The role of the precise definition of stiffness in designing codes for the solution of ODEs.[1]

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Abstract. The notion of *stiffness*, which originated in several applications of different nature, has dominated the activities related to the numerical treatment of differential problems in the last fifty years. Its definition has been, for a long time, not formally precise. The needs of applications, especially those rising in the construction of robust and general purpose codes, require nowadays a formally precise definition. In this paper, we review the evolution of such notion and we provide also with a precise definition that could be used practically.

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INTRODUCTION

The concept of *stiffness* is the counterpart in Mathematics of the struggle generated by the duality "short times–long times" which appear in many aspect of our culture [1]. Apart from a few forerunner papers [7, 8], there is a general agreement in placing the date of the introduction of stiff problems in Mathematics around 1960. They were the necessities of the applications to draw the attention of the mathematical community towards such problems, as the name itself testifies: "*they have been termed stiff since they correspond to tight coupling between the driver and the driven components in servo-mechanism*" ([9] quoting from [8]).

Both the number and the type of applications proposing difficult differential problems has increased exponentially in the last fifty years. In the early times, the problems proposed by applications were essentially initial value problems and, consequently, the definition of stiffness was clear enough and shared among the few experts, as the following three examples evidently show:

D1 : *Systems containing very fast components as well as very slow components* (Dahlquist [9]).

D2 : *They represent coupled physical systems having components varying with very different times scales: that is they are systems having some components varying much more rapidly then the others* (Liniger [15]).

D3 : *A stiff system is one for which λ_{max} is enormous so that either the stability or the error bound or both can only be assured by unreasonable restrictions on h. Enormous means enormous relative to the scale which here is $\bar{t}$ (the integration interval)...* (Miranker [16]).

The above definitions are rather informal, certainly very far from the precise definitions we are accustomed to in Mathematics, but, at least, they agree on a crucial point: the relation among stiffness and the appearance of different time-scales in the solutions (see also [11]).

Later on, the necessity to encompass new classes of difficult problems, such as Boundary Value Problems, Oscillating Problems, etc., has led either to weaken the definition or, more often, to define some consequence of the phenomenon instead of defining the phenomenon itself. In Lambert's book [14] five propositions about stiffness, each of them capturing some important aspects of it, are given.

Sometimes one has the feeling that stiffness is becoming so broad to be nearly synonymous of difficult.

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[1] Work developed within the project "Numerical methods and software for differential equations".

At the moment, even if the old intuitive definition relating stiffness to multiscale problems survives in most of the authors, the most successful definition seems to be the one based on particular effects of the phenomenon rather than on the phenomenon itself, such as, for example, the following almost equivalent items:

D4 : *Stiff equations are equations where certain implicit methods ...perform better, usually tremendous better, than explicit ones* [8].

D5 : *Stiff equations are problems for which explicit methods don't work* [10].

As it usually happens, describing a phenomenon by means of its effects may not be enough to fully characterize the phenomenon itself. For example, saying that fire is what produces ash would oblige firemen to wait for until the end of a fire to see if the ash has been produced. In the same way, in order to recognize stiffness according to the previous definitions, it would be necessary to apply first explicit methods and see if they work or not.

It is clear that this situation is unacceptable. In particular it is necessary to have the possibility to recognize *operatively* this class of problems, in order to increase the efficiency of the numerical codes to be used in the applications. *Operatively* is intended in the sense that the definition must be done in terms of *numerically observable* quantities such as, for example, norms of vectors or matrices. It was believed that, seen from the applicative point of view, a formal definition of stiffness would not be strictly necessary: *Complete formality here is of little value to the scientist or engineer with a real problem to solve* [11].

Nowadays, after the great advance in the quality of numerical codes, the usefulness of a formal definition is strongly recognised, also from the point of view of applications: *One of the major difficulties associated with the study of stiff differential systems is that a good mathematical definition of the concept of stiffness does not exist* [5]. Following the definitions given in previous papers [2, 13], a precise definition of stiffness has been recently introduced in [1]. In this paper we report in brief the main concept and few examples.

