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New sparsing approach for real-time simulations of stiff models on electronic control units

Thomas Loderer, Vincent Heuveline

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Affiliation of the Authors

Thomas Loderer[a,1], Vincent Heuveline[b]

[a] *Robert Bosch GmbH,*
Germany
[b] *Engineering Mathematics and Computing Lab (EMCL),*
Interdisciplinary Center for Scientific Computing (IWR),
Heidelberg University,
Germany
[1] *Corresponding Author: Thomas Loderer, thomas.loderer@de.bosch.com*

Impressum

Heidelberg University
Interdisciplinary Center for Scientific Computing (IWR)
Engineering Mathematics and Computing Lab (EMCL)

Im Neuenheimer Feld 205,
69120 Heidelberg
Germany

Zusammenfassung

For real-time simulations of stiff models on electronic control units, one important ingredient is to reduce computation time within differentiation of the right-hand side of the underlying differential equation. A sparsing method represents a powerful tool in this context. For a reliable use of a real-time simulation of a stiff model in safety-critical conditions, it is important to be able to detect, when sparsing leads to an improper influence on the considered system. In this work we propose an extension which aims at addressing this numerically challenging problem in the context of real-time simulation.

1 Introduction

This work focusses on the extension of a sparsing approach in the context of the computation of an inexact Jacobian matrix for the purpose of enabling a real-time capable simulation of stiff models on electronic control units. This work is strongly related to [8], where large parts of this work are excerpted from and where central ideas of this work have been developed and formulated.

Differential equations offer a concise description of dynamic processes. Regarding software functions in electronic control units, they are applied to describe models that are used in model-based control and diagnosis and in virtual sensors (cf. [1, 5]). In comparison to data-driven approaches, a model described by differential equations can have various advantages (cf. [16, 8]): it can admit comprehensible relations within the model and support an understanding of the model. Furthermore, the computational and memory needs of models described by differential equations can show a better scaling than several data driven approaches in the case of a large number of model parameters. Additionally, the effort of parameterizing can be small compared to data driven approaches, if the model parameters have physical meanings and can be measured with moderate effort, as it might be the case, e. g., for lengths and weights (cf. [11]). One further advantage of models described by differential equations is that they might lead to more plausible results when used in operating points, where no measurements would be available for a data-driven model (cf. [9]).

Especially in the case of models described by stiff differential equations, a real-time simulation in electronic control units leads to numerical challenges. This is due to requirement that a time step of the real-time simulation of the stiff differential equations within a software function in the electronic control unit has to be performed with a comparatively reduced computational effort, e. g., in a hundred microseconds of computation time of a core of a microchip like an Infineon TC29x that has two TriCore 1.6P with 300 MHz and one TriCore 1.6E with 200 MHz (cf. [12, 8]). For the simulation of a model with 25 to 75 states, as it is regarded in [8], it is therefore a central requirement to reduce the computational effort of a time step of a simulation, in order to enable a real-time capable simulation of a model described by an ordinary differential equation in a software function in an electronic control unit. Furthermore, it is essential to avoid instabilities in the simulation as this might have critical consequences in the software function that uses the simulation of the model.

In [8] a linearly implicit Euler method, i. e., an implicit Euler method that uses exactly one Newton step to solve the arising potentially nonlinear equation system, is used as integration method. It is an A-stable integration method of order 1 (cf. [4]) and leads to a computational effort that tends to be not larger or even smaller than in the case of other integration methods as other variants of the implicit Euler methods or exponential integrators. The computational effort consists of evaluating the right-hand side of the differential equation, differentiating respectively computing an approximation of the Jacobian matrix of the right-hand side and solving a linear equation system. For each part, there are approaches to reduce the computational effort.

One kind of methods that can affect both the differentiation and the solution of the linear equation system are sparsing methods. The underlying idea is to replace suitable entries of a Jacobian matrix of the right-hand side by zeros. If these entries are determined offline, it is not necessary to compute these entries of the Jacobian matrix during runtime. This can be used to reduce the computational effort of the differentiation. A further consequence is that the structure of the linear equation system is sparsed hereby, which gives the method its name and leads to a reduction of the computational effort of the solution of the linear equation system, in case that a structure exploiting solution method is used. Sparsing is described in more detail in the chapter 2.

A main challenge in sparsing is to identify entries that are suitable to be replaced by zeros and to be able to detect, when a chosen sparsing leads to improper influences on the system dynamics. For this, approximations can be used that quantify the impact of a sparsing on the system dynamics, as described in chapter 2. With regard to an application in real-time simulations on electronic units, it is necessary to

be able to detect improper influences reliably. For this purpose, an approximation is developed in chapter 3 that can be used to quantify the impact of a sparsing on the systems dynamics in conditions, where this is not case for an established approach and therefore increases the ability to detect improper influences of the system dynamics due to sparsing and increase the reliability of the usage of sparsing.

2 Related Work

In this chapter, an introducing overview about sparsing approaches that have been discussed in the context of real-time simulations in automotive applications, is given. Furthermore, related methods as mixed-mode integration respectively IMEX-integration that has the idea to use an implicit integration method only for some states and an explicit integration method for the remaining states and that can be regarded as a special case of a sparsing method, is described. Additionally, the approach of a colored Jacobian matrix that supports to exploit the sparsed structure of the Jacobian matrix for runtime reductions during differentiation, is summarized. Then, a sparsing approach by [14] that will be extended in chapter 3, is regarded in detail.

2.1 Sparsing approaches

So called W methods (cf. [17, 19]) are implicit integration methods that have the property that a reduction of the approximation order of the Jacobian matrix does not lead to a reduction of the convergence order of the integration method as their convergence order holds even when the Jacobian matrix is chosen arbitrarily except for trivial special cases. The underlying idea of sparsing is to reduce the computational effort of a solution of a stiff differential equation by using a W method as integration method, in order to reduce the computational effort for the solution of the arising linear equation system by sparsing its structure in a manner that the system dynamics is influenced only slightly. The sparsing of the linear equation system leads to a reduction of the computational effort, if a structure exploiting solution method is used for the linear equation system. A sparsing can be done in each time step. This is denoted dynamic sparsing. In the context of real-time simulations, a sparsing can be determined offline, in order to avoid the computational effort to evaluate sparsing criteria during runtime.

