CALCULATION OF SENSITIVITY TO PARAMETERS
IN SINGLE–PHASE NATURAL CIRCULATION FLOWS USING ADIFOR

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ABSTRACT

An automatic technique to get the sensitivity of a margin to instability in natural circulation flows with respect to physical and discretization parameters has been developed. It is based on the use of a tool for the automatic differentiation of FORTRAN codes. ADIFOR was the tool adopted to get the derivatives of model variables with respect to model parameters. In this paper, we present an alternative, simpler, procedure to the authors' previous analysis. It is based in obtaining the Jacobeans derivatives automatically. This procedure gives results coincident with the previous ones, allowing for obtaining the desired sensitivities in a somewhat complex problem. It is worth pointing out that the procedure is general enough and may also be applied to other problems.

INTRODUCTION

In previous work by the authors (e.g. [1]-[8]), it was shown how a methodology of analysis based on numerical discretization of partial differential equations governing fluid-dynamic problems might be useful to get information on the capabilities of numerical methods in accurately predicting stability. A key point of this methodology is the evaluation of Jacobean matrices of the algebraic relationships that characterize the numerical method and the related boundary conditions. It is in this perspective that the use of automatic code differentiation tools may play an interesting role.

The sensitivity of stability results to physical and discretization parameters is analyzed using a tool for the automatic differentiation of FORTRAN codes. This is due, needless to say, because FORTRAN is the programming language in use for thermal-hydraulic system codes. ADIFOR (meaning Automatic DIfferentiation of FORtran) [9] is the adopted tool that allows for evaluating the derivatives of model variables with respect to model parameters. Related bibliography may be found at the ADIFOR WWW site [10]. Some introductory examples may also be found in the WWW (see for example [11]-[12]).

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It will only be mentioned here that ADIFOR is a pre-processor code which, given a FORTRAN 77 code that computes a function, automatically generates another, augmented, FORTRAN 77 code. It must be considered that any code may be put in the form of a function, simply by introducing a call to a main routine after setting parameter values. The latter computes the function and the derivatives with respect to a list of variables. The user must specify the list of dependent and independent variables. After generating the augmented code that calculates the specified derivatives via ADIFOR, the user must provide a new driving FORTRAN 77 code that takes into account the new set of variables. Some hints to help on the very first use of ADIFOR may be readily found in [10]-[12]. Many references document the accuracy of the derivatives calculated in this way. This is neither the only way to apply ADIFOR, nor ADIFOR is the only tool: the reader is referred to the aforementioned literature.

We are now interested in showing the sensitivity of the neutral stability boundary to nodalization and system parameters in natural circulation flows. The results reported here deal with the pioneering work Welander [13], because the stability properties of this prototypical problem have been the subject of the above-mentioned analytical and theoretical studies.

ALGORITHM

This paragraph presents an alternative procedure to the one presented by the authors in [4] for the calculation of the margin to neutral stability ($\Delta\rho$) sensitivity to system parameters. In what follows the analysis leading to its definition will be sketched.

A finite-difference procedure may be written as

$$\mathbf{F}\left(\mathbf{y}^{n+1}, \mathbf{y}^{n}, \mathbf{p}\right) = 0 \tag{1}$$

where $\mathbf{y}$ is the vector of nodal unknowns, $\mathbf{p}$ the vector of parameters, n is the time step number such that $t^{n+1} = t^n + \Delta t^n$

Steady-state conditions for a given set of parameters satisfy the relationship:

$$\mathbf{F}\left(\mathbf{y}^{s}, \mathbf{y}^{s}, \mathbf{p}\right) = 0 \tag{2}$$

By assuming small perturbations around steady-state:

$$\mathbf{y}^n = \mathbf{y}^s + d\mathbf{y}^n \qquad\qquad \mathbf{y}^{n+1} = \mathbf{y}^s + d\mathbf{y}^{n+1} \tag{3}$$

