis method requires the choice of a subspace and a projector onto that subspace. For an arbitrarily chosen subspace-projector pair, existence of the true solution curve is not sufficient to guarantee the existence of the corresponding reduced basis solution curve. However, when the former curve exists, it has been shown in [A1] that there are infinitely many subspace-projector pairings, each utilizing an arbitrarily selected subspace, under which the reduced basis solution curve exists. Moreover, the resulting error estimates are of the same nature as those that apply in the more familiar case when a subspace is paired with its orthogonal projector.

1.2 Reduced Basis Additive Correction Methods. Additive Correction Methods have been considered by a number of authors as a means of accelerating slowly converging iterative processes (see, for example, [A2]-[A4]). Furthermore, it has been recognized that additive correction is central to the basic idea of multigrid methods [A4-A5]. Although the reduced basis method in its original form appears to have little in common with additive correction, a class of such methods has been developed using the reduced basis concept [1]. Furthermore, it has been shown that in their "two-grid" form, certain multigrid

methods are special cases of this class. The reduced basis point of view provides insight into the error reduction capabili, of such multigrid methods and suggests additive correction variants that may be more effective than those commonly employed in multigrid methods.

2. The Reduced Basis Method for Systems of Differential Equations

Error Estimates for the reduced basis method solution of differential and differential-algebraic equation systems are contained in the thesis [2]. These estimates are local in the following two senses. First, they apply on a nontrivial, but possibly very small interval. Second, they require some point of the reduced curve to lie on the true solution curve. The recent research reported in [18] has removed the interval length restriction in the differential equation case and extended the error analysis to global versions of the methods in [2], thus effectively eliminating the second local aspect of that work. Furthermore, this work also incorporates the effects of the errors resulting from the numerical integration of the reduced basis ODE systems.

3. Two-Fluid, Two-Phase Flow

Additional theoretical results on the nature of the void fraction have been incorporated into [A6] resulting in the revision [3].

4. Binary Gas Mixture Flow Through Combustors

In an attempt to reduce the development cycle costs associated with design of gas turbine engine combustors, mathematical combustor models are

being employed to provide information about performance trends and to predict velocity, pressure and thermodynamic property profiles in simulated practical combustion environments. It has been demonstrated that the dual variable method can be applied to the predictive model of the fluid dynamics associated with an axially symmetric centerbody combustor being studied at WPAFB. This work appeared in [4].

5. Error Estimation and Singularities

The central theme of this project concerns the discretization error for general nonlinear, parameter-dependent equations of the form $F(z,\lambda) = 0$ where F is a nonlinear mapping, z is the state variable representing the solution, and λ is a vector of parameters that characterize intrinsic properties of the system or extrinsic quantities influencing its behavior. In the case of fluid problems, the operator F may be generated, for example, by the time-independent Navier Stokes equations together with the necessary boundary conditions.

In general, the solution set of such parametrized equations constitutes a differentiable manifold of dimension equal to that of the parameter space. While this fact is, of course, well known, we appear to have been the first who have been using this fact as the basis for a consistent study of the numerical problems for these equations. Our results have begun to show clearly the value and power of this geometric approach.

For numerical considerations, an important aspect of this theory concerns the estimation of the "distance" between the manifolds defined by a given differential equation and by its discretization, respectively. This has been the

topic of a series of papers by J. P. Fink and W. C. Rheinboldt with partial support under this grant. See the earlier articles [A7], [A8] and then [6] and [16]. In particular, in the last-named paper [16] we have been the first to analyze the case of multi-dimensional manifolds which is of increasing importance in applications.

An essential aspect of these studies concerns the question as to the exact definition of the error between a solution manifold and its approximation. Obviously, the error depends on which points are to be compared. In the cited papers it was shown that this correspondence between the points on the two manifolds has to be defined by appropriate local coordinate systems. In other words, the resulting error is controlled by the choice of the local coordinate system, and, since the error measure must be physically meaningful, not all local coordinate systems are equally desirable. This question becomes particularly acute in the vicinity of singular points where the behavior of the solutions may be subject to change.