Dynamic sparsing

Dynamic sparsing is introduced in [10]. A threshold for the value of the elements of the Jacobian matrix of the right-hand side is used as sparsing criterion. Elements with a smaller value are replaced by zero. This approach leads to a significant sparsing, if several elements with small values are present. It has to be mentioned that the influence of the sparsing of an element of the Jacobian matrix of the right-hand side cannot or only in a loose manner be characterized by its value (cf. [13]). Therefore, this approach is in general not suitable to be used to sparse elements that do not have a very small value.

The sparsing described in [10] seems not to be beneficial for applications in real-time simulations in electronic control units for several reasons: Due to the fact that the sparsing is not due to a physical relation of the Jacobian matrix elements, but rather due to purely algebraic properties, the risk of an improper influence on the system dynamics arises, if the thresholds for the values of the elements are chosen too large. Otherwise, less elements are sparsed as it might be possible by other sparsing approaches that consider the properties of the system dynamics more appropriately and that are therefore able to suggest a more distinguished indicator for the sparsibility of an element.

Sparsing approaches for real-time simulations for automotive applications

With regard to real-time simulations for automotive applications, sparsing approaches are developed in [14] and [13]. There, sparsing is used within the solution of differential-algebraic equations in hardware-in-the-loop systems that have PC hardware. In this approach, the equation obtained by the integration method is linearized and transformed to block diagonal form that has triangle matrices on its block diagonal, by the QZ algorithm. For each element respectively subset of elements of the arising matrix, a criterion is used to decide, whether this element respectively subset of elements can be replaced by zero without influencing the system dynamics in a significant way. One benefit of this approach is that the sparsing criterion for each element of the Jacobian matrix of the right-hand side can be obtained essentially by the computation of a scalar product.

The sparsing in [14] is done during runtime, whereas the sparsing in [13] is done offline. Because there is plenty of computation time for an analysis, if it is done offline, in the latter work an effortful optimization algorithm is used to determine a proper sparsing. Besides that difference, the approaches in both works are substantially congruent.

The sparsing in [14] and [13] aims for differential-algebraic equations. In the following, the approach will be described in the case of an ordinary differential equation, as for an application in electronic control units, the latter one already leads to major challenges that have to be mastered. In the following, the solution of the system

$$\dot{x}(t) = f(t, x),$$

with a linearly implicit Euler method with step size Δt is regarded. The Jacobian matrix of the right-hand side is denoted by J_f and A denotes a sparsing of the Jacobian matrix.

To decide, whether the replacement of an Jacobian matrix element leads to a significant impact on the system dynamics, the changes of the eigenvalues of the matrix pair

$$(B, C) = (I - \Delta t A, I + \Delta t (J_f - A)),$$

induced by the linearized difference equation

$$(I - \Delta t A) x_{n+1} = (I + \Delta t (J_f - A)) x_n, \tag{1}$$

due to the integration by the linearly implicit Euler method are regarded. The discrete evolution in equation 1 is only partially determined by the eigenvalues, because neither the basis nor the corresponding eigenspaces are considered. Despite of this, it is sensible to use changes of the eigenvalues as indicators for the impact on the system dynamics: First, they are obtainable with a feasible computational effort. Second, it is plausible that if a sparsing of an element of $J_f(t, x)$ leads to a significant impact on the discrete evolution in equation 1, it will also affect the eigenvalues in many cases.

Mixed-Mode Integration

One relevant special case of sparsing is mixed-mode integration that is described in [15, 3] for the context of real-time simulations, and which is also referred to as IMEX integration in other contexts. The idea is that those states of a stiff differential equation are solved with an explicit integration method, where this leads to a stable result. Only the remaining states are solved with an implicit integration method. The resulting benefit is that the dimension of the arising equation system within the implicit integration method is decreased and therefore, the corresponding computational effort is reduced.

According to [15], mixed-mode integration can be beneficially applied to models, where dynamics of different time scales are present. This is widespread for models in automotive applications in electronic control units (cf. [8]). Therefore, mixed-mode integration is a suitable approach in this context.

To see that mixed-mode integration is a special case of sparsing, let I denote the set of indices of those components of a stiff differential equation that are solved with an explicit integration method within mixed-mode integration. Then, replacing all elements of each column of the Jacobian matrix of the right-hand side with index $i \in I$ and of each row with index $i \in I$ leads to an equation system that is equivalent to one that is obtained by mixed-mode integration.

Colored Jacobian matrix

In [7] colored Jacobian matrices are introduced. This approach is applicable in differentiation methods that use evaluations of directional derivatives, e. g., numerical differentiation and automatic differentiation. The intention of the coloring is to reduce the number of evaluations of directional derivatives that is required to determine a Jacobian matrix. This is achieved by choosing an appropriate set of directions for the directional derivatives. For example, a Jacobian matrix in diagonal form can be determined by computing only one directional derivative, if that direction has no component with value zero.

In general, the determination of suitable sets of directions for the directional derivatives can be formulated as a graph coloring problem, which leads to the name of the approach (cf. [7]). This problem is NP-hard and therefore for now not solvable with feasible computational effort. There are, however, suitable approximation methods available.

For sparse Jacobian matrices, this approach can lead to significant reductions of the computational effort of the differentiation within the solution of a differential equation. In [2] this approach is investigated for

two fluid models in the context of plants. There, runtime reductions between 50 % and 80 % are obtained. Also in [8], this approach was used to contribute to a significant runtime reduction in case of a real-time simulation of a pipe model that describes mass and enthalpy transport, in an application in an electronic control unit.

2.2 Approximation of the impact of sparsings

An approximation that is developed in [14], relates the sum $\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)$ of differences of the eigenvalues $\tilde{\lambda}_i$ obtained after sparsing to the eigenvalues λ_i that are obtained without sparsing, without computing the eigenvalues or eigenvectors explicitly. This is described in Theorem 4 in [14]:

Theorem 1. *Let (B, C) be a diagonalisable matrix pair with eigenvalues λ_i and left eigenvectors y_i and right eigenvectors x_i. Assume all eigenvalues to be algebraically simple and C to be regular. Let E be a sufficiently small $\mathcal{O}(\epsilon)$ perturbation matrix. Let $\tilde{\lambda}_i$ denote the eigenvalues of the perturbed matrix pair $(B + E, C + E)$. Then, a first order approximation for the sum of differences between perturbed and unperturbed eigenvalues is given by*

$$\sum_i \left(\tilde{\lambda}_i - \lambda_i\right) = tr\left(C^{-1}E\left(I - C^{-1}B\right)\right) + \mathcal{O}\left(\epsilon^2\right).$$

As a corollary, the following approximation is obtained for the matrix pair

$$(B, C) = \left(\left(I - \Delta t A\right), I + \Delta t\left(J_f - A\right)\right),$$

if the assumptions of the previous theorem are fulfilled:

$$\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right| \approx \left|\mathrm{tr}\left(\left(I - \Delta t J_f\right)^{-1} \Delta t \Delta J \left(I - \left(I - \Delta t J_f\right)^{-1}\left(I + \Delta t J_f\right)\right)\right)\right| \tag{2}$$

with $\Delta J = A - J_f$. This approximation is the foundation for determining a suitable sparsing.