Introducing this in (1) and expanding up to the 1st order:

$$\mathbf{F}\left(\mathbf{y}^{n+1}, \mathbf{y}^{n}, \mathbf{p}\right) = \mathbf{F}\left(\mathbf{y}^{s}, \mathbf{y}^{s}, \mathbf{p}\right) + \left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^n}\right|^{s} \delta\mathbf{y}^n + \left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n+1}}\right|^{s} \delta\mathbf{y}^{n+1} + \ldots = 0 \tag{4}$$

then, using (2) and (4), it is

$$\left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^n}\right|^{s} \delta\mathbf{y}^n + \left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n+1}}\right|^{s} \delta\mathbf{y}^{n+1} = 0 \tag{5}$$

and, finally:

$$\delta\mathbf{y}^{n+1} = -\left[\left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n+1}}\right|^{s}\right]^{-1} \cdot \left[\left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^n}\right|^{s}\right] \cdot \delta\mathbf{y}^n \tag{6}$$

Then, in the adopted notation:

$$\mathbf{A} = -\left[\left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^{n+1}}\right|^{s}\right]^{-1} \cdot \left[\left.\frac{\partial \mathbf{F}}{\partial \mathbf{y}^n}\right|^{s}\right] \tag{7}$$

The value of $\Delta\rho$ given by:

$$\Delta\rho = \rho(\mathbf{A}) - 1 \tag{8}$$

where $\rho(A)$ is the spectral radius of the matrix A. As told before, $\Delta\rho$ is used as a measure of the margin in excess to neutral stability and to quantify the degree of damping or amplification. It takes negative values for stable conditions and positive ones for unstable conditions.

The calculation of the sensitivity of $\Delta\rho$ to parameters is based on the following approach:
- Define A and A^T, respectively as the matrix relating perturbations at time steps n and n+1 and its transpose. This matrix may be specified using ADIFOR. However, second order derivation to get derivatives of A with respect to p_i is beyond the objective of this paper. Consequently, A will be specified analytically.
- Use of ADIFOR to automatically calculate the derivative of A with respect to system parameters
- Calculation of the eigenvalues of A, λ_i, and its eigenvectors, x.
- Calculation of the eigenvectors of A^T, v.
- Determination of the eigenvalue corresponding to the spectral radius of A, λ_i, and the corresponding eigenvectors of A and A^T.
- Calculation of the sensitivity of λ_i with respect to system parameters.
- Calculation of the spectral radius sensitivity with respect to system parameters.

In what follows, the above-mentioned steps will be expanded, specifying some details of the different procedures.

1 Calculation of A and its transpose

The algebraic expressions leading to A come from the standard Finite-difference method. The analysis was performed using the volumetric flow rate and the temperature as system variables. It is focused on the results obtained using the implicit coupling of the momentum and energy equations and the forward time, upwind-space finite-difference method (FTUS) for the momentum equation. It may be argued that the consequences of using this approximation on the results are well known, i.e. obtaining a first order accurate solution in the space and time increments. What is not too evident is the quantification of these effects (and those of the coupling) on the stability limits in systems working in the natural circulation flow regime.

It must be emphasized that this algorithm is general. No particular assumptions are made with respect to A, except being real, that is always the case in finite-differences models in Fluid Dynamics. Parameters are considered to be independent of time in this analysis; however, this condition may be released at the price of feasible, more laborious analysis. Given A, its transpose is also determined.

2 Use of ADIFOR to automatically calculate the derivatives of A

ADIFOR 2.0D has been used to generate the augmented FORTRAN code to calculate the derivatives of A with respect to system parameters. In a general system, there are several parameters p_k. In this paper, only two scalar parameters, namely C_{0U}, the cell Courant number ($\equiv Q.\Delta t/\Delta s$)=0.8 and ξ =1.75 ($\equiv 2-\theta$, where θ is the exponent in the friction law), will be considered. A is a real matrix, non-symmetrical and almost sparse. However, the momentum equation is a full row, relating node temperatures, flow-rate and heat transfer boundary conditions.

3 Calculation of the eigenvalues of A, λ_i, and its eigenvectors, x

The vector of complex eigenvalues of A has been obtained using the classical EISPACK routines in their complex variable version. It may be argued that A is real, but to avoid problems of de-packing complex eigenvalues, the complex version was the adopted package. Simultaneously, the complete set of eigenvectors, x, was calculated.