This connection between the choice of the local coordinate systems and the singularity behavior of a point has led us to a closer study of admissible coordinate systems at foldpoints. But the results in the papers [5] and [7] also suggested that the open questions about the proper choice of the coordinate system for physically meaningful error measures requires a much closer look at the characterization of foldpoints on manifolds and at the methods for their computations. This is the topic of the next subsection.

6. Detection and Computation of Singularities

In addition to its application to error estimation, singularity theory is also being used to develop methods for the detection and computation of

singular points on the solution manifold of a nonlinear parameter-dependent equation $F(z,\lambda) = 0$.

As noted in the previous subsection, the solution set of a parametrized equation $F(z,\lambda) = 0$ represents, in general, a differentiable manifold in the combined space of the state variable and the parameter vector. This requires a regularity assumption which is not very restrictive in applications, but which -- from the viewpoint of singularity theory -- implies the use of suitable "unfoldings". In most practical problems a host of very natural unfoldings suggest themselves. The particular choice of unfolding parameters affects the location and type of the resulting fold-points on the manifold and with it also the questions raised in the previous subsection.

In the past years, our work in this area concentrated first on the computation of foldpoints by means of one of the many possible forms of augmented equations. One approach in this direction was the use of the tangent map of differential geometry which was exploited in the already mentioned papers [5] and [7] and led there to a geometrically instructive and coordinate free treatment of fold points, in general.

But these results also pointed, once again, at the need for a more detailed study of the geometrical aspects of the singular points. In [21] it was shown that it is possible to reformulate in our setting some of the basic results of bifurcation theory related to computational aspects. The availability of solution manifolds opens up the various tools of differential geometry and provides a very natural framework for the desired reformulation of the theory. In particular, the bifurcation sets appear as cuts of the solution manifold. This, in turn, corresponds again to the consideration of augmented equations and hence, our new theory, does provide indeed a new

approach to the vexing problem of the properties of the numerous augumentation considered in the literature. In [21] the results were already used to analyze a particularly promising augmentation for the computation of an entire class of fold points. This work is now continuing. Some further results on this topic were presented in [19].

The general computational problem in this area is, of course, the determination of the principal characteristic features of the solution manifold of the given parametrized equation. This includes, in particular, the computation of the foldpoints, but covers also other features. The principal methods used today for analyzing such manifolds are the continuation methods. But before any such method can be applied in the case of a multi-dimensional manifold, the parameter dimension has to be reduced to one. Geometrically, such a reduction is equivalent with a restriction to some path on the manifold of the original equation. A continuation method then computes a sequence of points along such a path. Clearly, in general, it is not easy to develop a good picture of a p-dimensional manifold from information along one-dimensional paths. Thus, it is not surprising that there is growing interest in computational methods which generate multi-dimensional grids of solution points covering an entire portion of the manifold. In [22] a new method for this purpose was presented. It allows for the computation of the vertices of a simplicial triangulation of a p-dimensional solution manifold of a parametrized equation. An essential part of the method is a constructive algorithm for computing moving frames; that is, of orthonormal bases of the tangent spaces that vary smoothly with their points of contact. The triangulation algorithm uses these bases, together with a chord form of the Gauss-Newton process as corrector, to compute the desired vertices. The Jacobian matrix of the mapping is not required at all the vertices but only at the centers of certain local

"triangulation patches". Numerical experiments have already shown that the method is very efficient, even around singularities. This opens up new possibilities for determining the form and special features of such solution manifolds.

7. Finite Element Formulation of the Streamfunction-Vorticity Equations

The Navier-Stokes equations can be written in primitive variable formulation, in terms of the streamfunction as a fourth order problem or as two second order equations in the streamfunction-vorticity formulation. In the linear case the fourth order problem for the streamfunction is the well-known biharmonic equation. Although the primitive variable formulation has received the most attention, the streamfunction-vorticity formulation is also of considerable interest in two dimensional domains. That is partly due to the fact that only two, as opposed to three, fields are to be computed; but it is mainly due to the fact that the incompressibility constraint is avoided through the introduction of the streamfunction.