Properties The equation 2 approximates the sum of differences of eigenvalues of the discrete evolution of equation 1. If the perturbation of each eigenvalue is sufficiently small, the stability of the solution of the differential equation without sparsing is maintained in case that a sparsing is used. Additionally, the system dynamics is changed unessentially. The impact on the accuracy of the solution of the differential equation is considered insignificant in [14] with the following argument: By using a W method as integration method, using an inexact Jacobian matrix will not lead to a reduction of the order of consistency respectively order of convergence in case of a stable solution of the differential equation. For sufficiently small step sizes, an adequate accuracy is expectable also in case of using a sparsing.

One requirement for the validity of the approximation of equation 2 is that the nonlinear perturbation terms are small. For this, in [14] it is suggested to choose the diagonal blocks within the block diagonalization in a manner that different diagonal blocks do not contain eigenvalues that are close to each other. Concerning this, as described in [13], a triangularization of the matrix of the linearized discrete evolution in equation 1 is done first. Second, Givens rotations are used to obtain an appropriate clustering of the eigenvalues. Then, a block diagonalization corresponding to the clustering of the eigenvalues is performed.

Cancellation effects In [14], it is pointed out that cancellation effects within the approximation in equation 2 can lead to the situation that on the one hand, a sparsing has a strong and improper influence on the system dynamics despite this sparsing seems to have an insignificant impact on the system dynamics according to the approximation in 2. This can be caused by cancellation of the perturbations of different eigenvalues. This risk is generally present in this sparsing approach and according to [14] it is considered substantial in case of oscillating modes.

An extension of the approximation, where such cancellation effects do not occur, because instead of

$$\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)$$

the term

$$\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2$$

is approximated, is shown in chapter 3.

Results In [14], sparsing is applied to a real-time simulation of a model described by a differential equation. There, a considerable simplification of the structure of the linear equation systems arising in the solution of the differential equation is achieved. By this, a reduction of the runtime for the solution of the arising linear equation system by over 65 % is obtained.

3 Extension of a sparsing approach

Sparsing according to [13] and [14] is developed for real-time simulations. Determining a sparsing offline, as described [13], is suitable for real-time simulations of stiff models in software functions in electronic control units. The approximation in equation 2 suggests suitable Jacobian matrix elements that can be sparsed.

In the following, the theoretical foundation of sparsing according to [13] and [14] is described. This description of sparsing adapts the explanations in[14], where differential-algebraic equations are regarded, for the case of ordinary differential equations. The obtained theoretical framework will be used to develop an extension of the approach that enables detecting an improper influence on system dynamics due to a sparsing in conditions, where the original approach would not indicate that improper influence due to a sparsing: As described in 2.2, cancellation effects in the term $\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right|$ in equation 2 can cause a misleading indication of the suitability of a given sparsing. The term

$$\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2,$$

does not suffer from this risk of such cancellation effects. An approximation for that term will be given.

Solving the ordinary differential equation

$$\dot{x}\left(t\right) = f\left(t, x\right),$$

with a linearly implicit Euler method leads to the integration equation:

$$x_{n+1} = \left(I + \left(I - \Delta t J_f\right)^{-1} \Delta t J_f\right) x_n = F x_n. \tag{3}$$

Now, the Schur form of F is determined using a QR algorithm: Let $T = U^H F U$ with a unitary matrix U and a triangle matrix T. The diagonal elements of T are the eigenvalues of F. A transformation of T is performed, in order to obtain a triangle matrix, which has the eigenvalues of F on its diagonal in an order, so that they are clustered corresponding to their values. The aim of this clustering of the eigenvalues will be become clear in the further course of the explanation. Also, the requirement to this clustering of the eigenvalues into clusters S_i will be specified further.

This transformation of T corresponding to choice of the clusters S_i of eigenvalues is obtained by Givens rotations. Without loss of generality, this transformed matrix will also be denoted with $T = U^H F U$.

The next step is a block diagonalization of T. This is done in a manner that those subsets of columns of T that correspond to different clusters S_i of eigenvalues, are orthogonal. For this, the following algorithm from[13] is used:

Let $P_{i,j}$ denote the canonical projection on the space generated by $\{\, e_k |\, i \leq k \leq j\}$, i. e.,

$$P_{i,j} e_k = \begin{cases} e_k & \text{, if } i \leq k \leq j, \\ 0 & \text{otherwise.} \end{cases}$$

Let $T_1 = U_1^H F U_1$ and $T_2 = U_2^H F U_2$ be two Schur forms of F, where in T_1 all eigenvalues of a cluster S_{i_0} are contained in the leading k diagonal elements, whereas in T_2 all eigenvalues of the cluster S_{i_0} occur in the same order in T_2 as the last k diagonal elements. Let

$$\begin{aligned} Y_2 &= P_{k+1,n} U_1, \\ Y_1 &= P_{n-k+1,n} U_2, \\ X_1 &= P_{1,k} U_1, \\ X_2 &= P_{1,n-k} U_2. \end{aligned}$$

The set of columns is orthogonal for each of these matrices. Furthermore, it holds $Y_1^H F X_2 = 0$ and $Y_2^H F X_1 = 0$. This yields:

$$\begin{pmatrix} Y_1^H \\ Y_2^H \end{pmatrix} F \begin{pmatrix} X_1 & X_2 \end{pmatrix} = \begin{pmatrix} T^{(1)} & 0 \\ 0 & T^{(2)} \end{pmatrix}.$$

Analogously, $T^{(2)}$ can be obtained by a corresponding transformation for a further cluster $S_i \neq S_{i_0}$. By iteration, T can be transformed to block diagonal form with diagonal blocks that are in triangle form and that correspond to the clusters S_i of eigenvalues. If the matrix F is diagonalisable, matrices X and Y are obtained by this procedure, so that $Y^H F X$ is diagonal.