4 Calculation of the eigenvectors of A^T, v

In order to calculate the eigenvectors of A^T, it was necessary to perform once again the complete calculation of eigenvalues + eigenvectors, since no path in EISPACK (and LAPACK also) is available

-to authors' knowledge- to perform the simultaneous calculation for a matrix and its transpose. It did not pose problems in practice, because convergence of calculations was quite fast.

5 Determination of the eigenvalue corresponding to the spectral radius of A, λ_i, and the corresponding eigenvectors of A and A^T

The calculation of the spectral radius of A is quite obvious: it was a simple search for the maximum modulus of the eigenvalues vector. The interest of this search is also finding the index of the eigenvalue, denoted by i. The corresponding eigenvector, x_i, was found by simple correspondence of index. The corresponding eigenvector of A^T was found by an *ad hoc* routine performing the scalar product of the eigenvectors of A and those of A^T. It used the well-known property of their eigenvectors, namely:

$$x_i \cdot v_j = 0 \quad \text{if} \quad \lambda_i \neq \lambda_j$$

This procedure was needed because the eigenvalues of A^T are not necessarily calculated in the same order as those of A. In this way, computing the scalar products and letting the zero to almost machine precision, the corresponding eigenvector of A^T has been found without any trouble.

6 Calculation of the sensitivity of λ_i with respect to system parameters

This sensitivity is measured by the derivative of λ_i with respect to system parameters. It may be obtained from the following expression [14]:

$$\frac{\partial \lambda_i}{\partial p_k} = \frac{\partial \Re(\lambda_i)}{\partial p_k} + i \frac{\partial \Im(\lambda_i)}{\partial p_k} = \Re_{\partial_k} + i \cdot \Im_{\partial_k} = \frac{\left(\frac{\partial A}{\partial p_k} x_i, v_i \right)}{(x_i, v_i)}$$

where $\Re(\lambda_i)$ and $\Im(\lambda_i)$ are the real and imaginary part of the eigenvalue corresponding to the spectral radius, $\Re_{\partial_k}$ and $\Im_{\partial_k}$ are the real and imaginary part of the derivative of λ_i with respect to the k-th parameter and *(a, b)* indicates the scalar product between complex vectors. This formula may be deduced by application of the chain rule of derivation to the definition of the eigenvalue problem and a suitable permutation coming from the definition of the left eigenvalue problem. It constitutes a faster alternative to the direct calculation of $\Re_{\partial_k}$ and $\Im_{\partial_k}$ by automatic differentiation of the program calculating the eigenvalue. The latter was the approach adopted by the Authors in previous work [4].

7 Calculation of the sensitivity of the spectral radius with respect to system parameters

The sensitivity of the spectral radius of A (coincident with the sensitivity of the margin to instability) is calculated from:

$$\frac{\partial \Delta \rho}{\partial p_k} = \frac{\partial \rho(A)}{\partial p_k} = \frac{\Re(\lambda_i) \cdot \Re_{\partial_k} + \Im(\lambda_i) \cdot \Im_{\partial_k}}{\sqrt{\Re^2(\lambda_i) + \Im^2(\lambda_i)}}$$

This expression comes from the definition of the spectral radius and considering that the eigenvalues of A are generally complex.

RESULTS AND DISCUSSION

Figure 1 shows the stability map in the plane of α and ε, the system physical parameters. They measure, respectively the buoyancy and friction resistance in the loop. This map has been obtained using 31 nodes (dimensionless space increment $\Delta s = 1/30$), Courant number $C_{0u} \equiv Q.\Delta t/\Delta s = 0.8$ and the exponent of flow rate in the friction term of momentum equation given by $\xi = 1.75$. The selection

of these values for C_{OU} and ξ was not arbitrary: despite the low number of nodes, they ensure low numerical diffusivity while keeping the calculations stable, on one hand, and impose turbulent flow friction, on the other. The theoretical neutral stability boundary corresponds to Welander's analysis [13] and is shown as a reference.