Several theoretical and practical issues arising in the finite element approximation of the streamfunction-vorticity equations have been studied. Initially error estimates for the linear problem were investigated. Since the velocity is expressed in terms of the derivatives of the streamfunction, it is of practical concern to ascertain if these derivatives are optimally approximated for choices of elements. Previous analyses concerning this problem were improved upon and the optimality of the error verified in [A10].

Other issues arising in the finite element approximation of the streamfunction and vorticity include computations in multiply connected domains, the use of low order elements, the incorporation of a variety of boundary

conditions into the weak formulation, estimates for the errors in the finite approximations for the nonlinear problem and the recovery of the primitive variables. A preliminary report on computations in multiply connected domains using low continuity finite element spaces was presented in [11]. A comprehensive report dealing with all of the theoretical and practical issues mentioned above as well as presenting numerical examples is given in [12].

8. A Finite Element Analysis of MHD Flow

The equations governing the steady flow of incompressible electrically conducting fluids in the presence of a given magnetic field can be expressed as

$$- \frac{1}{n^2} \Delta \underline{u} + \frac{1}{N} (\underline{u}\nabla \underline{u}) + \nabla\phi - (\underline{B}\times\nabla\phi) - (\underline{u}\times\underline{B}\times\underline{B}) = 0$$

$$-\Delta\phi + \text{div}(\underline{u}\times\underline{B}) = 0$$

$$\text{div } \underline{u} = 0$$

where $\underline{u}$ is the velocity, p the pressure, ϕ the electric potential, $\underline{B}$ the magnetic field and N,M given dimensionless parameters. By rewriting certain terms using vector identities and using appropriate spaces, one can obtain a weak formulation for this problem that is similar to one for the Navier-Stokes equations written in terms of primitive variables (see [A11]). The purpose of using such a weak formulation is to take advantage of the results already proved in [A11]. Specifically, the weak formulation is to find $\underline{u} = (\underline{u},\phi) \in \underline{W}$, $p \in L_o^2$ such that

$$a(\underline{u},\underline{v}) + a_1(\underline{u},\underline{u},\underline{v}) + b(\underline{v},p) = (f,\underline{v}) \quad \text{for all } \underline{v} \in \underline{W}$$

$$b(\underline{u}, \chi) = 0 \qquad \text{for all} \quad \chi \in L_o^2$$

where

$$a(\underline{u}, \underline{v}) \quad = \frac{1}{n^2} \int \nabla \underline{u} : \nabla \underline{v} + \int \{\nabla \phi - (\underline{u} \times \underline{B})\}\{\nabla \psi - (\underline{v} \times \underline{B})\}$$

$$a_1(\underline{u}, \underline{u}, \underline{v}) = \frac{1}{2N} \int \{\underline{u} \nabla \ \underline{u}\underline{v} - u \nabla \ vu\}$$

$$b(\underline{v}, \chi) \quad = -\int \chi \ \text{div} \ \underline{v}$$

and $\underline{W} = \underline{H}_o^1 \times \underline{H}_o^1$, $L_o^2 = \{\phi \in L^2: \int_\Omega \phi = 0\}$.

The continuity and stability conditions necessary to guarantee existence and uniqueness of the solution of the weak problem have been proved. In addition, an error estimate for the finite element approximation of the weak problem has been obtained. These results, as well as a discussion of an iterative method for solving the discrete problem will be presented in [13].

9. Dual Variable Transformations

The dual variable method, originally developed in the context of finite difference discretizations of transient incompressible Navier-Stokes equations [A9], is a technique to considerably reduce the size of the linear system to be solved at each time step. The method involves

(1)   the determination of the rank of the discrete divergence operator, A,

(2)   the determination of a basis for the null space of A, and

(3)   the calculation of a particular solution of the discrete continuity equation.

In [8] a finite element implementation of the dual variable method is

presented using quadrilateral piecewise bilinear velocity/constant pressure elements. Algorithms for the determination of a basis for the null space of the discrete divergence operator and a particular solution are presented.

In [9] a finite difference discretization of the Navier-Stokes equations describing a compressible flow problem is viewed as a system defining flows on an associated network. This observation then provides a means of applying the dual variable method to economize on their numerical solution.