In the following, the impact of a perturbation ϵM of the matrix F on the eigenvalues will be characterized. It is assumed that F has only algebraically simple eigenvalues. In particular, F is diagonalisable. Let

$$\begin{pmatrix} Y_1^H \\ Y_2^H \end{pmatrix} M \begin{pmatrix} X_1 & X_2 \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}.$$

According to theorem 2.8 in [18], there exist transformation matrices $\tilde{X}$, $\tilde{Y}$ with

$$\tilde{Y}^H (F + \epsilon M) \tilde{X} = \begin{pmatrix} T^{(1)} + \epsilon M_{11} + \epsilon M_{12} P & 0 \\ 0 & T^{(2)} + \epsilon M_{22} + P \epsilon M_{12} \end{pmatrix},$$

where it is $\tilde{X}_1 = X_1 + P X_2$ and $\tilde{Y}_2 = Y_2 - Y_1 P^H$ with

$$\|P\| \leq 2 \frac{\|\epsilon M_{21}\|}{\operatorname{sep}\left(T^{(1)}, T^{(2)}\right) - \|\epsilon M_{22}\| - \|\epsilon M_{22}\|} \tag{4}$$

and

$$\operatorname{sep}\left(T^{(1)}, T^{(2)}\right) = \left(\inf_{\|Q\|=1} \left\| Q T^{(1)} - T^{(2)} Q \right\| \right) > 0. \tag{5}$$

Furthermore, the column vectors of $\tilde{X}_1$ respectively of $\tilde{Y}_2$ form a basis for the simple right respectively left invariant subspaces of $F + \epsilon M$. Equation 4 and equation 5 yield $\|P\| = \mathcal{O}(\epsilon)$ and therefore

$$\tilde{X}_1 = X_1 + \mathcal{O}(\epsilon) \frac{P}{\|P\|} X_2 \tag{6}$$

and

$$\tilde{Y}_2 = Y_2 - Y_1 \mathcal{O}(\epsilon) \frac{P^H}{\|P^H\|}. \tag{7}$$

Analogously, it is inferred

$$\tilde{X}_2 = X_2 + \mathcal{O}(\epsilon) \frac{\hat{P}}{\left\|\hat{P}\right\|} X_1 \tag{8}$$

and

$$\tilde{Y}_1 = Y_1 - Y_2 \mathcal{O}(\epsilon) \frac{\hat{P}^H}{\left\|\hat{P}^H\right\|}. \tag{9}$$

Altogether, the following equation can be concluded:

$$\tilde{Y}^H (F + \epsilon M) \tilde{X} = \begin{pmatrix} T^{(1)} + \epsilon M_{11} + \mathcal{O}\left(\epsilon^2\right) & \mathcal{O}\left(\epsilon^2\right) \\ \mathcal{O}\left(\epsilon^2\right) & T^{(2)} + \epsilon M_{22} + \mathcal{O}\left(\epsilon^2\right) \end{pmatrix}.$$

At this point, the choice of the clusters S_i of eigenvalues comes into effect. Due to the fact that the eigenvalues are clustered in different diagonal blocks corresponding to their value, different diagonal blocks do particularly not contain eigenvalues that are close to each other. Therefore, the linear parts of the perturbation terms are a good approximation of the perturbations and the nonlinear parts of the perturbation terms can be neglected (cf. [14, 18]). If there would be eigenvalues in different diagonal blocks that are close to each other, the nonlinear parts of the perturbation terms tended to be large.

As the nonlinear perturbation terms can be neglected in the given situation, it holds

$$\tilde{Y} (F + \epsilon M) \tilde{X} \approx \begin{pmatrix} T^{(1)} + \epsilon M_{11} & 0 \\ 0 & T^{(2)} + \epsilon M_{22} \end{pmatrix}.$$

In order to quantify the impact of the perturbation by the sparsing on the eigenvalues, it consequently suffices to quantify the impact of the perturbation by the sparsing on the eigenvalues of the corresponding diagonal block.

If F is diagonalisable and has only algebraically simple eigenvalues, a clustering, where each eigenvalue forms a separate cluster, leads to diagonal blocks that are single elements. For this case, particularly handy statements about the impact of a perturbation ϵM of the matrix F on the eigenvalues can be given.

Lemma 2. *Let the matrix F have only algebraically simple eigenvalues. Let Y respectively X be matrices that contain the left respectively right eigenvectors as column vectors, so that $Y^H F X$ and $Y^H X$ are diagonal. Then, the following statements hold for sufficiently small $\epsilon > 0$ and a matrix $\tilde{\Lambda}$ of eigenvalues $\tilde{\lambda}_i$ of the perturbed matrix $F + \epsilon M$:*

1. $\tilde{\Lambda} = X^{-1}(F + \epsilon M) X + \mathcal{O}(\epsilon^2)$. In particular, $X^{-1}(F + \epsilon M) X$ is diagonal up to auf $\mathcal{O}(\epsilon^2)$ terms.
2. $\tilde{\Lambda} - \Lambda = X^{-1} \epsilon M X + \mathcal{O}(\epsilon^2)$ for sufficiently small $\epsilon > 0$.
3. $\sum_i \left(\tilde{\lambda}_i - \lambda_i\right) = \mathrm{tr}(\epsilon M) + \mathcal{O}(\epsilon^2)$.

Beweis. Claim 1 follows from corollary 2 in [14] applied to the matrix pair $(A, B) = (F, I)$ with $(E, F) = (\epsilon M, 0)$.

Claim 2 is inferred from claim 1 due to the fact that the elements of $\tilde{\Lambda}$ depend continuously on ϵ, as, e. g., in corollary 2.3 in [18] yields, and that therefore the order of the eigenvalues in $\tilde{\Lambda}$ and Λ coincides.