DEFINITION OF STIFFNESS FOR LINEAR PROBLEMS

For initial value problems for ODEs, the concept of stability concerns the behavior of a generic solution $y(t)$, in the neighborhood of a reference solution $\bar{y}(t)$, when the initial value is perturbed. When the problem is linear and homogeneous, the difference, $e(t) = y(t) - \bar{y}(t)$, satisfies the same equation as $\bar{y}(t)$. For nonlinear problems, one resorts to the linearized problem which is described by the variational equation, which, essentially, provides valuable information only when $\bar{y}(t)$ is asymptotically stable. Such a variational equation can be used to generalize to nonlinear problems the arguments below which, for sake of simplicity, concerns only the linear case. The linearized problem to be considered is

$$y' = Ay, \qquad t \in [0,T], \qquad y(0) = \eta, \tag{1}$$

where $A \in \mathbf{R}^{m \times m}$ having all its eigenvalues with negative real part.

The following parameters have been defined in [1, 13]:

$$\kappa_c(T,\eta) = \frac{1}{\|\eta\|} \max_{0 \leq t \leq T} \|y(t)\|, \qquad \kappa_c(T) = \max_\eta \kappa_c(T,\eta),$$

$$\gamma_c(T,\eta) = \frac{1}{T\|\eta\|} \int_0^T \|y(t)\| dt, \qquad \gamma_c(T) = \max_\eta \gamma_c(T,\eta). \tag{2}$$

and the *stiffness ratio*:

$$\sigma_c(T) = \max_\eta \frac{\kappa_c(T,\eta)}{\gamma_c(T,\eta)}. \tag{3}$$

Let $A = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_m)$ with $\lambda_i < 0$ and $|\lambda_1| > |\lambda_2| > \ldots > |\lambda_m|$. The solution of problem (1) is $y(t) = e^{At}\eta$. In this case, we have that $k_c(T)$ is equal to 1, while $\gamma_c(T) = \frac{1}{T|\lambda_1|}$ and $\sigma_c(T) = T|\lambda_1|$.

The definition of stiffness is:

Definition 1.1 *The initial value problem (1) is* stiff *if $\sigma_c(T) \gg 1$.*
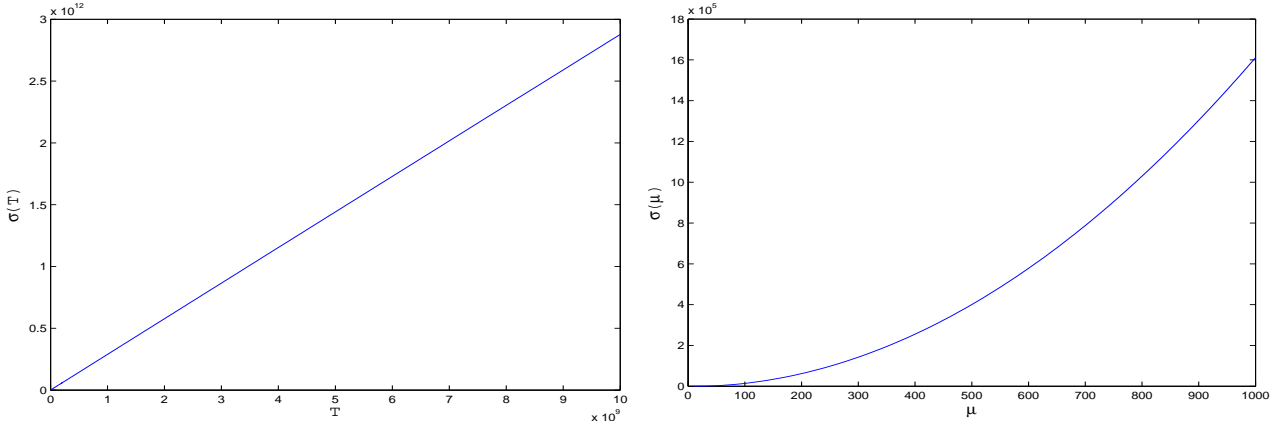
FIGURE 1. Estimated stiffness ratio of Robertson's problem (5) (left) and of Van der Pol's problem (6) (right).