The nature of the aerodynamics in and around such structures as cavities and deflectors or spoilers on various aircraft configurations was investigated using the dual variable method [10].

A summary of the dual variable method is given in [14].

Iterative methods are under investigation for the solution of the linearized finite difference discretizations involved in the dual variable method. The generic form of dual variable system suggests a splitting in which a Stieltjes matrix is to be solved at each step. The method has been implemented for two dimensional domains and convergence properties are being investigated as part of a Ph.D. thesis.

10. Fluid Flow on Curved Domains

A finite difference scheme was derived for two-dimensional, transient, incompressible Navier-Stokes problems in which the flow domain Ω is a bounded simply-connected region for which there exists a C^2 invertible mapping τ onto the unit square:

$$\tau : \Omega \to S = [0,1] \times [0,1]$$

The <u>transformed</u> Navier-Stokes problem is

$$\text{div } \underline{\phi} = \phi_{i,r_i} = 0$$

$$v_{i,t} + \frac{\phi_j}{|J|} v_{i,r_j} = -p_{r_j}r_{j,x_i} + \frac{\mu}{|J|} (\beta_{jk}v_{k,r_k})_{r_j} + f_i \quad i = 1,2$$

subject to initial condition

$$\underline{v}(\underline{r},0) = \underline{a}(\underline{x}(\underline{r})) \ , \ \underline{r} \in S$$

and boundary condition

$$\underline{v}(\underline{r},t) = \underline{0} \ , \ \underline{r} \in \partial S \text{ and } t > 0 \ ,$$

where, $\underline{v}(\underline{r},t)$ is velocity, p is pressure, the Jacobian matrix

$$J = [x_{i,r_j}],$$

$$[\beta_{ij}] = |J|J^{-1}(J^{-1})^T$$

$$\underline{\phi} = |J|J^{-1}\underline{v} \ .$$

The finite difference discretization of the above equations is proven to be unconditionally stable and convergent. They also reduce to the well known Krzhivitski and Ladyzhenskaya scheme [A12] for rectangular domains, e.g., r the identity. This work was the subject of a Ph.D. Dissertation [A13] and a recent technical report [17].

11. <u>Equilibrium Manifolds in Computational Mechanics</u>

Equilibrium problems arise naturally in continuum and fluid mechanics as a set of nonlinear equations of the form

$$\underline{F}(\underline{z},\underline{\lambda}) = 0 \tag{1}$$

where $\underline{z}$ is from the state space Z and $\underline{\lambda}$ is from a p dimensional parameter space. In general, F represents some boundary value problem and hence the state space Z is infinite dimensional. Let $X = Z \times \Lambda$ be the combined space, then the set of solutions to (1) in $D \subset X$,

$$M = \{(\underline{z}, \underline{\lambda}) \in D \mid F(\underline{z}, \underline{\lambda}) = 0\} \tag{2}$$

defines a surface or manifold of dimension p in X. M is called the equilibrium manifold.

The parameters $\underline{\lambda}$ and states $\underline{z}$ may also be required to satisfy a differential equation of the form

$$A(\underline{x})\dot{\underline{x}} = \underline{G}(\underline{x}) \tag{3}$$

where $\underline{x} = (\underline{z}, \underline{\lambda})$. We then interpret (3) as a differential equation on the manifold (2), DEM for short. Equations (1) and (3) together,

$$\begin{cases} F(\underline{x}) = 0 \\ A(\underline{x})\dot{\underline{x}} = \underline{G}(\underline{x}) \end{cases}$$

form what is called a differential-algebraic equation (DAE).

Two applications of interest to the investigators in which DEM's occur are:

(i) Incompressible Fluid Flow. The continuity equation is an algebraic constraint of the form (1) and the time-dependent Navier-Stokes equations are the differential equation.

(ii) Punch Stretching of Sheet Metal. The principle of virtual work provides a force equilibrium equation which defines an equilibrium manifold upon which one seeks solutions to differential constitutive laws of the form (3).