Moreover, it holds

$$\Lambda = \lim_{\epsilon \to 0} \tilde{\Lambda} = \lim_{\epsilon \to 0} \left(X^{-1}(F + \epsilon M) X + \mathcal{O}(\epsilon^2)\right) = X^{-1} F X.$$

Therefore, the following equation can be concluded:

$$\begin{aligned} \tilde{\Lambda} - \Lambda &= X^{-1}(F + \epsilon M) X + \mathcal{O}(\epsilon^2) - X^{-1} F X, \\ &= X^{-1} \epsilon M X + \mathcal{O}(\epsilon^2). \end{aligned}$$

Together with

$$\sum_i \left(\tilde{\lambda}_i - \lambda_i\right) = \mathrm{tr}\left(\tilde{\Lambda} - \Lambda\right) = \mathrm{tr}(\epsilon M) + \mathcal{O}(\epsilon^2),$$

this yields claim 3. □

As already described, this approximation leads to the risk that substantial changes of the eigenvalues are not detected due to cancellation effects. The following statement gives an approximation that avoids such cancellation effects in the case of real perturbation matrices.

Lemma 3. *Let F be a real matrix with only algebraically simple eigenvalues. Then the following equation holds for sufficiently small $\epsilon > 0$ and a matrix $\tilde{\Lambda}$of eigenvalues $\tilde{\lambda}_i$ of the perturbed matrix $F + \epsilon M$ with $\epsilon M \in \mathbb{R}^n$:*

$$\sum_{i=1}^{n} \left|\tilde{\lambda}_i - \lambda_i\right|^2 \leq tr\left(\epsilon^2 M^2\right) + \mathcal{O}\left(\epsilon^3\right).$$

Beweis. Choose matrices X and Y according to page 6 , so that $Y^H F X$ is diagonal. Due to $F \in \mathbb{R}^n$, the matrix U that arises during the determination of X and Y, is real. Therefore, X and Y are also real. Furthermore, X is regular. Choose $\tilde{X}$ and $\tilde{Y}$ according to page 6, so that $\tilde{Y}^H (F + \epsilon M) \tilde{X}$ is also diagonal. Then, $\tilde{X}$ and $\tilde{Y}$ fulfil the requirements of Lemma 2. Consequently, for sufficiently small $\epsilon > 0$ it holds

$$\tilde{\Lambda} - \Lambda = \tilde{X}^{-1} \epsilon M \tilde{X} + \mathcal{O}(\epsilon^2).$$

By complex conjugation of the overall setting, it can be concluded analogously that the following equation holds for sufficiently small $\epsilon > 0$:

$$\overline{\tilde{\Lambda} - \Lambda} = \overline{\tilde{X}^{-1} \epsilon M \tilde{X} + \mathcal{O}(\epsilon^2)}.$$

Equation 6 and equation 8 yield $\tilde{X} = X + \mathcal{O}(\epsilon)$. Because X is regular, $\tilde{X}$ is also regular for sufficiently small $\epsilon > 0$. Furthermore, it is $\tilde{X}^{-1} = X^{-1} + \mathcal{O}(\epsilon)$ and due to $X \in \mathbb{R}^n$, it therefore holds

$$\tilde{X}\overline{\tilde{X}^{-1}} = (X + \mathcal{O}(\epsilon))\,\overline{(X^{-1} + \mathcal{O}(\epsilon))} = I + \mathcal{O}(\epsilon).$$

For sufficiently small $\epsilon > 0$, the following equation can therefore be concluded

$$\begin{aligned}
\sum_i^n \left|\tilde{\lambda}_i - \lambda_i\right|^2 &= \operatorname{tr}\left(\left(\tilde{\Lambda} - \Lambda\right)\overline{\left(\tilde{\Lambda} - \Lambda\right)}\right), \\
&= \operatorname{tr}\left(\left(\tilde{X}^{-1}\epsilon M\tilde{X} + \mathcal{O}(\epsilon^2)\right)\left(\overline{\tilde{X}^{-1}\epsilon M\tilde{X}} + \mathcal{O}(\epsilon^2)\right)\right), \\
&= \operatorname{tr}\left(\tilde{X}^{-1}\epsilon M\tilde{X}\overline{\tilde{X}^{-1}\epsilon M\tilde{X}} + \mathcal{O}(\epsilon^3)\right), \\
&= \operatorname{tr}\left(\epsilon^2 M^2\right) + \mathcal{O}(\epsilon^3).
\end{aligned}$$

□

In the following, the previous results are used to determine the suitability of a sparsing of a subset of elements of a Jacobian matrix of the right-hand side within the solution of an ordinary differential equation with a linearly implicit Euler method.

Within a linearly implicit Euler method, where a sparsing is used, the equation

$$x_{n+1} = \left(I + \Delta t\,(I - \Delta t A)^{-1} J_f\right) x_n, \tag{10}$$

replaces the integration equation 3. Equation 10 can be regarded as integration equation within a linearly implicit Euler method, where F is perturbed by the matrix ϵM with

$$\begin{aligned}
\epsilon &= \left\|\Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f\right\|, \\
M &= \frac{\Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f}{\epsilon}.
\end{aligned} \tag{11}$$

This is confirmed by

$$\begin{aligned}
F + \epsilon M &= I + (I - \Delta t J_f)^{-1}\Delta t J_f + \Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f, \\
&= I + (I - \Delta t A)^{-1}\Delta t J_f.
\end{aligned}$$

It is mentioned that

$$\lim_{A \to J_f} \epsilon = 0,$$

so that ϵ is small in case of small perturbations of the Jacobian matrix. Altogether, the following theorem can be concluded.

Theorem 4. *Let λ_i be eigenvalues of the matrix $F = I + (I - \Delta t J_f)^{-1}\Delta t J_f$ and let $\tilde{\lambda}_i$ be eigenvalues of the matrix $I + (I - \Delta t A)^{-1}\Delta t J_f$. Let F have only algebraically simple eigenvalues. Moreover, let A and J_f be real and ϵ be defined according to equation 11. If $\epsilon > 0$ is sufficiently small, it holds:*

1. $\sum_i \left(\tilde{\lambda}_i - \lambda_i\right) = \operatorname{tr}\left(\Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f\right) + \mathcal{O}(\epsilon^2)$.
2. $\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2 = \operatorname{tr}\left(\left(\Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f\right)^2\right) + \mathcal{O}(\epsilon^3)$.