The interest in the analysis to follow is showing how the solution depends on the cell Courant number (C_{OU}) and ξ (=2-b, where b is the exponent in the friction law). This has been quantified by calculating the following derivatives: $\partial \Delta \rho / \partial C_{OU}$ and $\partial \Delta \rho / \partial \xi$.
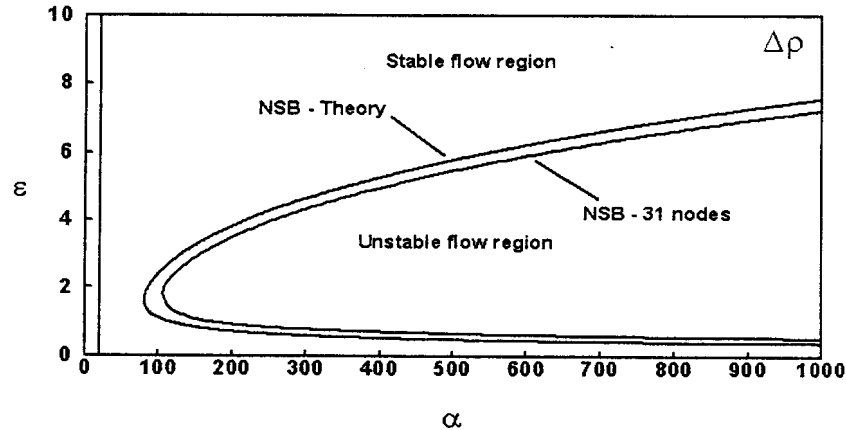

Figure 1 Map of $\Delta\rho$ for the first-order, explicit momentum, implicit temperature coupling, C_{OU}=0.8 and ξ=1.75, Δs = 1/30
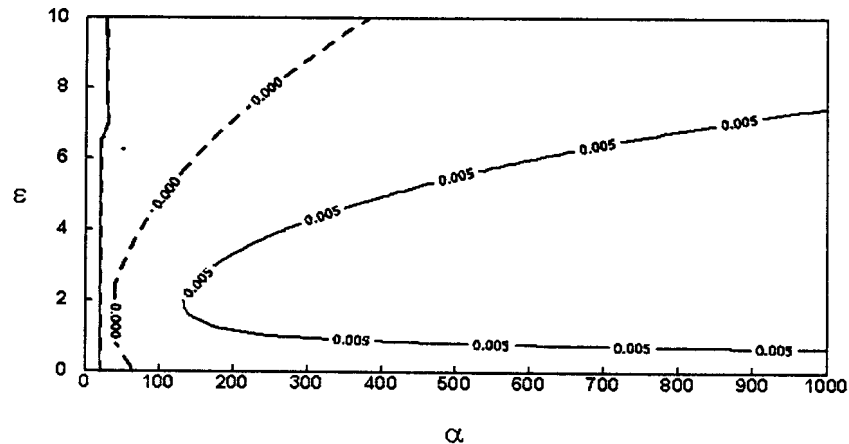

Figure 2 Sensitivity map of $\Delta\rho$ to cell Courant number ($\partial\Delta\rho/\partial C_{OU}$) for the first-order, explicit momentum and implicit temperature coupling. [C_{OU}=0.8, ξ=1.75 and Δs=1/30]

The results obtained were coincident with the ones in [4]. One of the maps, giving the variation of $\partial\Delta\rho/\partial C_{OU}$ is shown in Figure 2. However, the present algorithm leads to a much faster code than using ADIFOR to get the derivative of $\Delta\rho$.

CONCLUSIONS

A new algorithm has been developed, allowing for the calculation of the sensitivity of the margin to instability ($\Delta\rho$) to system parameters. It is based on the use of ADIFOR to evaluate the derivatives of the matrix of perturbations (A) and a formula relating this derivative and the eigenvalues and eigenvectors of this matrix and its transpose. The results so obtained are coincident with the ones previously reported by the authors [4], obtained with a more massive and, then, time-consuming use of ADIFOR. The procedure is now much faster and general. It may be stated that it may be applied to linear stability analysis based on the behavior of $\Delta\rho$ in a general case.

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