In [20], a new numerical method was presented for computer simulations of punch stretching of sheet metal. Most current approaches to finite element modeling of large deformation, elastic-plastic sheet metal forming use a rate form of the equilibrium equations and then must correct at each time step to insure that equilibrium is satisfied. Such methods are referred to as incremental methods. The new method, a DEM approach discretizes the more fundamental equilibrium equations in non-rate form and insures equilibrium of forces at each time step. Formulating the problem as a DEM or DAF also allowed for solution of the discretized system using off-the-shelf software such as LSODI. Numerical experimentation indicated that the DEM approach was computationally much more efficient than the incremental approach.

12. Energy Stability of Viscous Incompressible Flows

The problem of determining sufficient conditions for the flow of a viscous incompressible fluid to be stable under arbitrary disturbances was examined. This problem is of importance in the study of turbulence and the transition which occupies a region of space and subject to a prescribed velocity distribution on the boundary, will alter radically or only slightly in nature if it is perturbed at some instance.

The question of stability can be addressed by either standard linear perturbation techniques or by the energy method; the latter is chosen in this work. Although the great majority of stability calculations use linear stability analysis, the method has the drawback that it allows only perturbations which are infinitesimal in magnitude. This rules out perturbations of finite size and hence cannot give accurate information in many cases. The energy method allows arbitrary disturbances but its shortcoming is that the

disturbances do not necessarily satisfy the Navier-Stokes equations, and thus the stability criterion will be more restrictive than in the actual physical situation. However, the energy stability analysis is based on the Navier-Stokes equations and is nonlinear in nature due to the fact that no linearizations of the equations are done. The method is mathematically rigorous and does give insight into the physical situation.

The question of energy stability of a flow can be formulated as a linear generalized partial differential eigenvalue problem even though the analysis is based on the nonlinear Navier-Stokes equations. Essentially, the procedure is to obtain an equation for dK/dt where K is the kinetic energy of the disturbance, $\underline{u}$, and then to determine conditions which guarantee that the kinetic energy tends to zero as time increases. Using standard eigenvalue problem where stability is governed by the dominant eigenvalue. Specifically, we have that the flow is stable for Reynolds number less than $1/\lambda$ where λ is the dominant eigenvalue of the problem

$$\Delta \underline{u} - \text{grad } \phi = \lambda \underline{u} \ D$$

$$\text{div } \underline{u} = 0 \ , \tag{1}$$

$$\underline{u} = 0 \text{ on the boundary } .$$

Here D is the deformation tensor of the unperturbed flow.

A finite element method is used to approximate the dominant eigenvalue of (1). In particular, the weak form considered is to find nonzero $\underline{u} \in \underline{H}_o^1$, $\phi \in L^2$ and $\lambda \in R$ such that

$$\int \nabla \underline{u} : \nabla \underline{v} + \int \phi \text{ div } \underline{v} = \lambda \int \underline{u} D \underline{v} \quad \text{for all } \underline{v} \in \underline{H}_o^1$$
$$\int \chi \text{div } \underline{u} = 0 \qquad \text{for all } \chi \in L^2 \tag{2}$$

where L^2 is the space of all functions which are square integrable and $\underline{H}^1$, $\underline{H}^1_o$ denote the usual Sobolev spaces. To approximate the solution to the weak problem (2), finite dimensional subspaces $\underline{V}^h \subset \underline{H}^1_o$ and $W^h \subset L^2$ are chosen which depend upon a parameter $0 < h < 1$ tending to zero. The approximate problem is defined analogous to (2) where the solution is sought in the finite dimensional subspaces. Once bases for $\underline{V}^h$ and W^h are chosen, the approximate problem is equivalent to an algebraic generalized eigenvalue problem. An estimate for the error in λ and its Galerkin approximation is given in [A14].

As proposed, a code was developed which uses a mixed finite element method for approximating the dominant eigenvalue of (1). The program was used to determine a range of Reynolds numbers for which the flow is guaranteed to be stable for the examples of plane shear flow and Poisseuille flow.