Beweis. Choose matrices $\tilde{X}$ and $\tilde{Y}$ as described on page 6. Due to their existence, claim 1 can be inferred from lemma 2 and claim 2 from lemma 3 by applying them to

$$F = I + (I - \Delta t J_f)^{-1}\Delta t J_f$$

and

$$\epsilon M = \Delta t\left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f.$$

□

Some remarks have to be given on the previous theorem:

Claim 1 from theorem 4 is a slightly modified adaptation of the approximation according to theorem 4 in [14]. There, the impact of the perturbations of the Jacobian matrix by a sparsing are addressed via a formulation as a generalized eigenvalue problem. If the integration equation 1 is interpreted in this sense, then this theorem does not immediately yield a theorem that is analogous to theorem 4, because the matrix pair (E, F) would have to be chosen as $\left(I + (I - \Delta t A)^{-1} \Delta t J_f, 0\right)$. In theorem 1, only matrix pairs of the form (E, E) are admitted. The approximation that can be inferred from this theorem, is shown in equation 2.

By the approximation of $\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2$, it is possible to detect the occurrence of large differences $\tilde{\lambda}_i - \lambda_i$, even if they do not lead to large values of $\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)$. This detection is valuable. For a reliable application of sparsing, it has to be considered that the nonlinear perturbation terms are assumed to be negligible. This holds for sufficiently small $\epsilon > 0$. Furthermore, it can also hold for large valuesϵ, if the eigenvalues can be clustered appropriately. Therefore, this approximation is not restricted to the sparsing of Jacobian matrix elements with small values, if the eigenvalues of the integration equation of the linearly implicit Euler method are suitable.

Algorithm

In order to summarize the investigated sparsing approach, a description of the method is given in algorithm 1. Compared to the sparsing approach introduced in [14], the difference is given in steps ChoiceBounds and Check2. The choice of suitable bounds is discussed in section 3.

Algorithm 1 Proceeding of the investigated sparsing approach.

1: Determine Schur form F of Jacobian matrix of the right-hand side using QR algorithm.
2: Cluster eigenvalues into sets $S_1, \ldots, S_m$.
3: Obtain transformed Schur form $F^{(1)}$ with clustered eigenvalues on main diagonal according to $S_1, \ldots, S_m$ using Givens rotations.
4: **for** $i = 1$ **to** m **do**
5: Calculate two Schur forms $T_1^{(i)}$ and $T_2^{(i)}$ of $F^{(i)}$, where all eigenvalues of S_j are contained in the leading k diagonal elements in $T_1^{(i)}$ and in the last k diagonal elements in the same order in $T_2^{(i)}$.
6: Denoting P_{j_1,j_2} the corresponding canonical projection, calculate X and Y with $X = \begin{pmatrix} X_1 & X_2 \end{pmatrix}$ and $Y = \begin{pmatrix} Y_1^H \\ Y_2^H \end{pmatrix}$ and

$$\begin{aligned} Y_2 &= P_{k+1,n} U_1, \\ Y_1 &= P_{n-k+1,n} U_2, \\ X_1 &= P_{1,k} U_1, \\ X_2 &= P_{1,n-k} U_2. \end{aligned}$$

7: Obtain block diagonalization $\begin{pmatrix} T^{(1)} & 0 \\ 0 & T^{(2)} \end{pmatrix} = \begin{pmatrix} Y_1^H \\ Y_2^H \end{pmatrix} F \begin{pmatrix} X_1 & X_2 \end{pmatrix}$ of the Schur form $F^{(i)}$.
8: Set $F^{(i+1)} = T^{(2)}$.
9: **end for**
10: Choose bounds C_1 and C_2 suitably, e. g. $C_1 = \min_i (r_i)$ and $C_2 = \min_i \left(r_i^2\right)$ with $r_i = d\left(\lambda_i, \partial B_1(0)\right)$.
11: Check tr $\left(\Delta t \left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f\right) + \mathcal{O}\left(\epsilon^2\right) < C_1$.
12: Check tr $\left(\left(\Delta t \left((I - \Delta t A)^{-1} - (I - \Delta t J_f)^{-1}\right) J_f\right)^2\right) + \mathcal{O}\left(\epsilon^3\right) < C_1$.

For an application in real-time simulations, a promising candidate for the sparsing has to be determined at first. For this, different approaches are discussed in [8]. As described there, one central benefit of the considered sparsing approach is that it is a valuable support during the determination of such candidates as it offers enlightening insights to the system properties.

When a sparsing candidate is determined, the influence of the considered sparsing on the eigenvalues of the system can be examined by algorithm 1. The value of this influence serves as an indicator for

the suitability of the sparsing. In case of a strong influence on the eigenvalues, the sparsing tends to be insufficient. A small influence on the eigenvalues is desired. In this case, an elaborate validation of the chosen sparsing can be performed depending on the requirements regarding reliability. Therefore, a collateral benefit of the sparsing approach is that it enables a reduction of the validation effort for a sparsing as it enables a meaningful judgment with a comparatively small effort.

Choice of bounds

In the previous considerations, it is regarded, how the impact of a sparsing of a Jacobian matrix of the right-hand side within the solution of an ordinary differential equation on the eigenvalues of the linearized integration equation 3 can be approximated. This impact serves as indicator for the impact of a sparsing on the system dynamics. One question that arises, is, which changes of the eigenvalues in equation 3 can be considered admissible. With regard to a sparsing criterion, this corresponds to the choice of bounds C_1 and C_2, so that, if a sparsing of a Jacobian matrix fulfils the inequalities

$$\sum_i \left(\tilde{\lambda}_i - \lambda_i\right) \quad \leq \quad C_1, \tag{12}$$

$$\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2 \quad \leq \quad C_2, \tag{13}$$

the sparsing can be considered admissible.

Inherently, the bounds C_1 and C_2 depend on the ordinary differential equation that is solved, and on the requirements to the integration result. As described in [8], a stable solution is typically a requirement in the context of real-time simulation in software functions in electronic control units. Therefore, two heuristic inequalities for C_1 and C_2 can be justified:

The stability, i. e., the boundedness of the solution of an ordinary differential equation suggests that the eigenvalues in the matrix in equation 3 have to fulfil

$$\tilde{\lambda}_i \leq 1. \tag{14}$$

For this reason, it is natural to choose the bounds C_1 and C_2, so that inequality 14 is likely to hold. Let $r_i = d\left(\lambda_i, \partial B_1\left(0\right)\right)$. Then

$$C_2 = \min_i \left(r_i^2\right)$$

is a bound that yields stability in case of validity of theorem 4, so that the states of the solution remain bounded over the course of the simulation. For C_1, an analogous consideration yields

$$C_1 = \min_i \left(r_i\right), \tag{15}$$

where the corresponding criterion cannot be regarded assured due to potential cancellation effects. It is pointed out that it is necessary to be able to estimate the eigenvalues arising during real-time simulations of a model roughly offline in order to make use of this suggestion for a choice of the bound C_1.