How this definition reconciles with the most used definition of stiffness for the linear case, which considers into the play the "smallest" eigenvalue λ_m as well? The answer is already in Miranker's definition D3. In fact, usually the integration interval is chosen large enough to provide a complete information on the behavior of the solution. In this case, until the slowest mode has decayed enough, i.e. $T = 1/|\lambda_m|$, which implies

$$\sigma_c\left(\frac{1}{|\lambda_m|}\right) = \left|\frac{\lambda_1}{\lambda_m}\right|, \tag{4}$$

which, when much larger than 1, coincides with the most common definition of stiffness in the linear case. However, let us insist on saying that if the interval of integration is much smaller than $1/|\lambda_m|$, *the problem may be not stiff* even if $\left|\frac{\lambda_1}{\lambda_m}\right| \gg 1$.

The following examples show that Definition 1.1 is able to adequately describe the stiffness of nonlinear and/or non autonomous problems as well.

Example 1.1 *Let consider the well-known Robertson's problem:*

$$\begin{aligned}
y_1' &= -.04y_1 + 10^4 y_2 y_3, \\
y_2' &= .04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2, \qquad t \in [0, T], \\
y_3' &= 3 \cdot 10^7 y_2^2, \qquad\qquad\qquad y(0) = (1,\ 0,\ 0)^T.
\end{aligned} \tag{5}$$

Its stiffness ratio with respect to the length T of the integration interval, obtained through the linearized problem and considering a perturbation of the initial condition of the form $(0, \varepsilon, -\varepsilon)^T$, is plotted in Figure 1. As it is well-known, the figure confirms that for this problem stiffness increases with T.

Example 1.2 *Let consider the well-known Van der Pol's problem:*

$$\begin{aligned}
y_1' &= y_2, \\
y_2' &= -y_1 + \mu y_2(1 - y_1^2), \qquad t \in [0, 2\mu], \qquad y(0) = (2,\ 0)^T,
\end{aligned} \tag{6}$$

whose solution approaches a limit cycle of period $T \approx 2\mu$. It is also very well-known that, the larger the parameter μ, the more difficult the problem. In Figure 1 we plot the parameter $\sigma_c(\mu)$ for μ ranging from 0 to 10^3. Clearly, stiffness increases with μ.

In a similar way, when considering the discrete approximation of (1), for sake of brevity provided by a suitable one-step method over a partition π of the interval $[0, T]$, with subintervals of length h_i, $i = 1, \ldots, N$, the discrete problem will be given by

$$y_{n+1} = R_n y_n, \qquad n = 0, \ldots, N-1, \qquad y_0 = \eta, \tag{7}$$

whose solution is given by $y_n = \left(\prod_{i=0}^{n-1} R_i\right) \eta$. The corresponding discrete conditioning parameters are then defined by:

$$\kappa_d(\pi, \eta) = \frac{1}{\|\eta\|} \max_{0 \le n \le N} \|y_n\|, \qquad \kappa_d(\pi) = \max_\eta \kappa_d(\pi, \eta),$$

(8)

$$\gamma_d(\pi, \eta) = \frac{1}{T\|\eta\|} \sum_{i=1}^{N} h_i \max(\|y_i\|, \|y_{i-1}\|), \qquad \gamma_d(\pi) = \max_\eta \gamma_d(\pi, \eta),$$

and the *d*iscrete stiffness ratio:

$$\sigma_d(\pi) = \max_\eta \frac{\kappa_d(\pi, \eta)}{\gamma_d(\pi, \eta)}.$$

We say that the discrete problem (7), which is both defined by the used method and by the considered mesh, *well represent* the continuous problem (1) if

$$\kappa_d(\pi) \approx \kappa_c(T), \qquad \gamma_d(\pi) \approx \gamma_c(T).$$

(9)

The previous definitions naturally extend to the case of BVPs. In this case, innovative global mesh-selection strategies for the efficient numerical solution of stiff problems have been defined by requiring the match (9) (see, e.g., [3, 4, 6, 17]). It is advisable to extend to IVPs this mesh selection strategy, in order to construct codes that *measure* the reliability of the discrete problem with respect to the continuous one. In other words, we must be suspicious if the discrete problem provides parameters which are very different from the continuous ones. Since such parameters, for the discrete problem, depend on the chosen mesh, it is possible, for a fixed method, to vary the latter in order to be sure that the discrete parameters converge. This permits, for example, to recognize if the solution has two or more time scales in it. Indeed, this is the basic idea on which the mesh strategy for BVPs is based (see, e.g., [3, 4, 6, 17]).

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