The first example is the simple case of flow in a channel of width $0 < y < d$ where the initial velocity is given by the vector $(ky, 0)$, the deformation tensor is given by $D_{ij} = 0$ $i = j$ and $D_{ij} = .5k$ for $i \neq j$, $i, j = 1, 2$ the Reynolds number is kd^2/λ. The channel is assumed infinite in length. The computed Reynolds number for a channel of length L is given below.

1/L	1	1/2	1/3	1/4	1/5
Re No.	289.87	201.42	186.975	182.11	180.01

Using the above calculations the extrapolated value at $1/L = 0$ is 177.4 which is in good agreement with the value of 177 published by Orr.

The second problem of determining the stability of Poiseuille flow in a pipe is of more interest physically and has been studied by many authors. For this example the formulation (1) makes sense in an unbounded domain when the

solutions are single-valued in θ and periodic in z. To this end, the solution is assumed of the form $\underline{u}(r,\theta,z) = \underline{U}(r,\alpha,\beta)\ e^{i(dZ + \beta\theta)}$ where β is an integer. This form is substituted into (1) and the following system results

$$Lu - i\left[\frac{2\beta}{r^2}v\right] - \phi_r = -\lambda rw$$

$$Lv + i(2\beta/r^2\ u - \beta/r\phi) = 0$$

$$\hat{L}w - i\alpha\phi = -\lambda ru$$

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) + i\left(\frac{\beta}{r}v + dw\right) = 0$$

$$u,v,w \text{ bounded at } r = 0$$

$$u = v = w = 0 \text{ at } r = 1$$

where $\underline{U} = (u,v,w)$, $Lu = \frac{1}{r}\frac{\partial}{\partial r}(ru) - \left[\frac{\beta^2+1}{r^2} + \alpha^2\right]u$, $\hat{L}u = Lu + u/r^2$.

Note that these equations form a complex one-point boundary value problem with a singularity at the origin. The weak formulation must incorporate an appropriate boundary condition for the velocity at $r = 0$. The particular weak from considered is the following: Find $u,v,w \epsilon H_1$, $\phi \epsilon H_2$, $\lambda \epsilon R$ such that

$$\begin{cases} \int u_r\xi_r r\ dr + \int C_1\frac{u}{r}\xi dr + i\int \frac{2\beta}{r}v\xi dr - \int\phi\frac{\partial}{\partial r}(r\xi)dr = \lambda\int w\xi r^2 dr \quad \forall\ \xi\ \epsilon\ H_1 \quad \cdots \\[2mm] \int v_r\xi_r rdr + \int C_1\frac{v}{r}\xi dr - i\int\frac{2\beta}{4}u\xi dr + i\int\beta\phi\xi dr = 0 \quad\quad \forall\ \xi\ \epsilon\ H_1 \\[2mm] \int w_r\xi_r rdr + \int C_2\frac{w}{r}\xi dr + i\alpha\int\phi\xi rdr = \lambda\int u\xi r^2 dr \quad \forall\ \xi\ \epsilon\ H_1 \\[2mm] -\int\frac{\partial}{\partial r}(ru)\chi dr - i\int\beta v\chi dr - i\int\alpha w\chi rdr = 0 \quad\quad \forall\ \chi\ \epsilon\ H_2 \\[2mm] \text{where } C_1 = \beta^2 + 1 + \alpha^2 r^2\ ,\ C_2 = C_1 - 1 \end{cases}$$

for appropriate spaces H_1 and H_2.

With this weak formulation the condition imposed on the velocity at $r = 0$ is $ru_r = rv_r = rw_r = 0$, which is a natural boundary condition. This problem was discretized using piecewise linear elements. The results obtained agree with those of Joseph and Carmi [A15]. However, their numerical calculations were unnecessarily complicated. For example, different techniques for the various cases such as $\alpha = 0$ and $\alpha \neq 0$ had to be employed as well as using Frobenius series as starting values near the origin. Specifically, the value of 81.5 was obtained as a sure limit of stability and corresponded to the case $\alpha = 1$, $\beta = 1$. This agreed with Joseph and Carmi's result and confirmed the fact that the value of $R = 180$, which was previously believed to be a sure limit of stability, is incorrect. This work is discussed in a paper in preparation [23].

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