The requirement of a stable solution as described in [8] also demands that oscillations in the course of the simulation that are due to numerical integration, have to be small. Oscillations correspond to the arguments φ_j of the eigenvalues $\tilde{\lambda}_j = \left|\tilde{\lambda}_j\right| e^{i\varphi_j}$ of the matrix in equation 3, where it is $0 \leq \varphi_j \leq 2\pi$: If $|\pi - \varphi_j|$is small, then an oscillating dynamics of eigenvalue $\tilde{\lambda}_j$ is indicated. Therefore, in the case of oscillations due to numerical integration, it is advisable that a sparsing is not only chosen in a manner that inequality 14 holds, but also so that $|\varphi_j| \approx 0 \mod 2\pi$.

4 Numerical Experiment

The investigated sparsing approach is applied to a 1D pipe model that describes mass and enthalpy transport through a pipe. The model is originally developed in [6]. In [8], it is also described and several numerical approaches are examined with the aim of enabling a real-time capable simulation of the model on an electronic control unit. A simulation of the model can be used to enable the determination the temperature of a catalyst.

Term	Unit	Description
A	m^2	cross section area
c	$J\,K^{-1}\,kg^{-1}$	specific heat capacity of a solid phase
c_p	$J\,K^{-1}\,kg^{-1}$	specific heat capacity of a gas phase
d_h	m	hydraulic diameter
f	1	Darcy friction factor of pipe
h	$J\ kg^{-1}$	specific enthalpy
l	m	length
m	kg	mass
m_{mol}	$kg\,mol^{-1}$	molar weight
$\dot{m}$	$kg\,s^{-1}$	mass flow
Nu	1	Nusselt number
p	Pa	pressure
r	m	radius
T	K	temperature
R	$J\ mol^{-1}\,K^{-1}$	universal gas constant
Re	1	Reynolds number
Pr	1	Prandtl number
w_i	1	mass fraction of species i
α	$W\,m^{-2}\,K^{-1}$	convection coefficient
ϵ	1	emissivity
η	1	efficiency
λ	$W\,m^{-1}\,K^{-1}$	thermal conductivity
ρ	$kg\,m^{-3}$	density
σ	1	Boltzmann constant

Superscript	Description
A	ambience
B	bulk
C	canning

Tabelle 1: Notation for description of pipe model

The model equations are

$$\frac{pm_{\mathrm{mol}}}{RT_B}\frac{\partial w_j}{\partial t} = -\frac{\dot{M}}{A_B}\frac{\partial w_j}{\partial z}, \quad j = 1,\,2,\,3, \tag{16}$$

$$\frac{p}{T_B}\left(\frac{M_{\mathrm{mol}}c_{p,B}}{R}-1\right)\frac{\partial T_B}{\partial t} = -\frac{1}{A_B}\left(\dot{M}c_{p,B}\frac{\partial T_B}{\partial z}+\alpha_{B,C}l_B\left(T_B-T_C\right)\right), \tag{17}$$

$$\begin{aligned}\rho_C c_C\frac{\partial T_C}{\partial t} = {} & \lambda_C\frac{\partial^2 T_C}{\partial z^2}+\frac{1}{A_C}\Big(\alpha_{B,C}l_B\left(T_B-T_C\right)- \\ & \alpha_{A,C}l_C\left(T_C-T_A\right)-\epsilon_C l_C\sigma\left(\left(T_C\right)^4-\left(T_A\right)^4\right)\Big).\end{aligned} \tag{18}$$

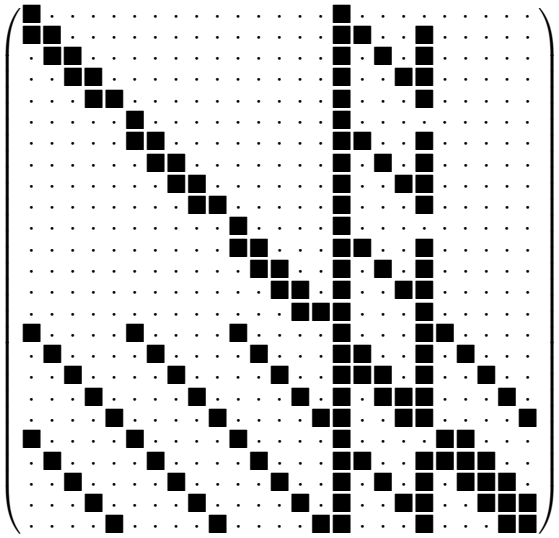
with notation according to table 1.

In this article, a semi-discretization of the pipe model with 5 spatial discretization cells is regarded. The structure matrix of the arising ordinary differential equation

$$\dot{x}\left(t\right) = f\left(t,x\right)$$

is shown in equation 19.

$$S = \left(\right) . \tag{19}$$



For the purpose of this investigation, one exemplary time step from a simulation with measured data is considered. The spectrum Λ_J of the Jacobian matrix $J_f\left(t_0, x_0\right)$ of the right-hand side at this time step is

$$\begin{aligned} \Lambda_J \quad \approx \quad & \big\{-1014.0, -1012.0, -1012.0, -1005.0, -1005.0 \\ & -0.03519, -0.03904, -0.04664, -0.05416, -0.05727, \\ & -748.5, -748.5, -748.5, -756.0, -756.0, \\ & -756.0, -750.4, -750.4, -750.4, -754.1, \\ & -754.1, -754.1, -752.2, -752.2, -752.2\big\}. \end{aligned} \tag{20}$$

It is pointed out that Λ_J does not contain multiple eigenvalues. Further specifications can be found in [8]. As shown in [8], a sparsing of the Jacobian matrix J_f to a sparsing matrix A with bidiagonal form, where the lower right 5×5 submatrix of A contains only zeros, is suitable.

Let

$$d_S = \left| \mathrm{tr}\left(\left(I - \Delta t J_f\right)^{-1} \Delta t \Delta J \left(I - \left(I - \Delta t J_f\right)^{-1} \left(I + \Delta t J_f\right) \right) \right) \right|$$

resp.

$$d_1 = \left| \mathrm{tr}\left(\Delta t \left(\left(I - \Delta t A\right)^{-1} - \left(I - \Delta t J_f\right)^{-1} \right) J_f \right) \right|$$

denote the approximation of $\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right|$ obtained according to equation 2 resp. statement 1 of theorem 4 and

$$d_2 = \sqrt{\mathrm{tr}\left(\left(\Delta t \left(\left(I - \Delta t A\right)^{-1} - \left(I - \Delta t J_f\right)^{-1} \right) J_f \right)^2 \right)},$$

the approximation of $\sqrt{\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|^2}$ obtained according to equation 2 of theorem 4. Furthermore, let d_r denote the actual value of $\sum_i \left|\tilde{\lambda}_i - \lambda_i\right|$. It can be seen from figure 1 that the approximation d_2 based on statement 2 of theorem 4 is able to describe the perturbation of the spectrum of the right-hand side matrix of the evolution equation 10 of the linearly implicit Euler method significantly more accurately than the approximation based on equation 2 for the regarded application. By comparing the values d_2 to the values d_1, it becomes clear that this has to be due to cancellation effects within the approximation in $\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right|$ due to general validity of the inequality

$$\sqrt{\sum_{i=1}^{m} \left|\tilde{\lambda}_i - \lambda_i\right|^2} \leq \sum_{i=1}^{m} \left|\tilde{\lambda}_i - \lambda_i\right|.$$

This shows that the approximation d_2 based on statement 2 of theorem 4 enables a detection of cancellation effects in the approximation $\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right|$ of based on equation 2 or statement 1 of theorem 4.

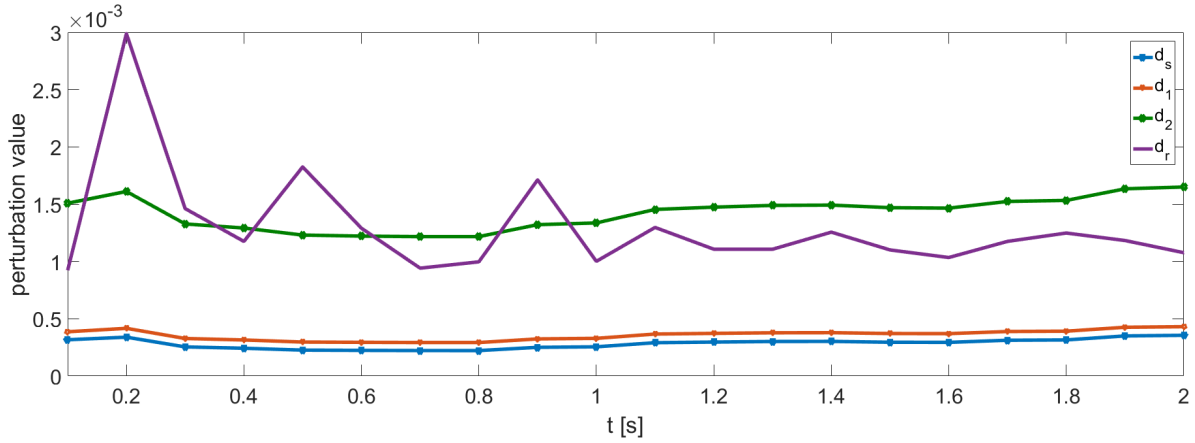


Abbildung 1: Plot of the course of different approximations for the perturbation of spectrum Λ_I for different time steps of a simulation based on measured data.

As pointed out in [14] resp. in section 3, the regarded approximations are only valid in case of the Jacobian matrix J_f of the right-hand side not having multiple eigenvalues. This is necessary to justify the neglection of the nonlinear perturbation terms. As shown in approximation 20, different simple eigenvalues of J_f lie close to each other. With regard to nonlinear perturbation terms, the investigated approximations have therefore to be used cautiously in the given application.

In [14], it is mentioned that critical cancellation effects with the investigated approximation of $\left|\sum_i \left(\tilde{\lambda}_i - \lambda_i\right)\right|$ are mainly expected in the context of oscillating modes and therefore in the context of eigenvalues with relevant imaginary parts. As it can be concluded rom figure 1, cancellation effects also occur in case of real spectra. By applying the approximation to variants of the investigated application, it seems indicated that this is not related to fact that for the measured data different eigenvalues of J_f lie close to each other.

Let m denote the dimension of x. Due to

$$\frac{1}{m}\sum_{i=1}^{m}\left|\tilde{\lambda}_i - \lambda_i\right| \leq \frac{1}{\sqrt{m}}\sqrt{\sum_{i=1}^{m}\left|\tilde{\lambda}_i - \lambda_i\right|^2} \leq \max_i \left|\tilde{\lambda}_i - \lambda_i\right|,$$

both d_1 and d_2 offer a possibility of estimating a lower bound for the maximal perturbation $\max_i \left|\tilde{\lambda}_i - \lambda_i\right|$ of an eigenvalue of Λ_I also in case of a large number of dimensions m.

As emphasized in [8], the investigated approximations can not only be used to approximate the perturbation of eigenvalues of Λ_I in the context of sparsing, but they can also be applied in the context of the determination of suitable inexact Jacobian matrices. This opens a wide field of applications in the context of real-time simulations of stiff models on electronic control units.

With regard to the choice of a bound C_1 of an acceptable value for the perturbation of an eigenvalue of Λ_I as described in inequality 12, the following observation is mentioned: From approximation 20, it can be seen that five eigenvalues of this spectrum have comparatively small absolute values. They might not have a central impact on the stiffness of the differential equation in this time step. However, they are decisive in a choice of C_1 according to equation 15. This is a general property of the given suggestion for choice of bounds. In order to avoid this, it is suggested to neglect those eigenvalues for the choice of C_1. In the context of the so-called mixed-mode integration, it is investigated how those eigenvalues can be identified (cf. [15, 8]). For the investigated application of sparsing to a pipe model, an appropriate subsystem of the original system not containing slow modes is identified in [8], so that Λ_J of this subsystem does not contain eigenvalues with small absolute values and the choice of the bound C_1 according to equation 15 yields meaningful values.

5 Conclusion

In this work, sparsing approaches for real-simulations of stiff models on electronic control units are considered. A dedicated numerical approach is proposed and allows to detect possible influences of the

sparsing of the Jacobian matrix on the computed dynamical system. This is enabled by an approximation of the sum of squares of the values of the differences between eigenvalues of the Jacobian matrix and the perturbed Jacobian matrix. The theoretical results are confirmed by numerical experiments.

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